Fracture pattern formation and wave propagation in particulate materials with rotational degrees of freedom

by

Maxim Esin

This thesis is presented for the degree of Doctor of Philosophy of

The University of Western Australia

School of Mechanical and Chemical Engineering

2016
Fracture processes occurring in particulate materials, whose constituents are able to rotate freely or under certain load, are paramount in engineering, especially when it comes to resource and construction industries. For instance, strain localisations in rocks resulting in macrofractures, shear and compaction bands often occur during mining operations leading to catastrophic consequences. An important (and somewhat underappreciated) feature of zones of strain localisation is the presence of substantial internal rotations (particle rotations). Therefore the consideration of rotational degrees of freedom is essential for understanding the mechanism of crack propagation in particulate materials.

Investigation of the rotational mechanism of crack propagation, analysis of strain localisations and pattern formation in presence of internal rotations, study the effect of negative stiffness on stability of and wave propagation in particulate materials due to rotation of non-spherical constituents under compression are the principal aims of this thesis.

We show that the microrotational mechanism of crack propagation supersedes the traditional one in particulate materials. This mechanism is based on mutual rotations of the particles leading to appearance of moment stresses and breakage of interparticle bonds between constituents. The mechanism is multiscale: the macroscopic scale corresponds to the macrocrack, the smaller scale corresponds to the grain rotations and the smallest scale corresponds to the microcracks formed in the bonds between particles. The bond breakage is initiated by their bending or twisting caused by the corresponding moments.

Modelling of particulate materials requires the use of non-standard continua. The Cosserat continuum being the simplest one accounting for the effect of internal rotations of and moment stresses is employed. For this, the original particulate material is treated as a statistically isotropic assembly of particles with translational and rotational degrees of freedom connected together by bonds to simulate the interparticle cementing substance. Then mathematical homogenisation of this discrete system leads to the Cosserat continuum.
Abstract

Since in the constitutive equations of the Cosserat continuum the elastic moduli associated with the force stress and elastic moduli associated with moment stress have different units, the length parameters (the Cosserat characteristic lengths) can be constructed. We show that in the continuum obtained by the homogenisation of the described discrete model these lengths are commensurate with the characteristic lengths of the original material, e.g. the grain size. We subsequently show that the Cosserat characteristic lengths must be much smaller than all distances in the Cosserat continuum that are interpretable in terms of the original particulate material. This leads to the asymptotics of small Cosserat lengths known as the small-scale Cosserat continuum.

The small-scale Cosserat continuum provides considerable simplification of the analysis of fracture propagation in particulate materials. We demonstrate that in the small-scale Cosserat continuum the relevant stress singularities at the crack tip are given by the intermediate asymptotics whereby only the distances much smaller than the fracture lengths, but much larger than the Cosserat characteristic lengths are considered. Furthermore, it is shown that the main term of the asymptotic solution of the system of Navier-Lamé equilibrium equations in the Cosserat continuum is delivered by the simple pseudo-Cosserat continuum with constrained microrotations (couple-stress theory). The higher asymptotic terms can be neglected due to the smallness of the Cosserat characteristic lengths. Therefore, formally the full Cosserat theory is reduced to the couple-stress theory, where the microrotations are no longer independent rather they are expressible through the displacements.

It is found that while the stress exhibits the conventional square root singularity at the crack tip for Mode I, II and III cracks, the moment stress has singularity of the power $-3/2$. The J-integral, however, is shown to be affected by the stress singularities only, while the moment stress singularities do not contribute to the energy release rate such that the J-integral is finite. Subsequently, the energy criterion of macrocrack propagation is formulated based on the conventional J-integral.

General features of the microfracturing associated with rotations are found. Firstly microfracturing is symmetric with respect to the macrocrack line. It explains the in-plane propagation of the macrocracks, in particular, Mode II cracks and Mode I anti-cracks, which cannot be explained by conventional mechanism of fracture propagation. Secondly, non-zero width of the microfractured areas leads to the band-like appearance of natural fractures. Finally, the microstresses created by the bending or twisting prevail
over the microstresses associated with the conventional stress singularities. On top of that, the geometry of damaging zones due to moment stresses in the case of cracks of different modes is obtained.

In addition to the analytical investigation, we conduct physical experiments accompanied by displacement and rotation measurements employing the photogrammetric technique based on the digital image correlation (DIC). The results are compared with the results of numerical simulation based on the discrete element method (DEM) studying Mode I crack in the idealised particulate material. The possibility of using the couple-stress theory instead of the general Cosserat continuum is confirmed.

Since accumulation of microcracks leads to pattern formation, we study the importance of internal rotations in the shear band formation and evolution in mono- and polydisperse particle assemblies. To this end, physical experiments accompanied by the DIC technique for recovering displacement and rotational fields are carried out. Also, numerical simulations using the DEM are conducted. Both experiments and simulations show that the average (over the assembly) values of the angles of rotation are insignificantly different from zero. Instead, the particle rotations exhibit clustering at the mesoscale (sizes larger than the particles but smaller than the whole assembly). Thus, rotating particles produce a structure on their own. This structure is different from the ones formed by particle displacements and force chains. This can give a rise to “moment chains” and indicate hidden aspects of the “Cosserat behaviour” of the particles.

In particulate materials under compression, rotating non-spherical particles produce the effect of negative stiffness. We consider wave propagation in such materials and demonstrate that the waves exist when the sum of the negative Cosserat shear modulus and the conventional shear modulus is positive. In the conventional isotropic Cosserat continuum the twist wave and one of the shear waves exist only at frequencies higher than a threshold. We show that when the Cosserat shear modulus is negative all waves exist at all frequencies.

The stability of materials with negative stiffness components is investigated by considering discrete mass-springs systems of particular configurations with fixed boundary particles. All other particles are assumed to have translational and rotational degrees of freedom. It is found that the system with negative stiffness springs can be
stable when the total number of negative stiffness springs does not exceed the total number of degrees of freedom in the system. For large systems the maximum relative number of negative stiffness springs tends to zero inversely proportional to the system size for 1D systems, while this number is constant for 2D and 3D systems, 1/2 and 3/5 respectively. The presence of negative stiffness springs leads to a decrease in the eigenfrequencies: the smallest eigenfrequency becomes zero when the absolute value of the negative stiffness spring reaches its critical value.
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The thesis is organised as a series of six journal papers. At present three papers are published, one is accepted, other two are submitted. The clear statement of the relative contributions of the candidate to each paper is presented below. All co-authors gave permission for the work to be included in this dissertation. The candidate and the coordinating supervisor signed the statement that permission has been obtained.

The candidate hereby declares that this submission is his own work and to the best of his knowledge it contains no materials previously published or written by another person, or substantial proportions of material which have been accepted for the award of any other degree or diploma at the University of Western Australia or any other educational institution, except where specific reference is made in the text to the work of others.

Chapter 2


Candidate contribution

The candidate performed an analysis of Mode I, II and III cracks in the developed small-scale Cosserat continuum. The candidate obtained the singular moment stress fields and compared them with the singular force stress fields near the crack tip. At the points where the moment stresses have maxima, the rotational mechanisms of microfailure (bond-twisting, bond-bending, echelon pattern, etc.) were investigated and the demonstrating figures produced. The candidate also developed the J-integral concept. All calculations were conducted by the candidate.

Chapter 3

Candidate contribution

The candidate planned the physical experiments in collaboration with Winthrop Professor Arcady Dyskin and Professor Elena Pasternak. The literature review, experiments, numerical simulations and all calculations were conducted by the candidate. The proprietary algorithm utilized in the work was developed by Ghulam Mubashar Hassan. Then it was modified significantly by the candidate. The paper was prepared by the candidate under the supervision of Professor Elena Pasternak and Winthrop Professor Arcady Dyskin.

Chapter 4


Candidate contribution

The physical experiments were planned by the candidate with the help of Winthrop Professor Arcady Dyskin and Professor Elena Pasternak. The literature review and physical modelling were conducted by the candidate. He also obtained the analytical solution for the Mode I crack. Numerical simulations were carried out by the candidate in corroboration with Yuan Xu. The proprietary algorithm utilized in the work was developed by the candidate. The paper was reviewed by Winthrop Professor Arcady Dyskin and Professor Elena Pasternak.

Chapter 5


Candidate contribution

The candidate performed the stability analysis of 1D, 2D and 3D discrete mass-spring systems. He obtained the necessary condition of stability for the systems containing negative stiffness elements. The stability of 1D dynamic system with viscous damping was also analysed. On top of that, the candidate analysed the eigenfrequencies, trajectories of motion and critical concentrations of negative stiffness springs. The papers were prepared by the candidate. Professor Elena Pasternak and Winthrop Professor Arcady Dyskin critically reviewed the papers.

Chapter 6


Candidate contribution

The candidate explored the effect of negative Cosserat shear modulus on wave propagation in isotropic Cosserat continuum. He generalised the expression for the wave velocities for the case of negative Cosserat shear modulus. Dispersion relationships for the twist and both shear-rotational waves were analysed and illustrated for the case of positive and negative Cosserat shear modulus. The candidate conducted all calculations. The paper was written by the candidate under the supervision of Professor Elena Pasternak and Winthrop Professor Arcady Dyskin.
Conference publications

Apart from the journal papers, three fully refereed conference publications showed below were written by the candidate and his supervisors. The results of these publications are reflected in the journal papers.


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PUBLICATIONS ARISING FROM THIS THESIS

Journal Articles


Conference papers


Publications arising from this thesis


Conference abstracts


ACKNOWLEDGEMENTS

I would like to take this opportunity to express many thanks to a number of people and institutions that helped me in various aspects over the course of my study.

First and foremost, I am deeply grateful to my supervisors Professor Elena Pasternak and Winthrop Professor Arcady Dyskin from whom I learnt many valuable research skills and knowledge. Their excellent scientific guidance, sustained support, encouragement, expertise and patience throughout all these years make me confident to continue my study until the end. I am thankful for the opportunity to conduct research under their supervision. I would like to express my appreciation to Soren Soe, for his helpfulness and for sharing his ample engineering and industrial experience with me.

I would like to thank fellow postgraduate students and colleagues from the University of Western Australia, including Iuliia Karachevtseva, Yuan Xu, Junxian He, Habibullah Chowdhury, Maxim Khudyakov, Maria Kuznetsova and Dr Igor Shufrin, for their support and precious friendship. The candidature would not have been such a joyful experience without it. Thank you all for your kindness, humour and everything that you have done for me.

I appreciate the financial support in the form of the Scholarship for International Research Fees, University Postgraduate Award, Overseas Travel Award and Safety-Net Top-Up Scholarship provided by the University of Western Australia. I would also like to acknowledge the Top-up Scholarship from the Deep Exploration Technologies Cooperative Research Centre. All this made my study possible in Australia.

I would like to express my gratitude to the administrative staff of the School of Mechanical and Chemical Engineering and Graduate Research and Scholarships Office, particularly John Pougher, Karen Leers and Jorja Cenin for their valuable assistance.

Most importantly, this thesis would not have been possible without unconditional love and constant support of my family. Words cannot express how grateful I am to my mother and father for all of the sacrifices that they have made on my behalf. Their endless love encouraged me throughout every step of my candidature. I thank my brother for his support and encouragement. I would like to express my deepest thanks to my best friend and beloved wife, Natasha, for allowing me the time to pursue
this thesis. Your unfailing love, understanding and warm support have motivated me throughout this study. I am thankful for having you around in my life.
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CHAPTER 1

General Introduction
Modelling of mechanical behaviour of solids whose microstructure is heterogeneous represents an actual and challenging problem. Since most of natural materials and a wide variety of engineering structural materials are non-homogeneous, this topic generates considerable interest. For example, geomaterials (e.g. rock, sand, clay) consist mostly of cemented grains or slightly cemented and unbound constituents thus possessing highly non-homogeneous microstructure. Concrete, mortar, ceramics, masonry and artificial interlocking structures are other examples of such materials. At large scale, the layered and blocky rock masses and the parts of the Earth’s crust containing tectonic blocks also represent heterogeneous solids.

Among the numerous properties of heterogeneity, internal microrotations play one of the crucial roles in mechanics of such materials. Microrotations result from the presence of unbalanced shear forces and moments in the medium with the moments responsible for relative rotations of the neighbouring constituents. Microrotations characterise the mechanical behaviour of particulate materials (materials whose constituents may rotate) at various scales and must be taken into account for adequate modelling. This is especially appropriate for the cases where internal rotations are observed as in the areas of strain localisations in granular materials (e.g. [1, 2]). Also, internal rotations could form a mechanism of formation and propagation of shear and compaction bands, cracks, fractures and damage zones.

Since most of geomaterials are subjected to compressive load, compaction and shear bands represent one of the main mechanisms of failure and arouse much interest from a practical standpoint. In resource (e.g. mining and petroleum) industry, these types of fracture and failure processes occur frequently. At large scale it could lead to catastrophic consequences involving the loss human life, destructions and financial losses, especially when the failure was not predicted and the appropriate actions were not taken. Despite the extensive research many aspects of these fracture and failure processes in heterogeneous materials remain unclear. The consideration of internal rotations may cast light on the mentioned failure mechanisms.

Numerous physical experiments corroborate the presence of considerable microrotations during pattern formation (e.g. shear and compaction bands) in particulate materials. Experimental investigations of shear bands use a variety of granular materials and different types of loading (e.g. biaxial, triaxial and shear laboratory experiments and in situ tests). Roscoe and Schofield [1] and Oda [2] were among the first scholars who...
realised the importance of microrotations on failures and observed rotations of sand particles during physical experiments. Oda et al. [3, 4], Calvetti et al. [5] and Misra and Jiang [6] carried out another type of experiment for observation and investigation of internal rotations using assemblies of relatively large circular or elliptical discs and oval cross-sectional cylindrical rods as granular material. With the development of non-destructive scanning techniques, experiments using sand and artificial materials with relatively small particles were conducted using various methods such as photogrammetry [7-9], gamma-rays [10], X-ray computed tomography [11-20], 2D microscopy [21], magnetic resonance imaging (MRI) [22], digital image correlation [16, 19, 23, 24] and ID-Track [13-15, 19]. Dynamics of shear bands formation in sand in tension was also experimentally investigated by using resistance sensors made of graphite powder [25, 26]. It was found that a characteristic feature of the emerging zones of strain localisation is the reduced sand density straight before the shear bands propagation. Moreover, the velocity of the shear bands propagation was determined (around 100 km/year in the conducted experiments), and this velocity does not depend on the sand deformation rate.

Rudnicki and Rice [27] theoretically investigated shear bands in terms of instability of homogeneous deformation and obtained the general conditions for a bifurcation. We note though that the bifurcation conditions are formulated based on the assumption that the strain localisation is occurring in a straight narrow strip, while the reasons for such a geometry remain unclear. This approach has become a major one for describing strain localisations in particulate materials. Later this method in combination with non-standard continuum modelling considering microrotations was used by Mühlhaus [28] and Mühlhaus and Vardoulakis [29]. Recently, other approaches of explanation of pattern formation have been developed, such as mean-field theory [30] and evolution of force chains [31-33].

Cundall [34] and Cundall and Strack [31] introduced a numerical tool, called the distinct element method (DEM), which is used to describe the mechanical behaviour of segmented heterogeneous materials. From the end of the 20th century this approach has been widely utilised for modelling and investigation of shear bands and became one of the dominant tools [35-49]. In particular, using this tool the critical role of particle rotations in mechanical behaviour of particulate materials was verified [35, 38, 39, 42].
It should be noted that in many cases authors used ideal spherical particles or circular discs to model the particulate material. Obviously, such a description of the material is far from reality, as the effects associated with rotation of non-spherical and non-circular constituents could not be described in this paradigm and were overlooked. It has been discovered by Pasternak et al. [50] and Dyskin and Pasternak [51-55] that rotation of non-spherical particles involving compressive loading can produce different mechanical effects, such as “elbowing”, negative stiffness and the emergence of large-scale characteristic lengths. It is suggested that the latter two effects are inseparably associated with manifestation of instability at macro-scale. On top of that, the formation of patterns where rotational zones are separated by non-rotational ones can also be explained by the non-spherical shape of particles [50]. However, it would be fair to mention that some papers about DEM were devoted to investigation of importance of the particle shape, as well as the resistance to particle rotation. The rolling resistance was defined either by incorporating the appropriate rolling resistance terms in contact laws (rheology-type rolling resistance model) or by explicit modelling of irregular particle shape [35]. Rothenburg and Bathurst [56, 57] conducted numerical simulations of planar assemblies composed of elliptical-shape particles in order to study the significance of particle shape on the mechanical behaviour of the assemblies at micro- and macro-scale. For biaxial compression tests the authors demonstrated how the stress-strain response of the considered assemblies changes when the value of particle eccentricities changes from 0 to 0.3. It was found that the assemblies consisting of elliptical particles have larger peak strengths and dilation rates than the assemblies composed of disk-shaped particles. On top of that, it was shown that the strength and dilation rates as well as the density increase with the eccentricity until it reaches 0.2, after which these parameters decrease. Later, Mirghasemi, Rothenburg and Matyas [58] numerically analyse the influence of the polygon-shaped particles with different angularities on the mechanical behaviour of the assemblies (e.g. density, compressibility, peak shear strength).

Tejchman and co-authors [59-64] employed another numerical simulation technique based on the finite element method (FEM) for study of pattern and shear band formation. The utilised FEM was based on the elastoplastic and hypoplastic constitutive equations enhanced by micro-polar terms. It has been shown that the effects of internal rotations are substantial in the shear band zones.
Recently comparative analysis of DEM and hypoplastic continuum modelling was conducted by Lin and Wu [65]. They demonstrated that results of the two different numerical techniques obtained for the same problem are in good agreement. Numerical solutions form a viable alternative to usually expensive and time-consuming experimental investigations and allow one to explore the pattern formation and strain localisation, which might be complicated to study experimentally, for instance, due to short durations of the band formation and re-compaction.

Shear and compaction bands can be considered as being a result of accumulation of microcracks at the scale microscopic to the scale of the band [66-69]. Due to the manifestation of significant internal rotations in zones of strain localisation, it conveys the suggestion that rotational mechanisms of failure can prevail over the traditional ones in some cases. For instance, it has been recognised [52] that rotation of particles influences the direction of fracture propagation. The rotational mechanism was also utilised for explaining why shear cracks and Mode I anti-cracks (i.e. shear and compaction bands) are able to grow in-plane under compression in particulate brittle materials though the physical experiments demonstrate kinking of shear cracks sometimes [52, 66, 70].

The importance of particle rotations in fracturing processes was recently shown by Teisseyre and Górski [71, 72]. Also it has been recognised that on top of the conventional stress singularities the moment stress singularities exist at the crack tip [73]. In addition, as mentioned above, the rotation of non-regular shaped single particles or cohesive clusters of particles (the existence of particle cluster rotating together was demonstrated by Rechenmacher et al. [24]) produces “elbowing” and an effect of negative stiffness, which have an influence upon the crack initiation and propagation and make the study even more curious. Thus, better understanding of the rotational mechanism of failure at micro-scale (which is common for shear and tensile cracks) has an invaluable practical significance for describing the mechanics of coalescence of microcracks into large-scale fractures, shear and compaction bands and other types of failure at macro-scale. This knowledge can help detecting and possibly predicting instability in mines and excavations, prevent natural shear failures, improve wellbores productivity and permeability by optimisation of the hydraulic fracturing processes, and so on.
We assume that microcracking leads to partial or complete grain de-bonding, which allows the grains to rotate and thus finalize grain detachment from the rest of the geomaterial and thus form propagating fracture. In rock testing, the de-bonding is accomplished at the point of reaching the peak load after which the random and almost uniform accumulation of microcracks is replaced with shear band formation and propagation [74]. It can be hypothesized that the latter corresponds to a collective grain detachment which propagates as a shear fracture or shear band. We suggest that the mechanism of grain detachment is the bond breakage caused by tensile microfractures created by grain rotations due to the action of bending and twisting moments. The independent grain rotations are enabled by intergranular damage developed in the preceding loading. The grain detachment and the subsequent independent rotations are suggested as a mechanism of in-plane propagation of macrofractures in geomaterials, which are macroscopically Mode I, II and III as well as Mode I anticracks.

Continuum modelling combined with linear elastic fracture mechanics is one of the approaches that allow studying the mechanical behaviour of fracture propagation in particulate materials. In the standard continuum the force acting at a point of the solid is defined by only force vector, while the moment vector is neglected. Consequently, the stress tensor is symmetric. Furthermore it is deemed to be sufficient to characterise the stress state. The absence of independent rotations in the standard continuum (each point has three translational degrees of freedom) makes the strain tensor symmetric as well. Subsequently, in the restrictions of the standard continuum it is not possible to fully take into account the microstructure of matter if the latter cases independent microrotations. Obviously, continuum modelling of particulate materials in the presence of independent grain rotations requires the use of the non-standard continuum theories. The first attempt to consider microstructure dates 1887, when Voight [75] proposed the description of continuum including both a central force and couples. Later this approach was developed extensively. There exists a number of non-standard continua, such as the Cosserat continuum (micropolar or asymmetric elasticity, Cosserat and Cosserat [76], Nowacki [77], Toupin [78], Eringen [79]), gradient theory of elasticity (e.g. Mindlin [80]), micromorphic elasticity (e.g. Mindlin [81], Eringen [79]), multipolar continuum (e.g. Green and Rivlin [82]) and non-local theories (e.g. Eringen [83], Kunin [84], Bažant and Jirásek [85]) more suitable for materials of this type.
We employ the Cosserat continuum in our study as the simplest theory accounting for internal rotations of particles. In this theory every point of continuum has three conventional translational degrees of freedom and, additionally three rotational degrees of freedom (in 2D there are two translational and one rotational degrees of freedom). As a result, kinematics is described by displacement and rotational vectors. Consequently, on top of the conventional stress (force stress) which becomes non-symmetrical the constitutive equations of the micropolar elasticity include moment stress (couple stress).

The finite element method based on the constitutive equations of the Cosserat continuum was used extensively for modelling particulate materials with strain localisations, in particular shear band formation in granular materials [28, 29, 59, 60, 62, 86, 87]. On top of that, using the concept of the asymmetric elasticity Teisseyre and Górski [71, 72] demonstrated the crucial role of particle rotations in fracture propagation.

In contrast to the standard continuum, where in the isotropic cases only two material constants (Lamé parameters, \( \lambda \) and \( \mu \)) are used in the constitutive equations, the Cosserat theory uses four additional moduli, \( \alpha, \beta, \gamma, \epsilon \) [77]. Note that the methods for determining these additional material constants based on experiments and analytical solution were also suggested (e.g. Lakes [88], Pasternak and Dyskin [89], Gauthier [90, 91] and Bigoni and Drugan [92]). The fact, that elastic moduli associated with the force stress and elastic moduli associated with couple stress have different units, leads to the emergence of characteristic lengths. The applicability of the Cosserat continuum is still limited due to the lack of methods for determining material constants and calibration of the characteristic lengths.

Microstructure of a real particulate material (Oolitic limestone [93] is chosen as an example) as seen under a microscope is demonstrated in Fig. 1a. Grains (pellets of calcium carbonate) of a different size and shape are binded together by cementing substance. Obviously, modelling of the mechanical behaviour of such non-homogeneous material is an intricate problem. The discretisation is one of the commonly known approaches to simplify this problem [89, 94-97]. In that case the material is treated as a statistically isotropic assembly of particles which are connected by elastic bonds to simulate the interparticle cementing substance (the material is assumed to be elastic in the scope of this study). Moreover, for the sake of simplicity, it
is often assumed that the particles in the discrete model have a spherical (circular in 2D) shape and the same diameter. The particles may have both translational and rotational degrees of freedom. Generally speaking, since the particles of real particulate materials are not spherical, this model only reflects the behaviour of the material related to internal rotations without the specifics of interaction associated with non-sphericity, such as “elbowing”, which under pressure manifests itself as negative stiffness [53-55]; these will be discussed separately.

The above consideration leads to the discrete model shown in Fig. 1b. The discrete model consists of a number of spherical non-deformable particles of the same diameter, $d$, with distance between the particles, $h$. The particles are connected with each other by a combination of normal, shear and rotational springs. The unit of the normal and shear springs stiffnesses is N/m, the unit of the rotational spring stiffness is N.m. Note that the packing of the particles can have an arbitrary configuration. The square packing is shown as an example in Fig. 1b.

**Fig. 1.** Models of particulate material and the characteristic lengths involved: (a) Real particulate material (Oolitic limestone [93] is chosen as an example, field of view 3 mm): grain sizes, $l_{\text{grain}}$, distances between grains, $l_{\text{distance}}$; (b) Discrete model: diameters of masses, $d$, initial spring lengths, $h$; (c) Cosserat continuum model: characteristic lengths, $l_1$, $l_2$, … can be expressed thought Lamé parameters and additional Cosserat elastic moduli or the spring stiffnesses of the discrete model.

The discretisation is a convenient way to describe the mechanical behaviour of particulate materials. However, it has some limitations [98]. First of all, this approach requires utilising the equations of motion for every particle. Since real particulate materials contain thousands and sometimes millions grains, implementation of such a model demands high computing power. Secondly, the discrete modelling requires
information about geometrical (if the discrete model consists of particles of different size and shape) and mechanical characteristics of all grains and interparticle spaces. Apparently, it is complex and time consuming to collect this information even using the advanced technology. These limitations can be (and often are) circumvented by homogenisation of the discrete model.

Homogenisation is a mathematical technique of representing the discrete system containing the rigid particles by a continuum (Fig. 1c). In the presence of the rotational degrees of freedom the discrete model transforms into a non-standard continuum, such as for instance the Cosserat continuum. Homogenisation consists of replacing the sets of displacements and rotations of particles (field variables) in the discrete system by homogenised continuous displacements and rotations in the continuum model. This is accomplished by averaging the sets of particle displacements and rotations as well as link forces and moments with averages over suitable representative volume elements (their properties are discussed below) [73]. Thus, homogenisation may significantly simplify the investigation of the initial discrete model. For example, the number of the equations of motion in the discrete model reduces dramatically to the number of degrees of freedom in continuum.

There are number of known homogenisation procedures: averaging over volume element adopted in the theory of effective characteristics [99-101], homogenisation method applied to materials with randomly varying elastic properties [102], homogenisation by differential expansions [103-105] and homogenisation by integral transformation [106, 107] (please see [95, 98] for more details about generalised homogenisation procedures for granular and layered materials). In this study we will use the equations of equilibrium and constitutive equations of the Cosserat continuum that were obtained by applying the method of homogenisation by differential expansions to the discrete model mentioned above [95, 96, 98]. As the name of the method suggests, the finite difference terms of the displacements and rotations in the expressions of the discrete model (e.g. potential energy density expression) are replaced by the corresponding differential expressions. Then the state and constitutive equations of the Cosserat continuum are derived by differentiation of the potential energy density with respect to the Cosserat deformation measures [95]. Thus, we move from the discrete to the continuum modelling. It is important to place emphasis once again on the fact, that
we homogenise the discrete model (Fig. 1b) rather than the initial particulate material (Fig. 1a).

The continuum model (Fig. 1c) obtained by the homogenisation procedure of the discrete model (Fig. 1b) is intimately connected with introduction of representative volume element (RVE) and the concept of separation of scales. The RVE characterises the scale of resolution of the continuum model and represents a point of the macroscopic continuum. Generally, the size of the RVE should be much larger than the characteristic size of the microstructure of the given material (in order to asymptotically satisfy the requirement for the RVE to be representative) but much smaller than the characteristic length of the variations of the external fields (in order to asymptotically satisfy the requirement for the RVE to be infinitesimal) [73, 95]. For that the difference between the microstructural size and the characteristic length of the variations of the external fields should be sufficient to ensure that the RVE satisfies the above properties. Such a situation is called the condition of separation of scales. The separation of scales allows modelling the given material as a continuum.

An important consequence is that while within the continuum one can formally consider any infinitesimal length, these lengths cannot be interpreted in terms of the original material. In other words, the consideration of sizes smaller than the RVE is not possible; the infinitesimal lengths in the continuum only exist asymptotically as the size of the RVE tends to zero. For example, a homogenised duct of grains under gravity shows near-boundary displacements (at the distances smaller than the spacing between the particles) in the directions against gravity, demonstrating the artefacts of the homogenisation procedure [87]. Thus, these infinitesimal lengths would be irrelevant in the continuum.

Now let us discuss the characteristic lengths of a real material and its mathematical representations in more details. As indicated above, we have an original particulate material (Fig. 1a). This material is represented as a discrete mass-spring system (Fig. 1b), which in turn is transformed into Cosserat continuum model (Fig. 1c) by a homogenisation procedure. The real particulate material has internal characteristic lengths associated with its microstructure, for instance, grain sizes, $l_{\text{grain}}$, and distances between grains, $l_{\text{distance}}$. The discrete model has its own characteristic lengths, such as a diameter of rigid masses, $d$, and a distance between the masses, $h$. On top of that as we discussed above, since the stiffnesses of different springs (e.g. shear and rotational
springs) have different units, other length-scale parameters can be constructed in the
discrete system. For instance, the square root of the ratio between the stiffness of the
rotational spring and the stiffness of the shear spring gives another characteristic length
in the discrete system.

As the next step, we homogenise the discrete system (Fig. 1b) by introducing a
representative volume element and move to the continuum model (Fig. 1c). Since the
representative volume element size in the Cosserat continuum should be much larger
than the characteristic lengths of the original discrete system, these lengths are beyond
the resolution in the Cosserat continuum.

On top of that the continuum model possesses its own characteristic lengths.
Two Cosserat characteristic lengths are usually introduced as combinations of Lamé
parameters and additional Cosserat elastic moduli. Since there is no unified approach
for defining characteristic lengths, the literature suggested different combinations (e.g.
Nowacki [77], Lakes [88], Pasternak et al. [96] and Dyskin and Pasternak [73]). We use
the following expressions for the Cosserat characteristic lengths in the current study
[73]:

\[ l^2 = \frac{(\mu + \alpha)(\gamma + \varepsilon)}{4\mu\alpha}, \quad l_z^2 = \frac{\gamma + \varepsilon}{4\alpha} \]  
(1.1)

Due to the fact that we employ the Cosserat continuum model which was
obtained by homogenisation of the discrete system, the Cosserat elastic moduli and,
consequently, the Cosserat characteristic lengths can be expressed through the spring
stiffnesses of the discrete model [73]:

\[ l^2 = \frac{1}{5} \frac{(k_n + 4k_\phi)(k_{n\phi} + 4k_{\phi\phi})}{k_n(2k_n + 3k_\psi)}, \quad l_z^2 = \frac{1}{10} \frac{k_{n\phi} + 4k_{\phi\phi}}{k_n}, \]  
(1.2)

where \( k_n \) denotes stiffness of the normal springs, \( k_\psi \) denotes stiffness of the shear
springs, \( k_{n\phi} \) and \( k_{\phi\phi} \) denotes stiffnesses of rotational springs around different directions.

It was shown in [73], that if elastic bonds (springs) between particles in the
discrete system are modelled as cylinders of height, \( h \), and radius, \( b \) (both parameters
are assumed to be order of the particle diameter, \( d \)) then the Cosserat characteristic
lengths read as:
\[ l^2 = \frac{1}{10} b^2 \left( E_b + 4G_b \right) \frac{(2E_b + G_b)}{(2E_b + 3G_b)G_b}, \quad l_z^2 = \frac{1}{20} b^2 \frac{2E_b + G_b}{G_b} \quad (1.3) \]

Here \( E_b \) and \( G_b \) are Young’s modulus and shear modulus of the material of the bonds respectively.

Interestingly, assuming that \( G_b \sim E_b \) and the radius of the cylinders, \( b \), is order of a particle diameter, it emerges that the Cosserat characteristic lengths are order of a particle diameter, i.e. \( l, l_z \sim d \). Thus, both characteristic lengths are much smaller than the representative volume size of the continuum. It means that the Cosserat characteristic lengths are beyond of the resolution of the Cosserat continuum model (similar to characteristic lengths of the original discrete model). This important conclusion will be used below when the mechanism of fracture propagation in particulate materials is considered. It should be noted that this conclusion is correct only in the case, when the Cosserat model is obtained by homogenisation of the discrete model described above.

Since the main objective of the thesis is the investigation of mechanism of fracture propagation in particulate materials, the multiscale nature of fractures (grain size, \( l_m \), are considerably smaller than the fracture length, \( L \)) may be used as a simplifying factor in the Cosserat continuum model. Introducing the RVE of size, \( H \), separation of scales in (Cosserat) continuum takes place \([108-111]\):

\[ l_m \ll H \ll L \quad (1.4) \]

This double inequality characterizes the scale of resolution of the Cosserat continuum model in presence of fractures. The double inequality leads to the following two asymptotics:

\[ H / L \to 0, \quad l_m / H \to 0 \quad (1.5) \]

The first asymptotic is the requirement for the RVE to be infinitesimal (the length of redistribution of the fields, e.g. fracture length, are larger than \( H \)), the second one is the requirement for the RVE to be representative. Consequently, two asymptotics in Eq. (1.5) result the following asymptotic:

\[ l_m / L \to 0 \quad (1.6) \]
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The validity of this asymptotic is the necessary condition for the use of the continuum modelling.

As discussed above, real particulate materials can be represented by a number of grains connected together by cement bonds. In this study the Cosserat continuum is based on a homogenisation procedure of this model. It was found that in this case the Cosserat characteristic lengths, $l_1$, $l_2$, are order of a grain size (generally speaking, the Cosserat lengths can be arbitrary depending on the model which is homogenised) [73, 94]. Hence the second asymptotic in Eq. (1.5) can be expressed as:

$$\frac{l}{H} \to 0$$

(1.7)

This situation corresponds to what is called the small-scale Cosserat continuum [52, 73, 94, 112]. The asymptotic in Eq. (1.6) can be rewritten in a similar way:

$$\frac{l}{L} \to 0$$

(1.8)

It is seen from Eq. (1.7) and the first equation in Eq. (1.5), that only distances $l << r << L$ (where $r$ is the distance to the crack tip, Fig. 2) can be considered relevant in the obtained Cosserat continuum. Consequently, we are thus led to the intermediate asymptotic:

$$\frac{r}{l} \to \infty, \quad \frac{r}{L} \to 0$$

(1.9)

Fig. 2. The range ($l << r << L$) of the intermediate asymptotic provided by the small-scale Cosserat continuum. Here $r$ is the distance from the crack tip, $L$ is the characteristic length of the crack, $l_m$ is the microscopic length, $l$ is the Cosserat characteristic lengths.

The stress singularities are referred to the stress distributions at distances from the crack tip much smaller than the fracture lengths [113, 114]. In contrast to that, the distances much smaller than the fracture lengths (the second asymptotic in Eq. (1.9)),
but much larger than the Cosserat characteristic lengths (the first asymptotic in Eq. (1.9) – outer solution) are related to an intermediate asymptotics.

The possibility of the intermediate asymptotic leads to a considerable simplification of the analysis and represents one of the key points of this study. Before we demonstrate it, let us write down the constitutive equations and the equations of equilibrium of the Cosserat medium. Hooke’s law for the Cosserat continuum read:

\[
\sigma_{ij} = (\mu + \alpha)\gamma_{ij} + (\mu - \alpha)\gamma_{ij} + \lambda\gamma_{kk}\delta_{ij} \\
\mu_{ij} = (\nu + \alpha)\kappa_{ij} + (\nu - \alpha)\kappa_{ij} + \beta\kappa_{kk}\delta_{ij}
\]  

(1.10)

Here \(\sigma_{ij}\) and \(\mu_{ij}\) are the components of the stress and moment stress tensor; \(\gamma_{ij}\) and \(\kappa_{ij}\) are the components of the strain and curvature-twist tensor; \(\delta_{ij}\) is the Kronecker delta function.

The equations of equilibrium in the absence of body forces and moments are expressed as:

\[
\sigma_{ji,j} = 0 \\
\mu_{ji,j} + \varepsilon_{kji}\sigma_{jk} = 0
\]  

(1.11)

where \(\varepsilon_{kji}\) is the alternating tensor.

For the following asymptotic analysis we assume that the characteristic length \(l\) has been normalised by the representative volume element size \(H\) such that \(l\) is dimensionless. The asymptotic solution of the system, Eq. (1.10) and Eq. (1.11), can be expressed for small \(l\) in the following form [73]:

\[
u = \nu^0 + \nu^1l^2 + ... \\
\phi = \phi^0 + \phi^1l^2 + ...
\]  

(1.12)

Here \(\nu\) is the displacement vector, \(\phi\) is the rotation vector.

It was shown in [73] that the main asymptotic terms, \(\nu^0\) and \(\phi^0\), are the solutions of the following system of equations:

\[
(\lambda + 2\mu)\text{grad div } \nu^0 - \mu \text{ rot rot } \nu^0 = 0 \\
\phi^0 = \frac{1}{2} \text{ rot } \nu^0
\]  

(1.13)
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The derived equations are identical to the equations of classical elasticity. Thus, the main asymptotic term, $u^0$ and $\phi^0$, can be determined from the couple stress theory (the pseudo-Cosserat continuum with constrained rotations). The solution given by the next asymptotic term will not be considered due to the smallness of the Cosserat characteristic lengths. Therefore, formally the full Cosserat theory is reduced to the couple-stress theory (otherwise called the pseudo-Cosserat continuum with constrained rotations), where the microrotations are no longer independent rather they are expressible through the displacements: $\phi = 1/2 \text{rot} u$. (This should not be confused with the reduced Cosserat continuum where displacements and rotations are independent, but couple stresses are equal to zero). This shows that the independence of internal rotations can only be reflected by the second order asymptotic terms, while the moment stresses obtained from the rotations are a part of the main term.

The possibility of this transformation to the pseudo-Cosserat continuum with constrained rotations is a key simplification factor in the analysis of fracture propagation in particulate materials and would be widely used in the current study. The couple-stress theory results in simplifying of the equations for the stress and moment stress singularity [52]. This simplification was used in [73, 94, 112] where the concept of small-scale Cosserat continuum was introduced and Mode I and Mode II cracks were considered. The crack propagation criteria were introduced based on comparing the average moment stresses with their critical values determined by initiating the bending-induced tensile microcracks.

Crack or fracture initiation and propagation in particulate materials are usually accompanied by generation of elastic waves. When fracture propagation occurs, it produces a sequence of impulses associated with the propagation steps. This manifests itself as acoustic (microseismic) emission whose temporal pattern contains the information of the fracture geometry, such as fractal dimension of the fracture. This information is important in both stability and fracture monitoring (e.g. hydraulic fracture).

Internal rotations affect the wave propagation in heterogeneous materials. For a conventional Cosserat continuum the types and velocity of planar waves are well-known (e.g. Nowacki [77]). There are a pressure wave, two shear waves, a twist wave and Rayleigh wave. On top of that, Kulesh et al. [115, 116] showed that two unique additional surface elastic waves exist in Cosserat continuum (these waves do not have
analogues in classical continuum). In contrast to the classical medium, all waves except the pressure wave show dispersion (the dependence of the wave velocity upon frequency). This property of wave propagation in the heterogeneous material can in principal be used for determining the material constants of Cosserat continuum, in particular for the case of large-scale rock masses when laboratory testing cannot be conducted.

Numerical analysis of wave propagation in the Cosserat elastic continuum was conducted by Sadovskaya and Sadovskii [117-119] and Varygina et al. [120]. The plane strain problem of uniform shear was considered in detail. It was demonstrated that the characteristic oscillations of particle rotations occur in the zone of shear. Moreover, it was found that materials with microstructure have the additional resonance frequency associated with the eigenfrequency of particle rotations and independent of size of the investigated region. The detailed computational results of Lamb’s problem for different types of loading (normal and tangential loads for 2D and 3D problems; torsional and rotational moments for 3D problem) are shown in [117-119]. Later, the micropolar continuum was used for investigating elastic wave propagation in blocky media composed of elastic blocks with compliant interlayers [121-123]. It was shown that the orthotropic Cosserat continuum is required to utilise due to arising anisotropy with the increasing thickness of interlayers. The eigenfrequency associated with rotation of the blocks in such structures was investigated [124]. It was discovered that the resonance frequency is independent of the interlayer thickness and the size of the block structure.

Combination of internal rotations and non-regular shapes of particles in the presence of compression has been shown to lead to the effect of negative stiffness by Dyskin and Pasternak [53-55]. It is another important point to consider, in particular when wave propagation in particulate materials is investigated. One of the main issues related to the systems with negative stiffness inclusions or elements is their stability. Since the work done on the negative stiffness element by the force is negative (the displacement is in the opposite direction to the force), according to thermodynamics the negative stiffness element should be unstable. Yet, materials and structures exhibiting negative stiffness may exist provided that they are stabilised with the aid of an encompassing system which makes the balance of the energy such that the total energy is positive definite. Thus, the system stabilising the negative stiffness element works as an energy reservoir. In the simplest case such a stabilising system can be replaced with
properly defined boundary conditions [51, 125, 126]. It is also found that a viscous damped system containing negative stiffness springs is stable when the system is tuned for high compliance [127]. Alternatively in continuous composite materials consisting of a positive stiffness matrix and negative stiffness inclusions the latter can be stabilised by the (positive stiffness) matrix, as long as the values of negative stiffness inclusions do not exceed particular thresholds [51, 55, 128-130].

We study the stability of heterogeneous materials with negative stiffness inclusions and wave propagation in it using two approaches: Cosserat continuum and discrete mass-spring models.

In the continuum modelling, the negative Cosserat shear modulus, \(\alpha\) (the modulus that couples translational and rotational degrees of freedom or, to be more precise, the non-symmetric part of shear stress and rotation), can represent the negative stiffness in Cosserat continuum taking place due to rotation of non-spherical particles in the presence of compression. Wave propagation in the Cosserat continuum with the positive Cosserat shear modulus is well known. There is a critical frequency above which additional shear wave and rotational waves appear [77]; this frequency is proportional to the Cosserat shear modulus. When the Cosserat shear modulus assumes negative values this can lead to different behaviour of wave propagation and instability. However, the mechanics of wave propagation in heterogeneous materials with negative Cosserat shear modulus has not been considered in the literature yet and hence needs special investigation.

Wave propagation can also be considered as motion of particles in discrete mass-spring models. In such systems the medium is represented as a set of spherical (circular in 2D) particles connected by the different types of springs with specified stiffness. Sometimes systems also include viscous dampers for more complex analysis. A number of structures were investigated that consist of negative stiffness elastic elements (e.g. Pasternak et al. [131], Wang and Lakes [127, 132, 133]). It should be highlighted, however, that the considered systems did not include rotational degrees of freedom. Thus, the results cannot sufficiently describe the mechanical behaviour of materials with microstructure. To model Cosserat type continuum, rotational degrees of freedom and associated rotational springs should be incorporated in the discrete mass-spring model. Rotation of non-spherical particles in the presence of compression will introduce negative values to the shear stiffness, \(k^S\), in the discrete system. This
parameter would be similar to the Cosserat shear modulus in continuum modelling. Consequently, it becomes possible to explore wave propagation in and stability of particulate materials with negative stiffness constituents by using simple discrete mass-spring models.

The main aims of this thesis are to: (a) investigate the multiscale rotational mechanism of Mode I, II and III cracks propagation in materials with rotational degrees of freedom, (b) analyse pattern and clustering formations at meso- and macro-scale caused by microrotations in particulate material, (c) explore the mechanical behaviour of and internal rotations in the cemented particulate material with a pre-existing crack and (d) study the effect of negative stiffness (e.g. negative Cosserat shear modulus) on wave propagation in and stability of particulate materials due to rotation of non-spherical particles during cracks and fractures growth.

The thesis is organised as a series of six journal papers and has the following structure.

Chapter 2 (Paper “Multiscale rotational mechanism of fracture propagation in geomaterials”) treats of the multiscale rotational mechanism of macrocrack propagation based on the breakage of bonds between mutually rotating grains. The bond breakage is initiated by their bending or twisting caused by the corresponding moments associated with the particle rotations. Modelling of this mechanism is based on the Cosserat theory. It is shown that when the Cosserat characteristic lengths are comparable with the grain sizes a pseudo-Cosserat continuum with constrained microrotations (small-scale Cosserat continuum) can be utilised. Cracks of different modes – tensile Mode I crack, compaction band (Mode I anticrack) and shear bands (Mode II and III cracks) – are investigated. Energy criterion of crack propagation in the small-scale Cosserat continuum is formulated based on the concept of $J$-integral.

Chapter 3 (Paper “Rotations and pattern formation in granular materials under loading”) narrates the observation of rotations at micro-scale and pattern formation (e.g. shear bands) at meso- and macro-scale in two-dimensional physical experiments and numerical simulation of non-cohesive granular material. Particles of the material are represented by smooth steel discs. In order to recover both displacement and independent rotation fields in the physical model we employ photogrammetry and the
digital image correlation method. Then we calibrate and determine the values of mechanical parameters needed for a numerical modelling based on discrete element method. We perform a special calibration of the experiments in order to determine the required input parameters (contact stiffness, friction coefficient, etc.) for the numerical modelling based on distinct element method with a potential to use the results for constructing a Cosserat continuum using an appropriate homogenisation method. The rotational behaviour and pattern formation are analysed for both monodisperse hexagonal packing assembly and polydisperse random packing assembly.

In Chapter 4 (Paper “Mode I crack in particulate materials with rotational degrees of freedom”) we investigate the mechanical behaviour of an idealised particulate material with a pre-existing fracture and determine the displacement and rotation fields around the Mode I crack using physical experiments accompanied by the digital image correlation technique of measuring particle rotations, numerical simulations based on discrete element method and analytical solution rested on the concept of the small-scale Cosserat continuum and the conventional equations of linear elastic fracture mechanics. Similarly to the previous chapter, the particulate material is represented by an idealised slightly cemented granular material where circular shaped thin discs are gluing together forming a square packing assembly. The glue is sufficiently flexible and delivers high movement capability. Thus, the adhesive bonds can transmit force moments and the discs are allowed to have relative rotation. The bonds between a few pairs of discs are removed to model the pre-existing fracture, and opening displacement is applied by using a thin wedge.

Chapter 5 considers stability of discrete systems with negative stiffness springs. It is comprised by two papers: “Stability of chains of oscillators with negative stiffness normal, shear and rotational springs” and “Stability of 2D discrete mass-spring systems with negative stiffness springs”. In the first paper the stability of a chain of particles is investigated. Each particle is assumed to have three degrees of freedom: two translational and one rotational. The particles are connected by normal (longitudinal), shear (transverse) and rotational springs with a possibility that stiffness of some springs can be negative. The chain ends are fixed. Different combinations of negative stiffness springs are explored. The stability analysis begins with consideration of a simple harmonic motion of a chain of linear oscillators connected in series by uncoupled normal and shear springs without an external time dependent force. Then masses
connected by coupled shear and rotational springs in the presence and absence of a driving force are studied. Finally, we consider the stability of dynamic system with viscous damping and show the influence of negative stiffness spring on the system’s behaviour.

The objective of the second paper is to analyse the stability of two-dimensional discrete mass-spring systems with negative stiffness springs. Each particle in such systems still has three degrees of freedom. The particles are connected by the same set of normal, shear and rotational springs. We obtain the necessary condition of stability by considering a few simple problems such as a system consisting of a single particle, a “channel” of two particles, two-by-two and three-by-three systems of particles. Then we generalise results for an arbitrary two-dimensional system. The stability is investigated in terms of the positive definiteness of the stiffness matrix, the eigenfrequencies and the trajectories of motion. On top of that, we discuss the necessary condition of stability for three-dimensional systems of particles.

In Chapter 6 (Paper “Wave propagation in materials with negative Cosserat shear modulus”) we explore the effect of negative Cosserat shear modulus on wave propagation in isotropic Cosserat continuum. It was discussed earlier, that rotation of non-spherical particles in the particulate materials under pressure can produce the effect of negative stiffness. We introduce the expression for the wave velocities in the conventional isotropic Cosserat continuum and then generalise them in terms of the negative Cosserat shear modulus. Dispersion relationship for the twist and both shear-rotational waves are analysed for the case of positive and negative Cosserat shear modulus. Furthermore, we consider the relations between velocities of shear-rotational waves and Cosserat shear modulus in order to demonstrate the possibility of wave propagation in solids with negative Cosserat shear modulus. We further discuss the possible practical application of the wave velocity measurements and detection of the twist wave and both shear-rotational waves in non-homogenous materials with the negative modulus.

