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**Exploring emergence of critical state and one-dimensional
compression through a granular micromechanics model**

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*"I imagined, I identified the obstacles in front of my imagination.
When I removed the obstacles, my imagination came true
spontaneously."*

Mustafa Kemal Atatürk

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Abstract

The mechanical behavior of granular materials, explored by frictional and collisional mechanisms, is elucidated with the stress-strain relations thanks to the properly modified for damage and plasticity phenomena under complex loading paths. In this thesis, a Granular Micromechanics Approach (GMA) based continuum model offers a fresh perspective to investigate the classical loading scenarios such the emergence of a critical state and one-dimensional uniaxial compression. Moreover, a continuum model is established based on elastic energy and dissipation potential definitions with regard to the grain-pair interactions in different orientations. A hemi-variational principle provides the basis for considering the evolution of damage and plasticity phenomena comprising grain-pair, respectively, with a decrease in stiffness and irreversible deformation. As a consequence, the Karush-Kuhn-Tucker (KKT)-type conditions are derived, which give the evolution equations for the irreversible phenomena. Notably, in this derivation, there is no invocation of flow rules and other similar assumptions of classical phenomenological continuum damage and plasticity. Further, Piola's ansatz is elaborated to kinematically connect granular micromechanics of grain-pair to the continuum description.

The mechanical response of granular materials is characterized by: i) a critical state, in which deformation occurs without change of material volume or stresses when subjected to large shear deformation; and ii) one-dimensional uniaxial compression, where the material is loaded with a monotonically increasing vertical compressive displacement until a specific threshold is reached. While the concepts of critical state analysis and one-dimensional compression have been handled with either phenomenological approaches or discrete numerical frameworks in a literature review, these concepts are examined within a micromechanics based continuum description in this thesis. The mechanical behavior of these concepts is shown to emerge as grain-pair related damage and plastic evolution, interacting in a competitive/collaborative manner during the imposed loading path.

This thesis also aims to explore the behavior of this model with a critical state concept by conducting a parametric study that varies the constitutive parameters over a wide range. The fundamental aspect is to present a comprehensive parametric study on a numerical model utilizing a GMA to explore the combination of constitutive parameters affecting a critical state with respect to the classical way in granular materials. A para-

metric study can clarify the further refinements in predicting the macro-scale behavior of granular materials, utilizing a numerical model to better capture experimental findings. The material properties of specimens with different initial density states are adapted according to dilatancy/compaction characteristics to achieve the idealized critical state behavior. The present model is then applied to simulate the stress and volumetric strain behaviors under varying characteristic compression constitutive parameters.

Uniaxial or one-dimensional compression is widely used in granular material processing to produce granular compacts and is a key experimental method for evaluating the compressibility of granular materials. Granular materials undergoing large deformations exhibit nonlinearity arising from both geometrical and material effects. To describe the stiffening behavior that elasto-frictional granular materials exhibit in confined compression, the elastic energy functional and dissipation potential were modified from previous versions of GMA-based models. Here, the earlier GMA-based continuum models are extended by enriching the grain-pair elastic energy functional and dissipation potential with new tangential terms and a coupling between normal and tangential parameters to better describe these nonlinear effects. In the first work of one-dimensional compression, the dissipation potential was also modified by incorporating coupling between plastic parameters that characterize plastic deformation accumulation as the grain-pair experiences compression and/or tension during loading process. The modified model, derived in the framework of geometrically nonlinear deformations, was then applied to replicate experimentally measured one-dimensional compression behavior of granular materials undergoing large compression. The results reveal nearly universal scaling with respect to the model parameters for predicting the behavior of granular materials composed of different particle types or initial density. A parametric study was conducted to determine the evolution of the microscale stored elastic energy and dissipation parameters in terms of grain-pair directions. In addition, this thesis provides a brief literature review of experimental observations and modeling approaches related to powder compaction behavior. In the second work of one-dimensional compression, the elastic energy of a generic grain-pair direction of a GMA is reformulated consisting of a complete quadratic and quartic (duffing) dependencies on normal and tangential relative displacements to capture various nuances of material nonlinearity. Further, the grain-pair dissipation potential formulation is modified by introducing (i) plastic dissipation in the tangential direction and (ii) coupling between the plastic dissipation in tension and compression. In this framework, these new terms are expected to better represent various deformation mechanisms that grains experience including grain crushing, rearrangement, rotation/rolling, sliding, loss of lateral support, neighborhood densification and strain localization. It is shown that the coupling of this nonlinear elastic and the damage-plastic behavior yields an appar-

ent molecular-type, such as Lennard-Jones type, potential for the granular system. A GMA framework is exploited to link the grain-scale behavior to the macroscopic response. To motivate the adoption of GMA framework, a brief review of grain-scale deformation mechanisms that lead to the emergent dissipative macroscale behavior and the evolution of induced anisotropy is presented. Classical behavior of lateral earth pressure coefficient, the ratio of lateral to axial stress, is predicted by the model. The obtained results are expounded with the aid of the evolution of two sets of parameters during the compaction process, one at the grain-scale and the other at the emergent macroscale. At the grain scale, the directional evolution of elastic energy, damage and plasticity is investigated. At the macroscale, the evolution of macroscale induced anisotropy is followed by considering the eigenvalues and harmonic decomposition of equivalent stiffness. The enriched model is used to simulate one-dimensional compression of elasto-frictional granular media.

The constitutive model is conducted in a stepwise manner to identify the evolution of damage and plastic irreversible variables related frictional grain-pair mechanism. As is typical in geomechanics, the simulations are performed assuming that specimen in such tests experience homogeneous deformations, such that the physical experiment can be represented by a single continuum material point. In this thesis, the emergence of critical state and one-dimensional uniaxial compression are investigated for the first time through the collaboration of coupled damage and plastic mechanics within a granular micromechanics based continuum description.

Keywords: critical state, one-dimensional compression, powder compaction, granular micromechanics, Karush-Kuhn-Tucker conditions, damage and plasticity mechanics, variational-based model, induced anisotropy, material nonlinearity, harmonic decomposition.

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List of Symbols

Geometrical and kinematical quantities

N	Set of grains
M	Set of grain–pair interactions
E^2	Two-dimensional Euclidean space
$\mathcal{B}$	Continuous body
$\mathbf{X}$	Position in the reference configuration
$\mathbf{x}$	Position in the current configuration
t	Time
χ	Placement function
$\mathbf{u}$	Displacement vector
$\bar{u}$	Applied displacement
$\hat{\mathbf{c}}$	Unit vector
L	Intergranular distance
$\mathbf{F} = \nabla \chi$	Deformation gradient
$\mathbf{G}$	Green–St. Venant strain tensor
$G_{ij,h}$	Gradient of Green–St. Venant strain tensor
$\mathbf{n}$	Outward unit normal vector
$\Theta(x)$	Heaviside function
$\mathcal{S}$	Region of the unit circle
$d\ell$	Infinitesimal element $d\theta$
$\mathbf{b}^{\text{ext}}$	External force on $\mathcal{B}$
$\mathbf{t}^{\text{ext}}$	External force on part $\partial_t \mathcal{B}$

Displacements and kinematic descriptors

u_η	Normal displacement
u_{τ_i}	Tangential displacement vector
u_τ^2	Square of tangential displacement
u_η^{el}	Elastic normal displacement
u_η^{pl}	Plastic normal displacement
u_τ^{2el}	Squared elastic tangential displacement
$u_\tau^{2pl} = \lambda_\tau^2$	Squared plastic tangential displacement
D_η	Normal damage variable
D_τ	Tangential damage variable

λ_η^t	Plastic multiplier in tension
λ_η^c	Plastic multiplier in compression

Stiffness parameters

k_η	Normal stiffness
k_η^t	Non-damaged normal stiffness in tension
k_η^c	Non-damaged normal stiffness in compression
k_τ	Tangential stiffness
$k_{\eta\eta}$	Non-damaged normal Duffing stiffness
$k_{\tau\tau}$	Non-damaged tangential Duffing stiffness
$k_{\eta\tau}$	Non-damaged coupling stiffness
$k_{\eta D}$	Damaged normal stiffness
$k_{\eta D}^t$	Damaged normal stiffness in tension
$k_{\eta D}^c$	Damaged normal stiffness in compression
$k_{\tau D}$	Damaged tangential stiffness
$k_{\eta\eta D}$	Damaged normal Duffing stiffness
$k_{\tau\tau D}$	Damaged tangential Duffing stiffness
$k_{\eta\tau D}$	Damaged coupling stiffness
k_{nn}	Normal Duffing stiffness coefficient
k_{tt}	Tangential Duffing stiffness coefficient
k_{nt}	Coupling Duffing stiffness coefficient

Energy functionals

$\mathcal{E}$	Action functional
U	Elastic energy
W	Total dissipation potential
W_D	Damage dissipation potential
W_D^η	Normal damage dissipation potential
W_D^τ	Tangential damage dissipation potential
W_{pl}	Plastic dissipation potential
W_{pl}^η	Normal plastic dissipation potential
W_{pl}^τ	Tangential plastic dissipation potential
U^{ext}	External energy

Specimen and experimental quantities

e	Void ratio
V_V	Void volume
V_S	Solid volume

G_V	Volumetric strain
G_{emp}	Empirical shear modulus
G_{VF}	Volumetric strain at failure
r	Specimen radius
S	Edge length
t	Pseudo-thickness
K_0	Lateral stress coefficient