The thesis ends up with conclusion and discussion about directions for further research.
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Reference

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CHAPTER 2

Multiscale rotational mechanism of fracture propagation in geomaterials
Multiscale rotational mechanism of fracture propagation in geomaterials

Arcady Dyskin\textsuperscript{a,*}, Elena Pasternak\textsuperscript{b} and Maxim Esin\textsuperscript{b}

\textsuperscript{a}School of Civil, Environmental and Mining Engineering, University of Western Australia, Perth, Australia; \textsuperscript{b}School of Mechanical and Chemical Engineering, University of Western Australia, Perth, Australia

(Received 21 October 2014; accepted 20 January 2015)

We consider rotational mechanism of macrocrack propagation based on breakage of the bonds between mutually rotating grains. The mechanism is multiscale with the macroscopic scale corresponding to the macrocrack, the next, smaller scale corresponding to the grain rotations and the smallest scale corresponding to the microcracks formed in the bonds whose propagation causes the bond breakage. The bond breakage is initiated by their bending or twisting caused by the corresponding moments. The sign of the moments only affects the side of the bond where the microfracturing starts. The independence of the microfracturing of the sign of the moment stresses provides a unified way of describing such apparently different types of fractures as tensile (Mode I) cracks, compaction bands (Mode I anticracks) and shear bands (Mode II and III). Modelling of this mechanism is based on the Cosserat theory. The bending/twisting moments are controlled by the corresponding components of moment stress. In the cases, when the Cosserat characteristic lengths are comparable with the grain sizes, the Cosserat theory is reduced to the couple-stress theory. It is found that the stress exhibits the square root singularity that coincides with the conventional ones, while the moment stress has singularity of the power $-3/2$. The $J$-integral, however, reflects only stress singularities, while the moment stress singularities do not contribute to the energy release rate. Subsequently, the energy criterion of macrofracture propagation can be based on the conventional $J$-integral and is not affected by the strong moment stress singularity.

Keywords: shear band; compaction band; particle rotation; Cosserat continuum; bending of bonds; twisting of bonds

1. Introduction

Fracture propagation in geomaterials happens at various scales. At large scales, it constitutes a mechanism of certain types of earthquakes. At smaller scales, it is a mechanism of rock mass instability in mining and petroleum. At the laboratory scale, the fracture propagation is behind failure of rock samples. On top of that, the fracture prop-

*Corresponding author. Email: arcady.dyskin@uwa.edu.au

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agation is a multiscale phenomenon in its own right involving accumulation of damage and formation of patterns of microfractures at different scales.

Often fracture propagation is observed to proceed in its own plane. The in-plane fracture propagation under tensile stress is natural and follows the load symmetry, unless the material heterogeneity or the speed of propagation makes the crack pass to deviate from the plane or bifurcate. In compression – the prevailing stress state in geomaterials – mostly shear fractures and compaction bands get developed. Their in-plane propagation is often observed at different scales [1–5]; however, the mechanics of in-plane propagation is not completely understood.

There is a tendency to treat the compaction bands as negative Mode I cracks (anticracks) when the conventional tensile stress singularity at the crack tip (contour in 3D) is replaced with similar compressive stress singularity (e.g. [6]). This apparent similarity becomes, however, less clear when one takes into account the non-symmetry in rock strength, whereby the compressive strength can be an order of magnitude higher than the tensile one. Furthermore, while the conventional tensile crack is free to open, the anticrack has to have some initial opening to produce the stress singularity. Replacing it with an elliptical soft inclusion, as suggested in e.g. [7], leads to weaker stress concentration and the difficulty in understanding further damage production given high compressive strength of geomaterials.

In-plane growth of shear fractures observed in compression tests of rocks (e.g. [4,8,9]) is even less clear, as the stress distribution caused by shear fractures is clearly asymmetric. Furthermore, in all direct experiments, cracks under applied shear load or inclined cracks under compressive load do not grow in their respective planes, but rather kink, e.g. [10]. Yet, in some cases, in-plane propagation of what looks like shear fractures or bands is observed.

Formation and propagation of shear and compaction bands are accompanied by microcracking that is accumulation of fractures/damage at the scale microscopic to the scale of the band, e.g. [4,11–14]. The observations of the multiple microcrack accumulation, however, fail to shed the light on the mechanics of their coalescence and formation of the step of large-scale fracture propagation. Indeed, the concepts of (micro) crack coalescence are essentially two-dimensional (2D), derived from either observations of rock sections or 2D experiments (e.g. [15–19]). However, three-dimensional (3D) generalization of (micro) crack coalescence is not straightforward, as it would essentially require all microcracks to grow parallel to each other and within a narrow zone to form a 3D surface of the future fracture.

These difficulties can be overcome if one assumes that the observed microcracks only lead to (at least partial) grain de-bonding, which allows the grains to rotate and thus finalize grain detachment from the rest of the geomaterial and thus form propagating fracture. In rock testing, the de-bonding is accomplished at the point of reaching the peak load after which the random and almost uniform accumulation of microcracks is replaced with shear band formation and propagation [8]. We hypothesize that the latter corresponds to the collective grain detachment which propagates as a shear fracture or shear band. We assume that the mechanism of grain detachment is the bond breakage caused by tensile microfractures created by grain rotations due to the action of bending and twisting moments, Figure 1. The independent grain rotations are enabled by intergranular damage developed in the preceding loading. The grain detachment and the subsequent independent rotations are suggested as a mechanism of in-plane propagation
of macrofractures in geomaterials, which are macroscopically Mode I, II and III, as well as Mode I anticracks.

Continuum modelling of deformation of geomaterials in the presence of independent grain rotations requires the use of the Cosserat continuum (e.g. [20]) that takes into account three rotational degrees of freedom on top of the conventional translational ones. A simplifying factor in such analysis is the multiscale nature of fracture propagation whereby the grain dimensions are considerably smaller than the fracture length. We assume that the separation of scales takes place, that is a representative volume element (RVE) of size, $H$, can be introduced for satisfying the following double inequality (e.g. [21–24]):

$$I_m \ll H \ll L$$

where $l_m$ is the characteristic size of the grains; $L$ is, in this case, the crack length. This permits the introduction of a continuum based on the stress–strain fields averaged over the RVE and subsequently the continuum description of fracture propagation. In this inequality, the asymptotics $H/L \to 0$ represents the replacement of the heterogeneous geomaterial with a continuum, while asymptotics $l_m/H \to 0$ makes the volume element representative. Eventually, the necessary condition of the use of continuum is the validity of asymptotics

$$l_m/L \to 0$$

As mentioned, the continuum which models the behaviour of particulate materials such as geomaterials with grains needs to be the Cosserat continuum in order to account for independent grain rotations. The fact that the translational and rotational degrees of freedom are represented by variables of different units – displacements (units of length) and rotations (dimensionless) lead to the emergence of characteristic lengths even in the elastic Cosserat continuum. (The conventional elastic continuum does not have characteristic lengths.)
The characteristic lengths can in principle be both large and small. However, there are cases when the characteristic lengths are of the order of the grain size. As shown in [25–28], this corresponds for instance to the case when the grains are connected by the elastically behaving binder which is sufficiently thick to negate the effect of grain shape. Then, the grains can be modelled by spheres and the binder – by a set of springs. (Rotating non-spherical particles can create elbowing [29] and apparent negative stiffness [30].) In this case, asymptotics (2) leads to a considerable simplification of the analysis formally reducing the full Cosserat theory to the couple-stress theory (the Cosserat continuum with constrained rotations). This results in simplifying of the equations for the stress and moment stress singularity [31].

This simplification was achieved in [21–24] where the concept of small-scale Cosserat continuum was introduced and Mode I and Mode II cracks were considered. The crack propagation criteria were introduced based on comparing the average moment stresses with their critical values determined by initiating the bending-induced tensile microcracks.

The current paper extends the above analysis to Mode III cracks. It also analyses $J$-integrals for all three crack modes and introduces the energy criterion of fracture propagation. Types of microcrack distribution for all three crack modes and the mechanisms of crack propagation are considered. The paper is organized as following. Section 2 is devoted to the introduction into the small-scale Cosserat continuum; Section 3 calculates the Mode I, II and III stress intensity factors; Section 4 analyses the $J$-integrals and formulates the energy criterion of fracture propagation; Section 5 considers the patterns of microfractures that accompany propagation of cracks of these three modes. Section 6 provides the discussion of peculiarities of these crack propagation mechanisms.

2. Asymptotics of small-scale Cosserat continuum

Consider a geomaterial consisting of grains connected by binder and suppose the grain centres are connected by vector $l_m = (l_1, l_2, l_3)$ whose length $l_m = |l_m|$ being a characteristic length of microstructure or microscopic length. In the isotropic geomaterials, we concentrate on, here, the characteristic length is usually the average grain diameter. At a larger scale, if a geomaterial has a blocky structure, the role of the characteristic scale will be played by the average block size. (In the case of regular block shapes, the geomaterial may cease to be isotropic.)

In modelling geomaterial as a continuum, each particle (grain) is assigned a displacement vector $u_i(x)$, associated with the particle centre $x$. After homogenizing, we obtain a continuum whereby the displacement becomes a smooth function of the point $x = (x_1, x_2, x_3)$ of the continuum. The conventional strain tensor – the symmetrical part of the tensor of displacement gradient – reads

$$
\varepsilon_{ij} = \frac{1}{2} (u_{ij} + u_{ji}) \approx \frac{1}{2} \left[ \frac{u_i(x + l_m) - u_i(x)}{l_{mj}} + \frac{u_j(x + l_m) - u_j(x)}{l_{mi}} \right], \quad i, j = 1, 2, 3. \quad (3)
$$

In the Cosserat continuum, each particle (grain) is also characterized by the rotation vector $\varphi_i(x)$. The Cosserat strain tensor is a combination of displacement gradients and rotations
The relative rotations of the particles are represented by components of the curvature-twist tensor, which at a point \( x = (x_1, x_2, x_3) \) reads

\[
\gamma_{ji} = u_{i,j} - \varepsilon_{kji} \varphi_k
\]

(4)

Their counterparts are the non-symmetric stress tensor \( \sigma_{ij} \) (force components per unit area of the faces of the RVE) and the moment stress tensor \( \mu_{ij} \) (components of the moment per unit area of the faces of the RVE). In the case of isotropic Cosserat medium, the stress and moment stress are related to the (Cosserat) strain and the curvature twist through the following constitutive equations [20]

\[
\begin{align*}
\sigma_{ji} &= (\mu + \varepsilon) \gamma_{ji} + (\mu - \varepsilon) \gamma_{ij} + \lambda \delta_{ij} \gamma_{kk}, \\
\mu_{ji} &= (\gamma + \varepsilon) \kappa_{ji} + (\gamma - \varepsilon) \kappa_{ij} + \beta \delta_{ij} \kappa_{kk},
\end{align*}
\]

(6)

where \( \mu \) and \( \lambda \) are the Lamé constants; \( \alpha, \gamma, \varepsilon \) and \( \beta \) are the Cosserat moduli.

The full set of governing equations is obtained by adding the equations of equilibrium that reflect the force and moment equilibrium:

\[
\begin{align*}
\sigma_{ji,j} &= 0, \\
\mu_{ji,j} + \varepsilon_{ijk} \sigma_{jk} &= 0,
\end{align*}
\]

(7)

where \( \varepsilon_{ijk} \) is the alternating tensor; it is equal to 1 if \( (ijk) \) is even, \(-1 \) if \( (ijk) \) is odd and \( 0 \) if \( (ijk) \) has indexes of the same values.

In the constitutive relationship (6), the moduli \( \mu, \lambda \) and \( \alpha \) have the units of stress, while \( \gamma, \varepsilon \) and \( \beta \) have the units of stress per square length. This gives rise to a number of Cosserat characteristic lengths, the most prominent being (e.g. [31])

\[
\begin{align*}
\ell^2 &= \frac{(\mu + \varepsilon)(\gamma + \varepsilon)}{4 \mu \alpha}, \\
\ell_2^2 &= \frac{\gamma + \varepsilon}{4 \alpha}, \\
\ell_2^2 &= \frac{\beta + 2\gamma}{4 \alpha}, \\
\ell_1^2 &= \sqrt{\ell^2 - \ell_2^2}
\end{align*}
\]

(8)

We now compare the characteristic length with the grain dimensions. To this end, we model, following [32,33], the isotropic geomaterial as an assembly of spherical particles of diameter \( D \sim l_m \) connected to each other by elastic bonds, randomly distributed over the particle surface with the coordination number \( k \). It is assumed that each bond is characterized by normal stiffness \( k_n \), the shear (tangential) stiffnesses \( k_s \), the same in both directions, a twist stiffness \( k_{\varphi n} \) and two equal bending stiffnesses \( k_{\varphi s} \).

The stiffnesses can be estimated by modelling the links as elastic cylinders and developing the stress distributions over the cylinder cross-section into Taylor series. Taking into account symmetry, the main terms responsible for classical stiffnesses, \( k_n \) and \( k_s \), are the first (constant) terms in the series, that is using uniform stress distributions. The main terms responsible for twist \( k_{\varphi n} \) and bending stiffnesses \( k_{\varphi s} \) are provided by the second (linear) terms of the distributions of the corresponding
shear and normal stress components. Assuming the bonds to be modelled by cylinders of height $h \sim D$ and radius $b \sim D$, one obtains the following expressions for the stiffnesses [31]:

$$
\begin{align*}
    k_n &\sim \pi l_m E_b, \\
    k_s &\sim \pi l_m G_b, \\
    k_{\phi_k} &\sim \frac{\pi l_m^3 E_b}{4}, \\
    k_{\phi m} &\sim \frac{\pi l_m^3 G_b}{2}
\end{align*}
$$

Here, $E_b$ and $G_b$ are the Young’s modulus and shear modulus of the material of the bond.

Using the homogenization by differential expansions [32,33], we obtain the following relationship between the Cosserat moduli and the bond stiffnesses:

$$
\begin{align*}
    l &\equiv \frac{k_m s}{C_24 l_m} (k_n + 3 k_s), \\
    \alpha &\equiv \frac{k_m s}{2 C_2 l_m} k_s, \\
    \lambda &\equiv \frac{k_m s}{2 C_2 D} (k_n - k_s) \\
    \gamma &\equiv \frac{k_m s}{2 C_2 D} k_{\phi k}, \\
    \varepsilon &\equiv \frac{k_m s}{2 C_2 D} k_{\phi m}, \\
    \beta &\equiv \frac{k_m s}{2 C_2 D} (k_{\phi n} - k_{\phi s})
\end{align*}
$$

Substituting (9) into (10) and the result into (8) leads, taking into account that $D \sim l_m$, to the following estimate:

$$
\begin{align*}
    l &\sim l_m, \\
    I &\geq I_1, I_2
\end{align*}
$$

The fact that the Cosserat length is of the order of the microscopic length together with (2) leads to the asymptotics $l/L \rightarrow 0$, which corresponds to what we call the small-scale Cosserat continuum [27–31]. The asymptotic solution of system (6), (7) can be expressed in the form $u = u^0 + u^1 l^2 + \ldots$, $\varphi = \varphi^0 + \varphi^1 l^2 + \ldots$. The main asymptotic form is given by $u^0, \varphi^0$, which are the solutions of the system:

$$
\begin{align*}
    (\lambda + 2 \mu) \text{grad div } u^0 - \mu \text{rot rot } u^0 &= 0 \\
    \varphi^0 &= \frac{1}{2} \text{rot } u^0
\end{align*}
$$

The first equation is the equation of the classical elasticity, while the second one is the classical expression of the rotation vector through the displacement gradients. Then, the stress and moment stress can be expressed through constitutive equations (6). Thus, the main asymptotic term is given by the couple-stress continuum (the Cosserat continuum with constrained rotations).

We now apply this asymptotics to crack problems. We firstly recall that cracks can be represented as a continuous and yet unknown distribution of dislocations (see details in [31]). Here, the edge dislocations represent the Mode I and II cracks, while the screw dislocations represent the Mode III crack. The couple-stress solutions for dislocations can be obtained using the correspondence theorem [34,35] which ensures that any solution of the equilibrium in displacements of classical elasticity (that is without couple-stresses) at the regular points (points without stress singularities) is also a solution of the corresponding equations of equilibrium in displacements in the couple-stress theory. It follows [31] that in order to obtaining the main asymptotic term for crack problems in the small-scale Cosserat continuum, one needs to solve the problem for a crack in the classical elastic continuum (or take an appropriate existing solution), take the
displacement field and find the field of rotations from the second equation of (12) and then using the Cosserat constitutive equations to find the moment stress distribution.

Essentially, this asymptotics provides the solution valid in a range of lengths which are largely compared to the microscopic length \( l_m \) (or the Cosserat characteristic length \( l \)) and the crack length \( 2L \), as conceptually shown in Figure 2. From this point of view, the small-scale Cosserat continuum is an intermediate asymptotics valid in the range identified.

In the following section we use this method to write the solutions for Mode I and II cracks (following [31]) and develop the solution for Mode III cracks.

3. Mode I, II and III cracks in small-scale isotropic Cosserat continua

Using the procedure outlined above, solutions for Mode I and II cracks in the asymptotics of small-scale isotropic Cosserat continuum can be obtained [31] (we drop the superscript ‘0’ indicating the main asymptotic term). The stress singularity for both crack modes coincides with the classical one (see Figure 2 and the coordinate frame shown there):

\[
\sigma_{22}(r) = \frac{K_I}{\sqrt{2\pi r}}, \quad \sigma_{21}(r) = \frac{K_{II}}{\sqrt{2\pi r}}
\]

where \( r = x_1 - L \) is the distance from the crack tip; \( K_I \) and \( K_{II} \) are the classical stress intensity factors. In particular, for the cracks of length \( 2L \) under uniform loads \( \sigma^0, \tau^0 \), they are \( K_I = \sigma^0 \sqrt{\pi L}, \quad K_{II} = \tau^0 \sqrt{\pi L} \).

The moment stress singularity is obtained by writing the displacement discontinuity at the crack tip for both crack modes:

\[
\begin{pmatrix}
\mu_1 \\
\mu_2
\end{pmatrix} = \frac{K_I}{2\mu} \sqrt{\frac{r}{2\pi}} \begin{pmatrix}
\cos \frac{\theta}{2} \left[ \kappa - 1 + 2 \sin^2 \frac{\theta}{2} \right] \\
\sin \frac{\theta}{2} \left[ \kappa + 1 - 2 \cos^2 \frac{\theta}{2} \right]
\end{pmatrix} + \frac{K_{II}}{2\mu} \sqrt{\frac{r}{2\pi}} \begin{pmatrix}
\sin \frac{\theta}{2} \left[ \kappa + 1 + 2 \cos^2 \frac{\theta}{2} \right] \\
- \cos \frac{\theta}{2} \left[ \kappa - 1 - 2 \sin^2 \frac{\theta}{2} \right]
\end{pmatrix}
\]

where for the plain strain case \( \kappa = 3 - 4\nu \).

Then, after differentiating the displacement discontinuity with respect to \( r \), setting \( \theta = 0 \) and substituting the results into the second equation of (12) and then into (6), we obtain the moment stress components at the crack tip in on the \( r \)-axis [31].
For Mode I crack:

\[ \mu_{13} = 0, \quad \mu_{23} = -\frac{2K_I l_2^2 \pi}{\sqrt{2\pi r^3/2}} \frac{1 - \nu}{\mu} \]  

(15)

For Mode II crack:

\[ \mu_{13} = \frac{2K_{II} l_2^2 \pi}{\sqrt{2\pi r^3/2}} \frac{1 - \nu}{\mu}, \quad \mu_{23} = 0 \]  

(16)

Here, \( l_2 \sim l \sim l_m \) is a Cosserat characteristic length. Hereafter, following \[31\], we use \( l_2 \) as a representative length.

We see that the moment stress has a strong and non-integrable singularity. It will be shown in the following section that these strong singularities do not affect the energy release rate.

Now, consider a Mode III crack that is a 2D crack in an infinite plane under uniform antiplane shear loading (Figure 3).

Using the first expression for deformation measures (4), we can find kinematic relations between the out-of-plane displacement \( u_3 \), rotation vector \( \varphi \) and, strain tensor \( \gamma_{ji} \) [36,37]:

\[ \gamma_{13} = \frac{\partial u_3}{\partial x_1} + \varphi_2, \quad \gamma_{31} = -\varphi_2, \quad \gamma_{23} = \frac{\partial u_3}{\partial x_2} - \varphi_1, \quad \gamma_{32} = \varphi_1, \]  

(17)

\[ \gamma_{11} = \gamma_{22} = \gamma_{33} = \gamma_{12} = \gamma_{21} = 0 \]

Taking into the account the dependence between the vector of rotation \( \varphi \) and the vector of displacements \( u \) (the second equation of (12)), non-zero components of strain tensor \( \gamma_{ji} \) and curvature-twist tensor \( \kappa_{ji} \) read:

\[ \gamma_{13} = \gamma_{31} = \frac{1}{2} \frac{\partial u_3}{\partial x_1}, \quad \gamma_{23} = \gamma_{32} = \frac{1}{2} \frac{\partial u_3}{\partial x_2}, \]  

\[ \kappa_{11} = -\kappa_{22} = \frac{1}{2} \frac{\partial^2 u_3}{\partial x_1 \partial x_2}, \quad \kappa_{12} = -\kappa_{21} = \frac{1}{2} \frac{\partial^2 u_3}{\partial x_1 \partial x_2}, \]  

(18)

In the case of antiplane problem, the Hooke’s law (6) reads:

Figure 3. A crack of length 2L in an infinite body under uniform antiplane shear loading under uniform load \( \tau_0 \).
\[
\begin{align*}
\mu_{12} &= (\gamma + \varepsilon)\kappa_{12} + (\gamma - \varepsilon)\kappa_{21}, \\
\sigma_{13} &= \sigma_{31} = 2\mu\gamma_{13}, \\
\sigma_{23} &= \sigma_{32} = 2\mu\gamma_{23}, \\
\mu_{11} &= -\mu_{22} = 2\mu\kappa_{11}, \\
\end{align*}
\]  
\tag{19}
\]
where \(\lambda\) and \(\mu\) are the Lamé constants; \(\varepsilon\) and \(\gamma\) are the Cosserat moduli.

Similarly to Mode I and II cracks (see above), for Mode III cracks, the main asymptotic terms of displacement and rotation discontinuities coincide with those for the classical crack, and the stress singularity at the crack tip coincides with the classical one. Thus, on the crack continuation (\(x_1\)-axis), the stress singularity has the usual form:

\[
\sigma_{23}(r) = \frac{K_{III}}{\sqrt{2\pi r}}
\]

where \(r = x_1 - L\) is the distance from the crack tip and \(K_{III}\) is the classical stress intensity factor. In particular, for the cracks of length \(2L\) under uniform load \(\tau^0\), it reads:

\[
K_{III} = \tau^0\sqrt{\pi L}.
\]

The displacement near the crack tip is taken from the classical solution for Mode III (e.g. [38]):

\[
u_3 = 2\frac{K_{III}}{\mu} \left(\frac{r}{2\pi}\right)^{1/2} \sin\frac{\theta}{2}
\]

Substituting (21) into (18) and (19) after some algebra, we obtain the moment stress singularities at the \(x_1\)-axis for Mode III cracks:

\[
\mu_{12} = \mu_{21} = 0, \quad \mu_{11} = -\mu_{22} = -\frac{K_{III}}{2\sqrt{2\pi r^{3/2}}} \frac{\gamma}{\mu}
\]

\tag{22}

It can be noted the main asymptotic term for moment stress has singularity \(-3/2\), while the main asymptotic term for stress has a classical square root singularity. It is the same type of singularity as for Mode I and II cracks and corresponds to the results [34,39,40].

### 4. Multiscale rotational mechanism of crack growth

The results presented in the previous section show that on top of the conventional stress singularities the cracks have the moment stress singularities. The latter can be responsible for crack growth mechanisms different from the conventional ones in that they are based on microfracturing initiated by mutual rotations of the grains. Figure 4 illustrates these mechanisms for Mode I crack and anticrack and for Mode II cracks. This mechanism is essentially multiscale. At the macroscale, the crack creates stress and moment stress singularities. At the next, smaller scale that is at the scale of the RVE these stresses are considered as uniform within the RVE (as per its definition). At this scale, i.e. at the scale of the material microstructure within the RVE different moment stress components (the stresses are not shown in Figure 4) impose mutual grain rotations leading to bending and/or twisting of the bonds. At the smallest scale bonds bending/
twisting produces tensile microcracks and microfailure and eventually a step of (macro) crack propagation.

We note that the described rotational mechanism of crack growth essentially creates microfailure ahead of the crack in its own plane, thus affecting macroscopic in-plane crack growth as usually observed in rock failure at different scales (see Introduction).

A criterion of macroscopic crack growth can then be proposed based on the magnitudes of the moment stress at a distance \( H \) from the crack tip, where \( H \) is the size of the RVE. Using asymptotics (1) to the limits, we can assume that \( H \sim l_m \) \cite{31,41}. Based on (11) and in order to be consistent with (15) and (16), we will use the Cosserat length \( l_2 \). Then, the stress (using the conventional solution, e.g. \cite{38}) and moment stress at distance \( l_2 \) for Mode I and Mode II respectively are \cite{31}:

\[
\sigma_{22} = \frac{K_I}{\sqrt{2\pi l_2}}, \quad \mu_{23} = -\frac{2K_I\sqrt{l_2}}{\sqrt{2\pi}} \frac{(1 - v)\pi}{\mu}, \quad \sigma_{21} = \frac{K_{II}}{\sqrt{2\pi l_2}}, \quad \mu_{13} = \frac{2K_{II}\sqrt{l_2}}{\sqrt{2\pi}} \frac{(1 - v)\pi}{\mu}
\]

(23)

As stated above, the bond breakage is assumed to be caused by the flexural crack initiated by the microscopic tensile stress induced by bond bending. The corresponding bending moment can be estimated by assuming the link to be of a cylindrical shape. The bending stress acts on the area of the order of \( \pi l_2^2/4 \), where we assumed, following \cite{31},
that the bond size is of the order of the grain size and hence of the order of the Cosserat length $l_2$. As a result, the maximum microscopic tensile stress caused by bending is

$$\sigma_m = \frac{32M}{\pi l_2^3}, \quad M = \frac{\pi}{4} \mu_3 l_2^2, \quad p = \begin{cases} 2 & \text{for Mode I crack} \\ 1 & \text{for Mode II crack} \end{cases} \quad (24)$$

Finally using (23) and assuming $1 - \nu \sim 1$, we obtain the following estimates of the microscopic stress causing the bond failure. (We use the absolute values for the stress intensity factors since the sign only controls which side of the bond is going to fracture.)

$$\sigma_m \sim \frac{|K_{I,II}|}{(2E_b/3G_b + 1)3\sqrt{2\pi l_2}} \quad (25)$$

We note that the expressions for the maximum microscopic stress are similar for Mode I and II cracks. Another observation is that the moment stress tends to zero as $l_2 \to 0$, while the conventional stress tends to infinity. Nevertheless, the influence of moment stress is far from being insignificant as the microscopic stress $\sigma_m$ in the bonds created by moment stress is an order of magnitude higher than the stress $K_{I,II}(2\pi l_2)^{-1/2}$ created at distance $l_2$ from the crack tip by the conventional stress singularity.

Similarly to Mode I and II, breaking of bonds between particles due to their mutual rotation is the additional crack growth mechanism in the case of Mode III crack. However, in contrast to Mode I and II where microcracks are created by bond bending, Mode III induces the bond twisting which leads to the development of multitude of microcracks inclined at $45^\circ$ to the crack plane, Figure 5.

According to (22), the absolute values of the moment stress $\mu_{11}$ and $\mu_{22}$ are equal to each other. But the singular term of moment stress $\mu_{11}$ created by a Mode III crack is negative, and the singular term of moment stress $\mu_{22}$ is positive.

![Figure 5. (colour online) Multiscale rotational mechanism of Mode III crack growth. The scales involved are the same as in Mode I and II cracks multiscale.](image-url)
As discussed, in the small-scale Cosserat continuum, the distances smaller than \( l_2 \) cannot be assigned physical meaning. We consider the criterion of crack growth based on calculating the stress and moment stress at distance \( l_2 \) from the crack tip. The non-zero stress and moment stress components acting on the line of Mode III crack continuation (\( x_1 \)-axis) at distance \( l_2 \) from the crack tip are:

\[
\sigma_{23} = \frac{K_{III}}{\sqrt{2\pi r}}, \quad \mu_{11} = -\mu_{22} = -\frac{K_{III} \sqrt{l_2}}{\sqrt{2\pi}} \frac{2\gamma}{(\gamma + \varepsilon)\mu}
\]

(26)

Using the concept developed for the Mode I and II cracks, we estimate the relative importance of the crack growth mechanisms based on the classical and moment stresses. In contrast to Mode I and II cracks where we had bond bending, here the bond breakage is caused by microcracks initiated by the normal microstresses induced by bond torsion. The bond torsion is caused by the torsion moment \( M \) in the inter-grain bonds. The torsion moment can be estimated by assuming again that the links have cylindrical shape. The torsion stress acts on the area of the order of \( \pi l_2^2 / 4 \). Then, the torsion moments are \( M_1 = \mu_{11} \pi l_2^2 / 4 \) and \( M_2 = \mu_{22} \pi l_2^2 / 4 \).

As the normal (principal) microstresses are created in this case by the maximum shear microstresses, we will compare the latter that are generated by the moment stress singularity and the conventional stress singularity. Assuming the maximum microscopic shear stress components caused by torsion being \( \tau_{m(1,2)} = M_{(1,2)}/W_p = 16 M_{(1,2)}/\pi l_2^2 \) and using (9) and (10), we obtain the following estimates. Since the sign of \( K_{III} \) only influences the direction of microcrack formation, we use absolute value of the stress intensity factor:

\[
\tau_m \approx \frac{|K_{III}|}{\sqrt{2\pi l_2}} \frac{20G_b(G_b/2 + 3E_b/8)}{(3G_b/2 + E_b)(G_b/2 + E_b)}
\]

(27)

In the conventional linear elastic fracture mechanics, the shear stress created by a Mode III crack is \( K_{III} (2\pi l_2)^{-1/2} \). From (27), the microscopic stress \( \tau_m \) in the bonds created by the moment stress is several times higher than the stress created at distance \( l_2 \) from the crack tip by the conventional stress singularity.

5. Energy release rate for Mode I, II and III cracks in the Cosserat continuum with constrained rotations

In the previous section, we have introduced the criteria of crack growth based on a rotational mechanism of microscopic failure. In many cases, it is convenient to use energy criteria, especially when the details of microscopic failure are not completely clear. We will now concentrate on formulating an energy criterion for cracks in the Cosserat continuum. In the process, we shall investigate whether the non-integrable moment stress singularity can lead to infinite energy release rate. To this end, we calculate the \( J \)-integral for Mode I, II and III cracks in the Cosserat continuum following [42–44]:

38
\[ J_m = \int_{\Gamma} (Wn - T_iu_i - M_i\phi_{i,m})ds - \int_{\tilde{V}_\Gamma} (f_iu_i + m_i\phi_{i,m})d\tilde{V} \]  

(28)

where \( W \) is the elastic energy per unit volume (strain energy density); \( \Gamma \) is the contour about the crack tip along which the \( J \)-integral is calculated; \( n \) is the outward normal to a contour \( \Gamma \); \( T_i = \sigma_jn_j \) and \( M_i = \mu_jn_j \) are the stress vector (traction) and the moment vector, respectively; \( f_i \) and \( m_i \) are the body forces and moments, respectively, acting throughout the volume of a body \( V_\Gamma \) bounded by the contour \( \Gamma \). The energy release rate is invariant with respect to the choice of contour \( \Gamma \) and volume \( V_\Gamma \).

Consider an arbitrary crack parallel the \( x_1 \)-axis in an infinite plane \((x_1, x_2)\) as shown in Figure 6. For the case of zero body forces and moments and after transformation to polar from Cartesian coordinates expression (28) reads:

\[ J_1 = \int_{-\pi}^{\pi} (W \cos \theta - T_iu_{i,1} - M_i\phi_{i,1})r d\theta, \quad J_2 = J_3 = 0 \]  

(29)

The strain energy density for the isotropic Cosserat continuum is a function of relative deformations \( \gamma_{ij} \) and twist-curvatures \( \kappa_{ij} \) [20,45]. In the absence of thermal components, the strain energy density is defined as:

\[ W = \frac{\mu + \alpha}{2} \gamma_{ij} \gamma_{ij} + \frac{\mu - \alpha}{2} \gamma_{ij} \gamma_{ij} + \frac{\lambda}{2} \gamma_{kk} \gamma_{nn} + \frac{\gamma + \epsilon}{2} \kappa_{ij} \kappa_{ij} + \frac{\gamma - \epsilon}{2} \kappa_{ij} \kappa_{ij} + \frac{\beta}{2} \kappa_{kk} \kappa_{nn} \]  

(30)

where \( \lambda \) and \( \mu \) are the Lamé constants; \( \alpha, \gamma, \epsilon \) and \( \beta \) are the Cosserat moduli. Also, it should be noticed that \( \lambda, \mu \) and \( \alpha \) have dimension of stress, but \( \gamma, \epsilon \) and \( \beta \) have dimension of stress times square of length.

Figure 6. The path for calculating the \( J \)-integrals.
In particular cases of the cracks under uniform tensile stress and uniform shear loading (Mode I and II) and under uniform antiplane shear loading (Mode III), the expressions for the strain energy density (30) become:

\[
W(I,II) = \frac{\mu + \alpha}{2} (\gamma_{11}^2 + \gamma_{22}^2 + 2\gamma_{11}\gamma_{22}) + \frac{\mu - \alpha}{2} (\gamma_{11}^2 + \gamma_{22}^2 + 2\gamma_{21}\gamma_{12}) + \frac{c}{2} \left( \kappa_{11}^2 + \kappa_{22}^2 + \kappa_{12}^2 + \kappa_{21}^2 \right), \tag{31}
\]

\[
W(III) = \frac{\mu + \alpha}{2} (\gamma_{23}^2 + \gamma_{13}^2) + \frac{\gamma + \epsilon}{2} \left( \kappa_{11}^2 + \kappa_{22}^2 + 2\kappa_{12}\kappa_{21} \right) + \frac{\beta}{2} \left( \kappa_{11}^2 + \kappa_{22}^2 + 2\kappa_{11}\kappa_{22} \right) \tag{32}
\]

where \( W(I,II) \) is the strain energy density for Mode I and II cracks, and \( W(III) \) is the strain energy density for Mode III crack.

Substituting these expressions into expression (29) for the \( J \)-integral, we obtain the final expressions for calculating the energy release rates for Mode I, II and III:

\[
J_{1}^{(I,II)} = \frac{1}{2\mu} \left( W(I,II) \cos \theta - T_1 u_{1,1} - T_2 u_{2,1} - M_3 \phi_{3,1} \right) \tag{33}
\]

\[
J_{1}^{(III)} = \frac{1}{2\mu} \left( W(III) \cos \theta - T_3 u_{3,1} - M_1 \phi_{1,1} - M_2 \phi_{2,1} \right) \tag{34}
\]

where the components of stress vector and the moment stress vector are

\[
T_1 = \sigma_{11} \cos \theta + \sigma_{21} \sin \theta, \quad T_2 = \sigma_{12} \cos \theta + \sigma_{22} \sin \theta, \quad T_3 = \sigma_{13} \cos \theta + \sigma_{23} \sin \theta
\]

\[
M_1 = \mu_{11} \cos \theta + \mu_{21} \sin \theta, \quad M_2 = \mu_{12} \cos \theta + \mu_{22} \sin \theta, \quad M_3 = \mu_{13} \cos \theta + \mu_{23} \sin \theta \tag{35}
\]

Substituting the expressions for the displacements near the crack tip (14), (21) into (33), (34) and integrating along the contour \( \Gamma \), we obtain the values of \( J \)-integral for Mode I, II and III cracks in the small-scale Cosserat continuum:

\[
J_{1}^{(I)} = \frac{K_I^2 (1 - \nu)}{2\mu}, \quad J_{1}^{(II)} = \frac{K_{II}^2 (1 - \nu)}{2\mu}, \quad J_{1}^{(III)} = \frac{K_{III}^2}{2\mu} \tag{36}
\]

It is easy to see that these expressions coincide with the corresponding expressions for the classic continuum (e.g. [38]). This means that in the asymptotics of the small-scale Cosserat continuum, the rotational degrees of freedom do not contribute to the \( J \)-integrals. Obviously, this is due to the fact that the displacement and rotation fields have been obtained using the equations of the classical continuum where only three translational degrees of freedom exist.
and hence only conventional stresses exist. As a consequence, the moment stresses do not contribute to the energy release rate. That is why the presence of non-integrable singularity in the expressions for the moment stresses does not affect the energy.

Now, the energy criterion of the (macroscopic) crack propagation can be expressed in the usual way by comparing the corresponding $J$-integral with the (macroscopic) specific fracture energy. In particular, according to [28] the energy criterion of the Mode I anticrack (the compaction band) is

$$\left(K_I^2 + K_{II}^2\right)\left(1 - \nu^2\right)E^{-1} = \gamma_b + \gamma_s + \gamma_c$$

(37)

where $\gamma_b$ is the specific fracture energy of fractured bonds, $\gamma_s$ is the specific energy related to shear of the new fracture surfaces and $\gamma_c$ is the specific energy related to compaction of the geomaterial due to rearrangement of the grains. Here, $E$ and $\nu$ are the Young’s modulus and Poisson’s ratio of the geomaterial. Furthermore, if we assume that the width of the bond is of the order of $l_2/2$, then the fracture area is $\sim l_2^2/4$ and $\gamma_b \sim v k \gamma_f/4$, where $v$ is volumetric fraction of the particles, $k$ is the coordination number and $\gamma_f$ is the specific fracture energy of the material of the bonds. The specific energy related to shearing of the new fracture surfaces $\gamma_s$ could be estimated if one knows the magnitude of compressive stress $p$ acting on the fracture plane and the friction coefficient $\mu$ associated with particle rolling. Then, $\gamma_s = \mu p$ times unit length in the direction of crack contour. In the case of compaction bands, the specific compaction energy is $\gamma_c \sim p V$, where $p$ is the compressive stress causing compaction and $V$ is the displacement discontinuity (convergence of the compaction band faces) due to re-compaction.

6. Stress, moment stress distribution around crack tip and the patterns of macrofractures

In Section 4, a possible mechanism of in-plane crack propagation based on bond breakage due to grain rotation was considered. Here, we are going to investigate the stress and moment stress distribution around the crack tip in an attempt to analyse a possibility of the rotation mechanism producing deviation from the in-plane propagation or even kinking. We will also consider possible microfracture patterns associated with the rotational mechanism of crack propagation.

We start with Mode I crack. Near the crack tip, the singular stress field for Mode I crack is expressed as [38]:

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{12} \\ \sigma_{22} \end{bmatrix} = \frac{K_I}{\sqrt{2\pi r}} \begin{bmatrix} 1 - \sin(\theta/2) \sin(3\theta/2) \\ \sin(\theta/2) \cos(3\theta/2) \\ 1 + \sin(\theta/2) \sin(3\theta/2) \end{bmatrix}$$

(38)

Near the crack tip, the singular moment stress field is easy to obtain by substituting the displacement vector (14) into the constitutive Equations (12) and (6):

$$\begin{bmatrix} \mu_{13} \\ \mu_{23} \end{bmatrix} = \frac{K_I B(1 - \nu)}{2\sqrt{2\pi}r^{3/2}} \begin{bmatrix} \sin(3\theta/2) \\ -\cos(3\theta/2) \end{bmatrix}$$

(39)
where $B = \gamma + \varepsilon$.

We now introduce dimensionless groups for stress and moment stress:

$$
\begin{bmatrix}
\sigma_{11}^D \\
\sigma_{12}^D \\
\sigma_{22}^D
\end{bmatrix}
= \frac{\sqrt{2\pi r}}{K_I} \begin{bmatrix}
\sigma_{11} \\
\sigma_{12} \\
\sigma_{22}
\end{bmatrix},
\begin{bmatrix}
\mu_{13}^D \\
\mu_{23}^D
\end{bmatrix}
= \frac{2\sqrt{2\pi r} \mu^3/2}{K_I B (1 - \nu)} \begin{bmatrix}
\mu_{13} \\
\mu_{23}
\end{bmatrix}
$$

The dimensionless stress and moments stress fields near the crack tip are shown in Figure 7 as functions of the polar angle $\theta$. As can be seen, the components of moment stress have the maximum magnitudes at $\theta = 0^\circ$, $\theta = \pm 60^\circ$ and $\theta = \pm 120^\circ$. In particular, moment stress component $\mu_{23}$ (we drop the subscript ‘0’ indicating the normalization) has the maximum magnitude at $\theta = 0^\circ$ that is in the crack plane thus affecting in-plane crack propagation by producing microcracks continuing the crack, Figure 8(a). The other component, $\mu_{13}$, while zero on the continuation of the crack has maxima of the magnitude (the sign of the moment stress only determines from which side the bond gets broken) at $\theta = \pm 60^\circ$. Since the magnitudes of maxima of $\mu_{13}$ are the same as of the maximum of $\mu_{23}$, the microfracturing will happen at both $\theta = 0^\circ$ and $\theta = \pm 60^\circ$. Furthermore, due to the nature of microfracturing created by component $\mu_{13}$, Figure 8(a), the microfracture pattern will be en-echelon tracing the (macro) crack from both sides, Figure 8(b). On top of that, component $\mu_{13}$ has maxima of its magnitude at $\theta = \pm 120^\circ$. This will create two arrays of collinear microcracks on both sides of the (macro) crack, straight behind the crack tip, Figure 8(b). Therefore, the rotational mechanism of Mode I crack growth will create a structure propagating in the plane of the macrocrack as a band. A similar situation should happen in the case of Mode I anticrack (compaction band) with the only difference that the bonds will bend in the directions opposite to Mode I crack.

As the expressions for the stress at the crack tip coincide with the conventional crack solution (e.g. [38]), the conventional criteria of Mode I crack propagation stay the same, predicting its in-plane growth.

We now proceed with Mode II and III cracks. Using the same technique, we obtain the following moment stress distributions around the crack tip:

**Mode II crack:**

![Figure 7. (colour online) Stress and moments stress near the crack tip for Mode I crack.](image)
Figure 8. (colour online) Full rotational mechanism of band-like Mode I crack propagation: (a) types of rotational bond breakage around Mode I crack tip; (b) the (micro) fracture pattern created by rotational bond breakage mechanism during the shear-band type propagation. Here (1) marks parallel (collinear) microfractures created by moment stress component $\mu_{23}$; (2) marks en-echelon pattern created by moment stress component $\mu_{13}$.

\[
\begin{align*}
\begin{pmatrix}
\mu_{13} \\
\mu_{23}
\end{pmatrix} &= \frac{K_{II}B(1 - v)}{2\sqrt{2}\pi \mu r^{3/2}} \begin{pmatrix}
\cos(3\theta/2) \\
\sin(3\theta/2)
\end{pmatrix}
\end{align*}
\]  

(41)

Mode III crack:

\[
\begin{align*}
\begin{pmatrix}
\mu_{11} \\
\mu_{12} \\
\mu_{22}
\end{pmatrix} &= \frac{K_{III}}{2\sqrt{2}\pi \mu r^{3/2}} \begin{pmatrix}
-\frac{\mu}{2} \cos(3\theta/2) \\
-\gamma \sin(3\theta/2) \\
\frac{B}{2} \cos(3\theta/2)
\end{pmatrix}
\end{align*}
\]  

(42)

In order to enable the comparison with the classical mechanisms of crack growth, we also add the stress distributions around the crack tip, which coincides with the conventional ones [38]:

Mode II crack:

\[
\begin{align*}
\begin{pmatrix}
\sigma_{11} \\
\sigma_{12} \\
\sigma_{22}
\end{pmatrix} &= \frac{K_{II}}{\sqrt{2}\pi r} \begin{pmatrix}
-\sin(\theta/2)[2 + \cos(\theta/2) \cos(3\theta/2)] \\
\cos(\theta/2)[1 - \sin(\theta/2) \sin(3\theta/2)] \\
\sin(\theta/2) \cos(\theta/2) \cos(3\theta/2)
\end{pmatrix}
\end{align*}
\]  

(43)
Mode III crack:

\[
\begin{Bmatrix}
\sigma_{13} \\
\sigma_{23}
\end{Bmatrix} = \frac{K_{III}}{\sqrt{2\pi r}} \begin{Bmatrix}
- \sin(\theta/2) \\
\cos(\theta/2)
\end{Bmatrix}
\] (44)

We again introduce the dimensionless groups for stress and moment stress:

Mode II crack:

\[
\begin{Bmatrix}
\sigma'_{11} \\
\sigma'_{12} \\
\sigma'_{22}
\end{Bmatrix} = \frac{\sqrt{2\pi r}}{K_{II}} \begin{Bmatrix}
\sigma_{11} \\
\sigma_{12} \\
\sigma_{22}
\end{Bmatrix}, \quad \begin{Bmatrix}
\mu'_{13} \\
\mu'_{23}
\end{Bmatrix} = \frac{2\sqrt{2\pi} \mu^{3/2}}{K_{II} B(1 - v)} \begin{Bmatrix}
\mu_{13} \\
\mu_{23}
\end{Bmatrix}
\] (45)

Mode III crack:

\[
\begin{Bmatrix}
\sigma''_{13} \\
\sigma''_{23}
\end{Bmatrix} = \frac{\sqrt{2\pi r}}{K_{III}} \begin{Bmatrix}
\sigma_{13} \\
\sigma_{23}
\end{Bmatrix}, \quad \begin{Bmatrix}
\mu''_{13} \\
\mu''_{23}
\end{Bmatrix} = \frac{2\sqrt{2\pi} \mu^{3/2}}{K_{III}} \begin{Bmatrix}
\frac{2}{5} \mu_{11} \\
\frac{2}{5} \mu_{12}
\end{Bmatrix}
\] (46)

Figure 9 shows the dependence of the moment stress singularity on the polar angle \( \theta \). It is clear from the plots that in Mode II crack, moment stress component \( \mu_{13} \) (we drop the subscript ‘0’ indicating the normalization) has the maximum magnitude at \( \theta = 0^\circ \) that is

![Figure 9](image_url)
in the crack plane thus affecting in-plane crack propagation by producing en-echelon type fracture pattern, see Figure 10(b). The other component, $\mu_{23}$, while zero on the continuation of the crack has maxima of the magnitude (the sign of the moment stress only determines from which side the bond gets broken) at $\theta = \pm 60^\circ$. Since the magnitudes of maxima of $\mu_{23}$ are the same as of the maximum of $\mu_{13}$, the microfracturing will happen at both $\theta = 0^\circ$ and $\theta = \pm 60^\circ$. Furthermore, due to the nature of microfracturing created by component $\mu_{23}$, Figure 10(a), the fracture pattern will resemble an array of parallel (collinear) microcracks tracing the (macro) crack from both sides, Figure 10(b). On top of that, component $\mu_{23}$ has maxima of its magnitude at $\theta = \pm 120^\circ$. This will create en-echelon microcracks on both sides of the (macro) crack, straight behind the crack tip, Figure 10(b). Therefore, the rotational mechanism of Mode II crack growth will also create a structure propagating in the plane of the macro-crack in a shear band fashion.

Comparing the rotational mechanism with the conventional mechanisms that control the direction of Mode II crack propagation, we note that in our case, the expressions for the stress at the crack tip coincide with the conventional crack solution (e.g. [38])
and the conventional criteria of Mode II crack propagation stay the same, predicting kinking no matter what criterion is used (e.g. [46] and a review in [47]). On the other hand, the distribution of the magnitudes of moment stress is symmetrical with respect to the crack line. From this point of view, the criterion based on the moment stress is the only one that predicts the in-plane growth of Mode II cracks. The fact that this criterion requires the existence of grain rotation (for instance enabled by the formation of damage during compressive loading) is the reason why in direct experiments the artificial Mode II cracks always kink while shear bands propagate in their own planes.