Material constitutive parameters

α	Regularization parameter
α_1	Additional constitutive parameter
B_η	Characteristic normal damage displacement
B_η^t	Characteristic normal damage displacement in tension
B_η^c	Characteristic normal damage displacement in compression
$B_\tau, B_{\tau 0}$	Characteristic tangential damage displacement
σ_η^t	Plastic yielding parameter in tension
σ_η^c	Plastic yielding parameter in compression
$\sigma_{\eta\eta}^t$	Plastic hardening/softening parameter in tension
$\sigma_{\eta\eta}^c$	Plastic hardening/softening parameter in compression
$\sigma_{\eta\eta}^{tc}$	Plastic coupling parameter
$\sigma_{\tau\tau}$	Tangential plastic yielding parameter

Stiffness tensors and harmonic decomposition parameters

$\mathbb{P}_{ij}$	Second-order pre-stress tensor
$\mathbb{C}_{ijab}$	Fourth-order stiffness tensor
$\mathbb{L}_{ijklcd}$	Sixth-order stiffness tensor
$\mathbb{N}_{ijklcdef}$	Eighth-order stiffness tensor
$\tilde{\mathbf{C}}$	Equivalent damage–elasto–plastic stiffness tensor
$\mathbf{S}$	Stress tensor
σ_{ij}	Experimental stress tensor
$\bar{S}$	Confining stress
λ	Lamé's first parameter
μ	Shear modulus
γ	Bulk modulus
β	Generalized shear modulus
λ_i	Eigenvalue
$\mathbb{J}, \mathbb{I}^4, \mathbb{K}$	Projection operators
I_1, I_2, I_3, J_1, J_2	Invariants

General introduction

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1.1 Motivation and objectives

A class of granular materials, commonly encountered as heaps of discrete particles or powders, has been extensively investigated across various industries for its unique flow, plastic deformation, and compaction behavior [1–4]. Granular materials span the spectrum from highly consolidated dense solids formed of particulate precursors to confined packing of particles to rapidly flowing colliding collection of grains. In this thesis, the class of frictional granular materials that is described as confined packing of non-cohesive (or lightly cohesive) particles, in which the external mechanical action is conveyed by particle contacts experiencing compression and shear mediated by frictional effects.

The unique mechanical properties of such elasto-frictional granular materials depend on a myriad of factors, including their initial density state (or solid fraction), heterogeneity, loading history, particle surface characteristics, and interparticle interaction behavior. Among these, the behavior of this class of granular materials is strongly influenced by the elasto-frictional contact between grains. The central theme of this thesis is to apply a Granular Micromechanics Approach (GMA) with appropriately formulated effective grain-scale elastic energy and dissipation potential functionals in order to investigate the emergence of critical state and one-dimensional compression. These effective energy functionals are formulated in the form of damage-elasto-plastic spring elements that represent the effective grain-pair interactions decomposed into the so-called normal, parallel to the grain-pair direction, and tangential, orthogonal to the grain-pair direction, directions.

In light of the following parametric studies, the mechanical response of granular materials is better understood by refining both energy equations and simulation parameters. These efforts strengthen the predictive capabilities of numerical model under different loading histories. Notably, the parametric study includes an optimization process that deepens understanding of how simulation parameter changes influence the material's overall behavior. By systematically varying the constitutive parameters, the new material properties are integrated into the model, affecting both the strength characteristics and the evolution of damage and plasticity. Additionally, a systematic approach enhances accuracy, consistency, and confidence in replicating experimental results, supporting the validation and calibration of model findings. This thesis not only advances the understanding of granular material behavior within a continuum framework but also establishes refined elastic energy and dissipation potential functionals to achieve more accurate and reliable predictions.

1.2 Structure of presentation

This thesis summarizes three years of research that led to the development of a novel constitutive model for exploring the macroscopic behavior of granular materials based on the typical experimental findings of classical concepts within a micromechanics-based continuum description. This thesis is organized as follows:

- Chapter 2 summarizes some of the relevant background literature.
- Chapter 3 presents the identification of homogenized energy terms based upon a grain-pair interaction and a hemi-variational principle to obtain the governing equations and corresponding Karush-Kuhn-Tucker (KKT) conditions. The conducted numerical study is presented with the considered samples to investigate the critical state, providing a sensitivity analysis to elucidate the effects of simulation parameters. The simulations are served for dense, mid-dense, and loose specimens with different initial density states with regard to the parametric studies to elucidate the effects of simulation parameters on the emergence of critical state. Conclusions and projections are drawn.
- Chapter 4 reports a GMA, including a new type of elastic energy and dissipation potential terms based on a generic grain-pair interaction and a hemi-variational method to derive KKT-type conditions for irreversible phenomena. The numerical investigations are presented by replicating experimental observations in one-dimensional

compression. The key findings are summarized, and the future research directions are discussed. A brief review of grain-scale deformation mechanisms responsible for the development of dissipative macroscopic behavior and induced anisotropy is presented. At the grain scale, the directional evolution of elastic energy, damage, and plasticity is examined. At the macroscale, the evolution of induced anisotropy is investigated through the eigenvalues and harmonic decomposition of the equivalent stiffness tensor.

Literature review

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A literature review on the representation of granular materials' behavior is presented based on two different viewpoints, namely critical state and one-dimensional uniaxial compression, in this chapter. While these concepts have been well accepted, their microscale (or grain scale) genesis and how the connections to macroscale can be incorporated into mathematical descriptions of the mechanical behavior of such granular materials remains open to further exploration.

Computational models are powerful tools for revealing the mechanical behavior of materials in diverse environments [5–10]. With the growing popularity of computational techniques, modeling and simulating granular materials has become crucial for exploring their complex characteristics. Recently, both discrete modeling and continuum-based approaches, as well as coupling strategies like discrete-continuum approaches, have proven valuable in studying granular materials from a mechanistic viewpoint. In particular, granular micromechanics frameworks link microscale interactions with macroscale observations, enabling the development of predictive constitutive models that account for the intrinsic heterogeneity and discrete nature of these materials [11, 12]. By integrating mi-

complementing continuum mechanics, this approach provides a robust foundation for analyzing key phenomena, including stress-strain relationships and anisotropic behavior, which are essential for accurately describing the deformation properties of granular media.

2.1 Mechanical behavior of granular materials

Granular media consists of assembly of such frictional materials related to interactions between particles under external loads, which are affected by the lack of strong bonding forces, leading to sliding of grains. The mechanical behavior of this class of frictional granular materials is of interest in a wide variety of engineering and scientific fields [13]. Applications range from understanding soil deformation in geomechanics and geotechnical engineering to improving particle handling in pharmaceutical and food manufacturing, supporting civil infrastructure, and assessing seismic and earthquake-related phenomena in geophysics. Additionally, estimating the pressure and loading exerted by slowly shearing grains is critical for industrial processing and material handling applications.

These materials exhibit complex behaviors, including nonlinear stress-strain responses, volumetric strain due to compaction and dilation, and anisotropy resulting from grain-grain interactions and frictional contacts [14–17]. These features present unique challenges in accurately modeling and predicting their responses under diverse loading conditions. Moreover, the tendency of granular materials to exhibit fluid-like flow further adds to the complexity of their mechanical response, necessitating advanced modeling approaches.

2.1.1 Deformation mechanisms and anisotropy evolution in granular materials

Numerous efforts have been dedicated to better understand the effect of deformation mechanisms upon the macroscale stress-strain relationship of granular materials. Under external loading, granular materials experience particle rearrangement, grain sliding, separation and collapse/buckling of particle chains, which are driven not only by elasto-frictional interactions but also by inelastic properties dictated by the particle characteristics and surface roughness through normal and tangential interactions including rolling [18–23]. For this deformation condition, grain-scale mechanism such as particle crushing, grain rearrangement, rotation/rolling or grain sliding, loss of lateral support, grain neigh-

borhood densification, and strain localization give rise to complex mechanical behavior. For example, particle crushing in granular materials results in irreversible deformations, and the material takes on a denser form through a reduction in initial void ratio. Interestingly, the so-called yield stress has been reported to increase due to crushing of granular material (refer to selected works for investigations into the stress-initial void ratio relationship [24, 25]). Indeed, the macroscopic behavior of granular assemblies is expected to be elucidated through grain-pair interactions. Under very high compressive loadings, particularly for brittle grains [26], particle crushing leads to reduction in particle size with the formation of finer grains resulting in increasing the material packing density (or stiffening) and decreasing permeability. These mechanisms generate typical stress-strain relationships, particularly under uniaxial compression and large shear deformations [25, 27, 28]. Notably, the energy in granular systems can be dissipated in both rate independent and dependent manner [29, 30], such as by frictional sliding and inelastic collisions at grain contacts. The consequence is that the emergent macroscale stress-strain response is influenced by the loading path [31, 32]. Further, the shear strength of these materials exhibit significant anisotropy due to the directional dependency of their resistance to deformation [33].

Anisotropy in granular materials emerges due to the microstructural arrangement of particles and the orientations of inter-particle contacts linked to the directional dependence of material's properties. Anisotropy and its evolution has been investigated by considering shape and arrangement of particles, inherent grain orientation, voids, and the contact orientations relative to the direction of imposed load or deformation [34–36]. Notably, granular material anisotropy has two distinct aspects, the inherent and the induced anisotropy [37]. The inherent anisotropy arises from the initial natural microstructure independent of any external loading effect. Its genesis may be traced to the deposition, compaction or sedimentation processes and is usually described using so called fabric tensors [38–41]. For example, Dafalias et al. [42] introduced a plasticity constitutive model incorporating the effect of inherent fabric anisotropy using a second-order symmetric fabric tensor to model variations in shear strength, dilatancy and the critical state line under monotonic loading. Cambou et al. [36] evaluated anisotropy in granular materials with respect to the roles of particle shape, contact distribution, and contact force-laws. Induced anisotropy, on the other hand, evolves during loading history and deformation growth as a result of the imposed loading condition, realignment of so called 'force chains' and contact interactions [43–46]. Effects of induced anisotropy have been widely investigated [47–50]. For example, anisotropic critical state theory for granular media has been presented to describe the effects of evolving fabric anisotropy on the stress-strain and dilatancy response of sands within the bounding surface plasticity model [51, 52]. Utilizing the discrete el-