Mode III crack develops distributions of moment stress whose magnitudes have maxima at $\theta = 0^\circ$, $\pm 60^\circ$ and $\pm 120^\circ$. The corresponding moment stress components produce both bond-twisting and bond-bending microfailure. Subsequently, the rotational mechanism of Mode III crack growth makes it propagate in a bond-like fashion, Figure 10, similarly to what happens in the Mode I and II cases. As the expressions for the stress at the crack tip coincide with the conventional crack solution (e.g. [38]), the conventional criteria of Mode III crack propagation stay the same, predicting its in-plane growth.

Figure 11. (colour online) Full rotational mechanism of shear band-like Mode III crack propagation: (a) types of rotational bond breakage around Mode II crack tip; (b) the (micro) fracture pattern created by rotational bond breakage mechanism during the shear band type propagation. Here (1) marks the microfractures created by moment stress component $\mu_{11}$ (torsion); (2) marks the microfractures created by moment stress component $\mu_{22}$ (torsion); (3) marks the microfractures created by moment stress component $\mu_{12}$ (bending).
7. Discussion

The multiscale rotational mechanism of crack propagation leads to a formation of a band-like fracture that is a feature with a width of the order of the grain size. For Mode I cracks, this is consistent with the presence of non-elastic, energy-dissipating zone around the crack tip observed in experiments with large cracks in concrete of different microstructures [48].

In Mode II, the formation of shear bands in rock failure is well documented (e.g. [4,49]). Furthermore, the alteration of microfracture patterns in front and behind the crack tip in the considered plane and antiplane (Mode III) situations, Figures 8, 10, 11, suggests that the rotational mechanism of fracture propagation leaves detached grains in the wake of a propagating crack. In the case of Mode II fractures, these detached grains may be behind the formation of the gouge observed in shear fractures in rock samples (e.g. [4,49]).

The rotational mechanism of crack propagation is essentially symmetrical. The asymmetry of the microfracture pattern observed by Reches and Lockner [4] after shear failure of rock samples can be explained by the superposition of the moment stresses with asymmetrical conventional stresses.

The above reasoning was based on the types of moment stress singularity at the crack tip. It is also necessary to investigate whether at the crack centre the signs of moment stress components remain the same as behind the crack tip. In addition, while the moment stresses at the crack tip in a continuum are formally singular, the stress and moment stress should be looked at a distance $l_2$ from the crack tip. Then, the magnitude of moment stress is finite and can be compared with that at the crack centre. We will conduct this analysis for a crack of Mode I by considering a crack of length $2L$ in an infinite plane under uniform tensile stress $\sigma$. The expressions for displacement field around the crack, assuming plane strain approximation, can for instance be taken from [50]. They read:

\[
\begin{align*}
    u_1 &= \frac{1-2\nu}{\mu} \frac{\partial \Re Z}{\partial x_1} - \frac{\nu}{\mu} \frac{\partial \Im Z}{\partial x_1} \\
    u_2 &= \frac{1-2\nu}{\mu} \Im Z - \frac{\nu}{\mu} \Re Z
\end{align*}
\]

where $Z$ is the complex stress function,

\[ Z = \frac{\sigma}{\sqrt{1 - (L/z)^2}}, \quad z = x_1 + i x_2 \]

Substituting displacements (47) into the second equation of (12) and then into the second equation of (6), we obtain:

\[ \mu_{13} = B \frac{1 - \nu}{\mu} \frac{\partial \Im Z}{\partial x_1}, \quad \mu_{23} = B \frac{1 - \nu}{\mu} \frac{\partial \Re Z}{\partial x_1} \]

where $B = \gamma + \varepsilon$.

Substituting (48) into (49), after some algebra one can find the moment stress in plain strain when $\nu = 0$ and $-L < x < L$:  

\[ 47 \]
Employing the same technique as in Section 4 and using (9) and (10), we can estimate the microscopic tensile stress induced by bond bending caused by moment stress $\mu_{13}$ at points $x_1 = 0$ (the centre of the crack) and $x_1 = L - l_2$ (the point behind the crack tip at a distance $l_2$ from it):

$$x_1 = 0 : \quad \sigma_m \sim 8 \frac{\mu_{13}^2}{L^2} \frac{|K_1|}{\sqrt{2\pi l_2}}$$

$$x_1 = L - l_2 : \quad \sigma_m \sim 3 \frac{|K_1|}{\sqrt{2\pi l_2}}$$

As can be seen from Figure 12, the signs of the moment stresses at the crack centre and at the crack tip behind it are the same. Furthermore, the highest magnitude of microscopic tensile stresses due to moment stresses at $y = 0$ is located near the crack tip [31] and equal to $11|K_1|/\sqrt{2\pi l_2}$. This is of course because by assumption $l_2<<L$. Obviously, it means that fracturing due to bond breakage is created in the crack tip zone and forms a band as the crack propagates.

In this paper, we have considered a mechanism of in-plane band-like fracture propagation often observed in particulate materials such as rock and concrete. At a macro-scale, the band may appear as a crack. Then, the bending/twisting mode of bond breakage can serve as microscopic triggers of the crack front/surface instabilities, especially in a mixed-mode loading (the conditions of instability of crack geometry are dis-
cussed elsewhere, e.g. [51,52]). Also in the mixed-mode loading, the band-like fracture propagation can still result in kinking if the ambient compression is insufficient to suppress out-of-plane crack growth initiated by the bond breakage.

8. Conclusions

The proposed multiscale rotational mechanism of propagation of macroscopic cracks of classical modes is based on breakage of the bonds between the grains or other relevant constituents of the material caused by their mutual rotation. These constituents form the next, finer scale. In the case of Mode I and Mode II cracks, the mutual rotations cause bending of the bonds followed by initiation and propagation of flexural microcracks in the bonds. The crack mode determines the orientations of the microcracks, while the signs of the corresponding $K_I$ and $K_{II}$ determine the direction of the microcrack growth, i.e. the side of the bond from which its breakage starts. In the case of Mode III cracks, the mutual rotations cause twisting of bonds located in front and behind the crack tip and a combination of bond twisting and bending at other locations. Bond twisting causes the development and propagation of tensile microcracks in the directions inclined at 45° to the bond directions. The microcracks developed during the bond bending/twisting form the smallest scale in the discussed rotational mechanism.

The common features of microfracturing associated with these types of rotations are: (1) the symmetry of the microfracturing with respect to the macrocrack, which ensures in-plane propagation of the macrocrack; (2) a certain width of the microfractured areas, which leads to a band-like propagation of the macroscopic crack; and (3) the microstresses created by the bending or twisting dominate the microstresses associated with the conventional stress singularities.

The first feature explains the often observed in-plane propagation of shear bands, which cannot be explained by modelling the shear bands as conventional Mode II cracks due to asymmetry of the associated stress concentration. On top of that, the third feature explains the dominance of the rotational mechanism over the conventional crack growth mechanisms. The second feature explains the band-like appearance of natural fractures. Furthermore, the independence of the microfracturing of the sign of the moment stresses provides a unified way of describing such apparently different types of fractures as tensile (Mode I) cracks, compaction bands (Mode I anticracks) and shear bands (Mode II and III).

Modelling of the rotational mechanism of macroscopic crack propagation requires the use of at least the Cosserat theory. We conduct the modelling for a specific case when the Cosserat characteristic lengths are of the order of microstructural size of the geomaterial. This, in particular, corresponds to the microstructure consisting of grains connected by elastic bonds. In this case, the Cosserat theory reduces to the couple-stress theory offering a considerable simplification. It is found that the stress exhibits the square root singularity that coincides with the conventional ones, while the moment stress has singularity of the power $-3/2$. The $J$-integral, however, reflects only stress singularities with moment stress singularities having no part in it. Therefore, the fact that the $-3/2$ singularity is not integrable does not affect the energy release rate which remains finite. Subsequently, the $J$-integral reflects the energy change caused by macroscopic crack propagation through the rotational mechanism. This gives rise to the energy criterion of crack propagation that involves grain rotations. In particular, the
energy criterion of the compaction band propagation of specific fracture energy consists of three terms: the fracture energy of the bonds (present in all types of fractures considered), specific energy of shear (for shear fractures/bands) and specific energy of compaction (for compaction bands).

Funding
The authors acknowledge support from the ARC Linkage Project Grant [grant number LP120100299]; AWE Ltd; Norwest Energy.

References


CHAPTER 3

Rotations and pattern formation in granular materials under loading
Rotations and pattern formation in granular materials under loading

Elena Pasternak\textsuperscript{a,c,*}, Arcady V. Dyskin\textsuperscript{b,c}, Maxim Esin\textsuperscript{a,c}, Ghulam M. Hassan\textsuperscript{d} and Cara MacNish\textsuperscript{d}

\textsuperscript{a}School of Mechanical and Chemical Engineering, University of Western Australia, Perth, Australia; \textsuperscript{b}School of Civil, Environmental and Mining Engineering, University of Western Australia, Perth, Australia; \textsuperscript{c}Deep Exploration Technologies Cooperative Research Centre, Adelaide, Australia; \textsuperscript{d}School of Computer Science and Software Engineering, University of Western Australia, Perth, Australia

(Received 16 November 2014; accepted 25 May 2015)

Shear band formation and evolution is a predominant mechanism of deformation patterning in granular materials. Independent rotations of separate particles can affect the pattern formation by adding the effect of rotational degrees of freedom to the mechanism of instability. We conducted 2D physical modelling where the particles are represented by smooth steel discs. We use the digital image correlation in order to recover both displacement and independent rotation fields in the model. We performed model calibration and determine the values of mechanical parameters needed for a DEM numerical modelling. Both mono- and polydisperse particle assemblies are used. During the loading, the deformation pattern undergoes stages of shear band formation followed by its dissolution due to recompaction and particle rearrangement with the subsequent formation of multiple shear bands merging into a single one and the final dissolution. We show that while the average (over the assembly) values of the angles of disc rotations are insignificantly different from zero, the particle rotations exhibit clustering at the mesoscale (sizes larger than the particles but smaller than the whole assembly): monodisperse assemblies produce vertical columns of particles rotating the same direction; polydisperse assemblies 2D form clusters of particles with alternating rotations. Thus, particle rotations produce a structure on their own, a structure different from the ones formed by particle displacements and force chains. This can give a rise to moment chains. These emerging mesoscopic structures – not observable at the macroscale – indicate hidden aspects of ‘Cosserat behaviour’ of the particles.

Keywords: granular material; digital image correlation; DEM model; shear bands

Introduction

Shear band formation is one of the most significant mechanisms of large deformation, instability and failure of granular materials. Understanding of this mechanism is important for safe structural design.

Experimental investigations of shear bands to date use a variety of granular materials and different types of loading. They include biaxial, triaxial and shear lab...
experiments and in situ tests. The use of sand and clay is very common, these granular materials were tested and analysed in numerous experiments [1–13]. It was shown that formation of shear band patterns in granular materials depends on many factors such as a mean particle diameter and size distribution, porosity, sample dimensions, water saturation, boundary conditions, etc. It is interesting that while a lot of parameters of shear bands formation (e.g. thickness of shear bands and angle of inclinations) were analysed, the effect of particle rotations did not receive similar attention. However, particle rotations were observed in zones of strain localisation in granular materials in direct physical experiments [10,14–16] and in discrete element method-type simulations [17–19].

A specific method of investigating the behaviour of granular materials is the 2D modelling. This is accomplished by either using rod-like particles [20] or thin discs [21–23]. In these experiments, shear band formation was observed as well as particle rotations or rolling. This indicated that the particle rotation mechanism might play an important in the formation of shear bands; however, no direct measurements of rotations of the particles were performed.

The above experiments used monodisperse particles. However, the granular materials are usually polydisperse. Formation of shear bands in polydisperse assemblies was studied in [24–27].

The numerical simulations of shear bands that allow one to recover the rotation of particles are based on two main methods [28]: the finite element method realising the equations of a Cosserat continuum [29,30] and the discrete element method [31,32]. These are viable alternatives to usually expensive and time-consuming experimental investigations and allow one to explore the formation of shear bands, which might be complicated to study experimentally, for instance, due to short durations of the band formation and re-compaction.

Papers [28,33–37] modelled shear bands in micropolar granular materials using the finite element method for both elastoplastic and hypoplastic models of the material behaviour. They showed that the Cosserat effects (the effects of mutual rotations of particles) are substantial in the shear band zones. Modelling of the formation of shear bands in granular materials with the discrete element method [38–42] indicated that their behaviour is controlled by both the particle rotations and the rolling resistance (and the corresponding couple stress) occurring in shear band zones [41,42].

In our paper, we develop further the approach proposed in [21–23] and include the measurements of rotations of each particle. We analyse the rotational behaviour of both mono- and polydisperse assemblies of particles. We use a DEM for simulating our laboratory tests. We conduct a special calibration of the experiments in order to determine the required input parameters (contact stiffness, friction coefficient, etc.) for the DEM with a potential to use them for constructing a Cosserat continuum using an appropriate homogenisation method [43]. We then simulate the emerging deformation patterns and re-compactions observed in our experiments.

**Physical model, loading device and measurements**

The 2D physical models we used are assemblies of mono- or polydisperse steel discs. The discs were made of steel and have thickness of 1.6 mm. The diameter of discs of the monodisperse assembly is 23.5 mm, and the mass of each disc is 5.45 g. This
model is similar to that of a model used in experiments conducted in [21,22], in which Japanese 10 yen coins (thickness is 1.5 mm, diameter is 23.5 mm and mass is 4.5 g) were used.

The monodisperse assembly (Figure 1(a)) contains 11 rows by 10 columns of smooth discs with speckles painted on them to enable the reconstruction of displacement and rotations using the DIC photogrammetric technique. The discs in the physical model were initially in contact with all the neighbouring discs forming hexagonal packing.

For the polydisperse assemblies (Figure 1(b)), we used three different sets of discs randomly packed into the assembly. The assemblies contained a mixture of 19, 38 and 33 discs with diameters of 20, 23.5 and 27 mm, respectively.

The loading device consists of a transparent PMMA frame and a slider to effect pressure on the assembly of the discs. The experimental set-up with a monodisperse assembly of the discs is shown in Figure 2. The experimental apparatus consisted of the slider which moves in and compresses the assembly. The slider is moved in by a rotating hand crank. The spring length is measured to determine the applied load using the spring stiffness. The latter was determined during the calibration, see below.

**Calibration**

The calibration stage was aimed at determining the following parameters of the physical model, which control its behaviour. It is the stiffness of the spring, the combined stiffness of the loading device (the slider and the walls) and stiffnesses of the disc contacts.

![Graph](image.png)

Figure 1. The physical model (a) The 10 × 11 array of coins, (b) the polydisperse assembly with random packing.
The spring stiffness was determined by conducting a separate test where the spring was loaded by known force and the resulting changes of the spring length were measured. Five repeat measurements conducted are shown in Figure 3. After averaging over the five measurements the spring stiffness was found to be 2.63 N/mm. In order to verify this value, the spring stiffness was also calculated by using the material parameters and the spring geometry. The shear modulus of the spring material (steel) is $G = 80$ GPa, the diameter of the spring wire is $d_W = 1.35$ mm, the mean coil diameter is $d_C = 8.26$ mm and the number of active coils is $n = 23$. Using a standard formula for calculation of the spring stiffness, the value 2.64 N/mm was obtained, which confirms the experimentally obtained stiffness.

Figure 2. The experimental apparatus with hexagonal packing of the discs: (1) Hand crank, (2) compression block, (3) compression spring ($k_{spring} = 2.63$ N/mm), (4) hollow cylinder, (5) slide mount, (6) slider, (7) roller bearings, (8) perplex plates, (9) physical model, (10) base.

Figure 3. (colour online) Calibration of the spring stiffness. The results of five tests are shown with markers - applied load, $F$, vs. change in the spring length, $u$. The line $F(u) = 2.63u$ shows a linear regression with a coefficient of determination $R^2 = 0.997$. 

$F(u) = 2.63u$, $R^2=0.997$
In order to determine the combined stiffness of the apparatus (the loading device), we conducted preliminary tests with monodisperse arrangements of discs in square packing.

The basis for this reconstruction is the theory of effective moduli of square packed assembly of monodisperse discs [44,45]:

\[ \begin{align*}
\sigma_{22} &= \frac{1}{b} k_n \gamma_{22}, \quad \sigma_{33} = \frac{1}{b} k_n \gamma_{33}, \quad \sigma_{23} = \frac{1}{b} k_s \gamma_{23}, \quad \sigma_{32} = \frac{1}{b} k_s \gamma_{32}, \\
\mu_{21} &= \frac{1}{b} k_t \kappa_{21}, \quad \mu_{31} = \frac{1}{b} k_t \kappa_{31}
\end{align*} \]  

(1)

Here \( b \) is the thickness of the discs; \( \sigma_{ij}, \mu_{ij} \) are the 2D stress and moment stress tensors (the Cartesian coordinates in [45] were chosen as following: axis \( x_1 \) is directed out of plane of the assembly; axes \( x_2 \) and \( x_3 \) are directed horizontally and vertically respectively (Figure 1), \( \gamma_{ij}, \kappa_{ij} \) are the 2D Cosserat strain and curvature tensors; \( k_n \) and \( k_s \) are the normal and shear stiffnesses of the contacts between the particles (discs in our case).

It is seen that in the case of square packing the effective modulus \( E_{\text{eff}} \) relating stress and strain components \( \sigma_{22} \) and \( \gamma_{22} \) depends only on the normal contact stiffness \( k_n \). Therefore, by starting the stiffness reconstruction from the square packing, we will be able to determine \( k_n \) independently.

The apparatus measures the force–displacement relationship of a combined system of the loading device–assembly. If \( k_a \) is the effective stiffness of the apparatus and \( k_L \) is the effective stiffness of the assembly of width \( L \), the linear approximation of the measured force–displacement relationship reads:

\[ u = F \left( \frac{1}{k_a} + \frac{1}{k_L} \right) \]  

(2)

where \( u \) and \( F \) are the measured displacement and force, respectively.

The effective stiffness of the assembly can be expressed through its effective modulus \( E_{\text{eff}} \) as:

\[ k_L = E_{\text{eff}} \frac{h b}{L} \]  

(3)

where \( L \) is the assembly width, \( h \) is its height, \( b \) is its thickness (Figure 4).

Equations (2) and (3) show that independent determination of both stiffnesses requires at least two measurements with different values of \( L \). We used two assemblies with 6 and 9 columns, respectively, and the corresponding lengths:

\[ L_6 = 12a, \quad L_9 = 18a \]  

(4)

where \( a \) is the disc radius.

This gives us two equations for determining stiffness \( k_a \) and modulus \( E_{\text{eff}} \) and then using (1), stiffness \( k_n \):

\[ \begin{align*}
\frac{u}{F}_6 &= \frac{1}{k_a} + \frac{L_6}{h b E_{\text{eff}}}, \\
\frac{u}{F}_9 &= \frac{1}{k_a} + \frac{L_9}{h b E_{\text{eff}}},
\end{align*} \]  

(5)
where \((F/u)_n\) is the slope of the force–displacement relationship for the assembly of \(n\) columns.

The force–displacement relationships for the assemblies of 6 and 9 columns are shown in Figure 5. The approximately linear force–displacement dependence indicates that the contacts between the discs and between the discs and the walls/slider behave linearly at least in the range of the loadings applied.

We obtain for the \(L_6\) assembly \(F = 30.048\) N, \(u = 1\) mm; for the \(L_9\) assembly \(F = 25\) N, \(u = 1\) mm. Given that \(h = 423\) mm, \(b = 1.6\) mm, we find \(E_{\text{eff}} = 15.5\) MPa, \(k_n = 50.4\) N/m. Then using (1) we determine the normal contact stiffness between the discs \(k_n = 24.8\) N/mm.

Thus, we can find the combined stiffness of the apparatus and using Equation (1) the normal contact stiffness. However, the model based on the effective characteristic does not allow the extraction of the stiffness of the contact between the discs and the apparatus walls since the theory of effective characteristics does not account for the boundary. We use discrete element modelling implemented in the Particle Flow Code (PFC2D), Itasca [46], for calibrating our model and the determination of this stiffness. The model is shown in Figure 6. The numerical model consists of an assembly of discs and three walls. The left vertical and horizontal walls are fixed. The linear contact model is used. It reproduces the mechanical behaviour of an infinitesimal, linear elastic and frictional interface that carries a point force [46].

Deformation is produced by horizontal displacements of the right wall with velocity \(v_2 = 0.01\) mm/s.
Assuming that the contact stiffness between the discs and the left wall is the same as with the right wall, in the numerical simulations we can assume the left wall stiffness infinite (we used a large value of $10^7$ N/mm for the task), while the right wall contact stiffness equals to the half of the sought contact stiffness. It was found that when the contact normal stiffness of the right wall is equal to 5.5 N/mm then the results of numerical simulation are close to the experimental ones, Figure 7. Subsequently, the sought normal contact stiffness between the disc and the wall is 11 N/mm. This is as twice as small as the inter-disc normal contact stiffness. Comparing this with the combined stiffness of the apparatus, $k_d = 50.4$ N/m, we can see that the loading device can be regarded as stiff as compared to the ‘sample’.

In order to estimate the shear stiffness of the inter-disc contacts, we conducted calibration tests using hexagonal packing and then the corresponding numerical simulations using PFC2D. The assembly contained 16 rows and 10 columns. The normal contact stiffnesses as well as apparatus stiffness were the same as determined in the square packing tests. The shear contact disc-to-disc and disc-to-wall stiffnesses where
determined to provide the best fit between the experiments and the simulations. The results of experimental tests and the fitted numerical simulations are shown in Figure 8.

Figure 6. (colour online) The numerical model with square packing of the discs. An assembly comprising 18 rows and 6 columns is shown. The left vertical and horizontal walls are fixed, right vertical wall moves with velocity $v_2 = 0.01$ mm/s.

Figure 7. (colour online) The results of numerical modelling – applied load, $F$, vs. displacement, $u$: (a) 18 rows by 6 columns and (b) 18 rows by 9 columns square packing assemblies. The crosses show experimental results for 18 rows by 6 columns assembly, the circles – for 18 rows by 9 columns assembly.
It has been determined that for reasonable correspondence of the experiment and numerical simulation the disc-to-disc and the disc-to-wall contact shear stiffnesses should be quite small, $k_s \sim 1$ N/mm.

The friction coefficients of inter-disc contact and contact between the discs and the walls were determined by conducting a separate test. Several discs were glued together in a row. This row was placed in the experimental apparatus. Then we tilted the apparatus with discs gradually and measured the angle when the row of discs began to move. It gave us the friction coefficient of the contact between the discs and the wall of apparatus. To find the friction coefficient of inter-disc contact, we glued further several discs in a row and placed them upon the first row. Then we fixed the first row in the apparatus, began to tilt gradually and measured the angle when the second row of discs began to move. After averaging over the several measurements the friction coefficients of inter-disc contact and contact between the discs were found to be approximately 0.22.

The list of the parameters determined is presented in Table 1. These parameters will be used in further DEM simulations using PFC2D. It is interesting to note that the determined normal and shear stiffnesses of particle contacts are low, in stark contrast to the values adopted (without prior measurements) in a number of papers devoted the DEM simulations of granular materials [40,47,48], which were several orders of magnitude higher than the values we obtained.

Figure 8. (colour online) The force–displacement diagrams obtained from the physical tests (data points) and numerical simulation (curve) for hexagonal packed assembly containing 16 rows by 10 columns.

<table>
<thead>
<tr>
<th>Table 1. The determined parameters of the assemblies.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normal stiffness of inter-disc contact, N/mm</td>
</tr>
<tr>
<td>Normal stiffness of disc – right wall contact, N/mm</td>
</tr>
<tr>
<td>Normal stiffness of disc – left wall contact, N/mm</td>
</tr>
<tr>
<td>Shear stiffness of inter-disc contact, N/mm</td>
</tr>
<tr>
<td>Density of discs, kg/m$^3$</td>
</tr>
<tr>
<td>Disc diameters, mm</td>
</tr>
<tr>
<td>Friction coefficient of inter-disc contact</td>
</tr>
<tr>
<td>Friction coefficient between the discs and the walls</td>
</tr>
</tbody>
</table>
As can be seen from Figure 8, the effective stiffness of the system does not remain the same, but reduces with loading. This is due to the fact that the discs go up and lose contacts with neighbouring discs during compression by the slider. By the time of the first re-compaction, discs lose all vertical contacts with neighbouring discs. These contacts make up 33% of the total number of contacts.

We note that the ratio between the spring stiffnesses determines the Poisson’s ratio for given geometry of the assembly. As in one of our micromechanical model for isotropic granular material [49] shown \( \nu = (k_n - k_s)/(4k_n + k_s) \) and the bounds for the Poisson’s ratio determined by the ratio of normal to shear stiffnesses were obtained as follows: \(-1 < \nu < 0.25\). According to the results presented in Table 1, \( \nu \approx 0.244 \).

**Measurement of displacements and rotations of discs**

One of the conclusions from the calibration is the presence of appreciable friction between the discs. This implies that mutual disc rotations may play an important role in the process of deformation. Subsequently, both displacements and rotations of each disc have to be measured and recorded. To this end, the discs were covered with speckles, Figure 9, such that the displacements and rotations of the discs could be recovered by taking successive photographs of the assembly with subsequent processing using the digital image correlation (DIC) technique. Furthermore, the displacements and rotations should be measured in every disc separately, such that the DIC should be simultaneously applied to each disc with the measurement areas set within each disc.

We used the DIC method implemented in VIC-2D™ software that recovers full-field displacement, strain and rotation data for areas-of-interest (comprising number of points) set by a user in the pre-processor. Figure 10 shows a result of a single calculation for the rotations.

Since the discs are assumed to move as rigid bodies (their stiffness is considerably higher than the contact stiffness) the corresponding displacement components are

![Figure 9. (a) Physical model during the first re-compaction, (b) close view of discs with speckles.](image)
determined as the displacements of the disc centres while the rotation is determined as the rotation field within a disc averaged over the area-of-interest. (In theory, the rotations within a disc must be uniform; however, the unavoidable errors of the reconstruction break the uniformity, Figure 10, which necessitates the averaging.)

The whole experiment is represented by thousands of such images and huge accompanying files containing information on displacements and rotations for many points in one disc and for all the discs in the assembly. Furthermore, post-processor features in VIC have certain limitations in visualising the results. For instance, as seen in Figure 10, the discs are coloured according to the rotations ranging from $-0.56$ to $0.57$ (in radians), which is restrictive. In order to overcome these limitations, we developed a proprietary algorithm to post-process the original images of the experiments and resultant data from VIC. This algorithm uses Hough transform for image analysis and identification of discs and their centre of mass. The algorithm organises the resultant data in convenient form for visualisation of mechanical behaviour and for further analyses. Then boundaries and the positions of the discs are identified and the rotations are then averaged within each disc. The disc images are filled with colour: green for counter clockwise rotation, blue for clockwise rotation, white for non-rotating discs. Discs with rotations within the measurement error $2^\circ$ are white. Hereafter, the experimental results were obtained using this algorithm.

During the progressive deformation the pictures were taken using a conventional still camera (Canon 5D Mark II). At the moments of re-compaction of the discs, which occurred very rapidly, a high-speed camera (1000 frames per second) was used.
Experiments with monodisperse hexagonal assembly

Loading of monodisperse square packing assemblies have not shown any re-compactions or instabilities within the whole range of allowable loadings. It is because the square packing assembly resists loading with virtually independent chains; the capacity of the loading device was insufficient to cause buckling of these chains. Subsequently, the force–displacement relationship is almost linear.

Displacement–control loading of monodisperse hexagonal packing assemblies shows a different picture. Figure 11 presents the force vs. slider displacement plots. No measurements were possible in the descending branches which correspond to almost instantaneous re-compaction. (Descending branches were plotted by connecting the last point of the previous ascending branch and the first point of the next ascending one.) It is seen that in the process of loading three re-compactions take place with typical post-peak softening parts of the loading curve corresponding to the re-compactions.

Figure 12(a) and (b) shows the details of the first and second re-compactions. We can distinguish four separate regions (I–IV) formed during the shear band formation at the time of the first re-compaction. Interestingly, several rhomboids ('lattice-like' pattern [23]) were observed during the second re-compaction (Figure 12(d)). This difference in patterns can be explained by small imperfections in the discs, their variable friction with the walls, small inclinations of the slider or other minor factors beyond the control of these experiments. The shear bands observed always form at 30°, which is consistent with the hexagonal packing of the discs. It is interesting that different tests produce qualitatively different deformation pattern in the second re-compaction. The differences between the regions will be explained later.

We determined the (negative) slopes of post-peak branches observed during the re-compactions from the graphs (Figure 11). The respective values of the slopes (stiffness of assembly during re-compactions) and the corresponding Young’s moduli are shown in Table 2. It is seen that as the re-compactions proceed the assembly softens.

Evolution of the monodisperse assembly during the first re-compaction is shown in Figure 13. The rotation of the discs is shown in Figure 13(a); the graphs connecting the

Figure 11. (colour online) Force vs. slider displacement graphs for three tests for the monodisperse assembly. Shear band formation during: (a) the first re-compaction, (b) the second re-compaction, (c) the third re-compaction.
centroids of discs rotating in mutually opposite directions (like gears) are shown in
Figure 13(b). In other words, each graph indicates the discs well contacted to each
other preventing mutual sliding. The percentages of the discs engaged in rotation in
these tests are, respectively, 45, 52, 75, 89, 97 and 86%.

The rate of first re-compaction was very high, so we had to use a fast camera (1000
frames per second) to ensure that increments of rotations between the frames are
sufficiently small to be able to use the DIC technique. The duration of the first re-
compaction was around 0.1 s. The slider velocity at the moment of re-compactions was
(13–6) mm/0.1 s = 70 mm/s (Figure 11) as the slider slid through 7 mm at 0.1 s. This is
due to the fact that the spring of the experimental set-up was accumulating energy dur-
ding the active loading (ascending branches of the force–displacement curve). This
energy was rapidly released as soon as the peak of the force vs. slider displacement
curve was reached. The durations of other re-compactions were around 0.1 s as well.

Figure 14 shows the rotation vs. slider displacement for two neighbouring discs
(Figure 12(a) and (b)). The circle markers (a) show the rotation of the disc #1, the cross
markers (b) shows the rotation of the disc #2. Fluctuations of rotations are due to the
noise associated with the DIC.

Figure 15 shows the final positions of the discs and their rotations after the first re-
compaction in the physical experiment. The small upright marks on each disc represent
the initial orientation (rotation is equal to zero). The radius vectors indicate rotations of
the discs. The numbers inside the discs show the angles of rotations in degrees. Positive
values indicate counterclockwise rotation, negative values – clockwise rotation.
Figure 13(a). (colour online) Evolution of the monodisperse assembly during the first re-compaction: rotation of the discs.

Figure 13(b). (colour online) Evolution of the monodisperse assembly during the first re-compaction: graph connects the centroids of discs rotating in mutually opposite directions (like gears). The percentages of these discs engaged in rotation left-to-right top-to-bottom are 0, 45, 52, 75, 89, 92, 97 and 86%. Green and blue colours indicate the anticlockwise and clockwise rotations respectively; the white colour indicates non-rotating discs (i.e. rotations within the measurement error of 2º).
Figure 14. (colour online) The disc rotations vs. displacement graphs: (a) the rotation of the disc #1, (b) the rotation of the disc #2, Figure 12(b). Markers – experimental results, lines – DEM results.

Figure 15. (colour online) The disc rotations after the first re-compaction. The small upright marks on each disc represent the initial orientation (rotation is equal to zero). The radius-vectors indicate rotations of the discs. The numbers inside the discs show the angles of rotations in degrees. Positive values indicate counter clockwise rotation, negative values – clockwise rotation.
Analysing the disc rotations in each region I–IV (cf. Figure 12(b)), we observe that the resultant angles of the disc rotations have the same sign in each vertical column within one region, but alternate signs between the columns. The values of the rotations are somewhat close. The only exception is region I, which contacts with both horizontal and vertical walls of the experimental apparatus. As a result, constrains on displacements and the friction force affect this region more than others. Most of the discs included in the region I rotate by smaller angles. As a result, most of the discs included in the region I rotate by smaller angles. It is also seen that for each side of the shear band between regions II, III and IV the signs of the disc rotations change when one goes from one region to another.

The rotations averaged over each of the four regions are found to be statistically insignificantly different from zero. This suggests that the shear band formation is accompanied by formation of oriented rotation patterns at the scale intermediate between the particle size and the region size.

The localised deformation and rotations observed in the experiments are qualitatively similar to those observed in experiments [21,22] except for the rhomboid pattern (Figure 12(d)). A similar rhomboid pattern was observed in our preliminary experiments [23].

**Discrete element modelling of monodisperse hexagonal packing assembly**

Using parameters from Table 1, we can carry out numerical simulation of our experiments. The evolution of the monodisperse assembly during the first re-compaction obtained by numerical simulation is shown in Figure 16. The simulations show the pattern similar to what we observe in the experiments: the formation of columns of the discs rotation in the same direction, rotations in the opposite directions between the neighbouring columns and discs rotating in the opposite directions across the shear bands.

Figure 17 compares the force–displacement curves obtained in an experiment and in the numerical simulation. It is seen that the simulation reproduces the experimental results in the ascending branches quite well, at least until the third re-compaction.

![Figure 16. Numerical simulation (discrete element method implemented in PFC2D) showing the evolution of the monodisperse assembly during the first re-compaction. Red and blue colours indicate the anticlockwise and clockwise rotations respectively.](image-url)
No measurements were possible in the descending branches that correspond to almost instantaneous re-compaction.) We note some accumulated shift of the numerical curve against the experimental one, especially visible at the third re-compaction. This could be attributed to small deviations of the shapes of the discs in the experiment from the ideal circular shape and non-uniform roughness of their contacted contours.

The post-peak (softening) slope following the first re-compaction is longer and shallower in the simulation. The post-peak (softening) slope following the second re-compaction is deeper in the simulation (Figure 17). There are always some differences between experiments and numerical simulations. This can be explained by imperfections of the experimental set-up such as: deviations in the disc shapes, friction between the apparatus’ walls and the discs, a slight tilt of the slider and possible buckling of the loading spring.

Figure 14 shows the rotation vs. slider displacement for two neighbouring discs (Figure 12(a) and (b)). The solid line (a) shows the rotation of the disc #1, the dotted

Figure 17. (colour online) Force vs. slider displacement for the monodisperse assembly. Shear band formation during: (a) the first re-compaction, (b) the second re-compaction, (c) the third re-compaction. The results of physical experiments are shown by the data points; the results of numerical simulation are shown by the curve.

(No measurements were possible in the descending branches that correspond to almost instantaneous re-compaction.) We note some accumulated shift of the numerical curve against the experimental one, especially visible at the third re-compaction. This could be attributed to small deviations of the shapes of the discs in the experiment from the ideal circular shape and non-uniform roughness of their contacted contours.

The post-peak (softening) slope following the first re-compaction is longer and shallower in the simulation. The post-peak (softening) slope following the second re-compaction is deeper in the simulation (Figure 17). There are always some differences between experiments and numerical simulations. This can be explained by imperfections of the experimental set-up such as: deviations in the disc shapes, friction between the apparatus’ walls and the discs, a slight tilt of the slider and possible buckling of the loading spring.

Figure 14 shows the rotation vs. slider displacement for two neighbouring discs (Figure 12(a) and (b)). The solid line (a) shows the rotation of the disc #1, the dotted

Figure 18. (colour online) Force vs. slider displacement for the monodisperse assembly (numerical simulation): (a) \( k_n = 15 \text{ N/mm} \), (b) \( k_n = 49.6 \text{ N/mm} \), (c) \( k_n = 150 \text{ N/mm} \).
line (b) shows the rotation of the disc #2. As can be seen, the simulation is in good agreement with the experimental results.

Figures 18–20 present the results of numerical simulations which show the effect of the main material parameters (Table 1) on the force–displacement curves. In Figures 18–20 the normal stiffness of inter-disc contact \( k_n \), shear stiffness of inter-disc contact \( k_s \) and the friction coefficient of the inter-disc contact \( \mu \) are varied. It can be seen that only the force–displacement curve obtained by using the parameters from Table 1 agree with the experimental results quite well. Changing the main material parameters \( k_n, k_s \) and \( \mu \) leads to both quantitative and qualitative mismatches in the curves.

**Deformation of polydisperse assemblies**

Figure 21 shows the experimentally obtained force vs. slider displacement graphs for polydisperse assemblies. Similarly to the monodisperse assembly, these graphs were

![Figure 19](image19.png)

Figure 19. (colour online) Force vs. slider displacement for the monodisperse assembly (numerical simulation): (a) \( k_s = 0.1 \text{ N/mm} \), (b) \( k_s = 1 \text{ N/mm} \), (c) \( k_s = 10 \text{ N/mm} \).

![Figure 20](image20.png)

Figure 20. (colour online) Force vs. slider displacement for the monodisperse assembly (numerical simulation): (a) \( \mu = 0.07 \), (b) \( \mu = 0.22 \), (c) \( \mu = 0.66 \).
Figure 21. (colour online) Force vs. slider displacement for three tests for the polydisperse assembly: (a) constant gradual re-compactions without significant drops in the force; (b) re-compactions with significant drops in the force.

Figure 22. (colour online) Original (a) and final (b) positions with the qualitative picture of the rotations of the discs in the polydisperse assembly. The graph connects the centroids of the discs rotating in opposite directions (as the gears). Green and blue colours indicate the anticlockwise and clockwise rotations respectively.
obtained from several tests. The most important feature of the polydisperse assemblies is that their behaviour depends on the packing. If packed randomly polydisperse assemblies can have quite different densities [50]. Obviously, the mechanical behaviour will be different as well.

In the tests we observed two types of re-compactions of the polydisperse assemblies: constant gradual re-compactions without significant drops in the force (Figure 21 (a)) and re-compactions similar to the graph for the monodisperse assembly (Figure 21 (b)). However, in the polydisperse assemblies, we did not observe shear band formation similar to what is observed in monodisperse assemblies. We can see a considerable dependence of the disc trajectories on the initial packing. We cannot exclude that this dependence is due to the boundary effect associated with insufficiently large dimensions of the assembly.

Figure 22 shows the original and final positions of the discs and their rotations after the re-compaction (the loading curve of type b in Figure 21; slider displacement 13–28 mm) of the polydisperse particle assembly in the physical experiment.

As before the green colour indicates the counter clockwise rotation, blue colour – clockwise rotation, white colour – non-rotating discs (discs with rotation angles within the measurement error 2°). In the experiment, the discs in the polydisperse assembly rotate in clusters rather than individually. To show the clusters, we connect the neighbouring contacting discs with opposite signs of rotations by red graphs. This indicates non-zero mutual gear-type disc rotations. In other words the clusters are the groups of particles (discs) whose rotations are correlated.

Figure 23(a). (colour online) Evolution of the polydisperse assembly during the first re-compaction (with significant drops in the force; the loading curve of type b in Figure 21): rotation of the discs.
Detailed evolution of the rotations and displacements in the polydisperse assembly during re-compaction is shown in Figures 23(a) and 23(b). It corresponds to slider displacements 13–28 mm shown in Figure 21(b). Steps between every two adjacent pictures in Figure 23 correspond to 1.5 mm of slider displacement. The rotations (Figure 23(a)) and displacement were determined using the frames obtained by a high speed camera. The radius vectors indicate rotations of the discs. The percentages of the discs engaged in rotation in these tests are, respectively, 0, 0, 33, 69, 68, 74, 80, 87, 91 and 93 (Figure 23(b)).

The above results indicate that during the re-compaction a number of clusters of synchronously rotating particles are observed forming at the mesoscale. Clusters of rotating particles/segments were previously observed at different scales from laboratory experiments in granular materials [10] to rotations of regions in the Earth’s crust as rigid domains [51,52]. The clusters in granular materials were also studied numerically in [39,53,54].

This paper focuses on the experimental aspects of rotations and pattern formation in granular materials. The full DEM modelling in the polydisperse case requires considerable computational efforts due to enormous number of possible realisations of the particle trajectories; it will be subject of further research based on the statistical physics – type simulations. Also larger numbers of disc will have to be included in the experiments in order to filter out the boundary effects.
Conclusions

Physical and discrete element modelling of the deformation of granular material in 2D give qualitatively similar results after proper calibration of the DEM. The calibration revealed very low values of interparticle particle-to-wall stiffnesses magnitudes, orders of magnitude lower than adopted in the literature for the discrete element modelling.

The results of physical experiments and discrete element modelling show that the deformation of assemblies of particles (discs) proceeds through alternating stages of evolutionary behaviour characterised by the ascending branches of the force–displacement curve and the re-compaction stages characterised by the descending branches of the force–displacement curve.

In monodisperse hexagonal packing assemblies, the re-compaction progresses through the development of shear bands forming either a wedge-like pattern or in some cases, the rhombus-like (lattice-like) pattern. The wedge-like pattern can be considered as a large-scale rhombus-like pattern that could not be realised due to the size restrictions of the model.

In polydisperse assemblies, the re-compaction does not produces visible shear bands. Also, depending on the realisation of the packing two types of re-compactions are observed: constant gradual re-compactions without significant drops in the force and re-compactions similar to the graph for the monodisperse assembly. A considerable dependence of the disc trajectories on the initial packing is observed perhaps caused by the boundary effect associated with insufficiently large dimensions of the assembly.

During the first re-compaction both mono- and polydisperse assembles get divided into separate regions between the shear bands. The process of deformation leads to considerable rotations of individual particles (discs). However, the average (over the area of the assembly) values of the angles of disc rotations are insignificantly different from zero. Instead the discs are separated into the groups of similarly rotating discs. In particular, in the monodisperse assemblies, alternating columns of discs rotating in one direction are formed with discs of neighbouring columns rotating in the opposite direction. Furthermore, upon crossing the shear band the rotations change the sign. It means that the rotations are microscopic (at the scale of the grain size), correlating at a mesoscale but do not proliferate to the macroscopic scale. In polydisperse assemblies, where the shear bands are not observed the clusters of mutually rotating (gear-like) discs are formed. Therefore, in both mono- and polydisperse assemblies, the formed rotation patterns are of a mesoscale nature: their size being larger than the particle size but yet smaller than the assembly dimensions.

It is important that at the mesoscale the particle rotations form clusters of particles rotating in the same directions and chains of particle rotating in the mutually opposite directions, i.e. without mutual sliding. Thus, particle rotations produce a structure on their own, a structure different from the ones formed by particle displacements and force chains. This can give a rise to moment chains. These emerging mesoscopic structures – not observable at the macroscale – indicate hidden aspects of ‘Cosserat behaviour’ of the particles. This new paradigm may shed further light on the deformation of granular materials.
Acknowledgement

The work has been supported by the Deep Exploration Technologies Cooperative Research Centre whose activities are funded by the Australian Government’s Cooperative Research Centre Programme. This is DET CRC Document 2015/664.

Disclosure statement

No potential conflict of interest was reported by the authors.

References

CHAPTER 4

Mode I crack in particulate materials with rotational degrees of freedom
A wide use of engineering and natural materials with microstructure makes it necessary to develop methods of describing mechanical behaviour of structures made of these materials. Yet, despite extensive research many aspects of fracture initiation and propagation in such materials remain unclear. We consider Mode I crack in particulate materials whose constituents are able to rotate. We model such materials in 2D as an idealised slightly cemented granular material where circular shaped thin discs are gluing together. In order to model the crack, the bonds between a few pairs of discs are removed with crack opening being introduced by a thin wedge. Rotations of the particles are analysed using physical experiments, an analytical model and a DEM numerical simulation. It is found that the DEM simulations give results very close to the experimental ones. Furthermore, the particle rotations during fracture propagation can be well described by the pseudo-Cosserat continuum with constrained microrotations.

4.1. Introduction

Materials with heterogeneous microstructure are ubiquitous in nature and widely used in engineering so this matter generates considerable interest. For instance, geomaterials consist mostly of cemented grains (e.g. rocks) or slightly cemented and unbounded constituents (e.g. clay, sand) thus possessing highly nonhomogeneous microstructure. Concrete, mortar, ceramics, masonry are other examples of such materials. Modelling of fracture initiation and propagation in these materials represents a challenging problem. A large number of parameters (e.g. porosity, particle size distribution and morphology, water saturation, ability of particles to rotate, boundary conditions, etc.) have an effect upon mechanical behaviour. All these aspects should be considered and taken into account for adequate modelling. In this study the primary focus is on rotation of particles and its importance on fracture behaviour in particulate materials – materials whose constituents may rotate.

Various forms of fractures and types of failure in geomaterials, such as single fractures, multiple interacting fractures, shear and compaction bands, damage zones under quasi-static and dynamic loading can be distinguished [1]. A number of papers have been devoted to experimental, numerical and analytical investigation of microrotations (particle rotations). Roscoe and Schofield [2] and Oda [3] realised the importance of microrotations on failures in particulate materials and observed rotations of sand particles during physical experiments. Later, Oda et al. [4, 5], Calvetti et al. [6] and Misra and Jiang [7] carried out special experiments for observation and
investigation of microrotations using assemblies of relatively large circular or elliptical discs and oval cross-sectional cylindrical rods as granular material (Rowe [8] designed and conducted a similar experiment earlier but microrotations were not studied).

Geomaterials are often subjected to compressive load leading to compaction and shear band formation, which represent the main mechanisms of failure. Consequently it is no wonder, that these types of failure attract much interest from a practical standpoint. This topic has been given much attention from the second half of the 20th century to the present day and discussed in the literature extensively. It has been established that shear and compaction bands are associated with strain localisation and accumulation of microcracks. With development of non-destructive scanning techniques, experiments using sand and artificial materials with relatively small particles were conducted using various methods to record the particle movement, such as photogrammetry [9-11], gamma-rays [12], X-ray computed tomography [13-22], 2D microscopy [23], magnetic resonance imaging (MRI) [24], photogrammetry with the digital image correlation [18, 21, 25, 26] and ID-Track [15-17, 21]. All experiments demonstrated the presence of considerable rotations in the regions of shear bands. Apart from the physical experiments, numerical simulations based on the finite element method (FEM) [27-30] and the discrete element method [27, 31-44] were carried out. The critical role of particle rotations as well as rolling resistance (associated with the particle shape) in mechanical behaviour of particulate materials was corroborated.

Due to heterogeneous microstructure and the presence of microrotations, the classical continuum whose every point possesses only three (two in 2D) translational degrees of freedom cannot describe satisfactorily the mechanical behaviour of particulate materials. A number of non-standard continua were proposed for the task such as the Cosserat continuum (micropolar or asymmetric elasticity), Cosserat and Cosserat [45], Nowacki [46], Toupin [47], Eringen [48]), micromorphic elasticity (e.g. Mindlin [49], Eringen [48]) and non-local theories (e.g. Eringen [50], Kunin [51, 52]; see also review in Pasternak and Mühlhaus [53, 54]) more suitable for materials of this type. The simplest theory accounting for internal rotations in the particulate materials is the Cosserat continuum. In this theory every point of continuum has three conventional translational degrees of freedom and additionally three rotational degrees of freedom (in 2D there are two translational and one rotational degrees of freedom). Consequently, on top of the conventional stress (force stress) which becomes non-symmetrical the
constitutive equations of the micropolar elasticity include moment stress (couple stress). Since elastic moduli associated with force stress and elastic moduli associated with couple stress have different units, the Cosserat continuum possesses the Cosserat characteristic lengths. These lengths are constructed by dividing the moduli relating the moment stresses and curvature twists by the moduli relating the stress with strain and rotation and then by taking square root of the ratios. Therefore, in contrast to the classical continuum the micropolar continuum is capable of addressing the scale of the material microstructure.