ement method (DEM), Kuhn et al. [50] investigated induced anisotropy to reveal that contact orientation responds most sensitively to loading and firmly correlates with stress and stiffness evolution while void anisotropy particularly influences permeability. Along similar lines, Zhao et al. [53] simulated the rolling resistance model in DEM to investigate particle shape effects and presented shear-induced fabric variation and anisotropy to highlight its limitations in accurately capturing the influence of particle elongation on contact normal anisotropy. The interplay between inherent and induced anisotropy has been investigated by considering the bedding plane angle and fabric evolution under repeated traffic loading [54].

2.1.2 Critical state phenomena

A key mechanical phenomenon exhibited by this type of granular materials is that of critical state at which deformation occurs without change of material volume or stresses as the material undergoes large shear deformation. See Chapter 6 Section 6.5 of [55] for some historical remarks regarding classical critical state observations based upon conventional triaxial compression and simple shear experiments on such granular materials composed of relatively stiff particles such as sands and glass beads. The need for further elaboration under more complex loading paths and for inclusion of additional microstructural measures for characterizing critical state have also been considered [56, 57]. However, direct experimental observations of such microstructural measures remain not only difficult, but confounded by intimate connection between the grain contact mechanics and interface conditions (microscale mechanical attributes), and microstructural arrangement of grains (measure of granular fabric). Although, notwithstanding the large variability and assumptions regarding microscale confounding factors (such as contact conditions), recent efforts of microscale characterization have been reported (see for example [58]). Indeed, the emergence of critical state in such granular systems can be expected to be an evolution in the interplay of grain-scale mechanics and microstructural arrangement of grains through loss/formation of grain contacts.

Such granular materials at relatively low solid fractions can exhibit a fluid-like behavior under large macroscale shearing deformations [59, 60], in which the elasto-frictional grain-grain contact may also include an inelastic collisional feature. At higher solid fractions, such granular materials often exhibit compaction-dilation behavior under large macroscale shearing leading to the so called 'critical state', in which grain-scale mechanism of grain sliding, separation, and collapse/buckling of particle chains mediated by

the elasto-frictional contacts have an important role [7, 8].

The emergence of macroscale critical state as a result of the evolution of grain-scale deformations involving elastic and dissipative processes have been rarely explored, even in discrete simulations, but more so in the context of continuum mechanics. For example, discrete simulations studies seldom explore the interconnections of the loss of contact (that is the evolution of coordination number), which can be interpreted as a loss of stiffness (or damage), and irrecoverable deformations of grain assembly, which can be interpreted as macroscale plastic deformations, although such interconnections have been observed (see the concluding remarks in [61], where comment is made about plastic deformations being associated with instabilities caused by loss of contacts). In conventional elasto-plastic constitutive frameworks, even those enhanced with fabric tensor evolution, such micro-macro interconnections could be difficult to evaluate. In this sense, a feasible methodology is provided by the continuum models based upon a Granular Micromechanics Approach (GMA), which seek micro-macro identifications of grain-scale and continuum kinematical parameters, elastic and dissipative energies [62–64]. In its simplest format, a GMA considers effective grain-pair as the building block. Since a continuum material point comprises many variously oriented effective grain-pairs, the macro-scale continuum model, within the format of classical Cauchy-type continuum theory, is obtained by integrating these interactions over the orientational space of the material point.

The resultant continuum model is used to simulate conventional biaxial loading test of an initial confining stage followed by shearing stage. Different initial density states (initial void ratio) are considered in these simulations. The effect of initial confinement is first considered for the density states to verify certain classical observations related to the dependence of volume strain at failure upon initial void ratio and confinement. The emergence of critical state is simulated for 5 initial density states illustrating their influence upon the dilative and compactive behavior of granular materials. The key concern is therefore to investigate the competitive/collaborative evolution of damage and plasticity as central to the emergence of critical state.

2.1.3 One-dimensional uniaxial compression

Under highly confined conditions, an important deformation condition is that of one-dimensional compression in which also the previously discussed grain-scale mechanisms play an important role depending upon the initial density state or solid fraction. In this

thesis, the compaction behavior of these materials under one-dimensional compression is discussed assuming the grains to be cohesionless or weakly cohesive, such that the grain-scale behavior is dominantly elasto-frictional.

It is worth to note that the introduced energy functional possesses, for the first time in this granular approach, quartic terms with respect to the normal displacement, in order to predict the desired elastic hardening behavior for the first work of one-dimensional compression. This part of thesis focuses on quantitatively results validating the model findings against the experiments for 3 different specimens with different initial void ratios and presenting the potency of the mathematical model in expressing the behavior of granular materials under uniaxial compression.

The focus of this thesis for the second work of one-dimensional compression is two-fold. One, to represent the effects of various microscale deformation mechanisms by reformulating the grain-pair elastic energy functional and dissipation potential with new tangential terms and a coupling between normal and tangential parameters to better describe the nonlinearity that arise from geometrical and material effects. And two, to investigate the directional evolution of elastic energy, damage and plasticity, and the evolution of consequent induced anisotropy, when the elasto-frictional granular material is subjected to one-dimensional (uniaxial) compression. The reformulated grain-pair elastic energy and dissipation potential are implemented in the framework of GMA-based continuum model. The one-dimensional (uniaxial) compression results obtained from the derived model are then analyzed to investigate the evolution of micro and emergent macro behavior. Particularly, eigenvalues and harmonic decomposition of equivalent stiffness are utilized to study the evolution of emergent macroscale anisotropy. Additionally, it is illustrated that the nonlinear elastic and the damage-plastic behavior encoded in this GMA based model yields an apparent molecular-type, such as Lennard-Jones type, potential for the granular system. Here, it is aimed to investigate, for the case of one-dimensional (uniaxial) compression, the stress-strain response, the evolution of irreversible phenomena and induced anisotropy, with particular emphasis on the representation of tangential plasticity for the first time in the adopted GMA framework.

2.1.3.1 Review of powder compaction

Powder compaction is a manufacturing technique for crafting robust and high-performance products capable of withstanding a range of loading conditions, whose performance depends upon the complex grain-scale interactions that evolve in granular materials under

uniaxial compression. Powder compaction increases the mass density while maintaining constant mass and in the process rearranging and deforming grains irrespective of stiff or soft interface properties. The packed microstructures emerge from densifying loose powders into solid entities, thereby acquiring the desired mechanical behavior of granular materials through compression causing volume reduction and consolidation of interparticle contact bonds. The compaction increases the stiffness as well as the shear strength and the fragmentation strength of the resultant grain pack. Powder compaction has been extensively used to fabricate a wide variety of products, these include pharmaceutical pills (see Wu et al. works [65, 66] and other selected works [67, 68] for investigation of pharmaceutical tablet compaction), metallurgy manufacturing [69–71], and ceramic green microstructures [72]. In particular, die compaction represents the compression of powdered materials to obtain dense and uniform structures, i.e. maximum compression pressure or minimum form separation, by placing powders under the defined boundary conditions in a die. To better understand the compaction process of ceramic powder, Niesz [73] has reviewed the pertinent factors and their association regarding green microstructure. Notably, the cohesive frictional behavior has a key role on fracture mechanism during powder compaction within a die (see for instance [74]). Bandara et al. [75] carried mechanical testing on proppant packs in oil/gas recovery processes, revealing significant plastic deformation during the first loading cycle. The lunar and martian regolith compaction behavior has also been experimentally explored by using powder simulants that are expected to have similar composition as that on Moon and Mars [76, 77]. Mechanical behavior of a range of granular materials has been examined based on experimental investigations, such as those of clayey sands and fine-grained soils [78, 79] and tailing dam material [80].

2.1.3.2 Nonlinear continuum model based upon energy principles

Variational techniques and energy principles form the fundamental framework for the development of mathematical models needed to investigate the mechanical behavior of materials [81]. The aim of these models are the predictions of materials physical properties, including their constitutive relations and governing equations. Further, these models form the basis for the discovery of scientifically designed exotic and innovative metamaterial applications [82], such as materials with pantographic [83–85] and granular motif [86–88], that exploit higher-gradient and higher-order formulations of continuum models, see e.g. [89, 90]. These novel mathematical models are also crucial for analyzing bone remodeling [91–93] and masonry structures [94–97], including rationally predicting the tension-compression asymmetric effects [98]. Further, by extending classical continuum

theories [99], the geometrical and material nonlinearity [100, 101] has been explored by these higher-gradient theories [102, 103] from both static [104, 105] and dynamic [106] points of view. In addition, energy-based criteria for damage and plasticity [107], failure [31] and fracture [108] have been successfully developed, which can be implemented along with methodologies for proper calibration of microstructural length [109] and use of advanced numerical integration schemes [110].

2.2 Modelling of granular materials

For describing the mechanics of such frictional granular systems, it is standard to resort to either discrete modelling (see selected works that also include a brief review [3, 21, 111–113]) or continuum modelling (limited citations are included here from numerous contributions as an initial guide to an inexperienced reader [55, 64, 114–117]) or some combination of the discrete-continuum approach (such as couplings discussed in [118–122]).