The Cosserat continuum was used extensively for modelling particulate materials with non-uniform deformation, in particular shear band formation in granular materials [28-30, 55-58]. On top of that, using the concept of the asymmetric elasticity Teisseyre and Górski [59, 60] demonstrated the crucial role of particle rotations in fracture propagation. Modelling of fracture propagation in Cosserat continuum, including 2D orthotropic continuum modelling layered materials with bending was conducted by Pasternak and Dyskin [61, 62], Mühlhaus and Pasternak [63], Pasternak et al. [64-66]. However, the applicability of the Cosserat continuum is still limited due to the lack of methods for determining material constants and calibration of the characteristic lengths.

Recently Dyskin and Pasternak [67, 68] and Pasternak and Dyskin [69] investigated a specific problem where the Cosserat characteristic length is commensurable with the characteristic size of the material microstructure (e.g. grain size). For this case the Cosserat continuum theory gets considerably simplified; it was named the small-scale Cosserat continuum. It was demonstrated that in this case the simple pseudo-Cosserat continuum with constrained microrotations could asymptotically be used instead of the general Cosserat continuum for the problem of fracture propagation [67-71]. In this asymptotic the microrotations are no longer independent rather they are expressible through the classical displacements:

\[
\varphi = \frac{1}{2} \text{rot} u \quad (4.14)
\]

Here \( \varphi \) is the rotation vector, \( u \) is the displacement vector.
Consequently, the rotation and couple stresses can be calculated using the displacement field obtained in the conventional crack problem and the Cosserat constitutive equations.

In this study we investigate the mechanical behaviour of an idealised particulate material with a pre-existing fracture and determine the displacement and rotation fields around a Mode I crack using physical experiment, numerical simulations and a simple analytical model based on the concept of small-scale Cosserat continuum. The chapter has the following structure. The detailed description of the physical model, the experimental apparatus and technique as well as the obtained results is given in Section 4.2. In Section 4.3 we use a known analytical solution for the considered type of pre-existing fracture and compare results with the experiment. Section 4.4 consists of numerical simulations based on the discrete element modelling (DEM) (we used a particular class of DEM implemented in PFC2D software [72] – the distinct element method), comparison of results and calibration of microparameters of the numerical model (e.g. normal and shear stiffness of bonds and particles, friction coefficients, etc.). The chapter ends up with conclusions about applicability of the pseudo-Cosserat continuum with constrained microrotations for modelling of fracture propagation in the particulate materials (Section 4.5).

4.2. Experiments

The physical model, the experimental apparatus and technique were reported elsewhere (see Pasternak et al. [73]). Here we give a brief description and dwell upon the modifications which have been made for the current experiments.

4.2.1. Physical model and experimental apparatus

We concentrate on two-dimensional models of granulate materials with rotations. We also presume that the particles/grains are represented by discs notwithstanding the fact that particle shape can qualitatively affect the behaviour of a particulate material (e.g. Pasternak et al. [74], Dyskin and Pasternak [75, 76]). Subsequently, the physical model consists of an assembly of monodisperse thin steel discs. The discs have the diameter of 23.5 mm, the thickness of 1.6 mm and the mass of 5.45 g (the calculated density of steel is 7.85·10³ kg/m³). Similar models with discs (actually, coins) were used in other experiments for investigation of particle rotations which were carried out by Tamura and Yamada [77] and Tamura [78].
The discs form a square packing assembly. The assembly consists of 15 rows by 8 columns. All discs are in contact with four neighbours. The discs are glued together by a sealant, as shown in Fig. 4.1, to simulate cement that binds grains of a real particulate material together. The gluing was performed as follows. The square packing assembly was placed on a non-adherent polyethylene film. Then the space between the discs was filled with sealant. Using a cutter, we manually removed the redundant sealant. As a result, the bonds geometry could vary slightly, but it was anticipated that this should not affect the results of the experiment greatly.

The adhesive for the assembly has been chosen to make sure that the sealant is sufficiently flexible and delivers high movement capability. As a result, the adhesive bonds can transmit a moment load and the discs are allowed to have relative rotations. On top of that, the bonding strength and adhesion need to be considerably high. The detailed characteristics of the selected sealant Sikasil® WS-305 CN are shown in Table 4.1.

**Table 4.1.** The basic sealant characteristics [79].

<table>
<thead>
<tr>
<th>Sealant type</th>
<th>Sikasil® WS-305 CN</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemical base</td>
<td>One-component silicone</td>
</tr>
<tr>
<td>Density</td>
<td>1490 kg/m³</td>
</tr>
<tr>
<td>Tensile strength</td>
<td>1 MPa</td>
</tr>
<tr>
<td>Elongation at break</td>
<td>900 %</td>
</tr>
<tr>
<td>Young’s modulus</td>
<td>0.4 MPa</td>
</tr>
</tbody>
</table>

**Fig. 4.1.** Gluing of the model particles: (a) steel discs are glued together by the silicone sealant; (b) geometry and dimensions of the bonds.
The experimental apparatus with the physical model is shown in Fig. 4.2. The square packing assembly is placed between two transparent acrylic glass (PMMA) walls. The transparent walls and the discs with speckles painted on them allow using the digital image correlation photogrammetric technique for measuring the assembly kinematics at micro-scale (particles displacement and rotation). The experimental apparatus includes a slider that limits the assembly displacement. By measuring the length of the spring one can calculate the force with which the assembly interacts with the slider. The spring stiffness was determined in the previous study [73]; it equals 2.63 N/mm.

![Fig. 4.2. The experimental apparatus with square packing assembly of the discs: (1) physical model, (2) compression spring ($k_{spring} = 2.63$ N/mm), (3) slider, (4) roller bearings, (5) acrylic glass plates, (6) additional device to explore opening of the crack, (7) base.](image)

The experiments are aimed to explore the mechanical behaviour of the square packing assembly with a pre-existing fracture. In order to implement the fracture into our physical model we removed the bonds between some pairs of the discs (to be more precise, between the discs of the 8th and the 9th rows from the bottom). Two fracture lengths were considered and several attempts of the experiment were carried out for each fracture length. First, we removed the bonds between two pairs of the discs and conducted the experiments. Then we cut off the bonds between one more pair of the discs and conducted the experiment with three pairs of the unbonded discs as shown in Fig. 4.3. Since the experimental technique is identical for both fracture lengths, in the following section we discuss experiments and demonstrate the results only for the case of three pairs of unbonded discs.
In contrast to the previous experiments where the same apparatus was used [73, 80], some modifications took place. In order to explore the crack opening, we designed and built an additional mechanical device which consists of a steel triangular wedge, a bolt with a hand knob and a mount (Fig. 4.4). The angle of the wedge was small and equal to 5° in order to minimise the horizontal reaction of the wedge on the assembly. The bolt thread (M8) with a pitch of 1.2 mm allowed controlling the wedge displacement. We cut a hole in the left wall of the apparatus and installed the device in such a way that a lower bound of the wedge was located exactly halfway between the 8th and the 9th rows in the assembly of the discs. We pushed the steel triangular wedge into the square packing assembly of the discs by turning the bolt. The wedge made the discs of three left columns go up. Thus, we simulated opening of the Mode I crack. In addition, we minimised the friction between the wedge and the assembly by applying powdered graphite on the wedge’s edges.

**Fig. 4.3.** The pre-existing fracture represented by three unbonded pairs of the discs.

**Fig. 4.4.** The crack opening device: (1) bolt with a hand knob, (2) mount, (3) steel wedge.
4.2.2. Experimental technique and results

The initial state of the physical model and the triangular wedge are shown in Fig. 4.5a. The experimental procedure consisted of two simple repetitive actions until the wedge reaches the crack tip, Fig. 4.5b: (1) a half-turn of the hand knob to ensure sufficiently small evolution of the assembly (small changes during an evolution are required for applicability of the digital image correlation technique); (2) taking a photograph of the physical model at the position achieved. We used an off-the-shelf camera Canon 5D Mark II with Sigma 70 mm macro lens, which ensures sufficiently high picture quality and resolution. Each experiment produces about one hundred images. These images were processed in VIC-2D software which employs the digital image correction method for reconstruction of displacement and rotation fields.

![Fig. 4.5. The physical model during the experiment: a) initial position; b) final position.](image)

The digital image correlation method recovers full-field displacement and rotation data for each disc (i.e. for each point within each area-of-interest) in all images taken during the experiment. Due to inevitable errors (e.g. image noise in a photography, camera shake during shutter release) the reconstructed rotation field is not uniform within each disc (see [73] for more details). The measurement error was determined; it is equal to 0.3 degrees. Since each disc represents a rotating rigid body, the rotation of the disc is obtained by averaging the rotation field within the area-of-interest. In order to achieve this we developed a proprietary algorithm which averages
the rotation within each area-of-interest using the resultant data exported from VIC-2D and then plot the results more transparent.

Fig. 4.6 presents the determined evolution of the assembly during the physical experiment when the wedge achieves the second pair of the unbonded discs (Fig. 4.6a), the third one (Fig. 4.6b) and the crack tip (Fig. 4.6c). We exclude the bonds between the discs from the figure to avoid demonstrating superfluous details. Rotation is indicated inside each disc. Negative values denote the clockwise direction. Rotations in both directions smaller than the measurement error of 0.3 degrees are not shown. Since the wedge height is relatively small, the discs above the wedge rotate slightly (maximum magnitude is 3.8 degrees), the discs near the right wall (slider) do not practically rotate. The wedge does not influence the discs below it.

The horizontal displacement of the slider is small (less than 0.5 mm) when the wedge reaches the crack tip. As a result, the calculated force in the spring is smaller than 1.3 N. This is due to the fact that the wedge scarcely creates the horizontal load. Furthermore, there are other reasons that resist the movement of the slider (e.g. friction in the roller bearings of the slider, friction between the discs and the bottom wall as well as the acrylic glass walls of the apparatus).

It is noteworthy that during the evolution of the assembly the wedge hardly has a contact with the discs along the upper fracture surface (except of the disc at the left boundary of the assembly). This shows that the opening of the Mode I fracture induces the rotations while the friction is not an important factor.
4.3. Simple analytical model

Particle rotations caused by wedging a crack can be modelled in the frame of small-scale Cosserat continuum. To this end, one needs to consider the crack in the frame of classical elasticity, determine the displacement field and then using Eq. (4.14) find the rotations. We consider a simplified analytical model whereby the wedge shown in Fig. 4.4 is replaced with a rectangular wedge. Then for the conventional elastic formulation we can use a known analytical solution (e.g. [81]). It concerns a semi-infinite crack in an infinite plane opened by a thin rigid rectangular wedge with thickness of $2h$, Fig. 4.7. The wedge is at a distance $b$ from the crack tip. Due to the symmetry, we consider the solution only for the upper half plane (i.e. $y > 0$).
Chapter 4. Mode I crack in particulate materials with rotational degrees of freedom

Fig. 4.7. A semi-infinite crack in an infinite plane opened by an inserted thin rigid wedge of thickness $2h$ at a distance $b$ from the crack tip [81].

While the configuration is cubic we will approximate the material as isotropic; the subsequent comparison with the experiment showed that this approximation gives errors commensurable with the general errors of this experiment and thus does not influence the main conclusion.

For the plane-strain problem the displacement field around the crack can be expressed as [81]:

$$\begin{align*}
2Gu &= (1-2\nu) \text{Re} \overline{Z} - y \text{Im} \overline{Z} \\
2Gv &= 2(1-\nu) \text{Im} \overline{Z} - y \text{Re} \overline{Z}
\end{align*}$$

(4.15)

where $Z$ is the Westergaard complex stress function, which for this crack reads:

$$Z(z) = \frac{Eh}{\pi} \frac{1}{\sqrt{z(z+b)}}, \quad z = x + iy$$

(4.16)

$\overline{Z}$ is the first integral of $Z$:

$$Z = \frac{d}{dz} \overline{Z}, \quad \overline{Z}(z) = \frac{Eh}{\pi} \text{sinh}^{-1} \frac{z}{\sqrt{b}}$$

(4.17)

For the case of plane-stress which corresponds to the physical model the same solution can be used if Poisson’s ratio, $\nu$, is replaced by $\nu/(1-\nu)$ and the Young’s modulus, $E$, is replaced by $E/(1-\nu^2)$. 

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In order to determine the correct branches of the square root functions in Eqs. (4.16) and (4.17), we express complex functions, $Z$ and $\overline{Z}$, in the polar form (see Appendix 4.A for details):

$$Z = \frac{Eh}{\pi} \frac{1}{\sqrt{\eta r_2}} \left[ \cos \left( -\frac{\theta_1 + \theta_2}{2} \right) + i \sin \left( -\frac{\theta_1 + \theta_2}{2} \right) \right]$$

(4.18)

$$\overline{Z} = \frac{Eh}{\pi} \sinh^{-1} \frac{\sqrt{\eta}}{b} \left[ \cos \left( \frac{\theta_1}{2} \right) + i \sin \left( \frac{\theta_1}{2} \right) \right],$$

(4.19)

where

$$\eta = \sqrt{x^2 + y^2}, \quad \theta_1 = \begin{cases} \arctan \left( \frac{y}{x} \right), & \text{when } x > 0, \quad y > 0 \\ \pi + \arctan \left( \frac{y}{x} \right), & \text{when } -b < x < 0, \quad y > 0 \end{cases}$$

$$r_2 = \sqrt{(b + x)^2 + y^2}, \quad \theta_2 = \arctan \left( \frac{y}{b + x} \right)$$

(4.20)

By substituting Eqs. (4.18) and (4.19) into Eq. (4.15), we obtain the displacement field.

As mentioned above, materials with microstructure require the use of non-standard continuum such as Cosserat continuum in order to find microrotations. However, as suggested in [67-69], the problem of moving and rotating elastically bonded discs can be considered in terms of small-scale Cosserat continuum as the Cosserat characteristic length is comparable with characteristic size of the material microstructure. Consequently, the pseudo-Cosserat continuum with constrained microrotations may be used instead of the general one. Thus, rotations become dependent on displacements. The rotation vector, $\phi$, can be easily found through the displacement gradients using the conventional equation from the classical continuum, Eq. (4.14).

Since we consider the plane problem there is only one component, $\phi$, in the rotation vector. Thus, the rotation field can be found as:

$$\phi = \frac{1}{2} \left( \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right)$$

(4.21)

Substituting Eq. (4.15) into Eq. (4.21) we obtain the rotation field.
Fig. 4.8 demonstrates the displacement and rotation fields for the upper half plane \((y > 0)\) assuming the Poisson’s ratio equal to 0.3. The geometrical dimensions are following: \(b = 62\) mm, \(2h = 10.8\) mm. This corresponds to the case when the wedge reaches the crack tip in the experiment (Fig. 4.7c). As can be seen from Fig. 4.8c, there is singularity in the rotation field at the crack tip \((x = 0, y = 0)\) and at the left side of the crack \((x = -b, y = 0)\).
**Fig. 4.8.** Analytical displacement and rotation fields near the crack: (a) horizontal displacement (along $x$-direction), $u$; (b) vertical displacement (along $y$-direction), $v$; (c) in-plane rotation, $\phi$. 
Chapter 4. Mode I crack in particulate materials with rotational degrees of freedom

We may assume that the angle of rotation of each disc can be calculated as a rotation field value at the centre of each disc (this proposition holds within the limits of the experimental accuracy). Fig. 4.9 illustrates analytical rotation of the discs in the same way as for experimental results (Fig. 4.6c). It is seen that the analytical solution for disc rotations near the crack tip (Fig. 4.9) is reasonably close to what we measured in the physical experiment (Fig. 4.6c). The difference in rotation of the discs within the dash-lined rectangle (Fig. 4.9) between the experimental results and analytical solution is up to 20 percent. This difference may be explained by inaccuracy of the physical modelling, for example, friction between the acrylic glass plates and the discs, slightly different bonds geometry, contacts between the wedge and the discs, the shape of the wedge.

It is important to note that the analytical solution does not take into account the external boundary conditions (constraints and friction due to the side walls, free surface at the top). Therefore, the analytically deducted rotation of the discs away from the crack tip (i.e. outside the dash-lined rectangle and close to the boundaries) and the results of the experiment differ markedly and cannot be compared.

![Fig. 4.9. Analytically calculated disc rotations. The number inside each disc indicates the angle of rotation in degrees (negative angles mean clockwise rotation). The dash-lined rectangle indicates a zone where analytical solution and experimental results are in good agreement.](image)
4.4. Discrete element model

A more accurate modelling requires the use of numerical methods. Here we study opening of Mode I crack using numerical modelling. The Particle Flow Code\textsuperscript{2D} (PFC2D) [72] realising the distinct element method [82] was utilized to conduct our modelling. In the PFC2D there are three main types of body: a particle, a clump and a wall. Particles and clumps are used to simulate particulate materials. A particle is represented by a disc with finite thickness and specified radius. A clump consists of number of particles and may have an arbitrary shape. A wall simulates the boundary constraint. Interactions between bodies are determined through specifying the behaviour of the contacts. The particles can be connected by a bond with finite bond strength and stiffnesses or simply not bonded but reacting with each other at contact point in compression. The distinct element method is, as well known, based on the combination of Newton’s second law and force-displacement law between two contacting pieces.

Two conventional built-in contact models in PFC2D are employed in our numerical simulation: the linear contact model and linear parallel bond model (PB model). The linear contact model provides linear elastic (no-tension) frictional behaviour of a contact between two bodies over a vanishingly small area. The contact behaviour is determined through a set of normal and shear springs with constant stiffnesses, $k_n$ and $k_s$, respectively. Since the contact acts on an infinitesimal area it can only transmit forces. In addition, damping is implemented in the linear contact model through dashpots with viscosities given in terms of the normal and shear critical-damping ratios, $\beta_n$ and $\beta_s$. The friction coefficient of the contact is denoted as $\mu$. The linear contact model is shown in Fig. 4.10a (see [72, 82] for more details).

Linear parallel bond model provides the behaviour of a cement-like matter that binds particles with other bodies. Linear parallel bond consists of two sets of springs that act in parallel: a set of linear springs with stiffnesses, $k_n$ and $k_s$ (like in the linear contact model), and a set of parallel bond springs with constant stiffnesses, $k_n$ and $k_s$ with finite bond tensile and shear strengths, $\sigma_f$ and $\tau_f$. The parallel bond springs can be considered as a set of springs that are uniformly distributed over a rectangular area in two-dimensional problem (over a circular area in three-dimensional problem). Thus, such a bond (the PB bond) can resist moments. Note that the unit of stiffness for linear contact spring is force/displacement while it is stress/displacement for parallel bond.
springs. Parallel bond breaks when either tensile or shear strength of the bond is exceeded. When parallel bond breaks, the set of parallel bond springs will be removed and the contact will behave like linear model. Similar to the linear contact model a friction coefficient, $\mu$, is implemented in the system. The PB model is shown in Fig. 4.10b (see [72, 83, 84] for more details).

![Fig. 4.10. Illustration of built-in contact models: (a) Linear contact model; (b) Linear parallel bond (PB) model.](image)

In our numerical modelling we use the linear parallel bond to represent the silicone sealant between the discs. To simulate the behaviour of the un-glued pairs of discs we utilize the linear contact model. Similar to our physical experiments, we investigated situations of two and three unbonded pairs of discs. However since the technique is the same, we only present the results and analysis of numerical simulation of the case of three unbonded pairs of discs here.

Fig. 4.11 illustrates our numerical model at the initial stage. The black lines between particles indicate the PB model while the linear contact model is represented by the white lines. The wedge was simulated by combination of two connected walls. Constant velocity of 0.5 mm/sec in the horizontal direction is applied to the wedge. Other walls are fixed. The wedge is moving until it does not achieve the crack tip.
Fig. 4.11. Discrete element model of a square packing assembly of discs. The wedge moves with horizontal velocity of 0.5mm/s, the walls are fixed. Black lines indicate parallel bonds between the discs and white lines represent the linear contacts (unbonded discs).

The micro-properties of the numerical model were calibrated and represented in Table 4.2. The calibration procedure was as follows. Initially, since the same discs and the similar experiment apparatus were used earlier, some parameters were taken from the previous study, namely the normal and shear stiffnesses of wall-to-disc and disc-to-disc contact, critical shear and normal damping ratio, friction coefficient of wall-to-disc and disc-to-disc contact [73]. The newly included micro-properties – normal and shear stiffnesses of PB model were estimated using the sealant’s mechanical properties (Table 4.1) and the geometry of gluing (Fig. 4.1b). The rough estimation for normal and shear stiffnesses of parallel bond springs can is:

\[
\bar{k}_n = \frac{E}{L} = 0.08 \text{MPa/mm} \\
\bar{k}_s = \frac{E}{2(1+\nu)L} = 0.03 \text{MPa/mm}
\]  

(4.22)

Here \(E\) is the Young’s modulus of the silicone sealant, \(L\) is a length of the bond, \(\nu\) is the Poisson’s ratio. The Poisson’s ratio was assumed to be equal to 0.3.

Since we do not study fracture propagation in the physical experiment due to the small size of the assembly, we set parallel bond tensile and shear strength to infinite (a large value of 10GPa is used for the task). Furthermore, as discussed in the experiment
section the powdered graphite was used as a lubricant so the friction coefficient between the wedge and discs was set to a small value as 0.01.

Table 4.2. The calibrated microparameters of the numerical model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normal stiffness of inter-disc contact</td>
<td>60 N/mm</td>
</tr>
<tr>
<td>Normal stiffness of disc – right wall contact</td>
<td>10 N/mm</td>
</tr>
<tr>
<td>Normal stiffness of disc – left wall contact</td>
<td>107 N/mm</td>
</tr>
<tr>
<td>Shear stiffness of inter-disc contact</td>
<td>1 N/mm</td>
</tr>
<tr>
<td>Density of discs, kg/m³</td>
<td>7850</td>
</tr>
<tr>
<td>Disc diameters, mm</td>
<td>23.5</td>
</tr>
<tr>
<td>Friction coefficient of inter-disc contact</td>
<td>0.3</td>
</tr>
<tr>
<td>Friction coefficient between the discs and the walls</td>
<td>0.3</td>
</tr>
<tr>
<td>Friction coefficient between the discs and the wedge</td>
<td>0.01</td>
</tr>
<tr>
<td>PB normal stiffness, MPa/mm</td>
<td>0.055</td>
</tr>
<tr>
<td>PB shear stiffness, MPa/mm</td>
<td>0.013</td>
</tr>
<tr>
<td>PB tensile strength, GPa</td>
<td>10</td>
</tr>
<tr>
<td>PB shear strength, GPa</td>
<td>10</td>
</tr>
</tbody>
</table>

During the calibration stage the microparameters were changed individually to provide the best fit between the experiments and the simulations. We discovered that some parameters such as PB normal and shear stiffnesses and friction coefficient between walls and discs are the most important micro-properties for the calibration. Changes in other parameters (e.g. wall and disc stiffnesses) do not significantly affect the assembly evolution.

The PFC2D solution scheme is based on the explicit finite-difference method which is sensitive to the time step. In our simulation we use the time step of $5 \times 10^{-4}$ sec. It was found that reducing the time step did not change the results, i.e. the solution is stable.

The horizontal contact force was tracked during the simulation and the maximum magnitude was appeared to be less than 1.3N as observed in the experiment. Moreover, the discs in the right boundary column have fairly small horizontal displacement within 0.5 mm, which is also in a good agreement with the physical experiment.

The evolution of rotations of the discs is shown in Fig. 4.12. The simulation produces the disc rotations similar to what we observed in the experiment. When the numerical simulation finished the first five columns of discs above the wedge had
relatively slight rotations in clockwise direction (maximum magnitude is 3.83 degrees). Other discs had rotation within 0.3 degrees. Similar to the experiments, during the evolution of the assembly the wedge practically does not have a contact with the discs along the upper fracture surface except of the disc at the left boundary of the assembly.

However, it can be seen from Fig. 4.12 that there is some difference with the physical experiment (Fig. 4.6c). The magnitudes of rotations of a few discs at the left boundary column are higher in the numerical simulation. This can be explained by the fact that in the physical experiment these discs were placed near the positions where the acrylic glass walls were fixed by bolts. This increases the friction between discs and apparatus walls and hence constrains rotations. The (relatively small) differences in rotations of other discs between experiment and numerical simulation can be attributed, similarly to discussed in the previous research [73], to not perfectly circular shaped discs, friction between the acrylic glass walls, slight tilt of the slider.

The rotation of disc I (shown in Fig. 4.11) vs. wedge displacement is presented in Fig. 4.13. The cross markers represent experimental results, the solid line gives the results of numerical simulation. These results are pretty close and confirm the selected microparameters of the numerical model.
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Fig. 4.12. Results of numerical simulation showing the evolution of the square packing assembly during the opening of Mode I crack. The number inside each disc indicates the angle of rotation in degrees (negative angles – clockwise rotation, positive angles – counter clockwise rotation). The rotation angles smaller than 0.1 degrees are not shown.

Fig. 4.13. Rotation of disc I (Fig. 4.11) vs. wedge displacement. Solid line represents the numerical simulations, cross markers give the experimental results.

4.5. Conclusion

Mechanical behaviour of an idealised slightly cemented granular material with a pre-existing fracture was investigated using different approaches such as physical
experiments accompanied by digital image correlation, numerical simulations based on discrete element modelling and analytical solution rested on the conventional equations of linear elastic fracture mechanics. The Mode I crack was simulated by using the wedge which produces the opening displacements. Due to the small size of the physical model we considered only the opening of the crack; the fracture propagation was beyond the scope of this study.

The analytical solution was obtained assuming that microrotations near the crack tip can be considered dependent on displacement gradients as in the classical continuum. In terms of continuum modelling of particulate materials it means that in the case of the crack problems the pseudo-Cosserat continuum with constrained microrotations can be used instead of the general Cosserat continuum. The comparison of rotation of the discs near the crack tip obtained by physical modelling and analytical approach demonstrates reasonably good agreement.

The discrete element modelling of opening of the Mode I crack also gives good agreement with the results of the experiments. The parametric analysis shows that some parameters (e.g. stiffnesses of parallel bond) influence on mechanical behaviour of the assembly more than others (e.g. stiffnesses of wall and particles) during the opening the Mode I crack. It is interesting that the back analysis yields low values of contact stiffnesses between the particles. These are several orders of magnitude lower than the ones typically used in the literature.
In order to convert complex functions $Z(z)$ and $\overline{Z}(z)$ to a polar form we express the complex arguments, $z$ and $z+b$, as:

$$z = \eta e^{i\theta_1}$$
$$z+b = r e^{i\theta_2}$$

Here, as shown in Fig. 4.A.1:

$$r_1 = \sqrt{x^2 + y^2}, \quad \theta_1 = \begin{cases} \arctan(y/x), & \text{when } x > 0, \quad y > 0 \\ \pi + \arctan(y/x), & \text{when } -b < x < 0, \quad y > 0 \end{cases}$$
$$r_2 = \sqrt{(b+x)^2 + y^2}, \quad \theta_2 = \arctan(y/b + x)$$

The square roots, $1/\sqrt{z(z+b)}$ and $\sqrt{z}$, in the complex functions, $Z$ and $\overline{Z}$, read:

$$\frac{1}{\sqrt{z(z+b)}} = \frac{1}{\sqrt{\eta e^{i\theta_1} r e^{i\theta_2}}} = \frac{1}{\sqrt{\eta r_2}} \left( \cos \left( \frac{-\theta_1 + \theta_2}{2} \right) + i \sin \left( \frac{-\theta_1 + \theta_2}{2} \right) \right)$$
$$\sqrt{z} = \sqrt{\eta e^{i\theta_1}} = \sqrt{\eta} \left( \cos \left( \frac{\theta_1}{2} \right) + i \sin \left( \frac{\theta_1}{2} \right) \right)$$
Thus, we can write the Westergaard complex stress function $Z$ and its first integral $\overline{Z}$ as:

\[
Z = \frac{Eh}{\pi} \frac{1}{\sqrt{r_1 r_2}} \left( \cos \left( -\theta_1 + \theta_2 \right) + i \sin \left( -\theta_1 + \theta_2 \right) \right)
\]

\[
\overline{Z} = \frac{Eh}{\pi} \sinh^{-1} \frac{\sqrt{r_1}}{b} \left( \cos \left( \frac{\theta_1}{2} \right) + i \sin \left( \frac{\theta_1}{2} \right) \right)
\]

(4.4)
Reference

Chapter 4. Mode I crack in particulate materials with rotational degrees of freedom


CHAPTER 5
Stability of discrete mass-spring systems
with negative stiffness springs
5.1. Stability of chains of oscillators with negative stiffness normal, shear and rotational springs
We consider chains of particles with fixed ends in planar movement such that each particle has three degrees of freedom: two translational and one rotational. The particles are connected by one normal (longitudinal), one shear (transverse) and one rotational spring with a possibility that stiffness of some springs can be negative. We showed that the necessary condition of stability is that such a chain is allowed no more than three negative stiffness springs. The allowable negative stiffness springs can be arranged in two ways: (i) the chain contains one normal, one shear and one rotational negative stiffness springs or; (ii) the chain contains one normal and two rotational negative stiffness springs. The absolute values of the negative stiffnesses should not exceed certain threshold values that depend upon the stiffnesses and the number of the other (positive) springs. The positions of normal and shear negative stiffness springs do not affect the critical values, however the positions of the negative rotational stiffness springs are found to be important. The modal frequencies reduce when one of the negative stiffnesses tends to the critical value; the smallest frequency tends to zero. Damped chains also exhibit similar decrease of damping frequencies, but the lowest frequency tends to zero while the chain is still stable. At this point the damping bifurcates and produces two branches: one increases with the increase in the value of negative stiffness, the other decreases. No giant damping is observed.

5.1.1. Introduction

Negative stiffness remains a relatively new concept in mechanics although it has received attention in recent years. The idea of negative stiffness is paradoxical and not obvious: when the applied force reduces the displacement increases. Negative stiffness can sometimes be found in nature. One example is the negative stiffness in hair-bundles in the ear [1]. Negative values of joint stiffness were reported in some cases [2, 3]. The post-peak softening observed in stiff loading of brittle materials such as rock and concrete [4, 5] when increase in strain causes stress decrease. The post-peak softening however is not reversible (the strain decrease causes further stress reduction) and strictly speaking cannot be regarded as a manifestation of negative stiffness. Yet, fracturing accompanying the post-peak softening suggests the presence of unstable phase of deformation. This is supported by the understanding that formally negative stiffness corresponds to the case when the work done by the force is negative, as it involves displacement in the direction opposite to the force. Therefore, the strain energy ceases to be positive definite and the system becomes unstable. This means that materials and
structures exhibiting negative stiffness can only be stable in the presence of an energy source/sink (energy reservoir [6]) which ensures the positive definiteness of the combined system consisting of the negative stiffness material/system and the energy reservoir. In many cases the role of the stabilising system can be modelled by the appropriate boundary conditions then it is the boundary conditions that stabilise the system [6-9]. For instance in the case of compression testing of brittle materials the role of the energy reservoir is played by the loading frame provided that it is sufficiently stiff. (If the loading frame is not stiff enough, the post-peak stage of loading cannot be observed; instead the sample fails, usually violently, which is a manifestation of instability.) The boundary conditions can then be represented by displacement-controlled loading.

One of the most known and well-studied mechanisms of negative stiffness is the post-buckling deformation of tubes. Bažant and Cedolin [10] considered negative stiffness associated with the deformation of post-buckled columns (“S” shape configuration), shells and L-frames. Later the mechanical behaviour of pre-buckled bonding silicone rubber shells (tubes) with silicone cement in a Reuss configuration was explored experimentally and theoretically [11, 12]. Other experiments showed that negative stiffness could be observed not only in pre-buckled macroscopic tubes but also with multiwalled carbon nanotubes [13-15].

Negative stiffness may emerge in discrete structures composed of other elastic elements such as: arches (the usage of arches in honeycomb structures is described below) [16], links and lever models with springs [17-20]. Different negative stiffness devices have already been designed and tested successfully, for instance, for seismic protection of structures, car seats suspensions. Also interlocking discrete structures of cubic elements [21, 22] are known to exhibit both negative stiffness and high damping attributed to contact change (the same effect is observed for buckled beams [23-26]). Dyskin and Pasternak [7, 27, 28] and Pasternak, Dyskin and Sevel [29] suggested another type of structures producing negative stiffness based on rotation of non-spherical particles involving compressive loading. It was suggested that rotations can form large-scale patterns [30] and may provide a mechanism of instability in granular materials, fragmented rocks and blocky rock masses [31-35].

In addition to the cases mentioned above, the phenomenon of negative stiffness may occur in distributed composite materials which have negative stiffness inclusions.
An analysis of the effects of negative stiffness inclusions in composite materials in the case when the interaction between the inclusions can be neglected was conducted by Lakes and Drugan [36]. It was shown that in this case negative stiffness may be stabilized by a positive-stiffness matrix (if inclusion stiffness is not excessively negative [37]). Further analysis of the stabilising effect of the matrix was conducted by Drugan [38], Kochmann and Drugan [39], Dyskin and Pasternak [6, 7].

Lakes [11, 12] suggested that the damping ratio for the rubber tube with negative stiffness could be orders of magnitude higher than for a common rubber under certain conditions. Obviously, these results are interesting from the point of view of practical application for effective decrease of vibrations and noise in structures. Recently Dong and Lakes [23, 24] designed stable axial damper modules consisting of PMMA and stainless steel columns. They established that negative structural stiffness and high damping can be achieved in the pre-buckled columns at large amplitude oscillations if the unattached flat-end columns are allowed to tilt at the edges. They also obtained that effective damping and the product of the Young’s modulus and the loss tangent significantly exceed these characteristics of the parent material. Wang and Lakes [40] suggested that systems containing negative stiffness elements could demonstrate very high damping. As a measure of damping they used the loss tangent. Kalathur and Lakes [25] conducted experiments with pre-buckled PMMA rods under small amplitude oscillations and demonstrated that when the rod ends are not glued high values of loss tangent (the tangent of phase shift) are observed. This was interpreted as high damping associated with negative stiffness. We note though that in a conventional single degree of freedom oscillator with damping, when the driving frequency coincides with the natural frequency, the phase shift becomes $-\pi/2$ (e.g. Main [41]). Therefore the absolute value of loss tangent can formally become infinite without the need in negative stiffness. Experimental investigations similar to Kalathur and Lakes [25] were further conducted by Kalathur, Hoang, Lakes and Drugan [26] and Fulcher, Shahan, Haberman, Seeppersad and Wilson [42].

It was also suggested by Lakes [11] that the presence of negative stiffness inclusions in a matrix can increase damping (again in terms of high values of the loss tangent). Lakes, Lee, Bersie and Wang [43] studied experimentally the mechanical properties of a composite material with negative stiffness inclusions made from single domains of ferroelastic vanadium dioxide ($\text{VO}_2$) in a pure tin matrix. It was shown that

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in addition to increasing loss tangent the negative stiffness inclusions enhance the effective composite stiffness even stronger than diamond inclusions [43, 44]. Other physical properties such as thermal expansion, piezoelectricity and pyroelectricity can also take extreme values in the presence of the negative stiffness phase in composite materials [37]. Later Wang, Ludwigson and Lakes [45] conducted a more detailed study of deformation of the composite material with negative stiffness inclusions of vanadium dioxide and compared its properties with other composites (SiC–InSn and Zinc). Jaglinski, Stone and Lakes [46] and Jaglinski, Frascone, Moore, Stone and Lakes [47] carried out a torsion testing of composites with VO$_2$ processed via powder metallurgy and indium (In) – thallium (Tl) binary alloy in martensitic phase transformation. They revealed internal friction anomalies over a broad range of temperatures. In summary, negative stiffness inclusions represent a potential effective tool for tuning wide range of various physical properties of the composite material.

Apart from composite materials and structures Lakes, Rosakis and Ruina [48] discovered that negative stiffness could be seen in cellular solids. They investigated solid foam and tetrakaidecahedron single-cell models. It was revealed that the stress-strain curve is monotonic for open-cell foam, but a force-deformation curve has regions of negative slope (i.e. negative stiffness) for single-cell models. Further research examined the energy absorption properties of a negative stiffness honeycomb structure [49, 50]. Prismatic cells of this honeycomb had special configuration and were created from curved beams. (Note, that clamped double curved beams under central loading demonstrate inherent negative stiffness behaviour [51]). On top of that, since curved beams provide elastic buckling, the honeycomb composed of curved beams is able to recover from large deformations in contrast to common honeycomb structures where plastic deformations occur. It was shown by Correa, Seepersad and Haberman [49] and Correa, Klatt, Cortes, Haberman, Kovar and Seepersad [50] that such honeycomb structure could have high energy absorption associated with buckling.

A number of structures were considered that consist of negative stiffness elastic elements [29, 40, 52, 53]. It was confirmed that systems with negative stiffness elements could be stable. In a spring system [52] extreme overall stiffness can be achieved when the system is metastable. (A similarity was noted with the diamond which is in a metastable state at ambient conditions.) The system can be stable if it is tuned for high compliance. These results are extended to two-dimensional systems [54,
55]. However, due to coupling between the modes the two-dimensional systems are less stable.

In order to gain insight into the conditions of stability of systems containing negative stiffness elements and their effect on damping, Pasternak, Dyskin and Sevel [29] considered a simple example of a 1D chain of \( n+1 \) masses (particles) connected in series by normal springs. The chain ends were fixed. The necessary and sufficient condition of stability has been found: a stable system can contain no more than a single negative stiffness spring and the absolute value of the negative stiffness spring should not exceed a certain critical value determined by all positive stiffnesses. Furthermore, the higher the number of masses or particles (the number of degrees of freedom) the lower is the critical value of negative stiffness spring. It was shown that as the negative stiffness tends to its critical value one of the model frequencies tends to zero, while other eigenfrequencies just reduce. Furthermore, no dramatic increase in damping suggested by Lakes [11] was observed.

The case considered by Pasternak, Dyskin and Sevel [29] includes springs of only one type – normal (longitudinal) springs, which corresponds to 1D systems with particles each having a single degree of freedom. A more general case would be to consider connections between the particles that involve both normal and shear resistance. Furthermore, if particles can independently rotate (as assumed for instance in the Cosserat theory) rotational springs should also be included. This chapter investigates two-dimensional motion of chains of \( n \) linear oscillators when each mass (particle) has three degrees of freedom, two translational and one rotational. The particles are connected by normal (longitudinal), shear (transversal) and rotational elastic springs. Such \( n+1 \)-mass systems are obviously characterised by \( 3(n+1) \) degrees of freedom.

We investigate different combinations of negative stiffness springs and obtain a criterion of stability for each case. We start our stability analysis by considering a simple harmonic motion of a chain of linear oscillators connected in series by uncoupled normal and shear springs without an external time dependent force, that is without excitation. Then we consider masses connected by coupled shear and rotational springs in the presence and absence of a driving force. Finally we study the stability of dynamic system with viscous damping and show the influence of negative stiffness spring on the system’s behaviour. The chapter is concluded with a discussion of the results.
5.1.2. Stability of chains of oscillators

Consider, following Abel [56] two-dimensional movement of oscillating particles assembled in a chain by connecting them through normal, shear and rotational springs. The movement of each particle is only characterised by two displacements, \( u_1 \) and \( u_3 \) and one rotation, \( \varphi_2 \) in the coordinate frame \( x_1, x_2, x_3 \) shown in Fig. 5.1.1. We start with a simplified problem without rotations and then add the rotations.

5.1.2.1. System with normal and shear springs

Consider a 2D model of a chain of particles (masses) connected to each other by one normal and one shear springs, Fig. 5.1.1.

We use the following notations:
- \( N_{ik} \) and \( S_{ik} \) are stiffnesses of the \( i \)-th normal and shear spring correspondingly,
- \( m_i \) is the mass of the \( i \)-th particle,
- \( u_{1i} \) and \( u_{3i} \) are translational displacements of the \( i \)-th particle in \( x_1 \) and \( x_3 \) directions correspondingly.

Assume that the end particles are fixed:
\[
\begin{align*}
    u_{10}(t) &= u_{30}(t) = 0 \\
    u_{30}(t) &= u_{3n}(t) = 0
\end{align*}
\] (5.1.1)

Since shear and normal springs work on different degrees of freedom the system with only shear springs is identical to the system consisting of only normal springs; the latter was studied in Pasternak, Dyskin and Sevel [29]. Equations of motion of the shear spring system are equivalent to those of the normal spring system with a change of notation. Therefore, it is apparent that the mechanical behaviour and, consequently, the stability criterion for the chains of oscillators consisting of only normal springs and the...
chains of oscillators with only shear springs should be the same. On top of that, the
stability criterion for the systems with both normal and shear springs (the combined
system) can be represented as a combination of the stability criteria for two independent
chains. Since the chains with normal springs were considered in detail in Pasternak,
Dyskin and Sevel [29], it is trivial to generalise the obtained results for the combined
systems. Let us briefly demonstrate it.

The system of differential equations for the chain with normal springs reads:

\[ m_i \ddot{u}_i + (k_i^N + k_i^{N,1})u_i - k_i^N u_{i-1} - k_i^{N,1} u_{i+1} = f_i \]  
(5.1.3)

Thus the system of differential equations for the chain with shear springs reads:

\[ m_i \ddot{u}_i + (k_i^S + k_i^{S,1})u_i - k_i^S u_{i-1} - k_i^{S,1} u_{i+1} = f_i, \]  
(5.1.4)

For both systems of differential equations, Eqs. (5.1.3) and (5.1.4), \( i = 1, \ldots, n-1 \) giving
all together \( 2(n-1) \) equations of motion.

The set of equations of motion for the system with normal and shear springs in
the matrix form reads:

\[ M \ddot{u} + Ku = f \]  
(5.1.5)

Here \( M \) is the mass matrix, \( u \) is the displacement vector, \( \ddot{u} \) is the acceleration vector,
\( f \) is the force vector, \( K \) is the matrix of stiffness:

\[
\begin{pmatrix}
m_1 & 0 & 0 & 0 & 0 & 0 \\
0 & \ldots & 0 & 0 & 0 & 0 \\
0 & 0 & m_n & 0 & 0 & 0 \\
0 & 0 & 0 & m_1 & 0 & 0 \\
0 & 0 & 0 & 0 & \ldots & 0 \\
0 & 0 & 0 & 0 & 0 & m_n\end{pmatrix}
\begin{pmatrix}
u_{11} \\
\vdots \\
u_{n-1} \\
u_{31} \\
u_{n-1} \\
u_{3n-1}\end{pmatrix}
\begin{pmatrix}
f_{11} \\
\vdots \\
f_{n-1} \\
f_{31} \\
f_{n-1} \\
f_{3n-1}\end{pmatrix}
\]  
(5.1.6)

\[
\begin{pmatrix}
k_i^N + k_i^S & -k_i^N & 0 & 0 & 0 & 0 & 0 \\
-k_i^S & k_i^N + k_i^N & \ldots & 0 & 0 & 0 & 0 \\
0 & \ldots & 0 & \ldots & \ldots & \ldots & \ldots & \ldots \\
0 & 0 & -k_i^{N,1} & k_{n-1}^N + k_i^S & 0 & 0 & 0 \\
0 & 0 & 0 & k_i^S & k_i^S & \ldots & \ldots & \ldots & \ldots \\
0 & 0 & 0 & 0 & 0 & \ldots & \ldots & \ldots & \ldots \\
0 & 0 & 0 & 0 & 0 & 0 & \ldots & \ldots & \ldots & \ldots \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -k_n^S & k_n^S \end{pmatrix}
\]  
(5.1.7)
Positive definiteness of elastic energy, which is a criterion of stability of the system, is equivalent to positive definiteness of the matrix of stiffness. The matrix of stiffness is a tridiagonal block matrix. It is clear from the set of the equations of motion, Eqs. (5.1.3) and (5.1.4), and the matrix of stiffness, Eq. (5.1.7), that the combined system is a simple extension of the system with only normal springs and the system with only shear springs. The matrix of stiffness of the system with uncoupled normal and shear springs, Eq. (5.1.7), is positive-definite when the block corresponding to the system with only normal springs and the block corresponding to the system with only shear springs are positive-definite. The condition of positive definiteness of the matrix of stiffness for the system with only normal springs was obtained in Pasternak, Dyskin and Sevel [29]:

\[
\sum_{i=1}^{n} \prod_{j=1}^{n} k_{ij}^{N} > 0 \tag{5.1.8}
\]

This condition was derived from the criterion that all main diagonal minors of the matrix of stiffness should be positive (the Sylvester’s criterion). Similarly we can write the condition of stability of the system with only shear springs:

\[
\sum_{i=1}^{n} \prod_{j=1}^{n} k_{ij}^{S} > 0 \tag{5.1.9}
\]

Combination of these two conditions, Eqs. (5.1.8) and (5.1.9), gives the necessary and sufficient condition of stability of the system with normal and shear springs.

It was further obtained in Pasternak, Dyskin and Sevel [29] that a stable chain consisting of only normal springs can have no more than one negative stiffness spring, \(k_{i}^{N}\). Obviously, it means that the maximum number of the negative stiffness springs in the combined system with normal and shear springs is two. Subsequently, the necessary condition of stability is that there can exist no more than one negative stiffness normal spring and one negative stiffness shear spring.

Acknowledging the fact that only one negative stiffness spring is allowed per degree of freedom and using conditions, Eqs. (5.1.8) and (5.1.9), the critical absolute values of negative stiffnesses (the maximum absolute values of negative stiffness when
the system becomes unstable) can be calculated for the combined system with \( n \) normal and \( n \) shear springs. Suppose the negative normal and shear springs have indexes \( i \) and \( m \). Then

\[
\begin{align*}
    k^N_{cr,i} &= \frac{\prod_{j=1}^n k^N_j}{\sum_{p=1}^n \prod_{j=p,i} k^N_j}, \quad k^S_{cr,m} = \frac{\prod_{j=1}^n k^S_j}{\sum_{p=1}^n \prod_{j=p,m} k^S_j}
\end{align*}
\] (5.1.10)

Subsequently the allowable values of negative stiffness are

\[
k^N_i > -k^N_{cr,i}, \quad k^S_m > -k^S_{cr,m}
\] (5.1.11)

It is seen that the critical negative stiffness for normal and shear springs is determined by the number and values of the positive stiffness springs. Positions of the negative stiffness springs do not affect the critical negative stiffness and stability of the system. In addition, the positions of the allowed negative stiffness shear and normal springs are independent. Since the combined system is uncoupled the shear and normal springs may be placed in the same or any other position and the system will remain stable.

5.1.2.2. System with coupled shear and rotational springs

Now we add a rotational degree of freedom represented in particle \( i \) by \( \varphi_{2i} \), which is the angle of rotation of the \( i \)-th oscillator about the \( x_2 \)-direction. We also add the related rotational springs resisting the relative particle rotations. We consider a system with shear and rotational springs (Fig. 5.1.2) neglecting, for the sake of simplicity, the normal springs as they obviously do not interact with shear and rotational springs. Stiffness of \( i \)-th rotational spring is denoted as \( k^\varphi_i \). Shear springs do not only react to displacements \( u_{3i} \) in the \( x_3 \) direction but also to rotations \( \varphi_{2i} \) about the \( x_2 \)-axis (Fig. 5.1.3). It means that shear and rotational springs in this system are coupled in contrast to the system consisting of normal and shear springs.
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Fig. 5.1.2. Chain of $n-1$ masses with fixed ends connected by $n$ shear and rotational springs.

To derive the equations of motion for this system we write the Lagrangian:

$$L = T - \Pi = \frac{1}{2} \sum_{i=0}^{n} \left( m_i \dot{u}_{3i}^2 + J_i \dot{\phi}_{2i}^2 \right) -$$

$$\frac{1}{2} \sum_{i=1}^{n} \left( k_i^s \left( u_{3i-1} - u_{3i-1} \right) + \frac{a}{2} \left( \phi_{2i-1} + \phi_{2i-1} \right) \right)^2 + k_i^r \left( \phi_{2i} - \phi_{2i-1} \right)^2,$$

where $J_i$ is the moment of inertia of the $i$-th oscillator; for spherical particles it is given by $\frac{2}{5} m_i r^2$, $r$ is the particle radius, $a$ is the distance between the particles.

Applying the Euler-Lagrange equation we obtain two sets of the equations of motion:

$$m_i \ddot{u}_{3i} - k_i^s u_{3i-1} + (k_i^s + k_{i+1}^s) u_{3i} - k_i^s u_{3i-1} + \frac{a}{2} k_i^s \phi_{2i} - \frac{a}{2} (k_i^s - k_{i+1}^s) \phi_{2i-1} = f_{3i} \quad (5.1.13)$$
For both systems of the differential equations, Eqs. (5.1.13) and (5.1.14), \( i = 1, \ldots, n-1 \), which gives \( 2(n-1) \) equations of motion.

These equations are in agreement with Pasternak and Mühlhaus [57] where the equations were obtained for the case when all stiffnesses are the same. The allowance for different stiffnesses provides a way to set negative stiffnesses for certain springs and investigate the stability of the system.

Similarly to the previous subsection, we assume that the end masses are fixed:

\[
u_{30}(t) = \dot{u}_{30}(t) = u_{3n}(t) = \dot{u}_{3n}(t) = 0 \\
\phi_{20}(t) = \dot{\phi}_{20}(t) = \phi_{2n}(t) = \dot{\phi}_{2n}(t) = 0
\]

The two sets of the equations of motion in the matrix form are identical to Eq. (5.1.5). The mass matrix \( \mathbf{M} \), the displacement vector \( \mathbf{u} \), the acceleration vector \( \mathbf{u}'' \), the force vector \( \mathbf{f} \) read:

\[
\mathbf{M} = \begin{pmatrix}
m_i & 0 & 0 & 0 & 0 & 0 \\
0 & \ldots & 0 & 0 & 0 & 0 \\
0 & 0 & m_{n-1} & 0 & 0 & 0 \\
0 & 0 & 0 & J_1 & 0 & 0 \\
0 & 0 & 0 & 0 & \ldots & 0 \\
0 & 0 & 0 & 0 & 0 & J_{n-1}
\end{pmatrix}, \quad
\mathbf{u} = \begin{pmatrix}
u_{31} \\
\ldots \\
u_{3n-1} \\
\phi_{2i} \\
\ldots \\
\phi_{2n-1}
\end{pmatrix}, \quad
\mathbf{f} = \begin{pmatrix}
f_{31} \\
\ldots \\
f_{3n-1} \\
M_{2i} \\
\ldots \\
M_{2n-1}
\end{pmatrix}
\]

The matrix of stiffness \( \mathbf{K} \) consists of submatrices and can be expressed as:

\[
\mathbf{K} = \begin{pmatrix}
\mathbf{K}_s & \mathbf{B} \\
\mathbf{B}^T & \mathbf{C}
\end{pmatrix}
\]

where \( \mathbf{K}_s \) is the stiffness matrix in the case when there are only shear springs in the system; submatrix \( \mathbf{B}^T \) is transposed to submatrix \( \mathbf{B} \).

The submatrices read:
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(5.1.19)

Using the Schur complement condition for positive definiteness and some algebra (see Appendix A for details) we derive the following criterion of stability of the system with shear and rotational springs. The system is stable if and only if:

\[ \sum_{j=1}^{n} \prod_{i=1 \atop i \neq j}^{n} k_j^S > 0 \]  \hspace{1cm} (5.1.20)

and

\[ \sum_{j=1}^{n} \prod_{i=1 \atop i \neq j}^{n} k_j^S + \frac{a^2}{\sum_{j=1}^{n} \prod_{i=1 \atop i \neq j}^{n} k_j^S} \sum(\text{adj}(K^o)) > 0, \]  \hspace{1cm} (5.1.21)

where \( \sum(\text{adj}(K^o)) \) is the sum of all elements of a adjugate of a square matrix \( K^o \), the matrix \( K^o \) is identical to the matrix \( K^S \) where the shear stiffnesses are replaced with the rotational ones.

More detailed analysis is possible if we restrict ourselves to a necessary criterion of stability. In particular we can determine the maximum allowable number of negative stiffness springs in the system. To this end, we construct a quadratic form using the stiffness matrix. We start with a simple case of chain with two masses and three shear and rotational springs in the chain, \( n = 3 \). For this particular case the stiffness matrix has the following form:

\[ K^S = \begin{pmatrix}
  k_1^S + k_2^S & -k_2^S & 0 & 0 \\
  -k_2^S & k_2^S + k_3^S & ... & 0 \\
  0 & ... & ... & -k_{n-1}^S \\
  0 & 0 & -k_{n-1}^S & k_{n-1}^S + k_n^S
\end{pmatrix}, \quad B = \begin{pmatrix}
  \frac{a}{2} (k_1^s - k_2^s) & -\frac{a}{2} k_2^s & 0 & 0 \\
  -\frac{a^2}{2} k_2^s & \frac{a}{2} (k_2^s - k_3^s) & ... & 0 \\
  0 & ... & ... & -\frac{a}{2} k_{n-1}^s \\
  0 & 0 & -\frac{a}{2} k_{n-1}^s & \frac{a}{2} (k_{n-1}^s - k_n^s)
\end{pmatrix} \]
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By constructing a quadratic form based on this matrix it can be shown that if the number of negative stiffness springs exceeds two, the system is not stable as the matrix is not positive definite (see Appendix B for details). The negative stiffness springs can be arranged in such a way that either (1) there is one negative stiffness shear spring and one negative stiffness rotational spring; or (2) there are two negative stiffness rotational springs. These rules can be generalized to the system with arbitrary number of masses and form a necessary condition of stability.

Despite the complexity of the system it is possible to obtain a critical value of negative stiffness in some cases. For instance, when one of the shear spring stiffness is negative (let it be spring number 1), \( k_1^s < 0 \), the remaining shear springs stiffnesses are positive and equal to the same value \( k_i^s = k^s \) \((i = 2, \ldots, n)\) and all rotational spring stiffnesses have the same positive value \( k_i^\varphi = k^\varphi \) \((i = 1, \ldots, n)\), then we can find the bounds for the negative stiffness from Eqs. (5.1.20) and (5.1.21):

\[
\begin{align*}
    k_1^s &> -\frac{k^s}{(n-1)} \quad \text{and} \quad k_i^s > -\frac{12}{n(n^2-1)\frac{a^2}{k^\varphi} + 12(n-1)\frac{1}{k^s}} \tag{5.1.23}
\end{align*}
\]

The second inequality in Eq. (5.1.23) is stronger than the first one. Thus the first inequality is redundant and the final bound for the negative stiffness is:

\[
    k_1^s > -\frac{12}{n(n^2-1)\frac{a^2}{k^\varphi} + 12(n-1)\frac{1}{k^s}} \tag{5.1.24}
\]

The position of the negative stiffness shear spring is unimportant. But the positions of negative stiffness rotational springs do affect the critical negative stiffness in the case of coupled system. For instance, if a chain consists of two masses connected
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by three shear and rotational springs with different values of stiffness then the criterion of stability, Eq. (5.1.21), can be formulated as:

$$k_1^o k_2^o + k_2^o k_3^o + k_1^o k_3^o + \frac{a^2 k_1^o k_2^o k_3^o}{k_1^o k_2^o + k_2^o k_3^o + k_1^o k_3^o} \left( k_1^o + 4k_2^o + k_3^o \right) > 0$$  (5.1.25)

It is seen, Eq. (5.1.25), the position of the negative stiffness rotational springs is essential for the stability analysis, though one can observe symmetry for the first and third springs in this case. The significance of the location of the negative stiffness springs is discussed in the following section. In particularly, in the case of chain with two masses we demonstrate in detail that the rotational negative stiffness springs have different critical values (when the system loses its stability) depending on their arrangement.

5.1.3. Eigen frequencies and trajectories of undamped chains

5.1.3.1. Trajectories of free chains

Now we consider the behaviour of the coupled systems in more detail by analysing a chain consisting of two masses connected by three shear and rotational springs, $n = 3$ (Fig. 5.1.4).

For the following it is convenient to write this system of the equations in dimensionless form. To this end we introduce the dimensionless groups:

$$\dot{u}_{3i} = \frac{m_i \ddot{u}_{3i}}{k_i^o a}, \quad \phi_{2i} = \frac{J \ddot{\phi}_{2i}}{k_i^o a}, \quad u_{3i} = \frac{u_{3i}}{a}, \quad k_i^o = \frac{k_i^o}{k_3^o}, \quad k_i^r = \frac{k_i^r}{k_3^r}, \quad k_i^ss = \frac{k_i^ss}{k_3^ss}, \quad f_{3i} = \frac{f_{3i}}{k_3^s a}, \quad M_{2i} = \frac{M_{2i}}{k_3^s a^2}$$  (5.1.26)

Subsequently, the equations of motion in the dimensionless form read:
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\[ \ddot{u}_{31}^* + (k_1^S + k_2^S)u_{31}^* - k_2^S u_{32}^* + \frac{(k_1^S - k_2^S)}{2} \varphi_{21}^* - \frac{k_2^S}{2} \varphi_{22}^* = f_{31}^* \]

\[ \ddot{u}_{32}^* - k_2^S u_{31}^* + (k_2^S + 1)u_{32}^* + \frac{k_2^S}{2} \varphi_{21}^* + \frac{(k_2^S - 1)}{2} \varphi_{22}^* = f_{32}^* \]

\[ \dot{\varphi}_{21}^* + \frac{(k_1^S - k_2^S)}{2} u_{31}^* + \frac{k_2^S}{2} u_{32}^* + \left( \frac{k_1^S + k_2^S}{4} + k_1^{\omega r} + k_2^{\omega r} \right) \varphi_{21}^* + \left( \frac{k_2^S}{4} - k_2^{\omega r} \right) \varphi_{22}^* = M_{21}^* \]

\[ \dot{\varphi}_{22}^* - \frac{k_2^S}{2} u_{31}^* + \frac{(k_2^S - 1)}{2} u_{32}^* + \left( \frac{k_2^S}{4} - k_2^{\omega r} \right) \varphi_{21}^* + \left( \frac{k_2^S}{4} + k_2^{\omega r} + k_3^{\omega r} \right) \varphi_{22}^* = M_{22}^* \]

These equations of motion with boundary conditions, Eqs. (5.1.15) and (5.1.16), according to which the end masses are stationary are used to analyse the oscillations.

The general solution to the homogeneous system is a linear combination of normal modes:

\[ \begin{pmatrix} u_{31}^* \\ u_{32}^* \\ \varphi_{21}^* \\ \varphi_{22}^* \end{pmatrix} = \sum_{j=1}^{4} \mathbf{e}_j \left[ C_j^+ \exp(i\omega_j t) + C_j^- \exp(-i\omega_j t) \right], \quad (5.1.28) \]

where \( C_j^\pm \) are arbitrary constants, \( \mathbf{e}_j \) are the eigenvectors of the dimensionless matrix of stiffness, Eq. (5.1.22), \( \omega_j \) are the eigenfrequencies.

To analyse the relationship between the first eigenfrequency, \( \omega_1 \) (the smallest one) and spring stiffnesses for a three-spring oscillator we consider two different sets of spring stiffnesses: (a) \( k_2^S = k_3^S = k_3^{\omega r} = 1 \) while \( k_1^S \) and \( k_1^{\omega r} \) are variable (Fig. 5.1.5a) and; (b) \( k_3^S = k_1^{\omega r} = k_3^{\omega r} = 1 \), while \( k_1^S \) and \( k_2^{\omega r} \) are variable (Fig. 5.1.5b). In other words, we assume that all positive shear stiffnesses are equal to the same value such that all the shear stiffnesses can be normalised by it. Furthermore, we normalise all positive rotational stiffnesses by the positive shear stiffness and by the distance between the masses; then the positive normalised stiffness is assumed to be equal to 1. Similarly to Pasternak, Dyskin and Sevel [29], the smaller the negative stiffness the smaller the eigenfrequencies. When the negative stiffness reaches its critical value, the first eigenfrequency (the smallest one) tends to zero. The eigenfrequency becomes imaginary when the absolute value of the negative stiffness exceeds its critical value. As a result,
the solution includes an exponential function with positive argument and hence the system becomes unstable.

The relationships between the first eigenfrequency and spring stiffnesses (Fig. 5.1.5) also demonstrate the importance of the positions of the rotational springs in the coupled systems. For instance, the critical absolute value of stiffness of the first rotational spring, $k_1^{\omega}$, which makes the system unstable, is equal to 1.15 (Fig. 5.1.5a), provided that other normalised spring stiffnesses are equal to 1. Due to symmetry of the considered system (Fig. 5.1.4) and the structure of the expression, Eq. (5.1.25), we can conclude that the critical values of stiffness of the first rotational spring, $k_1^{\omega}$, and the third one, $k_3^{\omega}$, are the same. Meanwhile, the critical absolute value of stiffness of the second rotational spring, $k_2^{\omega}$, is different and equal to 0.5 (Fig. 5.1.5b) under the same conditions. On top of that, it is found that the negative stiffness rotational springs attached to the boundaries can possess greater critical absolute value of stiffness than if they are placed in other positions (given that other spring stiffnesses are positive and equal to the same value). This result was also corroborated by numerical simulations of the coupled chains consisting of greater number of particles connected by shear and rotational springs. In particular, for the same normalised positive spring stiffnesses equal to 1, if the system contains 5 masses and 6 rotational and shear springs, i.e. $n = 6$, the rotational springs have the following critical absolute values of stiffness: $k_{cr1}^{\omega} = 0.76$, $k_{cr2}^{\omega} = 0.36$, $k_{cr3}^{\omega} = 0.22$; the critical absolute value of stiffness for the shear springs regardless of the position: $k_{cr}^{S} = 0.04$. When $n = 11$, the critical absolute values of stiffness are following: $k_{cr1}^{\omega} = 0.42$, $k_{cr2}^{\omega} = 0.29$, $k_{cr3}^{\omega} = 0.20$, $k_{cr4}^{\omega} = 0.14$, $k_{cr5}^{\omega} = 0.11$, $k_{cr6}^{\omega} = 0.10$, $k_{cr}^{S} = 0.008$. (Due to symmetry we presented the critical absolute values of stiffness for half of the system rotational springs.) Thus, the further from the boundary the negative stiffness rotational spring is placed the smaller critical absolute value of stiffness it can possess. In other words, the closer the negative stiffness spring to the boundary the higher the critical absolute value of the stiffness is. That is the boundary works as a stabiliser.

It is important to note that not only the first eigenfrequency $\omega_1$, but also all eigenfrequencies decrease with decreasing negative stiffness. Fig. 5.1.6 shows the dependence between the second eigenfrequency $\omega_2$ and spring stiffnesses.
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The behaviour of the system can also be illustrated through the trajectories of motion. This approach allows visualising the difference in oscillating of the particles (including unbounded response, i.e. instability) at different values of negative spring stiffnesses and at different number of negative stiffness springs.

We apply instantaneous unit displacement to the left mass \( u_1^*(0) = 1 \). Fig. 5.1.7 represents four plots with different sets of spring stiffnesses: (a) all spring stiffnesses are positive, \( k_1^{ss} = k_2^{ss} = k_3^{ss} = k_1^{os} = k_2^{os} = k_3^{os} = 1 \); (b) the stiffnesses of two springs are negative and their values do not exceed the critical values \( (k_{cr1}^{ss} = -0.123, k_{cr1}^{os} = -0.2) \), \( k_2^{ss} = k_2^{os} = k_3^{os} = 1, k_1^{ss} = k_1^{os} = -0.1 \); (c) the stiffness of one shear spring is negative and its value is above the (negative) critical value \( (k_{cr1}^{ss} = -0.25) \): \( k_2^{ss} = k_1^{os} = k_2^{os} = k_3^{os} = 1, k_1^{ss} = -0.26 \); (d) stiffness of one rotational spring is negative and above the critical value \( (k_{cr1}^{os} = -1.15) \). \( k_1^{ss} = k_2^{ss} = k_3^{os} = 1, k_1^{os} = -1.16 \).

Obviously the system with all positive spring stiffnesses is stable (Fig. 5.1.7a). The system with two negative stiffnesses Fig. 5.1.7(b) is still stable. When the negative stiffness becomes below the (negative) critical value we can see instability, which manifests itself as unbounded increase in displacement and rotation, Fig. 5.1.7(c) and (d).

![Fig. 5.1.5. Relations between the first eigenfrequency and normalised spring stiffnesses for a coupled oscillator:](image)

Fig. 5.1.5. Relations between the first eigenfrequency and normalised spring stiffnesses for a coupled oscillator: (a) \( k_2^{ss} = k_2^{os} = k_3^{os} = 1, k_1^{ss} \) and \( k_1^{os} \) are varying, the critical value of stiffness \( k_1^{ss} = -0.25 \) when \( k_1^{os} = 1, k_1^{ss} = -1.15 \) when \( k_1^{os} = 1 \); (b) \( k_2^{ss} = k_1^{os} = k_3^{os} = 1, k_1^{ss} \) and \( k_3^{ss} \) are varying, the critical value of the stiffness \( k_1^{ss} = -0.25 \) when \( k_2^{ss} = 1, k_2^{os} = -0.5 \) when \( k_1^{ss} = 1 \). All critical values are indicated by a thick line drown on the horizontal part of the plot.
Fig. 5.1.6. Relations between the second eigenfrequency and normalised spring stiffnesses for a coupled oscillator: (a) $k_2^{\omega^*} = k_2^{\varphi*} = k_3^{\omega*} = 1$, $k_1^{\omega*}$ and $k_1^{\varphi*}$ are variable; (b) $k_2^{\omega^*} = k_1^{\omega*} = k_3^{\omega*} = 1$, $k_1^{\omega*}$ and $k_2^{\omega*}$ are variable. The critical values are indicated by a thick line drawn on the horizontal part of the plot.

Fig. 5.1.7. Trajectories under instantaneous unit displacement of the left mass $u_1^*(0) = 1$ and in the absence of the driving force: (a) $k_1^{\omega^*} = k_2^{\omega^*} = k_3^{\omega^*} = k_3^{\varphi*} = 1$; (b) $k_2^{\omega^*} = k_2^{\varphi*} = k_3^{\varphi*} = 1$, $k_1^{\omega*} = k_1^{\varphi*} = -0.1$; (c) $k_2^{\omega^*} = k_1^{\omega*} = k_2^{\varphi*} = k_3^{\varphi*} = 1$, $k_1^{\omega*} = -0.26$, where $k_1^{\omega*}$ is below the (negative) critical value, so the system is in an unstable state; (d) $k_1^{\omega^*} = k_2^{\omega^*} = k_2^{\varphi*} = k_3^{\varphi*} = 1$, $k_1^{\omega*} = -1.16$, where $k_1^{\omega*}$ is below the (negative) critical value which also results in the system instability.
5.1.3.2. Trajectories of forced oscillations of the chain

Here we investigate a response of the chain to harmonic excitation with arbitrary driving frequencies considering the system from the previous part (two masses and three shear and rotational springs). Initially all masses are in the state of rest: \( u_{31}^*(0) = u_{32}^*(0) = \varphi_{21}^*(0) = \varphi_{22}^*(0) = 0 \). We assume that the non-homogenous system of the equations of motion, Eq. (5.1.27), includes only one non-zero sinusoidal force applied to the first particle, \( f_{31}^* = F_0^* \sin(\omega_F^* t) \), where \( F_0^* \) and \( \omega_F^* \) are the force amplitude and frequency respectively (both dimensionless). Thus the system of equations of motion reads:

\[
\begin{align*}
\ddot{u}_{31}^* + \left( k_{31}^{s*} + k_{32}^{s*} \right) u_{31}^* - k_{22}^{s*} u_{32}^* + \frac{k_{31}^{s*} - k_{32}^{s*}}{2} \varphi_{21}^* - \frac{k_{22}^{s*}}{2} \varphi_{22}^* &= F_0^* \sin(\omega_F^* t) \\
\ddot{u}_{32}^* - k_{22}^{s*} u_{31}^* + \left( k_{22}^{s*} + k_{23}^{s*} \right) u_{32}^* + \frac{k_{22}^{s*}}{2} \varphi_{21}^* + \frac{k_{22}^{s*} - 1}{2} \varphi_{22}^* &= 0 \ \\
\ddot{\varphi}_{21}^* + \frac{k_{22}^{s*} - k_{23}^{s*}}{2} u_{31}^* + \frac{k_{22}^{s*}}{2} u_{32}^* + \left( \frac{k_{22}^{s*} + k_{23}^{s*}}{4} + k_{12}^{s*} + k_2^{s*} \right) \varphi_{21}^* + \left( \frac{k_2^{s*} - k_2^{s*}}{4} \right) \varphi_{22}^* &= 0 \\
\ddot{\varphi}_{22}^* - \frac{k_{22}^{s*}}{2} u_{31}^* + \frac{k_{22}^{s*} - 1}{2} u_{32}^* + \left( \frac{k_{22}^{s*}}{4} - k_2^{s*} \right) \varphi_{21}^* + \left( \frac{k_2^{s*} + 1}{4} + k_2^{s*} + k_3^{s*} \right) \varphi_{22}^* &= 0
\end{align*}
\]

(5.1.29)

Fig. 5.1.8 represents trajectories of the particles when the driving frequency coincides with (a) the first and (b) the second eigenfrequency of the system. The set of spring stiffnesses includes one negative shear and normal stiffness springs: \( k_2^{s*} = k_2^{s*} = k_3^{s*} = 1 \), \( k_1^{s*} = k_1^{s*} = -0.1 \). The driving amplitude \( F_0^* \) is equal to 1. We see that the system exhibits a conventional resonance even in the presence of negative stiffness springs.
Fig. 5.1.8. Response to harmonic excitation with resonance frequency: (a) \( \omega_1^* = \omega_0^* = 0.1547 \); (b) \( \omega_2^* = \omega_0^* = 0.8724 \). The driving amplitude \( F_0^* = 1 \). Normalised spring stiffnesses: \( k^*_{22} = k^*_3 = k^*_1 = 1 \), \( k^*_1 = k^*_0 = -0.1 \).

Fig. 5.1.9 represents a response to a general sinusoidal driving force with frequency \( \omega_0^* = 2 \) for various sets of spring stiffnesses (similar to Fig. 5.1.7): (a) all spring stiffnesses are positive, \( k^*_1 = k^*_2 = k^*_3 = k^*_0 = 1 \); (b) the stiffnesses of two springs are negative and their values are below the (negative) critical values (\( k^*_{12} = -0.123 \), \( k^*_{31} = -0.2 \)): \( k^*_2 = k^*_0 = k^*_3 = 1 \), \( k^*_1 = k^*_0 = -0.1 \); (c) the stiffness of one shear spring is negative and its value is above the (negative) critical value (\( k^*_{12} = -0.25 \)): \( k^*_1 = k^*_2 = k^*_3 = 1 \), \( k^*_1 = -0.26 \); (d) stiffness of one rotational spring is negative and its value is above the (negative) critical value (\( k^*_{10} = -1.15 \)): \( k^*_1 = k^*_2 = k^*_3 = 1 \), \( k^*_1 = -1.16 \). Similarly to the previous case, the driving amplitude \( F_0^* \) is 1. Still, a system with negative stiffness whose value is above the (negative) critical one can be stable in the presence of driving force, Fig. 5.1.9 (b). However, when the value of negative stiffness is below the (negative) critical value, instability (unbounded displacements) occurs, Fig. 5.1.9(c) and (d).
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Fig. 5.1.9. Response to harmonic excitation with driven frequency $\omega_0^* = 2$ and driven amplitude $F_0^* = 1$: (a) $k_1^{S^y} = k_2^{S^y} = k_1^{S^\omega} = k_2^{S^\omega} = k_3^{S^\omega} = 1$; (b) $k_2^{S^\omega} = k_3^{S^\omega} = k_4^{S^\omega} = 1$, $k_1^{S^y} = k_4^{S^y} = -0.1$; (c) $k_2^{S^\omega} = k_3^{S^\omega} = k_4^{S^\omega} = 1$, $k_1^{S^y} = -0.26$, where $k_1^{S^y}$ is below the (negative) critical value, so the system is in an unstable state; (d) $k_1^{S^y} = k_2^{S^y} = k_3^{S^y} = k_4^{S^y} = 1$, $k_1^{S^\omega} = -1.16$, where $k_1^{S^\omega}$ is below the (negative) critical value which also results in the system instability.

5.1.4. Eigen frequencies and trajectories of free chains with linear damping

Behaviour of a system with normal positive and negative stiffness springs with damping was considered in Pasternak, Dyskin and Sevel [29]. Here we introduce damping in the chain of particles connected by shear and rotational springs and then compare the results with discrete linear viscoelastic system consisting of only normal springs.

For the sake of simplicity, we assume that all damping coefficients for translational and rotational motion are the same and equal to $\alpha$ and $\alpha^\omega$ respectively. The equations of motion in the presence of linear viscous damping read:

$$m_i \ddot{u}_i + \alpha \dot{u}_i + (k_i^{S^y} + k_i^{S^\omega}) u_i - k_i^{S^y} u_{i-1} + \frac{\alpha}{2} k_i^{S^\omega} \varphi_{2i-1} + \frac{\alpha}{2} (k_i^{S^y} - k_i^{S^\omega}) \varphi_{2i} - \frac{\alpha}{2} k_i^{S^\omega} \varphi_{2i+1} = f_i$$

(5.1.30)
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\[ J \ddot{\varphi}_{2i} + \alpha^v \dot{\varphi}_{2i} - \frac{\alpha}{2} k_i^s u_{3j-1} + \frac{\alpha}{2} (k_i^s - k_j^s) u_{3j} + \frac{\alpha}{2} k_{i+1}^s u_{3j+1} + \left( \frac{\alpha^2}{4} k_i^s - k_i^v \right) \varphi_{2i-1} + \left( \frac{\alpha^2}{4} (k_i^s + k_{i+1}^s) + k_i^v \right) \varphi_{2i} + \left( \frac{\alpha^2}{4} k_{i+1}^s - k_{i+1}^v \right) \varphi_{2i+1} = M_{2i}, \quad i = 1, \ldots, n - 1 \] (5.1.31)

Also, similarly to Eq. (5.1.27) we non-dimensionalise this system of the equations of motion. To this end we introduce two additional dimensionless groups associated with damping:

\[ \alpha^* u_{3j}^* = \frac{\alpha u_{3j}}{k_j^s a}, \quad \alpha^v \varphi_{2i}^* = \frac{\alpha^v \dot{\varphi}_{2i}}{k_i^s a^2} \] (5.1.32)

Using Eqs. (5.1.26) and (5.1.32) the equations of motion in the dimensionless form for the chain consisting of two masses and three shear and rotational springs, \( n = 3 \), can be written in the following form:

\[
\begin{cases}
\dot{u}_{31}^* + \alpha^* u_{31}^* + (k_1^s + k_2^s) u_{31}^* - k_3^s u_{32}^* + \frac{(k_3^s - k_2^s)}{2} \varphi_{21}^* - \frac{k_3^s}{2} \varphi_{22}^* = f_{31}^* \\
\dot{u}_{32}^* + \alpha^* u_{32}^* - k_2^s u_{31}^* + (k_2^s + 1) u_{32}^* + \frac{k_2^s}{2} \varphi_{21}^* + \frac{(k_2^s - 1)}{2} \varphi_{22}^* = f_{32}^* \\
\dot{\varphi}_{21}^* + \alpha^v \varphi_{21}^* + \frac{(k_1^s - k_2^s)}{2} u_{31}^* + \frac{k_2^s}{2} u_{32}^* + \left( \frac{k_1^s + k_2^s}{4} + k_1^v + k_2^v \right) \varphi_{21}^* + \left( \frac{k_2^s}{4} - k_2^v \right) \varphi_{22}^* = M_{21}^* \\
\dot{\varphi}_{22}^* + \alpha^v \varphi_{22}^* - \frac{k_2^s}{2} u_{31}^* + \frac{(k_2^s - 1)}{2} u_{32}^* + \left( \frac{k_2^s}{4} - k_2^v \right) \varphi_{21}^* + \left( \frac{k_2^s}{4} + k_2^v + k_3^v \right) \varphi_{22}^* = M_{22}^* 
\end{cases}
\] (5.1.33)

For the sake of simplicity we consider a particular case when \( \alpha^v = \alpha^* \). Then the fundamental solution reads:

\[
\begin{pmatrix}
u_{31}^* \\
u_{32}^* \\
\varphi_{21}^* \\
\varphi_{22}^*
\end{pmatrix} = \sum_{j=1}^{4} e_j \left[ C_j^* \exp \left( -\frac{\alpha^*}{2} t + i \omega_{j\alpha} t \right) + C_j^* \exp \left( -\frac{\alpha^*}{2} t - i \omega_{j\alpha} t \right) \right].
\] (5.1.34)

where \( C_j^* \) are arbitrary constants, \( e_j \) are the eigenvectors of the dimensionless matrix of stiffnesses, \( \omega_{j\alpha} \) are the damping frequencies.

Since the matrix of stiffness \( K \), Eq. (5.1.22), does not change in the viscoelastic system it can be concluded that damping does not affect the criterion of stability. It means that when frequencies of damped oscillators become imaginary the system can
remain stable although the oscillations become aperiodic. There are two situations possible: a frequency of damped oscillators $\omega_{ja}$ is real, so the oscillations are periodic and the damping coefficient is still $\alpha^*$, or a frequency of damped oscillators $\omega_{ja}$ is imaginary, then the oscillations become aperiodic and the damping coefficient changes:

$$
\alpha_j^* = \begin{cases} 
\alpha^* - \frac{\omega_{ja}^2}{2} & \omega_{ja}^2(\alpha^*) < 0 \\
\alpha^* & \omega_{ja}^2(\alpha^*) > 0 
\end{cases}, \quad \omega_j^* = \begin{cases} 
0 & \omega_{ja}^2(\alpha^*) < 0 \\
\sqrt{\omega_{ja}^2(\alpha^*)} & \omega_{ja}^2(\alpha^*) > 0 
\end{cases}, \quad j = 1, 2 \quad (5.1.35)
$$

To analyse dependencies between the normalised frequency $\omega_j^* / \omega_1$ ($\omega_1$ is the eigenfrequency that is the frequency of the system without damping) and spring stiffnesses for the viscoelastic chain of the oscillators we consider two different sets of spring stiffnesses: (a) $k_2^s = k_2^\sigma = k_3^s = 1$, while $k_1^s$ and $k_3^\sigma$ are variable (Fig. 5.1.10a); (b) $k_2^s = k_1^s = k_3^\sigma = 1$, while $k_1^\sigma$ and $k_3^\sigma$ are variable (Fig. 5.1.10b). We plot these dependencies for two values of the damping coefficient $\alpha^* = 0.2$ and $\alpha^* = 1$. It is seen that the first eigenfrequency (the real part) becomes zero at a lower absolute value as compared to the undamped system, while the critical negative stiffness obviously remains the same. It means that the system is still stable although the trajectories become aperiodic.
Fig. 5.1.10. Relations between the normalised frequency $\omega^* / \omega_1$ and normalised spring stiffnesses for the viscoelastic chain of the oscillators: (a) $k_2^{s*} = k_2^{p*} = k_3^{s*} = k_1^{s*}$ and $k_1^{p*}$ are variable (b) $k_2^{s*} = k_1^{p*} = k_3^{p*} = 1$, $k_1^{s*}$ and $k_2^{p*}$ are variable.

Fig. 5.1.11 represents the dependencies between the relative damping coefficient $\alpha^* / \alpha$ and spring stiffnesses $k_1^{s*}$ and $k_1^{p*}$ ($k_2^{s*} = k_3^{s*} = k_2^{p*} = k_3^{p*} = 1$): (a) $\alpha^* = 1$ (Fig. 5.1.11a); (b) $\alpha^* = 0.2$ (Fig. 5.1.11b). It is interesting and noteworthy that the relative damping coefficient can both grow and decrease while reducing the stiffness. With the first eigenfrequency $\omega_1$ tending to zero, the relative damping coefficients tend either to 2 or 0. Thus for stiffnesses smaller than a particular threshold the damping coefficient bifurcates into two coefficients, one increasing and another decreasing.
5.1.5. Discussion

In the previous study of Pasternak, Dyskin and Sevel [29] a chain of \( n + 1 \) particles connected by \( n \) normal (longitudinal) springs with the end particles fixed was considered. In such a chain each particle had only one degree of freedom, while the whole chain was characterised by \( n - 1 \) degrees of freedom. (As the end particles are fixed only \( n-1 \) particles can move.) It was shown that no matter how many particles (degrees of freedom) the chain possesses, no more than one negative stiffness spring is allowed for the chain to be stable. In this study we added two more degrees of freedom per particle, one degree of freedom related to the transversal displacement (that is in the direction normal to the chain) and another related to rotation assuming that the movement of particles in the chain is planar that is characterised by two displacements.
Essentially the movement of such a chain is a superposition of the longitudinal movement of the particles controlled by the normal (longitudinal) springs and the movement represented by displacement in the orthogonal direction and rotation (both coupled). Now the maximum allowable number of negative stiffness springs is 3, again independent of the number of particles. Superficially it looks as if one negative stiffness spring is allowed per a degree of freedom of a particle. However, the situation is more complex. While for the normal springs controlling the longitudinal particle movement indeed no more than one negative stiffness spring is allowed, the shear and rotational springs are essentially coupled. As a result, on top of the obvious necessary condition of no more than one shear and one rotational spring, another necessary condition of stability is that no more than two negative stiffness rotational springs are allowed, while all shear springs must have positive stiffness.

The restriction that no more than 3 negative stiffnesses are allowed, no matter how many particles the chain contains, means that the longer the chain the smaller the allowable concentration (fraction) of the negative stiffness springs that is the negative stiffness elements. If the chain contains \( n \) springs the fraction of negative stiffness springs (negative stiffness elements) \( c \) must satisfy the following inequality:

\[
c \leq c_{cr} = \frac{3}{n}
\]  

(5.1.36)

Thus the allowable fraction of negative stiffness elements is inversely proportional to the chain length as in the case of the simple chain with only normal springs considered by Pasternak, Dyskin and Sevel [29].

Another interesting finding concerns the systems with damping. Similarly to what was found for a single longitudinal chains as the value of negative stiffness springs reduces, there is a point (before the critical stiffness is reached) when the damping bifurcates such that simultaneously two types of movement develop: one with higher damping and another with lower damping. Obviously, the movement with lower damping will eventually dominate, so we can conclude that no gigantic increase in damping predicted by Dong and Lakes [23], Toru and Yoshitaka [13] and Yap, Lakes and Carpick [14] is observed in this exact analytical solution. This puts severe
limitations on the claims that the adding negative stiffness elements can considerably increase oscillation damping, which is not surprising in the light of the review given in Introduction.

Analysing the stability of systems with negative stiffness elements is important for the formulation of criteria of instability of particulate geomaterials in the presence of compressive loading and subsequently the failure criteria ranging, depending upon the scale, from the failure of foundations to catastrophic failures in mining excavations to earthquake generation. The constituents of the particulate materials are rarely spherical (as they are usually modeled); as mentioned in Introduction, rotation of non-spherical particles in the presence of compressive loading leads to the phenomenon of apparent negative stiffness. Such a particulate material can be represented as a discrete system of particles that are connected by bonds some of which have negative stiffness. The criterion of stability of this system is the criterion of stability of the particulate material as a whole, which has a potential to predict the failure processes in the material. The emergence of a low frequency resonance can be used as an indicator of approaching failure and become a basis for a new failure monitoring technique.

5.1.6. Conclusion

Materials and structures containing negative stiffness elements were modelled as chains of particles connected by springs whose stiffnesses can also be negative. The particles in the chain are only allowed planar movement such that each particle has three degrees of freedom: two translational and one rotational. The particles are connected by one normal (longitudinal), one shear (transverse) and one rotational springs. The end particles are fixed. We showed that in order to be stable such a chain allows no more than three negative stiffness springs. The concentration of allowable negative stiffness elements (springs) decreases inversely proportional to the chain length.

The three allowable negative stiffness springs can be arranged in two ways: (i) the chain contains one normal, one shear and one rotational negative stiffness springs and; (ii) the chain contains one normal and two rotational negative stiffness springs. In the second case no negative stiffness shear springs are allowed. The absolute values of the negative stiffnesses should not exceed certain threshold values that depend upon the stiffnesses and the number of the other (positive) springs. The positions of normal and shear negative stiffness springs do not affect the critical values and stability of the
system, however the positions of the negative rotational stiffness springs are found to be important.

When stable, the undamped chains with negative stiffness elements undergo oscillations. All mode frequencies reduce when one of the negative stiffnesses tends to the critical value; the smallest frequency tends to zero. Damped chains also exhibit similar decrease of damping frequencies, but the lowest frequency reaches zero while the chain is still stable (the absolute value of the negative stiffness is below the critical value). At this point the damping factor bifurcates and produces two branches: one increase with the increase in the value of negative stiffness, the other decreases. No giant damping is observed.
Appendix 5.1.A. Derivation of Eqs. (5.1.20) and (5.1.21)

Here we derive the criterion of stability of the system with coupled shear and rotational springs. According to Schur complement condition for positive definiteness the matrix of stiffness $K$, Eq. (5.1.18), is positive definite if and only if $K^S$ and Schur complement $S = C - B^T (K^S)^{-1} B$ are positive definite. The positive definiteness of $K^S$ leads to already obtained inequality, Eq. (5.1.9).

Conducting matrix multiplication and simple arithmetic operations in the Schur complement we obtain:

$$S = C - B^T (K^S)^{-1} B = K^o + pU,$$

where

$$p = \sum_{i=1}^{n} \prod_{j=1 \atop j \neq i}^{n} k_j^S, \quad U \text{ is a square matrix of ones, } U = \begin{bmatrix} 1 & 1 & \ldots & 1 \\ 1 & 1 & \ldots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \ldots & 1 \end{bmatrix}.$$

For positive definiteness all main diagonal minors of the Schur complement should be positive. Computing the determinant of the sum of the matrices $K^o$ and $pU$ we derive:

$$\det(S) = \det(K^o + pU) = \det(K^o) \left( 1 + p \sum_{i=1}^{n} \prod_{j=1 \atop j \neq i}^{n} k_j^S \right) = \det(K^o) + p \sum_{i=1}^{n} \prod_{j=1 \atop j \neq i}^{n} \det(\text{adj}(K^o)),$$

where $\sum(\text{adj}(K^o))$ is the sum of all elements of an adjugate of a square matrix $K^o$, $\sum(K^o)^{-1}$ is the sum of all elements of an inverse of a square matrix $K^o$.

Thus, Eq. (5.1.A.2) gives the second part of the criterion of stability:

$$\sum_{i=1}^{n} \prod_{j=1 \atop j \neq i}^{n} k_j^o \left( 1 + p \sum_{i=1}^{n} \prod_{j=1 \atop j \neq i}^{n} k_j^o \right) = \sum_{i=1}^{n} \prod_{j=1 \atop j \neq i}^{n} k_j^o + p \sum \left( \text{adj}(K^o) \right) > 0 \quad (5.1.A.3)$$
Appendix 5.1.B. Determination of the maximum allowable numbers of negative shear and rotational springs in a chain (necessary condition of stability)

First we consider the case with two masses and three shear and rotational springs in a chain, \( n = 3 \).

The quadratic form constructed using the stiffness matrix, Eq. (5.1.22), reads:

\[
\begin{align*}
\mathbf{z}^T \mathbf{K} \mathbf{z} &= (v_1 + w_1)^2 k_1^s + (-v_1 + v_2 + w_1 + w_2)^2 k_2^s + (v_2 - w_2)^2 k_3^s + \\
&\quad \frac{4}{a^2} \left( w_1^2 k_1^\phi + (w_1 - w_2)^2 k_2^\phi + w_2^2 k_3^\phi \right),
\end{align*}
\]

where \( \mathbf{z} = (v_1, v_2, 2w_1/a, 2w_2/a)^T \) is a non-zero vector, \( v_1, v_2, w_1, w_2 \) are arbitrary numbers.

We prove that not more than 2 rotational springs are allowed. Assume that we have all three rotational springs with negative stiffness: \( k_1^\phi < 0 \), \( k_2^\phi < 0 \) and \( k_3^\phi < 0 \).

Then, obviously the term in Eq. (5.1.B.1) which contains rotations will be negative. We now show that we can find displacements \( v_1, w_1, \ldots \), such that the quadratic terms that contain them are zero. This requirement corresponds to the following system of homogeneous equations:

\[
\begin{align*}
v_1 + w_1 &= 0 \\
-v_1 + v_2 + w_1 + w_2 &= 0 \\
v_2 - w_2 &= 0
\end{align*}
\]  

(5.1.B.2)

The rank of the system is smaller than the number of unknowns (i.e. the system has infinitely many solutions), so it has non-trivial solutions. Subsequently, we can always choose a non-zero vector \( \mathbf{z} \) such that the quadratic form is negative, e.g. \( v_1 = v_2 = w_2 = -1, w_1 = 1 \). This means that the quadratic form is not positive definite and the system is not stable.

Now we consider the situation when there are two shear negative stiffness springs in the system. Let us number the springs and masses in such a way that \( k_1^s < 0 \) and \( k_2^s < 0 \). This means that the first two terms in Eq. (5.1.B.2) are negative. We can choose displacements and rotations such that the remaining terms in Eq. (5.1.B.2) are zero. Indeed, this requirement leads the following homogeneous system:
Chapter 5.1. Stability of chains of oscillators with negative springs

\begin{align}
  v_2 - w_2 &= 0 \\
  w_1 &= 0 \\
  w_1 - w_2 &= 0 \\
  w_2 &= 0
\end{align}

(5.1.B.3)

One can see that there are three independent equations. The component \( v_1 \) of a non-zero vector \( z \) is not contained in these equations and can be arbitrary. For instance, a non-zero vector \( z = (1, 0, 0, 0)^T \) makes the quadratic form, Eq. (5.1.B.1), negative. Obviously, it is followed from this consideration that three negative stiffness springs are not allowed either.

In summary, we have shown that for the system with two masses the number of negative stiffness springs cannot exceed two to ensure that the system is stable. They can be arranged in such a way that either there are one negative stiffness shear and one negative stiffness rotational springs or two negative stiffness rotational springs.

Now we examine the maximum number of negative stiffness springs for the arbitrary number of masses \( n - 1 \) in the system. In a general case the quadratic form can be expressed as:

\[ z^T K z = (v_1 + w_1)^2 k_1^s + (-v_1 + v_2 + w_1 + w_2)^2 k_2^s + \ldots + (-v_{n-2} + v_{n-1} + w_{n-2} + w_{n-1})^2 k_{n-1}^s + (v_{n-1} - w_{n-1}) k_n^s + \frac{4}{a} \left( w_1^2 k_1^p + (w_1 - w_2)^2 k_2^p + \ldots + (w_{n-2} - w_{n-1})^2 k_{n-1}^p + w_{n-1}^2 k_n^p \right), \]

(5.1.B.4)

where \( z = (v_1, v_2, \ldots, v_{n-1}, 2w_1/a, 2w_2/a, \ldots, 2w_{n-1}/a)^T \).

The structure of this quadratic form is identical to Eq. (5.1.B.1). The number of unknown components of vector \( z \) is \( 2(n-1) \), the number of addends in the quadratic form is \( 2n \). It means that the number of negative stiffness springs should not exceed two to ensure that the system is stable. If the number of negative stiffness springs is greater than two then the terms that do not contain negative stiffnesses can be made equal to zero by a proper choice of \( z \). This is because the number of homogeneous equations similar to Eq. (5.1.B.2) will be smaller than the number of unknowns. For instance, if we assume that \( k_1^p < 0 \), \( k_2^p < 0 \) and \( k_n^p < 0 \), than the system of \( 2n - 3 \) homogeneous equations (the left hand sides are equal to the coefficients of the positive stiffnesses) read as:
\begin{align*}
\begin{cases}
    v_i + w_i = 0 \\
    -v_{i-1} + v_i + w_{j-1} + w_j = 0 \\
    v_{n-1} - w_{n-1} = 0 \\
    w_{j-1} - w_j = 0 \\
    w_{n-1} = 0
\end{cases}, \quad \text{where } i = 2 \ldots n - 1, \ j = 4 \ldots n - 1 \quad (5.1.B.5)
\end{align*}

The number of unknowns is \(2n - 2\), so the rank of the system \(2n - 3\) is smaller than the number of unknowns (i.e. the system has infinitely many solutions) and we can choose a non-zero vector \(z\) (e.g. \(v_1 = -1, v_2 = -1, v_i = 0, w_1 = 1, w_2 = -1, w_i = 0\) where \(i = 3 \ldots n - 1\)) such that the quadratic form is negative. Thus if the number of negative stiffness springs is greater than two the quadratic form is not positive definite and system is unstable. Since the structure of the quadratic form is identical to Eq. (5.1.B.1) we can conclude that if there is more than one negative stiffness shear spring in the chain the rank of the system will be also smaller than the number of unknowns.

Thus the number of negative stiffness springs in the system with the arbitrary number of masses should not exceed two to ensure that the system is stable. There can be no more than one negative stiffness shear and rotational springs or two negative stiffness rotational springs in the system for it to be stable.
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Reference

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5.2. Stability of 2D discrete mass-spring systems with negative stiffness springs
Negative stiffness elements (elements with direction of the force opposite to the
direction of the deformation) are unstable as the energy is no longer positive definite.
Nevertheless, materials and structures with negative stiffness elements can exist when
the element negative energy is compensated by the energy of the rest of the system or an
encompassing system that provide stabilisation. Here we study stability of two-
dimensional square packing discrete mass-spring systems with some spring stiffnesses
being negative. Each mass (particle) in the system has three degrees of freedom. The
particles are connected by normal, shear and rotational springs to simulate all possible
elastic interactions between the masses. The stability is investigated by considering
three simple problems: (i) a system consisting of only one particle, (ii) a “channel” of
two particles, (iii) two-by-two and three-by-three systems of particles. The particles are
connected to rigid external boundary. We found that two-dimensional square packing
systems with fixed boundary particles consisting of positive and negative stiffness
springs can be stable when the total number of negative stiffness springs does not
exceed the total number of degrees of freedom of the system. This necessary condition
is also generalized to three-dimensional cubic packing systems. The presence of
negative stiffness springs leads to a decrease in the eigenfrequencies: the smallest
eigenfrequency becomes zero when the absolute value of the negative stiffness spring
reaches its critical value.

5.2.1. Introduction

Hooke's law – a fundamental concept of mechanics – is a generalisation of the
fact that the force required to deform an elastic body is proportional to the body’s
deformation. The proportionality factor (the stiffness) is supposed to be positive
(otherwise the elastic energy loses its positive definiteness), which means that the
direction of the force coincides with the direction of the deformation.

However, there are known cases when stiffness can be negative. Negative
stiffness (negative slope in the force-displacement curve) is observed at post-peak
softening of brittle materials, for example, concrete and rock [1, 2] (stiff loading is
required for this phenomenon to be observed) and granular materials (see for instance
2D physical and discrete element modelling [3-5]). Interestingly, negative stiffness is
also observed in some parts of a human body, for instance, joints and hair-bundles in the
ear [6-8]. High effective stiffness associated with contact change is also observed in
topological interlocking structures of cubic elements [9, 10]. On top of that, it was
discussed in [11, 12] that when the Poisson ratio of a stable system tends to $-1$ then the local behaviour characteristic for the negative stiffness materials can be observed.

The concept of negative stiffness has been a subject of numerous studies in recent years. One of the reasons why the negative stiffness has attracted that much attention is a possibility of a range of practical applications. It was suggested that systems with negative stiffness inclusions might effectively decrease vibrations and noise in structures [13-15]. The damping ratio of the structures with negative stiffness constituents could be magnitudes higher than without these inclusions [16-20]. Furthermore, a number of structures exhibiting negative stiffness have been created for the use in car seats suspensions and driver vibration isolation [21, 22], seismic protection of structures (e.g. multi-story buildings, highway bridges) [23, 24] and structural vibration control (negative-stiffness dampers based on magnetism) [25]. Enhanced damping is not the only feature of the materials with negative stiffness constituents. Effective stiffness of the system, internal friction, thermal expansion, pyroelectricity and piezoelectricity are affected by the negative stiffness of the system components and can reach extreme values in metamaterials with negative stiffness phase [14, 26-30].