2.2.1 Discrete modelling

From the viewpoint of discrete modeling, numerous efforts have been made to study critical state in both 2D and 3D simulation of particle packing using the so called discrete element method (DEM). DEM can provide the evolution of macroscopic properties such as bulk density and shear strength. As the computational domain is represented by a set of particles in DEM, grain-level interactions of a range of complexity can be represented in the simulations. Also, DEM can potentially handle many types of heterogeneities present in granular media, such as random granular structure, grain shapes and sizes, but with increasing costs associated to not only computations but also to the interpretation of the results in the light of lack of information regarding all aspects of grain properties and granular microstructures. DEM based studies typically focus upon the evaluation of the effect on critical state of various grain characteristics, such as size and shape, as well as the evolution of microstructural measures such as void ratio, coordination number, contact normal distributions (represented by a second-order tensor), "force" chains, and grain clusters. Along these lines, Rothenburg and Krut [61] presented a micromechanical theory of critical state in terms of the coordination number evolution during shear deformations based upon 2D discrete element simulations of bi-axial compression tests.

They observed that critical state is related to the notion that plastic deformations of granular materials are associated with instabilities created by disintegration of contacts during shear deformations. Fabric evolution along with volume changes in dense and loose assemblies that have relevance to critical state was studied by [123]. Ng [124] studied the critical state of assemblages of ellipsoids in DEM based numerical drained tests. Further, to investigate the critical state in the perspective of localized and diffuse failure modes, mesoscale fabric was investigated for particle packing of different initial void ratios [125]. More recently, the fundamental role of critical state in the failure of granular materials was examined by Deng et al. [126] using biaxial and proportional strain loading path discrete simulation. While discrete models have been widely used, it is well-known that DEM frameworks are computationally-inefficient, especially when a large number of particles are included whose geometry, surface characteristics and mechanical behavior have to be accurately described for realistic simulations resembling physical granular systems. Moreover, the imposition of boundary conditions can be arduous and difficult to interpret from a continuum mechanics viewpoint in many cases (see for example discussion of continuum identification from discrete models [127]). Nevertheless, the micromechanical understanding gained from these simulations are insightful and can be utilized to inform continuum models. As an example, motivated by discrete simulation results, fabric tensor (as a representation of contact normal distribution) and its evolution has been recently introduced to describe an anisotropic critical state theory for granular media by adapting conventional elasto-plastic constitutive frameworks, as elaborated by Li and Dafalias [51] and Gao et al. [128].

DEM directly considers the grain-scale properties, such as stiffness, strength, shapes, and sizes, and can be used to investigate one-dimensional compression with the ability to monitor the micro-scale behavior including particle position and contact force, and local packing density. DEM has been used to study certain features of the compaction behavior of idealized granular systems. For example, Cheng et al. [129] have employed DEM to investigate the characteristics of crushable sands, using triaxial tests to validate the numerical simulations, and compared the simulation results with experiments conducted on silica sand. Minh and Cheng [130] have presented the effect of particle-size distribution on one-dimensional compression of granular packing with non-deformable particles and compared the outcome with experimental data. Several DEM simulations have been performed for crushable particles (see [131, 132] for the effect of particle fracture and plastic deformation). Bolton et al. [133] focused on mechanical behavior of irregularly packed agglomerates by comparing breakable and unbreakable assemblies. Along a fractal distribution of particles, McDowell and de Bono [134] have simulated one-dimensional compression and explored particle crushing mechanism and fractal particle size distri-

bution replacing the breaking particle with new smaller particles while preserving mass. To investigate cyclic loading phenomena for packs, Garcia and Medina [135] utilized a numerical simulation-based upon DEM showing decreased dissipation in a dense case. Wiącek et al. [136] have investigated the evolution of contact force in binary granular mixtures under uniaxial compressive load using 3D DEM simulations, however, the directional evolution of either the dissipation potential and elastic energy or the contact force were not presented. Discrete description (see selected works that also include a brief review on the micromechanics grain breakage under one-dimensional compression [137–142]) or a hybrid approach blending discrete and continuum methodologies are existing (such as the combined couplings explored in [118, 143, 144]). Finally, Ransing et al. [145] considered compression of powders consisting of ductile and brittle particles using DEM and compared with continuum approach.