Several methods of implementation of negative stiffness in metamaterials and structures can be distinguished. In continuous composite materials negative stiffness inclusions can be introduced by using single domains of ferroelastic vanadium dioxide (VO$_2$) in a pure tin matrix [14, 26, 27]. A number of papers was devoted to a comparison of properties of the composites having negative stiffness phase (VO$_2$) with other composites, e.g. SiC–InSn and Zinc [28], indium (In)–thallium (Tl) binary alloy [29, 31]. In discrete structures such elements as post-buckled columns [30, 32-34], L-frames [35], tubes (with silicone cement in a Reuss configuration) [16, 17] as well as arches [36], lever models with springs [24, 37] and curved beams [38] demonstrate negative stiffness. Interestingly, the phenomenon of negative stiffness appears not only in macroscopic tubes but also in nanotubes [18-20]. Cellular solids (e.g. solid foam and honeycombs) are another type of materials where negative stiffness mechanism can be found [39-41]. On top of that, it was recently proposed that rotation of non-spherical particles in granular materials and rock masses might be responsible for manifestation of negative stiffness in such materials [42-47].
One of the main issues related to the systems with negative stiffness inclusions or elements is their stability. Since the work done on the negative stiffness element by the force is negative (the displacement is in the opposite direction of the force) according to thermodynamics the negative stiffness element should be unstable. Yet, materials and structures exhibiting negative stiffness may exist provided that negative stiffness is stabilised with the aid of the rest of the system or an encompassing system which make the balance of the energy such that the total energy is positive definite. Thus the system stabilising the negative stiffness element works as an energy reservoir. In the simplest case such a stabilising system can be replaced with properly defined boundary conditions [48-50]. It is also found that a viscous damped system containing negative stiffness springs is stable when the system is tuned for high compliance [51]. In continuous composite materials, negative stiffness inclusions may be stabilised by the (positive stiffness) matrix, as long as the values of negative stiffness inclusions do not exceed particular thresholds [42, 48, 52-54]. In the Berglund’s work [55] an isotropic Cosserat continuum was used to analyse stability of a 2D discrete system which upon homogenisation should deliver an orthotropic continuum. Stability of materials with rotating non-spherical particles was also analysed in [56] by modelling such materials as a Cosserat continuum with negative Cosserat shear modulus (the modulus that relates the non-symmetric part of shear stress and rotation; in mass-spring systems with rotations this would correspond to negative shear stiffness $k^S$, see below). It was found that there also exists a threshold value of the negative Cosserat shear modulus beyond which the system is unstable. The practical benefits of these results are twofold. Firstly, knowing the allowable value of stiffness of shear negative springs in the mass-spring system, one can estimate the corresponding negative Cosserat shear modulus of micropolar continuum by using the relationships between the Cosserat moduli and the spring stiffnesses (e.g. [57]). Secondly, in the cases when the negative stiffness is caused by natural mechanisms, e.g. rotation of non-spherical particles/grains in particulate materials, the knowledge of the allowable values of negative stiffness gives a way of predicting global instability and resulting failure.

Our area of interest includes modelling of materials and structures containing negative stiffness elements as discrete mass-springs systems with negative stiffness springs and analysis of their stability. Chains of oscillators (one-dimensional (1D) problem) were studied in [58-60]. The necessary and sufficient conditions of stability were obtained for a chain where each particle had only one degree of freedom and the
particles (masses) were connected by normal (longitudinal) springs [58, 60]. It was found that these chains cannot have more than one negative stiffness spring. The necessary condition of stability was also obtained for the general case, when particles in the chain have three degrees of freedom (two translational and one rotational). The particles in such a chain were connected with each other by normal (longitudinal), shear (transversal) and rotational springs to simulate various interactions between particles in real material. For this case the number of negative stiffness springs cannot exceed three (two rotational and one normal springs or one shear, one rotational and one normal springs) to ensure that the system is stable [59, 60]. In addition to that, the values of negative stiffness should not exceed certain critical values.

In this study, we generalise the previous results and analyse the stability of two-dimensional (2D) square packing discrete mass-spring systems with negative stiffness springs. Since linear elastic systems are considered, we study their stability in terms of positive definiteness of the stiffness matrices. It differs from the systems described above which have hyperelastic or finite deformations (e.g. buckled structures) and where stability is analysed by checking the positive definiteness of incremental stiffness matrix.

Each particle in the system has three degrees of freedom (two displacements and independent in-plane rotation). The particles are connected by normal, shear and rotational springs. In Section 5.2.2 we describe this system in more detail, apply boundary conditions and derive the equations of motion. The criterion of stability is investigated in Section 5.2.3 by considering three simple problems: (i) a system consisting of only one particle, (ii) a “channel” of two particles, (iii) two-by-two and three-by-three systems of particles. In Section 5.2.4 we analyse eigenfrequencies of the systems (ii) and (iii). The stability is discussed in more detail with the use of the trajectory of motion. Further we compare the stability criterion for one- and two-dimensional systems and touch three-dimensional system in the discussion part (Section 5.2.5).

5.2.2. Equations of motion and boundary conditions of 2D discrete mass-spring systems

A 2D square packing discrete mass-spring model is shown in Fig. 5.2.1. Particles are connected with each other by normal (longitudinal), shear (transversal) and
Chapter 5.2. Stability of 2D discrete mass-spring systems with negative stiffness springs

Each particle has three degrees of freedom which are characterised by two translational displacements in the $x_1$- and $x_3$- directions, that is $u_{i_1}$ and $u_{i_3}$, and one in-plane rotation about the $x_2$- direction, $\phi$. We use the following notations: subscripts $i$ and $j$ characterise the position of particles and springs and refer to the order numbers of the column and the row, respectively. Thus $k_{ij}^{1N}$, $k_{ij}^{1S}$, $k_{ij}^{1\phi}$ are stiffnesses of the $ij$-th normal, shear and rotational spring correspondingly oriented in the $x_1$- direction, likewise $k_{ij}^{3N}$, $k_{ij}^{3S}$, $k_{ij}^{3\phi}$ are stiffnesses pointing in the $x_3$- direction, $m_{ij}$ is the mass of the $ij$-th particle, $u_{ij}$ and $u_{ij}$ are translational displacements and $\phi_{ij}$ is an in-plane rotation of the $ij$-th particle.

Normal springs $k_{ij}^{1N}$ and shear springs $k_{ij}^{3S}$ react to displacements $u_{ij}$ in the $x_1$- direction. It implies that normal springs $k_{ij}^{1N}$ and shear springs $k_{ij}^{3S}$ are coupled. Similarly, normal springs $k_{ij}^{3N}$ and shear springs $k_{ij}^{1S}$ are coupled and react to displacements $u_{ij}$ in the $x_3$- direction. Furthermore, both types of shear springs $k_{ij}^{1S}$ and $k_{ij}^{3S}$ react to rotations $\phi_{ij}$ about the $x_2$- direction (Fig. 5.2.2). Therefore shear springs $k_{ij}^{1S}$ and $k_{ij}^{3S}$, and rotational springs $k_{ij}^{1\phi}$ and $k_{ij}^{3\phi}$ are coupled as well.

![Fig. 5.2.1. 2D mass-spring system ($l$-columns and $n$-rows) with fixed boundary particles connected by normal, shear and rotational springs.](image-url)
Chapter 5.2. Stability of 2D discrete mass-spring systems with negative stiffness springs

We now derive the equations of motion for the system. To obtain the equations we write the kinetic and potential energies first. The kinetic energy, \( T \), of the system reads as the sum of the kinetic energies of each particle:

\[
T = \frac{1}{2} \sum_{i=0}^{n} \sum_{j=0}^{n} \left( m_{ij} \dot{u}_{ij}^2 + m_{ij} \dot{\varphi}_{ij}^2 + J_{ij} \dot{\varphi}_{ij}^2 \right) \quad (5.2.1)
\]

Here \( J_{ij} \) is the moment of inertia of the \( ij \)-th particle; for spherical particles it is given by \( 2/5 \ m_{ij} r^2 \), \( r \) is the particle radius (all particles are assumed to have the same radius).

The potential energy, \( \Pi \), of the system determined as the total of the potential energies of each spring is:

\[
\Pi = \frac{1}{2} \sum_{i=1}^{n+1} \sum_{j=1}^{n+1} \left( k_{ij}^{NS} \left( u_{ij} - u_{i,j-1} \right)^2 + k_{ij}^{NS} \left( \varphi_{ij} - \varphi_{i,j-1} \right)^2 \right)
+ \frac{a}{2} \left( \varphi_{ij} + \varphi_{i,j-1} \right)^2 + k_{ij}^{NS} \left( \varphi_{ij} - \varphi_{i,j-1} \right)^2 \quad (5.2.2)
\]

\[
\sum_{i=1}^{n+1} \sum_{j=1}^{n+1} \left( k_{ij}^{NS} \left( u_{ij} - u_{i,j-1} \right)^2 + k_{ij}^{NS} \left( \varphi_{ij} - \varphi_{i,j-1} \right)^2 \right)
+ \frac{a}{2} \left( \varphi_{ij} + \varphi_{i,j-1} \right)^2 + k_{ij}^{NS} \left( \varphi_{ij} - \varphi_{i,j-1} \right)^2 \right)
\]

where \( a \) is the distance between the particles. For the sake of simplicity, the distances between all the particles are assumed to be the same.

Hereafter we assume that the boundary particles are fixed:
Chapter 5.2. Stability of 2D discrete mass-spring systems with negative stiffness springs

\[ u_{_{ij}}(t) = \ddot{u}_{_{ij}}(t) = u_{_{ij}}(t) = \ddot{u}_{_{ij}}(t) = 0 \]
\[ u_{_{10}}(t) = \ddot{u}_{_{10}}(t) = u_{_{10}}(t) = \ddot{u}_{_{10}}(t) = 0 \]
\[ u_{_{0j}}(t) = \ddot{u}_{_{0j}}(t) = u_{_{0j}}(t) = \ddot{u}_{_{0j}}(t) = 0 \]
\[ u_{_{30}}(t) = \ddot{u}_{_{30}}(t) = u_{_{30}}(t) = \ddot{u}_{_{30}}(t) = 0 \]
\[ \phi_{_{ij}}(t) = \ddot{\phi}_{_{ij}}(t) = \phi_{_{ij}}(t) = \ddot{\phi}_{_{ij}}(t) = 0 \]
\[ \phi_{_{0j}}(t) = \ddot{\phi}_{_{0j}}(t) = \phi_{_{0j}}(t) = \ddot{\phi}_{_{0j}}(t) = 0 \]

where \( i = 0, ..., l, \ j = 0, ..., n. \)

Deriving the Lagrangian of the system, \( L = T - V \), and applying the Euler-Lagrange equation we obtain three sets of equations of motion:

\[
\begin{align*}
& m_{_{ij}} \ddot{u}_{_{ij}} - k_{y} u_{_{ij}} - k_{N} u_{_{ij}} + (k_{N} + k_{1} + k_{y} + k_{y}) u_{_{ij}} - \\
& k_{N} \ddot{u}_{_{ij}} + a \frac{k_{3}}{2} \phi_{_{ij}} + \frac{a}{2} (k_{y} - k_{y}) \phi_{_{ij}} - \\
& a k_{y} \phi_{_{ij}} = f_{_{ij}} \\
& m_{_{ij}} \ddot{u}_{_{ij}} - k_{y} u_{_{ij}} - k_{y} u_{_{ij}} - k_{y} u_{_{ij}} + (k_{y} + k_{y} + k_{y} + k_{y}) u_{_{ij}} - \\
& k_{y} \ddot{u}_{_{ij}} + a \frac{k_{3}}{2} \phi_{_{ij}} + \frac{a}{2} (k_{y} - k_{y}) \phi_{_{ij}} - \\
& a k_{y} \phi_{_{ij}} = f_{_{ij}} \\
& a \phi_{_{ij}} - \frac{a}{2} (k_{y} - k_{y}) + k_{y} + k_{y} + k_{y} \phi_{_{ij}} - \\
& (k_{y} - k_{y}) \phi_{_{ij}} + (\frac{a}{2} k_{y} + k_{y} + k_{y} + k_{y}) \phi_{_{ij}} + \\
& \frac{a}{2} (k_{y} - k_{y}) \phi_{_{ij}} + \frac{a}{2} (k_{y} + k_{y} + k_{y}) \phi_{_{ij}} + \\
& \frac{a}{2} (k_{y} + k_{y} + k_{y}) \phi_{_{ij}} + \frac{a}{2} (k_{y} - k_{y}) \phi_{_{ij}} = M_{_{ij}}
\end{align*}
\]

where \( i = 1, ..., l - 1, \ j = 1, ..., n - 1 \), which gives \( 3(l - 1)(n - 1) \) equations of motion.

In the matrix form, Eq. (5.2.4), for the 2D discrete mass-spring model is:

\[
\dot{M} u + Ku = f
\] (5.2.5)
Chapter 5.2. Stability of 2D discrete mass-spring systems with negative stiffness springs

Here \( \mathbf{u} \) is the displacement vector, \( \mathbf{\ddot{u}} \) is the acceleration vector, \( \mathbf{f} \) is the force-moment vector, \( \mathbf{M} \) is the mass matrix, \( \mathbf{K} \) is the matrix of stiffness:

\[
\mathbf{u} = \begin{pmatrix} u_{11} \\ \vdots \\ u_{1,l-1} \\ u_{21} \\ \vdots \\ u_{2,l-1} \\ \vdots \\ \vdots \\ u_{l,1} \\ \phi_{11} \\ \vdots \\ \phi_{l,1} \\ \phi_{1,l-1} \\ \vdots \\ \phi_{1,n-1} \\ \phi_{l,n-1} \end{pmatrix}, \quad \mathbf{\ddot{u}} = \begin{pmatrix} \ddot{u}_{11} \\ \vdots \\ \ddot{u}_{1,l-1} \\ \ddot{u}_{21} \\ \vdots \\ \ddot{u}_{2,l-1} \\ \vdots \\ \vdots \\ \vdots \\ \ddot{\phi}_{11} \\ \vdots \\ \ddot{\phi}_{l,1} \\ \ddot{\phi}_{1,l-1} \\ \vdots \\ \ddot{\phi}_{1,n-1} \\ \ddot{\phi}_{l,n-1} \end{pmatrix}, \quad \mathbf{f} = \begin{pmatrix} f_{11} \\ \vdots \\ f_{1,l-1} \\ f_{21} \\ \vdots \\ f_{2,l-1} \\ \vdots \\ \vdots \\ \vdots \\ f_{l,1} \\ M_{11} \\ \vdots \\ M_{l,1} \\ M_{1,l-1} \\ \vdots \\ M_{l,n-1} \end{pmatrix},
\]

(5.2.6)

Here the empty spaces refer to zero entries.

The form of the matrix of stiffness, \( \mathbf{K} \), is case-specific and depends on the size of the discrete particle-spring model. We consider this matrix in more detail in the following section.

**5.2.3. Stability of 2D discrete mass-spring systems**

Here we study the stability of three simple 2D discrete particle-spring systems and then summarise the results for 2D square packing systems of arbitrary size.

We begin with the simplest 2D case where the system consists of only one particle (Fig. 5.2.3), then consider a “channel” of two particles (Fig. 5.2.4), and finally study two-by-two (Fig. 5.2.5) and three-by-three systems of particles.
5.2.3.1 Stability of a 2D single particle system with negative stiffness springs

The system is shown in Fig. 5.2.3 and consists of one particle and four normal, shear and rotational springs connecting the particle to a fixed boundary.

According to Eq. (5.2.4), the equations of motion for this case read:

\[
\begin{align*}
    m_1 \ddot{u}_{h_1} + (k_{11}^{1N} + k_{21}^{1N} + k_{11}^{3S} + k_{12}^{3S}) u_{h_1} + \frac{a}{2} (k_{11}^{3S} - k_{12}^{3S}) \phi_{11} &= f_{h_1} \\
    m_1 \ddot{u}_{\eta_1} + (k_{11}^{1S} + k_{21}^{1S} + k_{11}^{3N} + k_{12}^{3N}) u_{\eta_1} + \frac{a}{2} (k_{11}^{1S} - k_{21}^{1S}) \phi_{11} &= f_{\eta_1} \\
    J_1 \ddot{\phi}_{11} - \frac{a}{2} ((k_{11}^{3S} - k_{12}^{3S}) u_{h_1} + (k_{11}^{1S} - k_{21}^{1S}) u_{\eta_1}) &= 0 \\
    \left(\frac{a^2}{4} (k_{11}^{1S} + k_{21}^{1S} + k_{11}^{3N} + k_{21}^{3N}) + k_{11}^{1p} + k_{21}^{1p} + k_{11}^{3p} + k_{21}^{3p}\right) \phi_{11} &= M_{11}
\end{align*}
\] (5.2.7)

These equations of motion in the matrix form are identical to Eq. (5.2.5). The acceleration vector \( \ddot{u} \), the displacement vector \( u \), the force-moment vector \( f \) and the mass matrix \( M \) read:

\[
\begin{align*}
    \mathbf{u} &= \begin{pmatrix} u_{h_1} \\ u_{\eta_1} \\ \phi_{11} \end{pmatrix}, \quad \ddot{\mathbf{u}} = \begin{pmatrix} \ddot{u}_{h_1} \\ \ddot{u}_{\eta_1} \\ \ddot{\phi}_{11} \end{pmatrix}, \quad \mathbf{f} = \begin{pmatrix} f_{h_1} \\ f_{\eta_1} \\ M_{11} \end{pmatrix}, \quad \mathbf{M} = \begin{pmatrix} m_{11} \\ m_{11} \\ J_{11} \end{pmatrix}
\end{align*}
\] (5.2.8)
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The matrix of stiffnesses is:

\[
\mathbf{K} = \begin{pmatrix}
  k_{11}^{N} + k_{21}^{N} + k_{11}^{S} + k_{12}^{S} & 0 & \frac{a}{2} (k_{11}^{S} - k_{12}^{S}) \\
  0 & k_{11}^{S} + k_{21}^{S} + k_{11}^{N} + k_{12}^{N} & \frac{a}{2} (k_{11}^{N} - k_{12}^{N}) \\
  \frac{a}{2} (k_{11}^{N} - k_{12}^{N}) & \frac{a}{2} (k_{11}^{S} - k_{12}^{S}) & \frac{a^2}{4} (k_{11}^{N} + k_{21}^{N} + k_{11}^{S} + k_{12}^{S}) + k_{11}^{\theta} + k_{21}^{\theta} + k_{11}^{\rho} + k_{12}^{\rho}
\end{pmatrix}
\] (5.2.9)

The system is stable when the matrix of stiffnesses is positive definite since it is equivalent to positive definiteness of elastic energy of the system. In 1D systems with normal and shear springs, the form of the matrix of stiffness (tridiagonal block matrix) allowed one to use the Sylvester’s criterion and formulate the concise condition of stability [58, 59].

For matrix of stiffnesses, Eq. (5.2.9), Sylvester’s criterion cannot give such a laconic formulation of the necessary and sufficient criterion of stability. This matrix of stiffnesses, Eq. (5.2.9), relates to the simplest case of 2D systems. It is then logical to assume that we will have similar or even more complicated situations for more complex systems. From now on we restrict ourselves to a necessary condition of stability and consider quadratic forms related to the matrices of stiffnesses and find the minimum numbers of positive stiffness springs (or maximum numbers of negative stiffness springs).

The quadratic form associated with stiffness matrix, Eq. (5.2.9), reads:

\[
z^T \mathbf{K} z = v_i^2 k_{11}^{N} + v_{i1}^2 k_{21}^{N} + (v_i + y_i)^2 k_{11}^{S} + (w_i - y_i)^2 k_{21}^{S} + w_i^2 k_{11}^{N} + w_{i1}^2 k_{12}^{N} +
\]

\[
(v_i + y_i)^2 k_{11}^{S} + (v_i - y_i)^2 k_{12}^{S} + \frac{4y_i^2}{a^2} (k_{11}^{\theta} + k_{21}^{\theta} + k_{11}^{\rho} + k_{12}^{\rho})
\] (5.2.10)

where \( z = (v_i, w_i, 2y_i/a)^T \) is a non-zero vector and \( v_i, w_i, y_i \) are arbitrary numbers.

We now show that quadratic form, Eq. (5.2.10), can be positive definite only if the system has no less than three positive stiffness springs. To prove it we assume that there are only two positive stiffness springs in the system. In this case we can always find a non-zero vector \( z \) that makes the quadratic form not positive. For instance, suppose the system has only two springs with positive stiffness \( k_{11}^{N} > 0, k_{11}^{\theta} > 0 \). Then only the terms in Eq. (5.2.10) that contain positive stiffness will be positive. To make them zero we assume that \( v_i \) and \( y_i \) are equal to zero while \( w_i \) is a non-zero arbitrary
number. Subsequently, we can choose a non-zero vector $z$ that makes the quadratic form non-positive definite, e.g. $z = (0, 1, 0)^T$.

Obviously, if the system has only one positive stiffness spring, the system will be unstable for the same reason.

Three arbitrary positive stiffness springs may be not sufficient to ensure that the system is stable. Indeed, if the system has three positive stiffness rotational springs $k_{11}^{1p} > 0$, $k_{21}^{1p} > 0$, $k_{11}^{3p} > 0$ then the same non-zero vector $z = (0, 1, 0)^T$ makes the quadratic form non-positive definite. This situation occurs when the rank of the homogeneous system of equations (the left hand side of these equations consists of the multipliers of positive stiffness values) is smaller than the number of unknowns (components of a non-zero vector $z$: $v_1$, $w_1$ and $y_1$). The homogeneous equation in the case of three positive stiffness rotational springs reads: $y_1 = 0$. The rank of the homogeneous system of equations is equal to the number of unknowns when the set of three positive stiffness springs contains one positive stiffness spring per each degree of freedom. For example, if $k_{11}^{1N} > 0$, $k_{11}^{3N} > 0$, $k_{11}^{1p} > 0$ then we cannot find such a non-zero vector $z$ that makes the quadratic form not positive definite. For this case it is required to know the values of stiffness to conclude if the quadratic form is positive or negative definite.

In summary, the minimum number of positive stiffness springs in the 2D system consisting of one particle is 3 (one per each degree of freedom). Consequently, the maximum number of negative stiffness springs is 9 to ensure that the system is stable.

5.2.3.2 Stability of the “channel” of two particles with negative stiffness springs

A “channel” of two particles ($l = 3$, $n = 2$) is shown in Fig. 5.2.4.
Chapter 5.2. Stability of 2D discrete mass-spring systems with negative stiffness springs

Fig. 5.2.4. “Channel” of two particles connected to the fixed boundary connected by normal, shear and rotational springs.

This system contains two particles and seven normal, shear and rotational springs. Since the total number of the springs is quite high the index form of the equations of motion is not convenient.

We use matrix form, Eq. (5.2.5), where the acceleration vector \( \ddot{\mathbf{u}} \), the displacement vector \( \mathbf{u} \), the force-moment vector \( \mathbf{f} \) and the mass matrix \( \mathbf{M} \) read:

\[
\mathbf{u} = \begin{pmatrix} u_{t1} \\ u_{t2} \\ u_{s1} \\ u_{s2} \\ \phi_{t1} \\ \phi_{t2} \end{pmatrix}, \quad \ddot{\mathbf{u}} = \begin{pmatrix} \ddot{u}_{t1} \\ \ddot{u}_{t2} \\ \ddot{u}_{s1} \\ \ddot{u}_{s2} \\ \ddot{\phi}_{t1} \\ \ddot{\phi}_{t2} \end{pmatrix}, \quad \mathbf{f} = \begin{pmatrix} f_{t1} \\ f_{t2} \\ f_{s1} \\ f_{s2} \\ M_{11} \\ M_{21} \end{pmatrix},
\]

\[
\mathbf{M} = \begin{pmatrix} \mathbf{M}_m & \mathbf{m}_m \\ \mathbf{m}_m^T & \mathbf{M}_j \end{pmatrix}, \quad \mathbf{M}_m = \begin{pmatrix} m_{11} \\ m_{21} \end{pmatrix}, \quad \mathbf{M}_j = \begin{pmatrix} J_{11} \\ J_{21} \end{pmatrix}
\]

The matrix of stiffnesses has the form:
Chapter 5.2. Stability of 2D discrete mass-spring systems with negative stiffness springs

\[ K = \begin{pmatrix}
  k^{11}_{11} + k^{11}_{21} + k^{13}_{21} & -k^{13}_{21} & 0 & 0 & \frac{a}{2}(k^{13}_{11} - k^{13}_{12}) & 0 \\
  -k^{13}_{21} & k^{11}_{11} + k^{11}_{21} + k^{13}_{21} & 0 & 0 & \frac{a}{2}(k^{13}_{11} - k^{13}_{12}) & 0 \\
  0 & 0 & k^{11}_{11} + k^{13}_{21} + k^{13}_{12} & -k^{13}_{12} & \frac{a}{2}(k^{13}_{11} - k^{13}_{12}) & -\frac{a}{2}k^{13}_{21} \\
  0 & 0 & -k^{13}_{12} & k^{11}_{11} + k^{13}_{21} + k^{13}_{12} & \frac{a}{2}k^{11}_{11} + \frac{a}{2}k^{13}_{11} & -\frac{a}{2}(k^{13}_{11} - k^{13}_{12}) \\
  \frac{a}{2}(k^{13}_{11} - k^{13}_{12}) & 0 & \frac{a}{2}(k^{13}_{11} - k^{13}_{12}) & \frac{a}{2}k^{11}_{21} & \frac{a^2}{4}k^{11}_{11} + \frac{a^2}{4}k^{13}_{11} & -\frac{a^2}{4}(k^{13}_{11} - k^{13}_{12}) \\
  0 & -\frac{a}{2}(k^{13}_{11} - k^{13}_{12}) & \frac{a}{2}(k^{13}_{11} - k^{13}_{12}) & \frac{a}{2}k^{11}_{21} & \frac{a^2}{4}k^{11}_{11} + \frac{a^2}{4}k^{13}_{11} & \frac{a^2}{4}(k^{13}_{11} - k^{13}_{12})
\end{pmatrix} \tag{5.2.12}
\]

where \( k^{11}_{11} = k^{1S}_{11} + k^{1S}_{21} + k^{3S}_{12} \), \( k^{13}_{21} = k^{1S}_{11} + k^{3S}_{21} + k^{3S}_{22} \), \( k^{13}_{12} = k^{1S}_{21} + k^{3S}_{12} + k^{3S}_{11} \), \( k^{1p}_{11} = k^{1p}_{11} + k^{1p}_{21} + k^{3p}_{12} \), \( k^{1p}_{22} = k^{1p}_{21} + k^{3p}_{21} + k^{3p}_{22} \).

Similarly to the previous section, we study the stability of the system using the quadratic form associated with stiffness matrix, Eq. (5.2.12):

\[ z^T K z = v_1^2 k^{11}_{11} + (v_1 - w_1)^2 k^{11}_{21} + w_1^2 k^{11}_{21} + (w_1 - y_1)^2 k^{13}_{21} + (v_2 + w_2 - y_1 + y_2)^2 k^{13}_{12} +
(v_2 - y_2)^2 k^{13}_{11} + y_2^2 k^{13}_{12} + y_1^2 k^{3S}_{11} + v_2^2 k^{3S}_{21} + v_2^2 k^{3S}_{22} + (v_1 + w_1)^2 k^{3S}_{12} + (v_1 - w_1)^2 k^{3S}_{21} +
(w_1 + y_2)^2 k^{3S}_{21} + (w_1 - y_2)^2 k^{3S}_{22} + \frac{4}{a^2}(w_2^2 k^{1p}_{11} + k^{3p}_{11} + k^{3p}_{12}) + y_2^2 (k^{1p}_{11} + k^{1p}_{21} + k^{3p}_{12}) + (w_2 - y_2)^2 k^{1p}_{21} \tag{5.2.13}
\]

where \( z = (v_1, w_1, y_1, v_2, 2w_2/a, 2y_2/a)^T \) is a non-zero vector and \( v_1, w_1, y_1, v_2, w_2, y_2 \) are arbitrary numbers.

The structure of quadratic form, Eq. (5.2.13), is identical to Eq. (5.2.10) except for the terms which are related to the springs between two particles: \( k^{1S}_{11}, k^{1S}_{21} \) and \( k^{1p}_{21} \).

However, this difference does not change the necessary condition of stability. Since non-zero vector \( z \) has six arbitrary components (it is equivalent that the system has six degrees of freedom), the minimum number of positive stiffnesses springs is equal to six provided that each particle has three positive stiffness springs (one spring per each degree of freedom). For example, a “bad” set of six positive stiffness springs (when the above rules are not met and the system is unstable) is \( k^{11S}_{11}, k^{11S}_{11}, k^{1p}_{11}, k^{1S}_{31}, k^{3S}_{31}, k^{3p}_{11} \).

Indeed, we can choose a non-zero vector \( z \) such that the quadratic form is negative, e.g. \( v_1 = w_1 = y_1 = w_2 = 0 \), \( v_2 = y_2 = 1 \).

If the necessary condition is satisfied then quadratic form, Eq. (5.2.13), might be positive definite in the presence of the appropriate values of spring stiffnesses. Thus, the minimum number of positive stiffness springs is 6 (maximum number of negative stiffness springs is 15) to ensure that the “channel” of two masses is stable.
5.2.3.3. Stability of the two-by-two system of particles with negative stiffness springs

A two-by-two system of particles \( (l = 3, \ n = 3) \) is shown in Fig. 5.2.5.

![Diagram of a two-by-two system of particles](image)

**Fig. 5.2.5.** 2D system consisting of two-by-two particles connected to the fixed external boundary by normal, shear and rotational springs.

There are four particles and twelve normal, shear and rotational springs in the system. The matrices and vectors present in the equations of motion in matrix form, Eq. (5.2.5), read:
The matrix of stiffnesses is a twelve-by-twelve square symmetric matrix which can be obtained using Eq. (5.2.4). Due to large number of components of this matrix we only show the quadratic form associated with this matrix. The quadratic form reads:

\[
\begin{align*}
\mathbf{z}^T \mathbf{K} \mathbf{z} &= v_1^2 k_{11}^{1N} + (v_1 - w_1)^2 k_{21}^{1N} + w_1^2 k_{31}^{1N} + y_1^2 k_{12}^{1N} + (v_2 - y_1)^2 k_{32}^{1N} + v_2^2 k_{33}^{1N} + \\
&\quad (w_2 + y_3)^2 k_{11}^{1S} + (v_4 - w_2 + y_2 + y_3)^2 k_{21}^{1S} + (v_4 - y_2)^2 k_{31}^{1S} + (v_5 + w_4)^2 k_{12}^{1S} + \\
&\quad (-v_3 + w_3 + w_4 + y_3)^2 k_{22}^{1S} + (w_3 - y_3)^2 k_{32}^{1S} + w_2^2 k_{11}^{3N} + y_2^2 k_{12}^{3N} + (v_3 - w_2)^2 k_{33}^{3N} + \\
&\quad (w_5 - y_2)^2 k_{22}^{3N} + v_2^2 k_{11}^{3N} + w_5^2 k_{32}^{3N} + (v_1 + y_3)^2 k_{12}^{3S} + (v_4 + w_1)^2 k_{21}^{3S} + \\
&\quad (-v_1 + w_4 + y_1 + y_3)^2 k_{22}^{3S} + (v_2 + v_4 - w_1 + y_4)^2 k_{12}^{3S} + (w_4 - y_1)^2 k_{31}^{3S} + \\
&\quad (v_2 - y_4)^2 k_{22}^{3S} + 4/\alpha^2 (y_3^2 (k_{11}^{1p} + k_{11}^{3p})) + (v_4 - y_3)^2 k_{21}^{1p} + v_2^2 (k_{31}^{1p} + k_{21}^{3p}) + \\
&\quad w_2^2 (k_{12}^{1p} + k_{13}^{3p}) + (w_4 - y_3)^2 k_{22}^{1p} + y_3^2 (k_{12}^{3p} + k_{23}^{3p}) + (w_4 - y_1)^2 k_{12}^{3p} + (v_4 - y_4)^2 k_{22}^{3p}
\end{align*}
\]

(5.2.15)

where \( \mathbf{z} = (v_1, w_1, y_1, v_2, w_2, y_2, v_3, w_3, 2y_3/a, 2v_4/a, 2w_4/a, 2y_4/a) \) is a non-zero vector, \( v_1, w_1, y_1, ..., v_4, w_4, y_4 \) are arbitrary numbers.

The structure of the quadratic form, Eq. (5.2.15), is analogous to the quadratic forms in the previous sections, Eq. (5.2.10) and Eq. (5.2.13). Evidently, the necessary condition of stability should be similar. For this particular case (Fig. 5.2.5) the minimum number of positive stiffness springs is 12 (three springs per each particle, one spring per each degree of freedom).
Similarly to Eq. (5.2.13), we have terms which are related to the springs between particles. Studying this quadratic form, we found that the positive stiffness springs cannot be isolated from the boundaries in the stable systems. Here we prove this additional part of the necessary condition of stability.

Assume that we have twelve positive stiffness springs in the system: \( k_{21}^{N}, k_{21}^{S}, k_{21}^{1p}, k_{22}^{1p}, k_{12}^{1p}, k_{12}^{3p}, k_{22}^{3p}, k_{22}^{3q} \) (highlighted in bold in Fig. 5.2.5).

According to the necessary condition of stability described above, this set of positive stiffness springs may make the system stable. However, let us consider the homogeneous system of equations (the left hand side of these equations consist of the multipliers of positive stiffness values):

\[
\begin{align*}
    v_1 - w_1 &= 0 \\
    v_4 - w_2 + y_2 + y_3 &= 0 \\
    v_4 - y_3 &= 0 \\
    \ldots \\
    v_4 - y_4 &= 0
\end{align*}
\] (5.2.16)

The rank of homogeneous system of equations, Eq. (5.2.16), is nine while the number of unknowns is twelve. It means that we can find a non-zero vector \( \mathbf{z} \) such that the quadratic form is negative, the matrix of stiffness is non-positive definite and the system is unstable, e.g. \( v_1 = w_1 = 0, v_2 = y_1 = 1, v_3 = w_2 = 1, w_3 = y_2 = 2, w_4 = y_3 = y_4 = v_4 = -0.5 \).

If we assume the first three springs (\( k_{21}^{N}, k_{21}^{S}, k_{21}^{1p} \)) in our spring combination negative, but keep \( k_{11}^{3N}, k_{11}^{3S}, k_{11}^{3p} \) positive then the rank of the new homogeneous system of equations will be equal to twelve which means that the system might be stable and values of the spring stiffnesses should be taken into account for further investigation.

It turns out that the minimum number of positive stiffness springs is 12 (the maximum number of negative stiffness springs is 24) in the stable two-by-two system of particles. On top of that, certain conditions in the arrangement of these springs should be satisfied.

5.2.3.4. Stability of the three-by-three system of particles with negative stiffness springs
Chapter 5.2. Stability of 2D discrete mass-spring systems with negative stiffness springs

Before generalising the results of previous sections to a two-dimensional system of arbitrary size we consider a three-by-three system of particles \((l = 4, n = 4)\). In contrast to the previous systems there is an inner mass, \(m_{22}\), which is not connected to any boundaries. It should be examined whether this feature affects the stability of the system.

The system is composed of nine masses and twenty four normal, shear and rotational springs.

The acceleration, displacement and force-moment vectors in Eq. (5.2.5) read:

\[
\mathbf{u} = \begin{pmatrix} u_{h1} \\ \vdots \\ u_{33} \\ \phi_1 \\ \vdots \\ \phi_{33} \end{pmatrix}, \quad \mathbf{\ddot{u}} = \begin{pmatrix} \ddot{u}_{h1} \\ \vdots \\ \ddot{u}_{33} \\ \ddot{\phi}_1 \\ \vdots \\ \ddot{\phi}_{33} \end{pmatrix}, \quad \mathbf{f} = \begin{pmatrix} f_{h1} \\ \vdots \\ f_{33} \\ M_{11} \\ \vdots \\ M_{33} \end{pmatrix}
\]

(5.2.17)

The mass matrix, \(\mathbf{M}\), compounds of submatrices, \(\mathbf{M}_m\) and \(\mathbf{M}_j\):

\[
\mathbf{M}_m = \begin{pmatrix} m_{11} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & m_{33} \end{pmatrix}, \quad \mathbf{M}_j = \begin{pmatrix} J_{11} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & J_{33} \end{pmatrix}
\]

(5.2.18)

The matrix of stiffnesses is a 27-by-27 square symmetric matrix. Similar to the previous section we analyse the stability using the quadratic form associated with this matrix. For the sake of further convenience a non-zero vector, \(\mathbf{z}\), is taken as:

\[
\mathbf{z} = \begin{pmatrix} v_1, w_1, y_1, \ldots, v_6, w_6, y_6, \frac{2v_2}{a}, \frac{2w_2}{a}, \frac{2y_2}{a}, \ldots, \frac{2v_9}{a}, \frac{2w_9}{a}, \frac{2y_9}{a} \end{pmatrix}^T
\]

(5.2.19)

Here \(v_1, w_1, y_1, \ldots, v_9, w_9, y_9\) are arbitrary numbers.

Then the quadratic form can be expressed as:
Despite the complexity of the expression, the quadratic form, Eq. (5.2.20), has the structure which is identical to the structure of the quadratic forms obtained in the previous sections, Eq. (5.2.10), Eq. (5.2.13) and Eq. (5.2.15). All multipliers (arbitrary numbers, \( v_i, w_j, y_k \)) are squared and do not affect the positive definiteness of the quadratic form as opposed to the spring stiffnesses. The stability of the system is defined by the same conditions obtained for the two-by-two system. Thus, the minimum number of positive stiffness springs is 27 (three springs per each particle, one spring per each degree of freedom).

We consider the case when all particles except the inner one, \( m_{22} \), are connected to the boundary by 27 positive stiffness springs, \( k_{11}^{1N}, k_{11}^{1S}, k_{11}^{1P}, k_{12}^{1N}, k_{12}^{1S}, k_{12}^{1P}, k_{13}^{1N}, k_{13}^{1S}, k_{13}^{1P}, k_{21}^{1N}, k_{21}^{1S}, k_{21}^{1P}, k_{22}^{1N}, k_{22}^{1S}, k_{22}^{1P}, k_{23}^{1N}, k_{23}^{1S}, k_{23}^{1P}, k_{31}^{1N}, k_{31}^{1S}, k_{31}^{1P}, k_{32}^{1N}, k_{32}^{1S}, k_{32}^{1P}, k_{33}^{1N}, k_{33}^{1S}, k_{33}^{1P} \). This number of springs is required for the stability. However, the particular arrangement of the springs should be examined.

Following the same procedure, the homogeneous system of equations consisting of the multipliers of positive stiffness values in the quadratic form reads:
\[
\begin{align*}
&v_4 = 0, \\
&v_1 + v_7 = 0, \\
&v_7 = 0, \\
&\ldots, \\
&w_7 = 0
\end{align*}
\] (5.2.21)

The number of unknowns is 27, while the rank of the homogeneous system of equations, Eq. (5.2.21), is 24. Therefore, a non-zero vector \( \mathbf{z} \) exists such that the quadratic form is negative. The system is unstable for this set of positive stiffness springs.

Nevertheless, the stability can be achieved with the same number of positive stiffness springs if we connect the inner mass to the neighbouring one by positive stiffness springs \( k_{22}^{3N}, k_{22}^{3S}, k_{22}^{3O} \) (the last three springs, \( k_{21}^{3N}, k_{21}^{3S}, k_{21}^{3O} \), become negative). In that case, the rank of the new homogeneous system of equations will be equal to the number of unknowns.

Consequently, the minimum number of positive stiffness springs is 27 (the maximum number of negative stiffness springs is 45) in the stable three-by-three system of particles. However, this does not guarantee the stability of the system. Certain conditions in the arrangement of the springs should be fulfilled.

Based on the above we can state that with further increase in the number of particles in the system, the quadratic form will have similar structure and the necessary condition of stability will remain the same.

To sum up, we can formulate the necessary condition of stability for 2D square packing systems of arbitrary size:

- The minimum number of positive stiffness springs in the system is equal to the number of particles multiplied by the number of degrees of freedom;
- Positive stiffness springs cannot be isolated from the boundaries.

In Section 5.2.5 we discuss this condition in more detail and consider how it relates to 1D and 3D systems.

We used quadratic forms to investigate the stability of the systems. This approach makes it possible to rather easily analyse the positive definiteness of the
stiffness matrix. Moreover, comparing the structure of the quadratic forms for the different size systems we can generalise results for a two-dimensional system of arbitrary size. Another method that could in principle be used would be a brute-force approach that is considering all possible combinations of springs, perhaps by using a mathematical package. However, the number of springs rises rapidly as the number of masses increases. Furthermore, the number of possible arrangements of the negative stiffness springs rises exponentially. Investigation of the stability and generalisation of the results requires calculating a large number of combinations. Suppose for simplicity that the stiffness of each spring in the two-dimensional system is set to be slightly negative or very large positive (four orders of magnitude higher). The system consists of \( n + 2 \) columns and \( l + 2 \) rows of particles (end particles are fixed). The total number of springs is equal to \( 6nl + 3(n + l) \). For instance, let us consider the case of \( n = 5 \) and \( l = 5 \). It gives \( 2^{6 \cdot 5 + 3(5+5)} = 2^{180} \) combinations of the stiffness matrix. Then Sylvester’s criterion requires calculating \( 3nl \) lead minors for each combination. Thus, the brute-force approach is not applicable (even if symmetry is taken into account) as computationally the problem becomes exponentially complex. That is why we only consider here the simple systems, such as one single mass, the “channel”, two-by-two and three-by-three systems, analysed their quadratic forms and then generalized results.

5.2.4 Eigenfrequencies and trajectories

Here we study the “channel” of two particles and the two-by-two system of particles in more detail. We use the following dimensionless groups:

\[
\begin{align*}
  u_{y}^{*} &= \frac{u_{y}}{a}, \quad \phi_{y}^{*} = \phi_{y}, \quad \ddot{u}_{y}^{*} = \frac{m_{y} \ddot{u}_{y}}{k_{31} a}, \quad \ddot{\phi}_{y}^{*} = \frac{J_{y} \ddot{\phi}_{y}}{k_{31} a^{2}}, \\
  k_{ij}^{1N*} &= \frac{k_{ij}^{1N}}{k_{31}}, \quad k_{ij}^{1S*} = \frac{k_{ij}^{1S}}{k_{31}}, \quad k_{ij}^{0*} = \frac{k_{ij}^{0}}{k_{31} a}, \\
  f_{ij}^{*} &= \frac{f_{ij}}{k_{31} a}, \quad M_{y}^{*} = \frac{M_{y}}{k_{31} a^{2}},
\end{align*}
\]  

(5.2.22)

where \( i = 1, \ldots, l - 1 \), \( j = 1, \ldots, n - 1 \); \( l = 3 \), \( n = 2 \) for the “channel” of two particles and \( l = 3 \), \( n = 3 \) for the two-by-two system of particles.
Normalisation of the terms related to the $x_3$-direction is expressed in a way similar to the terms related to the $x_1$-direction, Eq. (5.2.22). As a result, system of the equations of motion, Eq. (5.2.4), will be expressed in a dimensionless form.

The general solution of this system reads:

$$\mathbf{u}^* = \sum_{j=1}^{3(l-1)(n-1)} \mathbf{e}_j \left[ C_j^+ \exp(i\omega_j^* t) + C_j^- \exp(-i\omega_j^* t) \right],$$

(5.2.23)

where $\mathbf{e}_j$ are the eigenvectors of the dimensionless matrix of stiffness, $C_j^\pm$ are constants, $\omega_j^*$ are the eigenfrequencies.

5.2.4.1. The “channel” of two particles with negative stiffness springs

Fig. 5.2.6 shows the relationship between all eigenfrequencies and one varying spring stiffness, $k_{11}^{\text{LN*}}$, for a “channel” of two particles (Fig. 5.2.4). Other values of spring stiffnesses are set to be equal to 1. Similarly to the previous studies [58, 59], the smallest eigenfrequency, $\omega_1^*$, tends to zero when the negative stiffness exceeds its critical value ($k_{11,\text{cr}}^{\text{LN*}} = -2.75$). When it happens, the solution, Eq. (5.2.23), tends to infinity and the system loses stability. In contrast to papers [14, 27] where enhancement of the effective stiffness in the system with negative stiffness inclusions was observed, here one can see that the effective stiffness only decreases.

Fig. 5.2.6. Relationship between eigenfrequencies and different values of spring stiffness, $k_{11}^{\text{LN*}}$, for the “channel” of two particles. Other values of spring stiffnesses are equal to 1.
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It is of particular interest to note that the order of eigenfrequencies remains unchanged regardless of the value of the spring stiffness, e.g. $\omega_1^*$ always remains the smallest eigenfrequency, $\omega_6^*$ always remains the biggest one. As a consequence, from this point on we consider only the smallest and the biggest eigenfrequencies. Other eigenfrequencies are always located between these two so their consideration is unnecessary for analysis. On top of that, due to the symmetry of the system we confine ourselves to varying three stiffnesses of normal, shear and rotational springs: $k_{11}^{1N^*}$, $k_{11}^{3N^*}$, $k_{11}^{1S^*}$, $k_{21}^{1S^*}$, $k_{11}^{1\omega^*}$, $k_{11}^{2\omega^*}$, $k_{21}^{3\omega^*}$.

Fig. 5.2.7 shows the relationships between eigenfrequencies $\omega_1^*$ and $\omega_6^*$ and different values of (a) normal, (b) shear and (c) rotational springs. Note that the critical stiffness of the springs between the particles is always much higher than the critical stiffness of boundary springs, e.g. $k_{11}^{1N^*} = -2.75$, $k_{11}^{3N^*} = -2.7$, $k_{21}^{1\omega^*} = -1.5$, Fig. 5.2.7(a).
Fig. 5.2.7. The smallest and largest eigenfrequencies, $\omega_1^*$ and $\omega_6^*$, and different values of spring stiffness for the “channel” of two particles. Other values of spring stiffnesses are equal to 1.

The trajectories of motion demonstrate the behaviour of the system. This is another approach to determine if the system with negative stiffness springs is stable. We use this method as an illustration of the obtained necessary condition of stability (e.g. minimum number of positive stiffness springs) and eigenfrequency analysis (i.e. the
critical value of a certain negative stiffness spring). At the initial time we apply instantaneous unit displacement to the left particle in the $x_3$–direction $u_{31}^*(0)=1$. Fig. 5.2.8 shows the trajectories of motion (translational displacements of the particles in $x_3$–direction, $u_{31}^*$ and $u_{32}^*$) for the different sets of spring stiffness. When the system has one negative stiffness spring ($k_{11}^{1S} = -2$) (other spring stiffnesses are equal to 1) and its absolute value does not exceed the critical value ($k_{11r}^{1S} = -2.14$) the system remains stable (Fig. 5.2.8 (a)). When the absolute value of the negative stiffness spring ($k_{11}^{1S} = -2.15$) is above the critical value, the system loses stability, Fig. 5.2.8 (b).

Fig. 5.2.9 (a) demonstrates the stability of the system when there are only six positive stiffness springs in the “channel” $k_{11}^{1NS} = k_{11}^{1S} = k_{11r}^{1S} = k_{31}^{1NS} = k_{31}^{1S} = k_{31r}^{1S} = 1$, other spring stiffnesses being negative and equal to -0.1. If we assume that one of the positive stiffness springs is negative and the value is very small, e.g. $k_{11}^{1S} = -10^{-10}$, the system loses stability, Fig. 5.2.9(b).

The trajectories were calculated numerically using a regular mathematical package. We established by changing the time step that the trajectories stabilise numerically such that the obtained instability has the physical nature. This supports our statement about the necessary condition of stability that the minimum number of positive stiffness springs is 6 for the “channel” of two particles.

![Fig. 5.2.8. Trajectories produced by the initial instantaneous unit displacement of the left particle $u_{31}^*(0)=1$. All spring stiffnesses are equal to 1 except one: (a) $k_{11}^{1S} = -2$ – the system is stable, (b) $k_{11}^{1S} = -2.15$ – the system loses stability since $k_{11}^{1S}$ is above the critical value, $k_{11r}^{1S} = -2.14$.](image)
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Fig. 5.2.9. Trajectories caused by the initial instantaneous unit displacement of the left particle $u_{31}^*(0) = 1$:

(a) $k_{11}^{NS} = k_{11}^{IS} = k_{11}^{I\omega} = k_{31}^{NS} = k_{31}^{IS} = k_{31}^{I\omega} = 1$, other spring stiffnesses are negative and equal to -0.1,

(b) $k_{11}^{NS} = k_{11}^{IS} = k_{11}^{I\omega} = k_{31}^{NS} = k_{31}^{IS} = k_{31}^{I\omega} = 1$, $k_{11}^{I\omega} = -10^{-10}$, other spring stiffnesses being negative and equal to –0.1.

5.2.4.2 The two-by-two system of particles with negative stiffness springs

Due to symmetry we can confine ourselves to consideration of only two normal, shear and rotational springs in the two-by-two system (Fig. 5.2.5) of particles: $k_{11}^{NS}$, $k_{21}^{NS}$, $k_{11}^{IS}$, $k_{21}^{IS}$, $k_{11}^{I\omega}$, $k_{21}^{I\omega}$.

Similarly to Fig. 5.2.7, Fig. 5.2.10 shows the relationships between eigenfrequencies (the smallest, $\omega_1^*$ and the biggest, $\omega_2^*$) and different values of

(a) normal, (b) shear and (c) rotational springs.

One can see that the critical stiffness of the boundary springs is far smaller than the absolute values of the critical stiffnesses of the springs between the neighbouring particles, e.g.

$\ k_{11}^{NS} = -2.37, \ k_{21}^{NS} = -1.38, \ $ Fig. 5.2.10(a).
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Fig. 5.2.10. Relationship between the smallest and largest eigenfrequencies, \( \omega_1^* \) and \( \omega_{12}^* \), and different values of spring stiffness for the two-by-two system of particles. Other values of spring stiffnesses are equal to 1.

Fig. 5.2.11 shows the trajectories of motion of the particles, \( u_{3j}^* \), when the system has the minimum number (twelve) of positive stiffness springs
\[
k_{11}^{\text{NS}} = k_{11}^{\text{IS}} = k_{11}^{\text{OS}} = k_{21}^{\text{NS}} = k_{21}^{\text{IS}} = k_{21}^{\text{OS}} = k_{12}^{\text{NS}} = k_{12}^{\text{IS}} = k_{12}^{\text{OS}} = k_{22}^{\text{NS}} = k_{22}^{\text{IS}} = k_{22}^{\text{OS}} = 1,
\]
other stiffnesses of the springs being negative and equal to \(-0.1\). The system is still stable.
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Fig. 5.2.11. Trajectories under instantaneous unit displacement of the top left particle $u_3^* (0) = 1$, $k_{31}^{NS} = k_{31}^{SR} = k_{31}^{RN} = k_{31}^{LR} = k_{12}^{NS} = k_{12}^{SR} = k_{12}^{RN} = k_{12}^{LR} = 1$, other stiffnesses of the springs being negative and equal to –0.1.

5.2.5. Discussion

We studied the stability of 2D square packing discrete mass-spring systems with rotations. We note that adding rotational degrees of freedom to the system implies including the corresponding rotational springs, otherwise the system becomes unstable (mechanically indeterminate) [61, 62] independently of the sign of spring stiffnesses. We now compare the results with the already investigated one-dimensional systems (chains of particles) [58, 59]. It was found that the maximum number of negative stiffness springs is equal to 1 in the chains consisting only of normal springs [58], and to 3 in the chains where particles are connected by normal, shear and rotational springs [59]. Evidently, the maximum number of negative stiffness springs does not depend on the number of particles in the chains. It may seem that the conditions of stability for 1D systems are different from the 2D systems, where the number of negative stiffness springs depends on the number of particles.

In order to investigate this difference further, consider a chain of $n + 1$ particles connected by $n$ normal springs. The end particles are fixed and $n − 1$ particles can move. According to the conditions of stability obtained in this study (the minimum number of positive stiffness springs equals the number of particles times the number of degrees of freedom) there should be minimum $n − 1$ positive stiffness springs in the system (since each particle has one degree of freedom). Consequently, the maximum number of negative stiffness spring is always equal to 1 regardless of the number of
masses. The situation will be identical for the chains consisting of normal, shear and rotational springs. Thus the conditions of stability obtained for 2D systems are also true for the chains of particles.

The critical concentration (fraction) of negative stiffness springs for 1D systems with only normal springs when the systems can still be stable is [58]:

\[
c_{cr}^{1D} = \frac{1}{n}
\]  

(5.2.24)

Now we calculate the critical fraction of negative stiffness springs for 2D systems, \(c_{cr}^{2D}\). Assume that the model consists of \(n+2\) columns and \(l+2\) rows of particles (end particles are fixed). The total number of springs is equal to \(N_{total}^{2D} = 6nl + 3(n+l)\). The minimum number of the positive stiffness springs is equal to \(N_{min}^{2D} = 3nl\), the maximum number of negative stiffness springs is \(N_{max}^{2D} = 3nl + 3(n+l)\). The system may be stable if the fraction of negative stiffness springs, \(c^{2D}\), satisfies the following inequality:

\[
c^{2D} \leq c_{cr}^{2D} = \frac{3nl + 3(n+l)}{6nl + 3(n+l)}
\]  

(5.2.25)

Thus in 2D systems the critical fraction of negative stiffness springs tends to \(1/2\) with increasing of the number of particles.

Following this logic, the necessary condition of stability can be extended to three-dimensional (3D) cubic packing systems. Each particle will have six degrees of freedom (three translational displacements in the \(x_1, x_2, x_3\) – directions and three rotations around these directions) and will be connected to 30 springs (6 normal springs, 12 shear and rotational springs). If a system consists only of one particle there should be six positive stiffness springs (one per each degree of freedom) to ensure that that system can be stable. Assume that the system has \(n+2\) columns, \(l+2\) rows and \(h+2\) layers of particles (boundary particles are fixed) then the minimum number of positive stiffness springs is equal to \(N_{min}^{3D} = 6nlh\) provided that these springs are not isolated from the boundaries. The total number of springs is equal to \(N_{total}^{3D} = 15nlh + 5(nl + hl + hn)\). Consequently, the maximum number of negative stiffness springs:
The critical fraction of negative stiffness springs in the model reads as:

\[ c_{cr}^{3D} = \frac{9nlh + 5(nl + hl + hn)}{15nlh + 5(nl + hl + hn)} \]  

(5.2.26)

The system is stable when \( c_{cr}^{3D} \leq c_{cr}^{3D} \) provided that stiffnesses of springs and their position are taken into account. The critical fraction of negative stiffness springs tends to \( 3/5 \) with increasing of the number of particles in the system.

Consider a single mass system. In the case of 1D system the mass has 3 DOF (two translational and one rotational) and can be connected by up to 6 springs (two shear, normal and rotational springs). The same mass has 3 DOF (two translational and one rotational) and can be connected by up to 12 springs (four shear, normal and rotational springs) in 2D. In the 3D case the mass has 6 DOF (three translational and three rotational) and can be connected by up to 30 springs (six normal, twelve shear and rotational springs). It is apparent that the number of springs is increasing more rapidly than the number of DOF. It has been established that the mass may be stable if at least one positive stiffness spring per DOF is attached to it. Thus, the mass can be stable when it has 3 negative stiffness springs in 1D, 9 negative stiffness springs in 2D and 24 negative stiffness springs in 3D. The calculated critical fraction of negative stiffness springs is 0.5 for 1D, 0.75 in 2D and 0.8 for 3D. This explains why the larger dimension of the system the greater the critical fraction of negative stiffness springs.

The obtained formulae of the critical fraction of negative stiffness springs for the 2D and 3D systems, Eq. (5.2.25) and Eq. (5.2.26) are only based on the necessary condition of stability. The particular arrangements of springs and values of spring stiffness are essential and should be examined. In contrast, the critical concentration of negative stiffness springs for the 1D systems with only normal springs, Eq. (5.2.24), does not depend on the arrangement of springs.

It is interesting to note that while the critical fraction of negative stiffness springs for 1D systems tends to zero with the increase in the system length, in 2D and 3D systems the critical fraction of negative stiffness springs tends to positive numbers albeit different for 2D and 3D. In a way, 2D and 3D systems seem to be more forgiving than the 1D systems; perhaps the presence of the fixed boundary from more than one
directions imposes a stabilising effect. This is supported by the fact that the critical fraction of negative stiffness springs in 3D is greater than that in 2D. The reason is that the presence of the fixed boundary in three directions provides greater stabilisation that the fixed boundary presented in only two directions. From this point of view, one should be careful when generalising observations from 1D systems to 2D and 3D systems.

5.2.6. Conclusion

The necessary condition of stability was established for mass-spring systems of the particular configuration (specific arrangement of springs, Fig. 5.2.1; square packed particles in 2D; cubic packed particles in 3D) with fixed boundary particles. The systems with negative stiffness springs (both translational in the coordinate directions and rotational) can be stable, when the number of negative stiffness springs does not exceed a certain critical number. For large systems the maximum relative number (the critical fraction) of negative stiffness springs is constant, 1/2 for 2D square packing systems and 3/5 for 3D cubic packing systems. This property is in stark contrast with the 1D systems where the critical fraction of negative stiffness springs tends to zero inversely proportional to the system size. This difference can be attributed to the fact that the presence of fixed boundary in two and three directions imposes additional stabilisation opposite to only two fixed ends in 1D chains. The obtained necessary condition of stability and the critical fractions of negative stiffness springs are correct only for the considered configurations of mass-spring systems. The influence of different system configurations (particles packing types and springs arrangements) on the criterion of stability was beyond the scope of this study.

The presence of negative stiffness springs in 2D system leads to a decrease in the eigenfrequencies: as soon as the absolute value of the negative stiffness spring reaches its critical value, the smallest eigenfrequency becomes zero, while all other eigenfrequencies decrease to certain minimum values. It is noteworthy that the order of frequencies (from the smallest to the largest) remains the same in the region of negative stiffnesses. Further increase in the absolute value of the negative stiffness makes the system unstable leading to the appearance of unbounded trajectories. This property is similar to that of 1D systems.
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CHAPTER 6

Wave propagation in materials with negative Cosserat shear modulus
Wave propagation in materials with negative Cosserat shear modulus

E. Pasternak*, A.V. Dyskinb,*, M. Esina

a School of Mechanical and Chemical Engineering, University of Western Australia, Perth, Australia
b School of Civil, Environment and Mining Engineering, University of Western Australia, Perth, Australia

A R T I C L E  I N F O

Article history:
Received 9 August 2015
Revised 2 November 2015
Accepted 21 November 2015

Keywords:
Cosserat continuum
Frequency threshold
Rolling of non-spherical particles
Shear-rotational waves

A B S T R A C T

Materials with negative elastic moduli are unstable, but can be stabilised by specific boundary conditions. In particulate materials under compression, rotating non-spherical particles produce the effect of negative Cosserat shear modulus. We consider wave propagation in such materials and demonstrate that when the sum of the negative Cosserat shear modulus and the conventional shear modulus is positive the waves can propagate. In the conventional isotropic Cosserat continuum the twist wave and one of the shear waves exist only at frequencies higher than a threshold. When the Cosserat shear modulus is negative all waves exist at all frequencies; observing the twist and shear waves one can detect and investigate the negative moduli.

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1. Introduction

Positive definiteness of the elastic potential energy is a thermodynamic requirement. It also ensures the uniqueness of elastic solution and, consequently, the stability of the corresponding material or the system. This imposes certain conditions on the values of the elastic constants. For instance in isotropic elasticity, the condition of positive definiteness imposes the following condition on the bulk and shear moduli, \( \kappa > 0, \mu > 0 \) (Landau & Lifshitz, 1986), while the first Lame constant can be negative, as long as \( \lambda > -2\mu/3 \). This also includes negative Poisson’s ratio (see for instance Pasternak & Dyskin, 2012 and the literature review therein), as long it is greater than \(-1\).

In what follows the term negative stiffness will explicitly refer to the cases when the negative values of the corresponding moduli do violate the positive definiteness of the energy. For example, if a spring with negative stiffness is loaded, the loading device does work on loading while the elastic energy reduces. This contradiction manifests itself in instability of such a system. Nevertheless the negative stiffness systems or materials can still be stable in a certain range of values of negative stiffness if the stability is maintained by appropriate boundary conditions (Dyskin & Pasternak, 2012a, 2012b; Kochmann & Milton, 2014). Thereafter we only consider the case when the stability is maintained by the appropriate boundary conditions. This paper does not consider the metamaterials in which peculiarities of wave propagation such as the presence of wave bands are interpreted in terms of negative dynamic modulus (Cheng, Xu, & Liu, 2008; Ding, Liu, Qiu, & Shi, 2007; Fang et al., 2006; Lee, Park, Seo, Wang, & Kim, 2009; Morvan, Tinel, Hladky-Hennion, Vasseur, & Dubus, 2010), negative mass/density (Ding et al., 2007; Park, Park, Lee, & Lee, 2015) or negative refraction index (Guenneau, Movchan, Petursson, & Ramakrishna, 2007; Lee, Ma, Lee, Kim, & Kim, 2011). A notion was put forward of a possibility of breakage of the second law of thermodynamics at very small scale and very short times, see Ostoj-Starzewski and Malyarenko (2014) for details. Notwithstanding this possibility we consider a macroscopic (effective) negative stiffness that can be exhibited by some structures.
We base our consideration on the fact that a number of mechanisms and material elements have been found to exhibit negative stiffness in a certain range of magnitudes of the loading and under appropriate boundary conditions. An obvious example is the post-peak softening of the rocks and concrete where the stability is clearly controlled by the stiffness of the loading device, that is by the boundary conditions (Cook, 1965; Salamon, 1970; Tarasov & Dyskin, 2005). Systems with negative stiffness include systems of elastic springs, arches, links and certain link and lever mechanisms (Carrella, Brennan, & Waters, 2008; Champneys, Hunt, & Thompson, 1999; Hunt, Muhlhaus, & Whiting, 1997; Park & Liu, 2007; Thompson & Hunt, 1973; Wang & Lakes, 2004). Negative shear modulus is exhibited by a cell comprised of four masses mutually connected by pre-loaded elastic springs of different stiffnesses (Lakes & Drugan, 2002). Tubes and columns pre-buckled to an S-shaped configuration (Bazant & Cedolin, 1991; Lakes, 2001) and nanotubes (Yap, Lakes, & Carpick, 2008) show negative stiffness. Negative stiffness is observed in single foam cells (Lakes, Rosakis, & Ruina, 1993) and was recently detected in hair-bundles in the ear: the negative stiffness is believed to be the basis of an amplification mechanism in hearing (Martin, Mehta, & Hudspeth, 2000). Phase transformations can produce an effect of negative stiffness (Roytburd, 1996). Rotating levers give another example of a mechanism producing negative stiffness (Tarasov & Randolph, 2008). Plate-like interlocking structures of cubic elements constrained by a rigid frame show negative stiffness in the post-peak stage (Estrin et al., 2004; Schaare et al., 2008).

Recently, the first two authors proposed yet another mechanism of apparent negative stiffness based on rotation of non-spherical particles, Fig. 1(a) (Dyskin & Pasternak, 2011, 2012b, 2012c). The effect is apparent from the consideration of moment equilibrium about the point of particle contact. The particle rotation is resisted by compressive load $P$ that creates a moment balancing the moment from the shear force. Subsequently, as the particle rotates the arm of application of the compressive force reduces thus reducing the resisting moment, Fig. 1(b). The importance of this mechanism is in its ubiquity: it can work in granular materials as well as in rocks at different scales (Dyskin & Pasternak, 2012c) and concrete at advanced stages of loading when the accumulated damage leads to grain/aggregate detachment enabling their independent rotation. (We note that modelling of granular materials, rocks and concrete is usually conducted under the assumption that the grains are spherical, which erases the effect of negative stiffness.) Furthermore, the considered negative stiffness mechanism is reversible: the reduction of the displacement causes increase in the shear force.

According to Dyskin and Pasternak (2011), (2012b), (2012c) the infinitesimal dependence between the displacement and force is given by

$$dT = kdu; \quad k = -\frac{P}{d\sin^3\theta}$$

This dependence is characterised by a negative stiffness, $k < 0$. Subsequently, the rotating non-spherical particle gives an example of a simplest system with structural negative stiffness.

Relationship (1) between the shear force, $T$, and shear displacement, $u$, was interpreted in Dyskin and Pasternak (2011), (2012b), (2012c) as the effect of negative shear modulus. We note however, that the mechanism of such a relationship is in the rotation of the (non-spherical) grain. We now rewrite this relationship in terms of shear force, $T$, vs. the grain rotation angle, $\varphi$. It reads

$$dT = k'd\varphi; \quad k' = -\frac{P}{\sin^3\theta}$$

We see that stiffness $k'$ (it has dimensions of force, which is different from the dimensions of $k$) relating the shear force and rotation is negative. This brings us to the notion of negative Cosserat shear modulus, the modulus that relates the non-symmetrical part of the Cosserat stress tensor and the Cosserat rotations.
While formally relating the tangential force and displacement, Fig. 1(b), this mechanism involves independent grain rotation that constitutes an additional (rotational) degree of freedom. In continuum modelling this corresponds to the appearance of the vector field of rotations independent of the vector field of displacements such that each point has 6 degrees of freedom (three translational and three rotational). This requires the use of the Cosserat theory for its description. The above effect of negative stiffness concerns the relation between the non-symmetric part of the shear stress (observe the non-symmetry of the shear force shown in Fig. 1(a)) and the (independent) rotation. This type of relation is controlled by what is called the Cosserat shear modulus, which can now be negative. Furthermore, Fig. 1 provides a simple example of a structure which when stabilised (that is undergoes displacement-controlled loading) exhibits negative Cosserat shear modulus. The present paper considers the effect of negative Cosserat shear modulus on wave propagation in isotropic Cosserat continuum.

2. Isotropic Cosserat continuum

As mentioned above, modelling materials with independent internal rotations (e.g., rotating particles) requires the introduction of a Cosserat continuum whereby the internal rotations add three more degrees of freedom on top of three classical ones associated with displacements. This isotropic formulation is the simplest theory that relates independent rotations and shear stress and that is the reason why we have chosen it from numerous other high order formulations. Subsequently, the presence of rotations calls for a set of deformation measures richer than in the classical continuum. These are strain and curvature-twist tensors defined as (e.g., Nowacki, 1970)

\[ Y_{ji} = u_{i,j} - \varepsilon_{e_{ji} \phi_i}; \quad \kappa_{ji} = \psi_{i,j} \]  

where \( \phi_i \) is the rotation vector. One can see that the new strain tensor, \( Y_{ji} \), is non-symmetric; its non-diagonal components include both displacement gradients and the components of the vector of internal rotations. The symmetrical part of the Cosserat strain tensor gives the classical strain tensor. On top of that an additional deformation measure is introduced, the curvature-twist tensor, \( \kappa_{ji} \), which is the tensor of rotation gradients.

The reciprocal quantities are the non-symmetric stress tensor, \( \sigma_{ji} \), and moment stress tensor, \( \mu_{ji} \), which combine forces and moments per unit area of the faces of the corresponding volume element. The Cosserat equations of motion read

\[
\sigma_{ji,j} = \rho \ddot{u}_i, \\
\mu_{ji,j} + e_{ki} \sigma_{kj} = J \ddot{\psi}_i
\]  

where \( \rho \) is the material density, \( J \) is the density of inertia moment. Here, the body forces and body moments are neglected.

The Hooke's law for isotropic Cosserat continuum can be expressed as (e.g., Nowacki, 1970)

\[
\sigma_{ji} = (\mu + \alpha) Y_{ji} + (\mu - \alpha) Y_{ji} + \lambda \gamma_{kk} \delta_{ij}
\]

\[
\mu_{ji} = (\gamma + \varepsilon) \kappa_{ji} + (\gamma - \varepsilon) \kappa_{ji} + \beta \kappa_{kk} \delta_{ij}
\]  

where \( \lambda, \mu \) are the Lame constants, \( \alpha \) is the shear Cosserat modulus, \( \gamma, \varepsilon, \beta \) are the Cosserat moduli.

In order to find the conditions of stability of isotropic Cosserat continuum consider the strain energy density for the isotropic Cosserat continuum as a function of relative deformations \( Y_{ij} \) and twist-curvatures \( \kappa_{ij} \). In the absence of thermal components the strain energy density is expressed as (e.g., Nowacki, 1970)

\[
W = \frac{\mu + \alpha}{2} Y_{ij} Y_{ji} + \frac{\mu - \alpha}{2} Y_{ij} Y_{ji} + \frac{\lambda}{2} Y_{kk} Y_{km} + \frac{\gamma + \varepsilon}{2} \kappa_{ji} \kappa_{ij} + \frac{\gamma - \varepsilon}{2} \kappa_{ji} \kappa_{ij} + \beta \kappa_{kk} \kappa_{mn}
\]  

We rewrite this representation in the following form:

\[
W = \frac{\mu}{2} Y_{ij} Y_{ji} + \frac{\alpha}{2} Y_{ij} Y_{ji} - \frac{\mu + \alpha}{4} Y_{ij} Y_{ji} + \frac{\lambda}{2} Y_{kk} Y_{km} + \frac{\gamma + \varepsilon}{2} \kappa_{ji} \kappa_{ij} + \frac{\gamma - \varepsilon}{2} \kappa_{ji} \kappa_{ij} - \frac{\varepsilon}{4} \kappa_{jj} \kappa_{ij} + \beta \kappa_{kk} \kappa_{mn}
\]  

Here

\[
Y_{ij} = \frac{1}{2} (Y_{ij} + Y_{ji}), \quad Y_{ij} = \frac{1}{2} (Y_{ij} - Y_{ji}), \quad \kappa_{ij} = \frac{1}{2} (\kappa_{ij} + \kappa_{ji}), \quad \kappa_{ij} = \frac{1}{2} (\kappa_{ij} - \kappa_{jj})
\]  

are the symmetric and antisymmetric parts of strain and curvature twist tensors respectively. It is important that the antisymmetric parts are independent from both the symmetric parts and the traces \( (\gamma_{mn} \text{ and } \kappa_{mn}) \). It is clear from (9) that if \( \alpha \leq 0 \), the energy is not positive definite. (Indeed, if \( \alpha \leq 0 \) then by choosing the deformation with \( Y_{ij} \) and \( \kappa \) equal to zero one has \( W = (\alpha/2) Y_{ij} Y_{ij} \leq 0 \).)

Now we see that the thermodynamics requires that \( \alpha > 0 \). The case we attempt to consider, \( \alpha < 0 \), which is thermodynamically inadmissible (yet structures with apparent negative stiffness do exist, see Introduction). We interpret this in the sense that an isotropic material with negative Cosserat shear modulus can exist (be stable), but only under certain boundary conditions (or, more generally as a part of an encompassing mechanical system such that the total energy of the material + system is positive definite, Dyskin and Pasternak (2012a,b,c).

In what follows we consider an infinite solid with \( \alpha < 0 \) assuming that at infinity the applied boundary conditions are such that the solid is stable. We now consider planar waves in such a solid propagating along an \( x_1 \) axis and determine the types and velocity of the waves. For a conventional Cosserat continuum the types and velocity of planar waves are known.
(e.g., Nowacki, 1970): there are a pressure wave, two shear waves (we will later see that they are in fact shear-rotational waves (Pasternak, 2002; Pasternak & Muhlhaus, 2005), since they involve both displacements and rotations) and a twist wave, all waves except the pressure wave show dispersion (the dependence of the wave velocity upon frequency). The following chapter will introduce the expressions for the wave velocities in the conventional isotropic Cosserat continuum and then generalise them to the case of negative Cosserat shear modulus.

3. Planar waves

3.1. Planar waves in conventional isotropic Cosserat continuum

The dynamic equations of motion with respect to displacement and rotation vectors are obtained by substituting the constitutive Eqs. (5) and (6) into the equations of motion (4). It is convenient to write, following Nowacki (1970), the obtained equation in the vector form. Neglecting the temperature variations caused by deformation the equations of motion can be expressed as

\[
(\lambda + 2\mu)\text{grad}\ \text{div}\ u - (\mu + \alpha)\ \text{rot}\ \text{rot}\ u + 2\alpha\ \text{rot}\ \phi = \rho \ddot{u}
\]

\[
(\beta + 2\gamma)\text{grad}\ \text{div}\ \phi - (\gamma + \varepsilon)\ \text{rot}\ \text{rot}\ \phi + 2\alpha\ \text{rot}\ u = \rho \ddot{\phi}
\]

(10)

Representing the displacement and rotation vectors, \(u, \phi\) through scalar and vector potentials, \(\Psi, H\)

\[
u = \text{grad} \Phi + \text{rot} \Psi, \quad \text{div}\ \Psi = 0
\]

\[
\phi = \text{grad} \Sigma + \text{rot} H, \quad \text{div} H = 0
\]

(11)

and directing the \(x_1\) axis along the direction of propagation of the planar wave such that the displacement, rotation and potentials are the functions of \(x_1\) only, one obtains the following wave equations with respect to the potentials (Nowacki, 1970):

\[
\square_1 = 0, \quad \square_3 \Sigma = 0, \quad \Omega \Psi = 0, \quad \Omega H = 0
\]

(12)

where the differential operators in (12) have the following form:

\[
\square_1 = (\lambda + 2\mu)\nabla^2 - \rho \partial_t^2, \quad \square_3 = (\beta + 2\gamma)\nabla^2 - 4\alpha - J\partial_t^2
\]

\[
\square_2 = (\mu + \alpha)\nabla^2 - \rho \partial_t^2, \quad \square_4 = (\gamma + \varepsilon)\nabla^2 - 4\alpha - J\partial_t^2
\]

\[
\Omega = \square_2 \square_4 + 4\alpha^2 \nabla^2
\]

(13)

It is seen that Eq. (10) get reduced to four separate equations with respect to potentials, \(\Phi, \Sigma, \Psi\) and \(H\). Furthermore, equations for \(\Psi\) and \(H\) have identical form. Now we can count the wave types. The first two waves are given by

\[
u = \text{grad} \Phi, \quad \phi = \text{grad} \Sigma
\]

(14)

The first one is the wave with displacement vector parallel to the direction of wave propagation. This is the familiar \(p\)-wave (pressure wave). Another wave is the wave with rotation vector parallel to the direction of wave propagation. This is what is called the twist wave as the rotation proceeds about axis parallel to the direction of wave propagation.

The other two types of waves are given by

\[
u = \text{rot} \Psi, \quad \phi = \text{rot} H
\]

(15)

These are waves with displacement and rotation vectors normal to the direction of wave propagation. The waves with displacement vectors normal to the direction of wave propagation are known as shear waves. However, since both waves are governed by equations having the same form (the last two equations in (12)) their velocities coincide. That is the reason for merging them into the same type and call them the shear-rotational waves (Pasternak, 2002; Pasternak & Muhlhaus, 2005; in these papers the wave with the rotation vector normal to the direction of its propagation was called rotational-shear to distinguish it from the wave with the displacement vector called shear-rotational. The reason was that in the orthotropic continuum considered there the velocities of these two types of waves were different.). (In Nowacki (1970), these waves are referred to as shear waves. We find this terminology confusing as it ignores the rotational part of the waves.)

Now we find the wave velocities assuming that the waves are monochromic and following Nowacki (1970). We assume the potentials in the form

\[
\Phi = A \exp (-i\omega t + ikx_1), \quad \Sigma = B \exp (-i\omega t + ikx_1)
\]

\[
\Psi = C \exp (-i\omega t + ikx_1), \quad H = D \exp (-i\omega t + ikx_1)
\]

(16)

where \(\omega\) is the frequency.

Substituting (16) into (12) one obtains three characteristic equations for the wave number \(k\) (equations obtained using \(\Psi\) and \(H\) coincide).

The first equation is equation for the \(p\)-wave (pressure wave) in which the material points oscillate in the direction coinciding with the direction of wave propagation. The velocity, \(c_1\), turns out to be the same as in the classical continuum

\[
c_1^2 = \frac{\lambda + 2\mu}{\rho}
\]

(17)
Isotropic Cosserat continuum produces two dispersionsal shear-rotational waves. They involve the displacement and rotation of the material points in the directions normal to the direction of wave propagation. Their velocities are derivable from the wave number given by the following characteristic equation (Nowacki, 1970) common for the shear and rotational components:

\[ c_2^2 c_4^4 k^4 + \left[ \omega_2^2 c_3^2 - \omega^2 (c_2^2 + c_4^2) \right] k^2 - \omega^2 (\omega_2^2 - \omega^2) = 0 \]  

(18)

Here \( c_2^2 = (\mu + \alpha)/\rho \), \( c_4^2 = (\gamma + \varepsilon)/J \), \( c_5^2 = \mu/\rho \), \( k \) is the wave number, \( \omega \) is the frequency and

\[ \omega_2^2 = \frac{4\alpha}{J}, \quad c_3^2 = \frac{\beta + 2\gamma}{J} \]  

(19)

Frequency \( \omega_2 \) is a threshold frequency: when \( \omega < \omega_2 \) only one shear-rotational wave exists (Eq. (18) has only one real solution). Its velocity tends to the velocity of the classical shear wave as frequency tends to zero. When \( \omega > \omega_2 \) the second shear-rotational wave (second real solution of Eq. (18)) appears.

For the following it is convenient to rewrite (19) in a dimensionless form. To this end we introduce the dimensionless groups (similar to the ones introduced in Pasternak & Dyskin, 2010; Pasternak & Dyskin, 2014)

\[ s_5 = c_2^2 c_5^2 = \frac{\omega^2}{k^2 c_5^2}, \quad s_2 = c_2^2 c_4^2 = 1 + \frac{\alpha}{\mu}, \]
\[ s_4 = c_2^2 c_5^2 = (\gamma + \varepsilon)\rho/\mu, \quad w = \frac{\omega_2^2}{\omega^2} = \frac{4\alpha}{\omega^2} = z \frac{\alpha}{\mu}, \quad z = \frac{4\mu}{\omega^2} \]

(20)

Subsequently, in the dimensionless form Eq. (18) reads

\[ (w - 1)s_2^2 + [w - (s_2 + s_4)]s - s_2 s_4 = 0, \]

or

\[ \left( z \frac{\alpha}{\mu} - 1 \right) s^2 - z \frac{\alpha}{\mu} - \left( 1 + \frac{\alpha}{\mu} + s_4 \right) s - \left( 1 + \frac{\alpha}{\mu} \right) s_4 = 0. \]  

(21)

The fourth wave type is the twist wave which involves rotations around the direction of wave propagation (the rotation vector coincides with the \( x_1 \) axis). For the frequencies higher than the threshold frequency, \( \omega > \omega_2 \), the twist wave velocity in the isotropic Cosserat continuum is

\[ c_t = \frac{c_3}{\sqrt{1 - \left( \frac{\omega}{\omega_2} \right)^2}} \]

(22)

This relationship is shown in Fig. 2(a). It is seen that as frequency \( \omega \to \omega_2 + 0 \) the wave velocity tends to infinity.

Fig. 2. Dispersion relationship for the twist wave in a Cosserat continuum: (a) with positive (\( \alpha > 0 \)) and (b) with negative Cosserat shear modulus (\( \alpha < 0 \)).
3.2. Planar waves in the presence of negative Cosserat shear modulus

We now consider the case of negative Cosserat shear modulus, \( \alpha < 0 \). We introduce the following notations:

\[
\alpha = -\alpha_n, \quad \omega_2^* = -\frac{4\alpha_n}{J}, \quad \omega_2^n = -\omega_2^* \tag{23}
\]

It can be seen that Eq. (17) for velocity \( c_1 \) of the p-wave does not depend on \( \alpha \) and will therefore not change. Eq. (22) for velocity \( c_t \) of the twist wave will change

\[
c_t = \frac{c_3}{\sqrt{1 + \left( \frac{\omega_n}{\omega_2^*} \right)^2}} \tag{24}
\]

The first unusual result of the presence of negative Cosserat shear modulus is the disappearance of the threshold frequency. Instead, the dispersion relation is controlled by a characteristic frequency \( \omega_n \). Now the twist waves can be generated at all frequencies, even at very low ones. This suggests a potential method of detecting the negative Cosserat shear modulus; its presence is indicated by the presence of low frequency twist waves and, as will be seen later, the second shear-rotational wave.

The dispersion relationship for the twist wave for \( \alpha < 0 \) is shown in Fig. 2(b). It is seen that the twist wave velocity reduces as frequency decreases. Furthermore, according to Eq. (24), as \( \omega \to 0 \), the twist wave velocity vanishes, \( c_t \to 0 \).

Let us now consider shear-rotational waves. In the case of negative Cosserat shear modulus, \( \alpha < 0 \) the corresponding characteristic equation (an analogue of characteristic Eq. (22) associated with the conventional positive Cosserat shear modulus) reads

\[
(z + 1)s^2 - \left[ z \frac{\alpha_n}{\mu} + \left( 1 - \frac{\alpha_n}{\mu} + s_4 \right) \right] s + \left( 1 - \frac{\alpha_n}{\mu} \right) s_4 = 0, \tag{25}
\]

where

\[
\begin{align*}
s & = \frac{c_2}{c_5} = \frac{\omega^2}{k^2 c_5^5}, \quad s_2 = \frac{c_2}{c_5} = 1 - \frac{\alpha_n}{\mu}, \quad s_4 = \frac{c_4}{c_5} = \frac{(\gamma + \varepsilon)J}{f\mu}, \\
c_2 & = \frac{\mu - \alpha_n}{\rho}, \quad w = \frac{\alpha_n^2}{\omega^2} = -\frac{4\alpha_n}{J\omega^2} = -z \frac{\alpha_n}{\mu}, \quad z = \frac{4\mu}{f\omega^2} \tag{26}
\end{align*}
\]

As can be seen from expression (26) for \( s_4 \), the admissible values of modulus \( \alpha_n \) are between 0 and \( \mu \). It means that the values of negative Cosserat modulus when the waves exist and the hence material is stable are in the range \(-\mu < \alpha < 0\).

The dispersion relations for the shear-rotational waves for \(-\mu < \alpha < 0\) are shown in Fig. 3. Again, due to the absence of the threshold frequency both shear-rotational waves are present at all frequencies. It is seen that as the frequency decreases the shear-rotational wave velocities reduce. It can easily be shown from the first equation of (25) that as \( \omega \to 0 \), one of the shear rotational wave velocities vanishes, \( c_{i1} \to 0 \), while the other one tends to the velocity of a conventional shear wave, \( c_{i2} \to c_5 \).

Combining the solutions for both equations we find the relation between the normalised velocities of shear-rotational waves and the normalised Cosserat shear modulus \( \alpha / \mu \), Fig. 4.

As can be seen, when \( z \alpha / \mu < 1 \) (it means \( \omega_2^2/\omega^2 < 1 \), that is the frequency is greater than the controlling frequency, \( \omega_n \)), we have two shear-rotational waves. This includes both the regions of negative and positive modulus \( \alpha \).
On the other hand, there is only one shear-rotational wave when \( z\alpha/\mu > 1 \) (it means \( \omega_n^2/\omega^2 > 1 \), that is the frequency is smaller than the controlling frequency, \( \omega_n \)) and modulus \( \alpha \) is always positive.

It is seen from Fig. 4, 5 that for the dependence of the shear-rotational wave velocities on the Cosserat shear modulus, the value \( \alpha = \mu/z = 1/4J\omega^2 \) is a discontinuity point in the relation between one of the wave velocities (the one which is the highest when the Cosserat shear modulus is negative) and the Cosserat shear modulus. In order to see the physical meaning of the discontinuity we need to recall that the plots in Fig. 4, 5 correspond to a certain frequency. The value \( \alpha = \mu/z = 1/4J\omega^2 \) of the Cosserat shear modulus is the value at which the frequency used in Fig. 4, 5 reaches the threshold after which the second shear wave appears. This manifests itself as a discontinuity.

Fig. 4. Relations between normalised velocities of shear-rotational waves and normalised Cosserat shear modulus \( \alpha \) \((z = 4\mu J^{-1} \omega^{-2} \) is varied, \( s_4 = c_4^2c_5^2 = 5)\).
When the Cosserat shear modulus $\alpha$ tends to infinity the value of the normalised velocity of this shear-rotational wave tends to the following limiting value:

$$
\frac{c_s}{c_5} = \sqrt{z - 1 + \frac{1 - 2z + 4s_4 + z^2}{2z}}
$$

(27)
4. Discussion

Dispersion relationships characteristic for shear-rotational and twist waves can be instrumental in determining parameters of the Cosserat continuum, which are not easy to measure otherwise. A key point to it is the fact that high frequency waves in heterogeneous materials are hard to detect as the wave length should considerably exceed the microstructural length to avoid wave scattering and attenuation (e.g., Pasternak & Dyskin, 2010; Pasternak & Dyskin, 2014). Furthermore when the frequency is below the threshold only the dispersion relation of a single shear-rotational wave is accessible, which is not sufficient for the full determination of the Cosserat moduli (Pasternak & Dyskin, 2010; Pasternak & Dyskin, 2014).

The situation changes drastically when the Cosserat shear modulus is negative (but within the stability range). In this case both shear-rotational waves and twist wave exist at low frequencies and hence can be detected. Furthermore, as seen in Figs. 3–5, both shear-rotational waves have considerably different velocities, which potentially permits detecting them by conventional shear wave transducers utilising the difference in the arrival times (for large enough samples). This paves a way for detecting the negative stiffness effect and determining the value of the negative Cosserat shear modulus. Then using the model depicted in Fig. 1 or a more sophisticated model that accounts for the resistance of the surrounding material to the dilation generated by rotations of non-spherical particles (Pasternak & Dyskin, 2013) one can analyse the mechanism of negative stiffness. Furthermore, when the rotating non-spherical constituents are used to develop hybrid materials with engineered microstructure (Pasternak, Dyskin, & Sevel, 2014) the wave measurements can be used for monitoring their state.

The analysis can further capitalise on the discontinuous relation between the Cosserat shear modulus and the shear-rotational wave velocities. In the cases when the Cosserat shear modulus can be varied by an external parameter, such as the magnitude of compressive load $P$ in the example shown in Fig. 1 and Eq. (2) the abrupt appearance of the second shear-rotational wave (if detected) will signal the approaching transition point to the negative Cosserat shear modulus. Furthermore the velocity of the wave can be used to determine the transition point more accurately. The transition of the Cosserat shear modulus to negative values can indicate approaching instability and failure. The identification of the negative modulus effect opens a new application of the measurement of shear (shear-rotational) wave dispersion (so far the main proposed application was the determination of the moduli of conventional Cosserat continuum, e.g., Pasternak & Dyskin, 2010, 2014; Pasternak, Muhlhaus, & Dyskin, 2003). The detection of the negative modulus effect and determination of its value can be used in failure monitoring for instance in geomaterials, where the instability is often associated with the presence of post-peak (softening) branch of the loading curve (Cook, 1965), which can be interpreted in terms of negative stiffness. This might revitalise the currently used microseismic methods of failure monitoring.

5. Conclusions

Materials with negative moduli violating the second law of thermodynamics can in some cases be stabilised by the boundary conditions or, more generally, by including them in an encompassing system such that the total energy is positive definite. In particular, in propagation of planar waves in ‘infinite’ isotropic Cosserat continuum (that is the waves with wavelengths much smaller than the dimensions of the material under consideration), the Cosserat shear modulus (the modulus relating the non-symmetrical part of shear stress and internal rotations) is allowed to assume negative values as long as its value does not exceed the value of the standard (positive) shear modulus. In this case the continuum still supports planar waves.

The longitudinal wave ($p$-wave) coincides with that of the classical continuum and hence is unaffected by the sign of the Cosserat shear modulus. For positive Cosserat shear modulus the twist wave and one of the shear-rotational waves exist only at high frequencies, higher than a certain threshold frequency, while the other shear-rotational wave exists for all frequencies and its velocity tends to the classical shear wave velocity as the frequency tends to zero. Opposite to this, in the case of negative Cosserat shear modulus the isotropic Cosserat continuum supports the twist wave and both shear-rotational waves at all frequencies. There exists a frequency-dependent positive critical value of the Cosserat shear modulus: above this value only single shear-rotational wave exists, below this critical value the second shear-rotational wave appears with very high velocity. As the value of the Cosserat shear modulus becomes negative another wave – the twist wave appears.

The wave velocity measurements and detection of the twist wave and the second shear-rotational can provide a method of determining the Cosserat moduli and identifying the presence and measuring the value of negative Cosserat shear modulus.

Acknowledgment

The authors acknowledge the financial support through ARC Discovery grant DP120102434.

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CHAPTER 7

General conclusions and suggestions for further research
In General Introduction the principal aims of the dissertation were identified as:
(a) investigate the multiscale rotational mechanism of Mode I, II and III cracks propagation in materials with rotational degrees of freedom; (b) analyse pattern and clustering formations at meso- and macro-scale caused by microrotations in particulate materials; (c) explore the mechanical behaviour of and internal rotations in the cemented particulate material with a pre-existing crack and (d) study the effect of negative stiffness (e.g. negative Cosserat shear modulus) on wave propagation in and stability of particulate materials due to rotation of non-spherical particles during cracks and fractures growth.

In this section we summarise the results and conclusions obtained according to these aims and outline the directions for further research.

7.1. Conclusions

This research has been devoted to the investigation of crack propagation and the corresponding stress concentrations in particulate materials. It has been recognised that consideration of internal rotational degrees of freedom and particle shapes is essential for better understanding of mechanical behaviour of these materials, especially when it comes to the mechanics of patterns formation such as creation of zones of strain localisation, and the formation and propagation of fractures, shear and compaction bands.

Four principal methodological approaches were employed: (a) analytical and asymptotics modelling based on non-standard continuum accompanied by the analysis of scales; (b) analytical discrete mass-spring modelling and stability analysis of systems with negative stiffness components, which model the effect of rotation of non-spherical particles; (c) physical experiments accompanied by non-destructive scanning techniques, such as digital image correlation for recovering displacement and rotational fields and (d) numerical simulation using the discrete element method (we used a particular class of DEM implemented in PFC2D software – the distinct element method).

We began with analytical investigation of multiscale rotational mechanism of propagation of macroscopic cracks of Modes I, II and III. Modelling of the mechanical behaviour of materials, whose constituents are able to rotate, required the use of non-standard continuum theories. Cosserat continuum was chosen as simplest one
accounting for internal rotations of particles or segments. We conducted the modelling for a specific case where the Cosserat characteristic lengths are commensurate with the characteristic size of the material microstructure (e.g. grain size). This, in particular, corresponds to the microstructure consisting of grains connected by elastic bonds. For this case the Cosserat continuum theory permits considerable simplification resulted in the so-called small-scale Cosserat continuum. Using asymptotic analysis it was demonstrated that when the Cosserat characteristic lengths are commensurate with the characteristic size of the material microstructure, the simple pseudo-Cosserat continuum with constrained microrotations provides the main term of asymptotics of small Cosserat characteristic lengths. Subsequently, we used this asymptotics in place of the general Cosserat continuum while investigating fracture propagation in particulate materials.

The small-scale Cosserat continuum was used to investigate the proposed multiscale rotational mechanism of crack propagation based on breakage of the bonds between the material constituents; the latter caused by bond bending due to relative rotation of the material constituents. These constituents correspond to the micro-scale of cracks propagation. It was found that in the case of Mode I and Mode II cracks, the relative rotations cause bending of the bonds followed by initiation and propagation of flexural microcracks from a side of the bonds. The crack mode determines the orientations of the microcracks, while the signs of the corresponding stress intensity factor determine the side of the bond from which its breakage starts. For the Mode III cracks the mutual rotations cause twisting of bonds located in front and behind the crack tip and a combination of bond twisting and bending at other locations. Bond twisting causes the development and propagation of tensile microcracks in the directions inclined at 45° to the bond directions. The microcracks developed during the bond bending or twisting form the smallest scale in the multiscale rotational mechanism of fracture propagation.

Microfracturing associated with rotations has the following common features: (a) the symmetry of the microfracturing with respect to the macrocrack line, which ensures in-plane propagation of the macrocrack even in Mode II; (b) a certain non-zero width of the microfractured areas, which results in a band-like propagation of the macroscopic crack; and (c) the microstresses created by the bending or twisting dominate the microstresses associated with the conventional stress singularities.
The first feature explains why shear bands in particulate materials (or heavily fractured heterogeneous materials) often demonstrate in-plane propagation, which cannot be explained by modelling the shear bands as conventional Mode II cracks due to asymmetry of the associated stress concentration. The second feature explains the band-like appearance of natural fractures. The third one expounds why the rotational mechanism dominates over the conventional crack growth mechanisms. Furthermore, the independence of the microfracturing of the sign of the moment stresses provides a unified way of describing such apparently different types of fractures as tensile (Mode I) cracks, compaction bands (Mode I anti-cracks) and shear bands (Mode II and III).

It was found that in the small-scale Cosserat continuum the stress singularity at the crack tip has the power $-1/2$, which coincides with the classical one, while the moment stress has singularity of the power $-3/2$ for cracks of all modes. It was also shown that the J-integral reflects only the stress singularities, while the moment stress singularities have no effect on the energy release rate. Therefore, the fact that the $-3/2$ singularity is not integrable does not affect the energy release rate which remains finite. Subsequently, the J-integral reflects the energy change caused by macroscopic crack propagation through the combination of the classical tensile and rotational fracture mechanisms. Based on this, we established the energy criterion of crack propagation in particulate materials. Specifically, in the energy criterion of the compaction band propagation the specific fracture energy consists of three terms: the fracture energy of the bonds (present in all types of fractures considered), specific energy of shear (for shear bands and shear fractures) and specific energy of compaction (for compaction bands, Mode I anti-crack).

In order to investigate the mechanism of formation of emerging patterns and their elements such as cracks, fractures, shear and compaction bands, we conducted physical experiments and numerical simulations for detailed investigation of importance of particles rotation for pattern formation and the effect of rotational degrees of freedom on the mechanism of instability. The physical modelling consisted of two-dimensional experiments, where smooth steel discs represented the particles of the particulate material. The discs of three different sizes were utilised for modelling mono- and polydisperse particle assemblies. The qualitatively different types of behaviour of these assemblies were established. In monodisperse hexagonal packing assemblies, the re-compaction progresses through the development of shear bands forming either a wedge-
like pattern or the rhombus-like pattern. The wedge-like pattern can be considered as a large-scale rhombus-like pattern that could not be realised due to the size limitations of the model. In polydisperse random packing assemblies, no shear bands accompanying re-compactions could be identified. Two types of re-companion in polydisperse assemblies were observed depending on the initial packing: constant gradual re-compactions and instantaneous re-compactions (similar to the monodisperse hexagonal packing assemblies). A considerable dependence of the disc trajectories on the initial packing is observed probably caused by the boundary effect associated with insufficiently large dimensions of the assembly.

Analysis of magnitudes of rotation on different scale levels was conducted. The process of deformation led to considerable rotations of individual particles. Interestingly, it was found that the average values of the angles of disc rotations over the area of the assembly are insignificantly different from zero. Instead the discs get separated into the groups of similarly rotating discs. In particular, in the monodisperse assemblies, alternating columns of discs rotating in one direction are formed with discs of neighbouring columns rotating in the opposite direction. Furthermore, upon crossing the shear band the rotations change the sign. It means that the rotations are microscopic (at the scale of the particle size), correlating at a mesoscale, but these patterns do not proliferate to the macroscopic scale. In polydisperse assemblies, where the shear bands were not observed, the clusters of mutually rotating discs are formed. Consequently, particles form rotational patterns at mesoscale level in both mono- and polydisperse assemblies. It is important that at the mesoscale the particles form clusters of particles rotating in the same directions and chains of particle rotating in the mutually opposite directions, i.e. without mutual sliding. Thus, particle rotations produce a structure on their own. The structure is different from the ones formed by particle displacements and force chains. This can give a rise to “moment chains” at mesoscale.

Physical and numerical modelling of the deformation of the monodisperse assembly gave qualitatively similar results after proper calibration of the discrete element model. In addition the calibration revealed very low values of particle stiffness, orders of magnitude lower than adopted in the literature for the discrete element modelling. This feature can be explained by the fact that the size of the disks utilized in our experiments is much larger than the size of the particles used for numerical modelling of rock samples.
Finally it was found in both physical and numerical modelling that the shear bands appear instantaneously rather than propagate.

Next, Mode I crack in the idealised slightly cemented granular material has been investigated by usage the same experimental apparatus with some modifications. Due to the small size of the physical model we considered only opening of the crack; its propagation was beyond the scope of this study. The comparison of rotation of the particles near the crack tip obtained by physical modelling and the analytical approach based on the propositions of small-scale Cosserat continuum demonstrated reasonably good agreement. Thus, the physical experiments confirmed the possibility of usage the simplified small-scale Cosserat continuum with constrained microrotations asymptotically for the crack problems in particulate materials. The discrete element modelling of opening of the Mode I crack also gave good agreement with the results of the experiments. The parametric analysis showed that some parameters (e.g. stiffnesses of parallel bond) influence the mechanical behaviour of the assembly stronger than others (e.g. stiffnesses of wall and particles) during the opening the Mode I crack. Thus both physical modelling and numerical modelling confirm the applicability of the small-scale Cosserat continuum for modelling cracks in particulate materials with microrotations.

In addition, we explored the importance of particle shape on the mechanical behaviour of particulate materials. It was indicated that combination of internal rotations and non-spherical (non-circular in 2D) shapes of particles leads, in the presence of compression to the effect of negative stiffness. This effect can interpreted as either negative stiffness shear springs in discrete mass-spring systems or negative Cosserat shear modulus in a continuum.

During crack and fracture growth waves are generated. The effect of negative stiffness occurring due to rotation of non-spherical particles under compression on wave propagation was investigated. On top of that, since materials with negative elastic moduli are unstable (but can be stabilised by the boundary conditions or, more generally, by including them in an encompassing system) we conducted the stability analysis.

The negative stiffness occurring due to rotation of non-spherical particles was implemented as the negative Cosserat shear modulus in isotropic Cosserat continuum.
We found that this modulus is allowed to assume negative values as long as its value does not exceed the value of the standard (positive) shear modulus. In this case the continuum still supports planar waves.

The longitudinal wave ($p$-wave) coincides with that of the classical continuum obviously unaffected by the sign of the Cosserat shear modulus. It is well-known that for positive Cosserat shear modulus the twist wave and one of the shear-rotational waves exist only at high frequencies, higher than a certain threshold frequency, while the other shear-rotational wave exists for all frequencies and its velocity tends to the classical shear wave velocity as the frequency tends to zero. In contrast to this, it was found that in the case of negative Cosserat shear modulus the isotropic Cosserat continuum supports the twist wave and both shear-rotational waves at all frequencies.

There exists a frequency-dependent positive critical value of the Cosserat shear modulus: above this value only single shear-rotational wave exists, below this critical value the second shear-rotational wave appears with very high velocity. As the value of the Cosserat shear modulus becomes negative another wave – the twist wave – appears.

It was proposed that the wave velocity measurements and detection of the twist wave and the second shear-rotational can provide a method of determining the Cosserat moduli and identifying the presence and measuring the value of negative Cosserat shear modulus.

Another approach to study the effect of negative stiffness on the material stability involved modelling such materials and structures as discrete systems containing a set of rigid particles connected by the different types of springs (normal, shear and rotational) with specified stiffness. Thus, we were able to explicitly introduce negative stiffness elements in the system. In the case of the one-dimensional problem the system (chain of particles) we also included viscous dampers.

We established the necessary condition of stability for one-, two- and three-dimensional systems of particular configurations with fixed boundary particles. We found that the system of particular configuration consisting of positive and negative stiffness springs can be stable when the total number of negative stiffness springs does not exceed the total number of degrees of freedom of the system. The absolute values of the negative stiffnesses should not exceed certain threshold values that depend upon the
stiffnesses and the number of the other (positive) springs. On top of that, certain conditions in the arrangement of negative stiffness springs should be satisfied.

For large systems the maximum relative number (the critical fraction) of negative stiffness springs is constant, 1/2 for two-dimensional square packing systems and 3/5 for three-dimensional cubic packing systems. This property is in stark contrast with one-dimensional systems where the critical fraction of negative stiffness springs tends to zero inversely proportional to the system size. This difference can be attributed to the fact that the presence of fixed boundary in two and three directions imposes additional stabilisation opposite to only two fixed ends in one-dimensional chains.

It was revealed that the presence of negative stiffness springs in one- and two-dimensional systems leads to a decrease in the eigenfrequencies: as soon as the absolute value of the negative stiffness spring reaches its critical value, the smallest eigenfrequency becomes zero, while all other eigenfrequencies decrease to certain minimum values. It is noteworthy that the order of frequencies (from the smallest to the largest) remains the same in the region of negative stiffnesses. Further increase in the absolute value of the negative stiffness makes the system unstable leading to the appearance of unbounded trajectories.

To sum up, the importance of internal rotations and particle shape in mechanical behaviour of materials with microstructure was corroborated. The main conclusions of this research are: (1) the rotational mechanism can prevail over the traditional one, especially in the case of strain localisations. The rotational mechanism of fracturing has an intrinsic multiscale nature. (2) It is possible to use fairly simple asymptotics for modelling the behaviour of particulate materials with microrotations. It leads to the applicability of a pseudo-Cosserat continuum with constrained microrotations (the small-scale Cosserat continuum) instead of the general Cosserat continuum for the problem of fracture propagation in particulate materials. (3) The effect of negative stiffness occurring due to rotation of non-spherical particles on wave propagation can be modelled using Cosserat continuum with negative Cosserat shear modulus. It was found that all waves (p-wave, twist wave and two shear waves) exist at all frequencies when Cosserat shear modulus in negative. (4) The necessary condition of stability of the systems with negative stiffness constituents was formulated and the critical concentration of negative stiffness elements was calculated.
These results can be potentially used in engineering, especially in resource industry, for optimisation of intentional fracturing processes (e.g. hydraulic fracture) and prediction of undesirable failure processes. On top of that, the obtained knowledge about the rotational mechanism of fracture propagation can probably help to improve methods of earthquake forecasting.

7.2. Recommendation for further research

In the course of this research, we tried to enhance the knowledge about the mechanism of crack and fracture propagation in materials with microstructure. However, many questions remain open. Taking into account the principal aims, results and conclusions of the thesis, the directions for further research can be identified. Four main areas of further study include the following: (a) more comprehensive experimental and numerical investigation of areas of strain localisations, such as cracks of different modes, shear and compaction bands; (b) study the role of negative stiffness in the elements of pattern formation (e.g. shear bands); (c) detection and monitoring of waves related to micropolar continuum with eventual negative modulus and measurement of their characteristics; (d) detailed analysis of two- and three-dimensional discrete mass-springs systems. Below we suggest the specific issues on which further research would be beneficial.

**Cracks of Mode II, III and higher modes associated with rotational degree of freedom**

Cracks of Mode I, II and III were contemplated in details analytically. Moreover, the experiments and numerical simulations were conducted for investigation of Mode I crack. For this type of cracks we corroborated the ideas of small-scale Cosserat continuum that pseudo-Cosserat continuum with constrained microrotations can asymptotically be used instead of the conventional Cosserat continuum. The use of this significant simplification is needed to be verified for Mode II and III cracks by conducting additional experiments. Ideally, the physical model should represent an assembly consisting of irregular shaped particles of different diameters. Apart from that, the discrete element modelling is viable alternatives to experimental investigations and allows altering geometry and physical properties easily and simply. However, it requires the initial calibration. On top of that, rotational degrees of freedom introduce higher mode cracks. Similarly, mechanism of higher modes crack propagation ought to be examined by physical and numerical modelling.
Mechanism of formation of shear bands

In investigating shear bands it is essential to distinguish between the cases when the shear band is instantaneously initiated to its full length and the cases when it propagates from a smaller initial crack. The physical modelling conducted in the course of this study had some limitations. For example, the high-speed camera used was not fast enough to distinguish between the progressive and instantaneous modes of fracture/band formation. Furthermore, the experimental apparatus was not sufficiently big, and the number of discs was relatively not sufficiently large for the purpose. These experimental limitations did not allow us to identify the mechanism of shear band formation. Perhaps, a new experimental apparatus should be designed and built for resolving this issue. In addition to physical modelling, numerical simulations should be carried out by using discrete element method.

Wave propagation in particulate materials

Interesting conclusions about wave propagation in materials whose (non-spherical) constituents are able to rotate and produce the effect of negative stiffness were obtained in this work. However, it should be pointed out that these results are theoretical. The next substantial step would be experimental confirmation of findings, detection and monitoring of waves and subsequent measurement of their characteristics. Potentially, it will give a method to determine the Cosserat elastic constants.

Discrete mass-spring systems

We considered one- and two-dimensional mass-spring systems and touched three-dimensional one. For each type of systems the necessary condition of stability was established. However, only the one-dimensional mass-spring system including viscous damping was fully investigated. The influence of negative stiffness springs on the mechanical behaviour of two- and three-dimensional systems containing viscous dampers should be examined. Finally, it is important to obtain both the necessary condition of stability and the sufficient condition and design a physical model necessary for more detailed investigation of the mechanics of instability.
Appendix. Source codes
1. Calculation of J-integral for Mode I, II and III cracks in the Cosserat continuum

```
syms K1 K2 K3 teta r mu nu k

% MODE I
sigma11=K1*cos(teta/2)*(1-sin(teta/2)*sin(3*teta/2))/sqrt(2*pi*r);
sigma22=K1*cos(teta/2)*(1+sin(teta/2)*sin(3*teta/2))/sqrt(2*pi*r);
sigma12=K1*cos(teta/2)*sin(teta/2)*cos(3*teta/2)/sqrt(2*pi*r);

u=K1*sqrt(r/(2*pi))*cos(teta/2)*(k-1+2*(sin(teta/2))^2)/(2*mu);
v=K1*sqrt(r/(2*pi))*sin(teta/2)*(k+1-2*(cos(teta/2))^2)/(2*mu);

du1dx1=diff(u,r)*cos(teta)-diff(u,teta)*sin(teta)/r;
du1dx2=diff(u,r)*sin(teta)+diff(u,teta)*cos(teta)/r;
du2dx1=diff(v,r)*cos(teta)-diff(v,teta)*sin(teta)/r;
du2dx2=diff(v,r)*sin(teta)+diff(v,teta)*cos(teta)/r;

eps11=diff(u,r)*cos(teta)-diff(u,teta)*sin(teta)/r;
eps22=diff(v,r)*sin(teta)+diff(v,teta)*cos(teta)/r;
eps12=(diff(v,r)*cos(teta)-diff(v,teta)*sin(teta)/r+diff(u,r)*sin(teta)+diff(u,teta)*cos(teta)/r)/2;

beforeJ1=(sigma11*eps11+sigma22*eps22+2*sigma12*eps12)*r*cos(teta)/2;
J1=simplify(int(beforeJ1,teta,-pi,pi));

beforeJ2=-((sigma11*cos(teta)+sigma12*sin(teta))*du1dx1+(sigma12*cos(teta)+sigma22*sin(teta))*du2dx1)*r;
J2=simplify(int(beforeJ2,teta,-pi,pi));

J_I=simplify(J1+J2);

% MODE II
sigma11=K2*sin(teta/2)*(2+cos(teta/2)*cos(3*teta/2))/sqrt(2*pi*r);
sigma22=K2*cos(teta/2)*sin(teta/2)*cos(3*teta/2)/sqrt(2*pi*r);
sigma12=K2*cos(teta/2)*(1-sin(teta/2)*sin(3*teta/2))/sqrt(2*pi*r);

u=K2*sqrt(r/(2*pi))*sin(teta/2)*(k+1+2*(cos(teta/2))^2)/(2*mu);
v=-K2*sqrt(r/(2*pi))*cos(teta/2)*(k-1-2*(sin(teta/2))^2)/(2*mu);
```
\[\begin{align*}
d_{11}x_{1} &= \text{diff}(u, r) \cdot \cos(\theta) - \text{diff}(u, \theta) \cdot \sin(\theta) / r; \\
d_{11}x_{2} &= \text{diff}(u, r) \cdot \sin(\theta) + \text{diff}(u, \theta) \cdot \cos(\theta) / r; \\
d_{22}x_{1} &= \text{diff}(v, r) \cdot \cos(\theta) - \text{diff}(v, \theta) \cdot \sin(\theta) / r; \\
d_{22}x_{2} &= \text{diff}(v, r) \cdot \sin(\theta) + \text{diff}(v, \theta) \cdot \cos(\theta) / r; \\
\epsilon_{11} &= \text{diff}(u, r) \cdot \cos(\theta) - \text{diff}(u, \theta) \cdot \sin(\theta) / r; \\
\epsilon_{22} &= \text{diff}(v, r) \cdot \sin(\theta) + \text{diff}(v, \theta) \cdot \cos(\theta) / r; \\
\epsilon_{12} &= \text{diff}(v, r) \cdot \cos(\theta) - \text{diff}(v, \theta) \cdot \sin(\theta) / r + \text{diff}(u, r) \cdot \sin(\theta) + \text{diff}(u, \theta) \cdot \cos(\theta) / r) / 2; \\
\text{before} J_{1} &= (\sigma_{11} \cdot \epsilon_{11} + \sigma_{22} \cdot \epsilon_{22} + 2 \cdot \sigma_{12} \cdot \epsilon_{12}) \cdot r \cdot \cos(\theta) / 2; \\
J_{1} &= \text{simplify} \left( \text{int} \left( \text{before} J_{1}, \theta, -\pi, \pi \right) \right); \\
\text{before} J_{2} &= -((\sigma_{11} \cdot \cos(\theta) + \sigma_{12} \cdot \sin(\theta)) \cdot d_{11}x_{1} + (\sigma_{12} \cdot \cos(\theta) + \sigma_{22} \cdot \sin(\theta)) \cdot d_{22}x_{1}) \cdot r; \\
J_{2} &= \text{simplify} \left( \text{int} \left( \text{before} J_{2}, \theta, -\pi, \pi \right) \right); \\
J_{\text{II}} &= \text{simplify} (J_{1} + J_{2}); \\
\% \text{ MODE III} \\
\sigma_{13} &= -K_{3} \cdot \sin(\theta/2) / \sqrt{2\pi} \cdot r; \\
\sigma_{23} &= K_{3} \cdot \cos(\theta/2) / \sqrt{2\pi} \cdot r; \\
w &= 2 \cdot K_{3} \cdot \sqrt{r/(2\pi)} \cdot \sin(\theta/2) / \mu; \\
d_{33}x_{1} &= \text{diff}(w, r) \cdot \cos(\theta) - \text{diff}(w, \theta) \cdot \sin(\theta) / r; \\
d_{33}x_{2} &= \text{diff}(w, r) \cdot \sin(\theta) + \text{diff}(w, \theta) \cdot \cos(\theta) / r; \\
\epsilon_{13} &= d_{33}x_{1} / 2; \\
\epsilon_{23} &= d_{33}x_{2} / 2; \\
\text{before} J_{1} &= (2 \cdot \sigma_{23} \cdot \epsilon_{23} + 2 \cdot \sigma_{13} \cdot \epsilon_{13}) \cdot r \cdot \cos(\theta) / 2; \\
J_{1} &= \text{simplify} \left( \text{int} \left( \text{before} J_{1}, \theta, -\pi, \pi \right) \right); \\
\text{before} J_{2} &= -((\sigma_{13} \cdot \cos(\theta) + \sigma_{23} \cdot \sin(\theta)) \cdot d_{33}x_{1}) \cdot r; \\
J_{2} &= \text{simplify} \left( \text{int} \left( \text{before} J_{2}, \theta, -\pi, \pi \right) \right); \\
J_{\text{III}} &= \text{simplify} (J_{1} + J_{2}); \\
J &= (J_{\text{I}} + J_{\text{II}} + J_{\text{III}}); \\
\end{align*}\]

2. Post-processing the original images of the experiments and resultant data from VIC

function [resB, files] = CD3()
file = uigetfile('*.bmp','Please select reference image only');
img_filename = file;
name = strsplit(file,'.');
csv_filename = [name{1,1} '.csv'];
im = imread(img_filename);
img = rgb2gray(im);
imbw = im2bw(img,graythresh(img));
[centers, radii, metric] = imfindcircles(imbw,[20
60],'Method','TwoStage');
figure; imshow(im)

centers_round = [round(centers(:,1)) round(centers(:,2))];
[num txt raw] = xlsread(csv_filename);
ind = find(strcmp(raw,raw{1,1}));
for ii = 1:length(centers_round)
    for jj = 1:length(ind)
        if jj == length(ind)
            block = num(ind(jj):length(num),:);
        else
            block = num(ind(jj):ind(jj+1)-3,:);
        end
        VICxy = block(:,1:2);
        dist = sqrt((VICxy(:,1) - centers_round(ii,1)).^2
+ (VICxy(:,2) - centers_round(ii,2)).^2);
        pres = find(dist<(radii(ii)/2));
        if length(pres) > 1
            blockCenter = find(dist == min(dist));
            result(jj,:) = [jj centers_round(ii,:) radii(ii) block(blockCenter(1),:) length(block)
mean(block(:,3)) mean(block(:,4)) mean(block(:,10))
std(block(:,3)) std(block(:,4)) std(block(:,10))];
        end
    end
end
resB{1,:,:} = result;

str = [date ' ' num2str(now)];
mkdir(str);
viscircles(result(:,2:3), result(:,4),'EdgeColor','b');
text(round(result(:,2))-15,round(result(:,3))-5,num2str(result(:,1)),'FontSize',14,'Color','white');
cd(str);
saveas(gcf,img_filename);
close(gcf)
cd ..

files = uigetfile('*.bmp','MultiSelect','on');

for ii=1:length(files)
    name = strsplit(files{1,ii},'.');
    im = imread([name{1,1} '.bmp']);
    img = rgb2gray(im);
    imbw = im2bw(img,graythresh(img));
    [centers, radii, metric] = imfindcircles(imbw,[20 60], 'Method', 'TwoStage');
    centers_round = [round(centers(:,1)) round(centers(:,2))];
    result_tmp = [];
    for jj = 1:length(centers_round)
        dist = sqrt((result(:,2) - centers_round(jj,1)).^2 + (result(:,3) - centers_round(jj,2)).^2);
        if min(dist) < radii(jj)
            pos = find(dist == min(dist));
            result_tmp(pos,:) = [result(pos,1) centers_round(jj,:) radii(jj)];
        end
    end
    centers_round(jj,:) radii(jj); end

[num txt raw] = xlsread([name{1,1} '.csv']);
ind = find(strcmp(raw, raw{1,1}));
for kk = 1:length(ind)
    if kk == length(ind)
        block = num(ind(kk):length(num),:);
    else
        block = num(ind(kk):ind(kk+1)-3,:);
    end
    pos = find(block(:,1)==result(kk,5) & block(:,2)==result(kk,6));
    if isempty(pos)
        if length(block)<1
            result_new(kk,:) = [result_tmp(kk,:)
            result(kk,5:6) zeros(1,15)];
        else
            result_new(kk,:) = [result_tmp(kk,:)
            result(kk,5:6) zeros(1,8) length(block) mean(block(:,3))
            mean(block(:,4)) std(block(:,3))
            std(block(:,4))];
        end
    else
        result_new(kk,:) = [result_tmp(kk,:)
        result(kk,5:6) zeros(1,8) length(block) mean(block(:,3))
        mean(block(:,4)) mean(block(:,10)) std(block(:,3))
        std(block(:,4))];
    end

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end
else
    result_new(kk,:) = [result_tmp(kk,:),
    \end
end
result = result_new;
resB{ii+1,:,:} = result;
figure; imshow(im)

viscircles(result(:,2:3), result(:,4),'EdgeColor','b');
text(round(result(:,2))-15,round(result(:,3))-5,num2str(result(:,1)),'FontSize',14,'Color','white');
cd(str);
saveas(gcf,files{1,ii});
close(gcf)
end

function nr = normalradius()
resBR=resB;
pixtoMM=0.35957;
xres=900;
yres=1280;
for i=1:length(resB)
    resBR{i}(:,4)=resB{i}(:,4)*pixtoMM;
    resBR{i}(:,2)=resB{i}(:,2)*pixtoMM;
    resBR{i}(:,3)=-resB{i}(:,3)*pixtoMM;
end
for j=1:length(resB(1))
    for i=1:length(resB{1})
        if resBR[j](i,4)>22/2 && resBR[j](i,4)<24.5/2
            resBR[j](i,4)=23.5/2;
        elseif resBR[j](i,4)>19/2 && resBR[j](i,4)<21/2
            resBR[j](i,4)=20/2;
        elseif resBR[j](i,4)>24.8/2 && resBR[j](i,4)<28/2
            resBR[j](i,4)=27/2;
        end
    end
end
for j=1:length(resB)
resBR{\text{j}}(:,4)=resBR{1}(:,4);
end

for \text{j}=2:length(resB)
    for \text{i}=1:length(resB{1})
        if resBR{\text{j}}(\text{i},18)==0
            resBR{\text{j}}(\text{i},18)=resBR{\text{j}-1}(\text{i},18);
        end
    end
end

\text{files = uigetfile('*\'.bmp', 'MultiSelect', 'on');}
\text{filesNEWIMAGE=files;}
for \text{i}=1:length(files)
    filesNEWIMAGE{\text{i}}{7:9}='png';
end

for \text{j}=1:length(resB)
    figure
    for \text{i}=1:length(resB{1})
        if resBR{\text{j}}(\text{i},18)>0.03
            filledCircle([resBR{\text{j}}(\text{i},2),resBR{\text{j}}(\text{i},3)],resBR{\text{j}}(\text{i},4)+0.4,1000,[0 0.6 0]);
        elseif resBR{\text{j}}(\text{i},18)<0.03 \\&& resBR{\text{j}}(\text{i},18)>-0.03
            filledCircle([resBR{\text{j}}(\text{i},2),resBR{\text{j}}(\text{i},3)],resBR{\text{j}}(\text{i},4)+0.3,1000,[1 1 1]);
        else
            filledCircle([resBR{\text{j}}(\text{i},2),resBR{\text{j}}(\text{i},3)],resBR{\text{j}}(\text{i},4)+0.3,1000,'b');
        end
    end
    hold on
end
axis equal
axis([14*pixtoMM 713*pixtoMM -1280*pixtoMM 0*pixtoMM]);
hold on
for \text{i1}=1:length(resB{1})
    if resBR{\text{j}}(\text{i1},18)>0.03 \\| resBR{\text{j}}(\text{i1},18)<-0.03
        for \text{i2}=1:length(resB{1})
            if resBR{\text{j}}(\text{i2},18)>0.03 \\| resBR{\text{j}}(\text{i2},18)<-0.03
            if
                sign(resBR{\text{j}}(\text{i1},18))\neq sign(resBR{\text{j}}(\text{i2},18))
            \end
\end
\end
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3. Displacement and rotation fields in the problem of a semi-infinite crack in an infinite plane opened by an inserted thin rigid wedge

function myfun(d, b, h, E, nu, G, hh)

step=b/50;
[x, y] = ndgrid(-b+1:step:b, 0:step:b);
fi1 = atan2(y,x);
fi2 = atan2(y,b+x);

r1=sqrt(x.^2+y.^2);
r2=sqrt((x+b).^2+y.^2);
Z_line = (E*2*h/(2*pi*(1-nu^2)))*asinh(sqrt((r1.*(cos(fi1)+sin(fi1)*1i))./b));
Z = (E*2*h/(2*pi*(1-nu^2)))*(1./sqrt(r1.*r2)).*(cos(- (fi1+fi2)./2)+sin(-(fi1+fi2)./2).*1i);
u = ((1-2*nu)*real(Z_line)-y.*imag(Z))/(2*G);
v = (2*(1-nu)*imag(Z_line)-y.*real(Z))/(2*G);

fil1_xplus = pi+atan(y./(x+hh));
fil2_xplus = atan(y./(b+x+hh));
r1_xplus=sqrt((x+hh).^2+y.^2);
r2_xplus=sqrt((x+hh+b).^2+y.^2);
Z_line_xplus = (E*2*h/(2*pi*(1-nu^2)))*asinh(sqrt((r1.*(cos(fi1)+sin(fi1)*1i))./b));
Z_xplus = (E*2*h/(2*pi*(1-nu^2)))*(1./sqrt(r1.*r2)).*(cos(- (fil1+fil2)./2)+sin(-(fil1+fil2)./2).*1i);
u_xplus = ((1-2*nu)*real(Z_line)-y.*imag(Z))/(2*G);
v_xplus = (2*(1-nu)*imag(Z_line)-y.*real(Z))/(2*G);
fil1_xminus = pi+atan(y./(x-hh));
fi2_xminus = atan(y.)/(b+x-hh));
r1_xminus = sqrt((x-hh).^2+y.^2);
r2_xminus = sqrt((x-hh+b).^2+y.^2);
Z_line_xminus = (E*2*h/(2*pi*(1-nu^2)))*asinh(sqrt((r1.*(cos(fil)+sin(fil)*1i))./b));
Z_xminus = (E*2*h/(2*pi*(1-nu^2)))*(1./sqrt(r1.*r2))*cos(-(fil+fi2)./2)+sin(-
(fi1+fi2)./2).*1i);
u_xminus = ((1-2*nu)*real(Z_line)-y.*imag(Z))/(2*G);
v_xminus = (2*(1-nu)*imag(Z_line)-y.*real(Z))/(2*G);

fil1_yplus = pi+atan((y+hh)./(x+hh));
fi2_yplus = atan((y+hh).)/(b+x+hh));
r1_yplus=sqrt((x+hh).^2+(y+hh).^2);
r2_yplus=sqrt((x+b+hh).^2+(y+hh).^2);
Z_line_yplus = (E*2*h/(2*pi*(1-nu^2)))*asinh(sqrt((r1.*(cos(fil)+sin(fil)*1i))./b));
Z_yplus = (E*2*h/(2*pi*(1-nu^2)))*(1./sqrt(r1.*r2))*cos(-
(fi1+fi2)./2)+sin(-(fi1+fi2)./2).*1i);
u_yplus = ((1-2*nu)*real(Z_line)-(y+hh).*imag(Z))/(2*G);
v_yplus = (2*(1-nu)*imag(Z_line)-(y+hh).*real(Z))/(2*G);

dvdx=(v_xplus-v_xminus)./(2*hh);
dudy=(u_yplus-u_yminus)./(2*hh);
fi=(dvdx-dudy)/2;

transp=0.7;
figure()
hSurface1=surf(x,y,u);
set(hSurface1,'FaceColor',[0 0 1],'FaceAlpha',transp);
set(gca,'FontSize',45, 'FontName', 'Times New Roman')

figure()
hSurface2=surf(x,y,v);
set(hSurface2,'FaceColor',[0 0 1],'FaceAlpha',transp);
set(gca,'FontSize',45, 'FontName', 'Times New Roman')

figure()
hSurface3=surf(x,y,fi);
set(hSurface3,'FaceColor',[0 0 1],'FaceAlpha',transp);
set(gca,'FontSize',45, 'FontName', 'Times New Roman')

4. Stability of chains of oscillators with negative stiffness normal, shear and rotational springs

% Eigen frequencies of undamped chains
function eigenfreq(m, J, n)

minstif=-2;
maxstif=1;
kOth=1;
incr=(maxstif-minstif)/100;
[kVar1, kVar2]=ndgrid(minstif:incr:maxstif);
kVar1=kVar1(:,1); kVar2=kVar2(:,1);

K=zeros(2*n,2*n,length(kVar1));
k=zeros(length(kVar1),2*(n+1));
freq=zeros(length(kVar1),2*n);
for i=1:length(kVar1)
    k(i,:)=[kOth kOth kVar1(i) kVar2(i) kOth kOth];
end

M=[m 0 0 0; 0 m 0 0; 0 0 J 0; 0 0 0 J];
for i=1:length(kVar1)
    K(:,:,i)=[k(i,1)+k(i,2), -k(i,2), (k(i,1)-k(i,2))/2, -k(i,2)/2;
              -k(i,2), k(i,2)+k(i,3), k(i,2)/2, (k(i,2)-k(i,3))/2;
             (k(i,1)-k(i,2))/2, k(i,2)/2, k(i,4)+k(i,5)+(k(i,1)+k(i,2))/4, -k(i,5)+k(i,2)/4;
                -k(i,2)/2, (k(i,2)-k(i,3))/2, -k(i,5)+k(i,2)/4, k(i,5)+k(i,6)+(k(i,2)+k(i,3))/4];
    freq(i,:)=sqrt(eig(M\K(:,:,i))); %for i=1:length(kVar1)
end

[kVar1, kVar2]=ndgrid(minstif:incr:maxstif);
freq1=reshape(freq(:,1),length(kVar1),length(kVar1));
freq2=reshape(freq(:,2),length(kVar1),length(kVar1));
freq3=reshape(freq(:,3),length(kVar1),length(kVar1));
freq4=reshape(freq(:,4),length(kVar1),length(kVar1));
surf(kVar1, kVar2, real(freq1));
figure() surf(kVar1, kVar2, real(freq2));

% Relations between the normalised frequency and normalised spring stiffnesses for the viscoelastic chain of the oscillators
function mydamp1(m, J, n)

alphaU = 0.5;
alphaFi = 0.5;
minstif=-1.5;
maxstif=1;
incr=(maxstif-minstif)/40;
[ks1, kff1]=ndgrid(minstif:incr:maxstif);
ks1=ks1(:); kff1=kff1(:);
kf2=1;
q_orig = zeros(8,length(ks1));
q = zeros(8,length(ks1));
q2 = zeros(8,length(ks1));
syms lambda
for i=1:length(ks1)
    mat = [1+alphaU*lambda+m*lambda^2+ks1(i), -1, -
          1/2+ks1(i)/2, -1/2;
          -1, 2+alphaU*lambda+m*lambda^2, 1/2 0;
          -1/2+ks1(i)/2, 1/2,
          1/4+alphaFi*lambda+J*lambda^2+ks1(i)/4+kf1(i)+kf2, 1/4-kf2;
          -1/2, 0, 1/4-kf2, 3/2+alphaFi*lambda+J*lambda^2+kf2];
eq=det(mat);
    q(:,i)=solve(eq==0,lambda);
end
[sorted, idx] = sort((abs(imag(double(q)))));
for i=1:length(ks1)
    q2(:,i) = q(idx(:,i),i);
end
q2=sort(q2(1:2,:));
[kss1, kff1]=ndgrid(minstif:incr:maxstif);
freqq1=reshape(-q2(1,:),length(kss1),length(kff1));

kVar1=kss1(:); kVar2=kff1(:);
K=zeros(2*n,2*n,length(kVar1));
k=zeros(length(kVar1),2*(n+1));
freq=zeros(length(kVar1),2*n);
for i=1:length(kVar1)
    k(i,:)=[kVar1(i) 1 1  kVar2(i) 1  1];
end
M=[m 0 0 0; 0 m 0 0; 0 0 J 0; 0 0 0 J];

for i=1:length(kVar1)
    K(:,i,:)=[k(i,1)+k(i,2), -k(i,2), (k(i,1)-k(i,2))/2, -
              k(i,2)/2;
              -k(i,2), k(i,2)+k(i,3), k(i,2)/2, (k(i,2)-
              k(i,3))/2;
              (k(i,1)-k(i,2))/2, k(i,2)/2,
              k(i,4)+k(i,5)+(k(i,1)+k(i,2))/4, -k(i,5)+k(i,2)/4;
              -k(i,2)/2, (k(i,2)-k(i,3))/2, -k(i,5)+k(i,2)/4,
              k(i,5)+k(i,6)+(k(i,2)+k(i,3))/4];
Appendix. Source codes

freq(i,:)=sqrt(eig(M\K(:,:,i))); end

[kVar1, kVar2]=ndgrid(minstif:incr:maxstif);
freq1=reshape(freq(:,1),length(kVar1),length(kVar1));
f1=imag(freq1);
f1_orig=real(freq1);
ff=zeros(length(f1),length(f1));
for i=1:length(freq1)
    for j=1:length(freq1)
        if f1(i,j)<0.01
            ff(i,j)=0;
        else
            ff(i,j)=f1(i,j)/f1_orig(i,j);
        end
    end
end

hSurface=surf(kVar1, kVar2, ff);
sel(hSurface,'FaceColor',[0 0 1], 'FaceAlpha',0.8);
xlabel('\it{k}^s_1','FontSize',65, 'FontName','Times New Roman')
ylabel('\it{k}^\phi_1','FontSize',65, 'FontName','Times New Roman')
zlabel('\omega_1*/\omega_1','FontSize',65, 'FontName','Times New Roman')
set(gca,'FontSize',60, 'FontName','Times New Roman')

% Relations between the relative damping coefficient and normalised spring stiffnesses

function mydamp2(m, J, n)
alphaU = 0.7;
alphaFi = 0.7;
minstif=-1.15;
maxstif=1;
incr=(maxstif-minstif)/10;
incl=(1+0.25)/40;
inc2=(1+1.15)/40;
[kss1, kff1]=ndgrid(-0.25:incl:1, -1.15:inc2:1);
ks1=kss1(:); kf1=kff1(:);
kf2=1;
q_orig = zeros(8,length(ks1));
q = zeros(8,length(ks1));
q2 = zeros(8,length(ks1));
syms lambda
for i=1:length(ks1)
    mat = [1+alphaU*lambda+m*lambda^2+ks1(i), -1, -1/2+ks1(i)/2, -1/2; -1, 2+alphaU*lambda+m*lambda^2, 1/2 0;];
\[-\frac{1}{2} + k_1(i)/2, 1/2,\]
\[1/4 + \alpha \phi_i \lambda + J \lambda^2 + k_1(i)/4 + k_f(1) + k_f(2); \]
\[-1/2, 0, 1/4 - k_f(2), 3/2 + \alpha \phi_i \lambda + J \lambda^2 + k_f(2);\]
\[eq = det(mat);\]
\[q(:,i) = solve(eq == 0, \lambda);\]
\end

[sorted, idx] = sort((abs(imag(double(q))));
for i = 1:length(k_1);
q_2(:, i) = q(idx(:, i), i);
end
q_2 = sort(q_2(1:2, :));
[k_s_1, k_f_1] = ndgrid(-0.25:inc_1:1, -1.15:inc_2:1);
freqq_1 = reshape(-q_2(1,:), length(k_f_1), length(k_s_1));
for i = 1:length(freqq_1)
\begin{verbatim}
    for j = 1:length(freqq_1)
        if freqq_1(i, j) < 0.01
            freqq_1(i, j) = 0;
        end
    end
end
\end{verbatim}
freqq_2 = reshape(-q_2(2,:), length(k_f_1), length(k_s_1));
freqq_2 = freqq_2;
freqq_2(:, :) = 0;
for i = 1:length(freqq_2)
\begin{verbatim}
    for j = 1:length(freqq_1)
        if \real(freqq_2(i, j)) / \real(freqq_2(length(freqq_2), length(freqq_2))) > 2
            freqq_2(i, j) = 2;
        else
            freqq_2(i, j) = \real(freqq_2(i, j)) / \real(freqq_2(length(freqq_2), length(freqq_2)));\n        end
    end
end
\end{verbatim}
hSurface = surf(k_s_1, k_f_1, 
\real(freqq_1) / \real(freqq_1(length(freqq_1), length(freqq_1))));
set(hSurface, 'FaceColor', [0 0 1], 'FaceAlpha', 0.8);
xlabel('\it{k}^s_1', 'FontSize', 65, 'FontName', 'Times New Roman';
ylabel('\it{k}^\phi_1', 'FontSize', 65, 'FontName', 'Times New Roman';
zlabel('\omega_1*/\omega_1', 'FontSize', 65, 'FontName', 'Times New Roman');
set(gca, 'FontSize', 60, 'FontName', 'Times New Roman');
xlim([-0.25 1]);
ylim([-1.15 1]);
5. Stability of 2D discrete mass-spring systems with negative stiffness springs

% Relationship between eigenfrequencies and different values of spring stiffness for the channel of two particles

function myeigen(mm, J, n, m)

minstif=-10;
maxstif=10;
n=1;
m=2;
incr=(maxstif-minstif)/10000;
kVar=minstif:incr:maxstif;
K=zeros(3*n*m,3*n*m,length(kVar));
freq=zeros(length(kVar),3*n*m);

% Stiffness
k1n11=kVar;
k1f11=ones(1,length(kVar));
k1n12=-1*ones(1,length(kVar));
k1s11=ones(1,length(kVar));
k1f12=ones(1,length(kVar));
k1n13=ones(1,length(kVar));
k1s12=ones(1,length(kVar));
k1f13=ones(1,length(kVar));
k3n11=ones(1,length(kVar));
k3s11=ones(1,length(kVar));
k3f11=ones(1,length(kVar));
k3n12=ones(1,length(kVar));
k3s12=ones(1,length(kVar));
k3f12=ones(1,length(kVar));
k3n21=ones(1,length(kVar));
k3s21=ones(1,length(kVar));
k3f21=ones(1,length(kVar));
k3n12=ones(1,length(kVar));
k3s12=ones(1,length(kVar));
k3f12=ones(1,length(kVar));
k3n22=ones(1,length(kVar));
k3s22=ones(1,length(kVar));
k3f22=ones(1,length(kVar));

for i=1:length(kVar)
    K(:,:,i)=[k1n11(i)+k1n12(i)+k3s11(i)+k3s21(i), -k1n12(i), 0, 0, 0.5*k3s11(i)-0.5*k3s21(i), 0; -k1n12(i), k1n12(i)+k1n13(i)+k3s12(i)+k3s22(i), 0, 0, 0.5*k3s12(i)-0.5*k3s22(i); 0, 0, k1s11(i)+k1s12(i)+k3n11(i)+k3n21(i), -k1s12(i), 0.5*k1s11(i)-0.5*k1s12(i), -0.5*k1s12(i);];
end
0, 0, -k1s12(i),
k1s12(i)+k1s13(i)+k3n12(i)+k3n22(i), 0.5*k1s12(i),
0.5*k3s11(i)-0.5*k3s21(i), 0, 0.5*k1s11(i)-
0.5*k1s12(i), 0.5*k1s12(i),
0.5*k3s11(i)-0.5*k3s21(i), 0.5*k1s12(i)-0.5*k1s13(i), 0.5*k1s12(i), -0.5*k1s12(i),
0.25*k1s11(i)+0.25*k1s12(i)+0.25*k3s11(i)+0.25*k3s21(i)+k1f
11(i)+k1f12(i)+k3f11(i)+k3f21(i), 0.25*k1s12(i)-k1f12(i);  
freq(i,:)=sqrt(eig(M\K(:,:,i))); 
end

plot(kVar, freq(:,1),kVar, freq(:,2),kVar, freq(:,3),kVar,
freq(:,4),kVar, freq(:,5),kVar, freq(:,6))

% The smallest and largest eigenfrequencies and different 
values of spring stiffness for the "channel" of two 
particles 

function myeigen2(mm, J, n, m)

minstif=-10;
maxstif=10;
incr=(maxstif-minstif)/100000;
KVar=minstif:incr:maxstif;
K=zeros(3*n*m,3*n*m,length(kVar));
freq=zeros(length(kVar),3*n*m);

% Stiffness

k1n11=ones(1,length(kVar));
k1s11=ones(1,length(kVar));
k1f11=ones(1,length(kVar));
k1n12=ones(1,length(kVar));
k1s12=ones(1,length(kVar));
k1f12=ones(1,length(kVar));
k1n13=ones(1,length(kVar));
k1s13=ones(1,length(kVar));
k1f13=ones(1,length(kVar));
k3n11=ones(1,length(kVar));
k3s11=ones(1,length(kVar));
k3f11=ones(1,length(kVar));
k3n21=ones(1,length(kVar));
k3s21=ones(1,length(kVar));
k3f21=ones(1,length(kVar));
k3n12=ones(1,length(kVar));
k3s12=ones(1,length(kVar));
k3f12=ones(1,length(kVar));
k3n22=ones(1,length(kVar));
k3s22=ones(1,length(kVar));
k3f22=ones(1,length(kVar));
Appendix. Source codes

\[
M = \begin{bmatrix}
mm & 0 & 0 & 0 & 0 & 0 \\
0 & mm & 0 & 0 & 0 & 0 \\
0 & 0 & mm & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & J & 0 \\
0 & 0 & 0 & 0 & 0 & J
\end{bmatrix};
\]

\[
figure() \\
\text{legendary} = ['k1n11'; 'k1n12'; 'k3n11']; \\
\text{for } t = 1:3 \\
\quad \text{if } t == 1 \\
\quad \quad rr = k1n11; \\
\quad \quad k1n11 = kVar; \\
\quad \quad \text{colour} = 'r'; \\
\quad \text{elseif } t == 2 \\
\quad \quad k1n12 = kVar; \\
\quad \quad \text{colour} = 'b'; \\
\quad \text{else} \\
\quad \quad k3n11 = kVar; \\
\quad \quad \text{colour} = 'g'; \\
\quad \text{end} \\
\quad \text{for } i = 1: \text{length(kVar)} \\
\quad \quad K(:,:,i) = \begin{bmatrix}
k1n11(i) + k1n12(i) + k3s11(i) + k3s21(i), -k1n12(i), 0, 0, 0.5*k3s11(i) - 0.5*k3s21(i), 0; 
-k1n12(i), k1n12(i) + kl13(i) + k3s12(i) + k3s22(i), 0, 0, 0.5*k3s12(i) - 0.5*k3s22(i); 
0, 0, kl11(i) + k1s12(i) + k3n11(i) + k3n21(i), -k1s12(i), 0.5*k1s11(i) - 0.5*k1s21(i), -0.5*k1s12(i); 
0, 0, -k1s12(i), k1s12(i) + k1s13(i) + k3n12(i) + k3n22(i), 0.5*k1s12(i); 
0.5*k3s11(i) - 0.5*k3s21(i), 0, 0.5*k3s11(i) - 0.5*k3s21(i), 0, 0.5*k3s11(i) - 0.5*k3s21(i); 
0.25*k1s11(i) + 0.25*k1s12(i) + 0.25*k3s11(i) + 0.25*k3s21(i) + k1f11(i) + k1f12(i) + k3f11(i) + k3f21(i), 0.25*k1s12(i) - k1f12(i); 
0, 0.5*k3s12(i) - 0.5*k3s22(i), 0.5*k3s12(i) - 0.5*k3s22(i), -0.5*k1s12(i), 0.5*k1s12(i) - 0.5*k1s13(i), 0.25*k1s12(i) - k1f12(i), 0.25*k1s12(i) + 0.25*k1s13(i) + 0.25*k3s12(i) + 0.25*k3s22(i) + k1f12(i) + k1f13(i) + k3f12(i) + k3f22(i)
\end{bmatrix}; \\
\quad \quad \text{freq(i,:)} = \sqrt{\text{eig}(M \backslash K(:,:,i))}; \\
\quad \text{end} \\
\quad \text{plot(kVar, freq(:,1),colour,kVar, freq(:,6),colour, 'LineWidth',3)} \\
\quad \text{grid on} \\
\quad \text{hold on} \\
\quad \text{set(gca,'FontSize',53,'FontName', 'Times New Roman')} \\
\quad \text{set(findall(gcf,'type','text'),'FontSize',53,'FontName', 'Times New Roman')} \\
\quad \text{xlim([-2.75,5])} \\
\quad \text{ylim([0,3])} \\
\quad k1n11=\text{ones(1,}\text{length(kVar)}); \\
\quad k1n12=\text{ones(1,}\text{length(kVar)}); \\
\quad k3n11=\text{ones(1,}\text{length(kVar)}); \\
\quad \text{plot([0 0], [0 3], 'k', 'LineWidth',1.5)} \\
\text{end}
6. Waves in the Cosserat continuum

% Dispersion relationship for the twist wave in the Cosserat continuum

function fig2(x)

SOL=sqrt(1./(1-x));
plot(x, SOL, 'linewidth', 2.5);
xlabel( '$\omega_n^2 / \omega^2$', 'fontsize', 40,'Interpreter','latex' );
y=ylabel('$\frac{c_t}{c_3}$', 'fontsize', 55, 'Rotation',0,'Interpreter','latex');
set(gca,'FontSize',25);
grid on

% Dispersion relationships for both shear-rotational waves in the Cosserat continuum with negative Cosserat shear modulus

function fig3()

syms s w s2 s4
SOL=solve((1+w)*s^2-(w+(s2+s4))*s+s2*s4,s)
w=0:0.01:5;

s2=0.1; s4=2;
SOL1=subs(SOL)
s2=0.5; s4=2;
SOL3=subs(SOL);
s2=0.5; s4=5;
SOL4=subs(SOL);
s2=0.9; s4=2;
SOL5=subs(SOL);
s2=0.9; s4=5;
SOL6=subs(SOL);

set(0,'DefaultAxesFontName', 'Times New Roman')
plot(w,sqrt(SOL1),'r',w,sqrt(SOL3),'k',w,sqrt(SOL4),'b',w,sqrt(SOL5),'g',w,sqrt(SOL6),'m','LineWidth',2)
set(gca,'FontSize',40);
xlabel( '$\omega_n^2 / \omega^2$', 'fontsize', 45,'Interpreter','latex');
y=ylabel('$\frac{c_s}{c_5}$', 'fontsize', 65, 'Rotation',0,'Interpreter','latex');
set(y, 'Units', 'Normalized', 'Position', [-0.14, 0.5]);
grid on;
axis square

% Relations between normalised velocities of shear-rotational waves and normalised Cosserat shear modulus
function fig5()

syms w s alfaN s z

SOL=solve(((z*alfaN-1)*s^2-((z*alfaN-((1+alfaN)+s4))*s-(1+alfaN)*s4,s));
z=2;
alfaN=-1:0.013:2;
s4=0.5;
SOL1=subs(SOL);
s4=2;
SOL2=subs(SOL);
s4=5;
SOL3=subs(SOL);
s4=10;
SOL4=subs(SOL);

figure;
plot(alfaN,sqrt(SOL1(1,:)),'r',alfaN,sqrt(SOL1(2,:)),'b','LineWidth',2);
xlabel( '$\frac{\alpha}{\mu}$', 'fontsize', 60,'Interpreter','latex' );
y=ylabel('$\frac{c_s}{c_5}$', 'fontsize', 80, 'Rotation',0,'Interpreter','latex');
hold on;
plot([0 0],[0 20],'k');
grid on;
set(y, 'Units', 'Normalized', 'Position', [-0.12, 0.5]);
title('$z=2:\:s_4=0.5$', 'fontsize', 60, 'Units', 'Normalized', 'Position', [0.17, 0.85], 'Interpreter','latex');
ylim([0 5]);
annotation('textarrow',[0.65,0.52],[0.65,0.47],...
'String','$\frac{\alpha}{\mu} = \frac{1}{z} = 0.5$', 'fontsize', 60,'Interpreter','latex');
set(gca,'FontSize',50,'FontName', 'Times New Roman');

figure;
plot(alfaN,sqrt(SOL2(1,:)),'r',alfaN,sqrt(SOL2(2,:)),'b','LineWidth',2);
xlabel( '$\frac{\alpha}{\mu}$', 'fontsize', 60,'Interpreter','latex' );
y=ylabel('$\frac{c_s}{c_5}$', 'fontsize', 80, 'Rotation',0,'Interpreter','latex');
hold on;
plot([0 0],[0 20],'k');
grid on;
set(y, 'Units', 'Normalized', 'Position', [-0.12, 0.5]);
title('$z=2:\:s_4=2$', 'fontsize', 60, 'Units', 'Normalized', 'Position', [0.17, 0.85], 'Interpreter','latex');
ylim([0 5]);
annotation('textarrow',[0.65,0.52],[0.65,0.47],...
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\begin{verbatim}

figure;
plot(alfaN, sqrt(SOL3(1,:)),'r', alfaN, sqrt(SOL3(2,:)),'b', 'LineWidth',2);
xlabel( '$\alpha / \mu$', 'FontSize', 60, 'Interpreter','latex' );
ylabel('$\frac{c_s}{c_5}$', 'FontSize', 80, 'Rotation',0,'Interpreter','latex');
hold on;
plot([0 0],[0 20],'k');
grid on;
set(gca,'FontSize',50,'FontName', 'Times New Roman')

end

end

\end{verbatim}