2.2.2 Continuum modelling

Continuum modeling remains the most feasible approach for describing the mechanical behavior of complex materials in which the stress–strain response exhibits non-standard behavior that could be dependent upon the sequence of loading or loading paths. Variational methods are a fundamental framework for deriving the governing equations for various physical systems (see [146–149]). To this end, variational and energy-based methods, which trace their origins to the earliest efforts at describing mechanical systems, have proven to offer particularly robust solutions. dell’Isola and Misra [82] discussed the principle of virtual work, which is a powerful tool that enables an effective micro-macro identification process and introduces the homogenization schema to explore exotic and innovative metamaterials. Variational techniques are vital for appropriately modelling and unraveling the complex mechanical properties of metamaterials (see [150] for investigating the nonlinear wave dynamics of tensegrity metamaterials, [151] for dynamic analysis of periodic material structures, and [152–154] for composite materials), as these approaches take into account not just conventional case but also dissipative processes (see selected work considering dissipative systems [92, 155–157]). Further, these methods have been harnessed to develop models beyond classical elasticity theory to accurately predict the behavior of complex multi-scale structures (see for example strain-gradient [85, 158–163] or higher-gradient [102, 103, 164–166] theory). These approaches offer a way of affirming the strain-gradient constitutive parameters for mechanical metamaterials that exhibit non-identical behaviors (see [167, 168]). In particular, asymptotic homogenization technique was utilized to determine the metamaterial constitutive parameters by linking the micro-

and macro-scale characteristics with strain gradient theory in [162], and also through solving a boundary value problem with FEM in [169]. Innovative experimental-numerical methodologies have been proposed to predict material characteristics by incorporating experimental tests and numerical simulations using artificial neural networks [170–172], as well as a combination of digital image analysis and FEM simulations [173–175]. Additionally, Ramaglia et al. [94, 176] conducted the numerical investigations focusing on the understanding and effectiveness of fiber-reinforced strengthening strategies for masonry structures. Moreover, continuum models treat the materials as continuous medium, focusing on predicting the macroscopic behavior of such pantographic metamaterials [177–183].

Several attempts have been made with regard to the representation of critical state within continuum models of frictional granular materials. The earliest efforts in this regard is the application of plasticity theory to develop the Cam-clay models and their modifications (see [55] for discussion on these models). Sheng et al. [184] discussed the numerical issues related to the finite element method (FEM) implementation of two generalized critical state soil models, namely Cam-clay model and unified clay and sand model. Along a different approach, Wu et al. [185] have obtained constitutive relationships that incorporate critical state conditions within a hypoplastic framework without recourse to classical concepts of yield surface, plastic potential, flow/hardening rules and elastic-plastic decomposition. Saberi et al. [186] proposed an elasto-plastic constitutive model based on two-surface plasticity theory, which is also suitable for critical state concept, to reveal the behavior of gravelly soil-structure (loose and dense) interfaces under monotonic and cyclic loading. Other advances in the application of plasticity theory to describe critical state includes bounding surface models [187] and further modifications to include effects of fabric evolution (see among a series of articles by Dafalias and coworkers [51, 52, 115, 128]). Liu et al. [188] utilized a high-fidelity discrete model for experimental database extension to illustrate a machine learning approach for identification of these types of critical state plasticity models. In addition, continuum models with microstructural motivations have also been presented to describe the critical state phenomena [189–191].

Numerical analysis of powder compaction has been explored by using continuum FEM or DEM or through coupled FEM-DEM approaches, as exemplified in the following works [145, 192, 193]. There are several studies that explore the macroscopic response of one-dimensional compression of granular mechanics grounded in continuum mechanics. The macro-scale behavior consists of elastic and dissipative phenomena resulting from the development of grain-scale deformations. Also, an early pioneering study served by Roscoe and Burland [194] that is the modified Cam-clay model, provides a predictive manner for the stress-strain link by utilizing elastic and plastic components. In elasto-plastic theory,

which is commonly conducted in this concept, plastic deformation occurs according to the loading path (see referred works [195, 196]). For example, Chang and Hicher [189] have established the elastic-plastic model by following Hertz-Mindlin's elastic law and Mohr-Coulomb's plastic law to derive the relation between stress and strain tensors by mobilizing particle contact. Einav has introduced continuum breakage mechanics to model crushable granular materials in a series of articles (see how addressed the dissipative process in Part 1 [197] without plasticity and Part 2 [198] including plasticity), incorporating the concept of breakage related to the hardening phenomenon through energy calculation and grain size distribution measurement. Chong and Santamarina [199] proposed the soil compressibility model to satisfy the asymptotic void ratios by modifying the existing models and functions at both low and high effective stress levels. Further, Cocks [200] and Cocks and Sinka [201] have constructed the constitutive models of plastically deforming powder compaction (metal), sintering (ceramic), and flow processes by offering valuable insights into the evolution of the actual yield surface. Alternatively, Russell [202] has proposed that the energy dissipation, which involves plastic work due to the creation of surface area of the fragments and load distribution and adapted this mechanism into a Cam-clay type energy equation. Park et al. [203] have proposed a yield criterion by modeling of metal powder die compaction which facilitates handling of bulk materials. Many other models of powder compaction using continuum approach have been considered (see for example [204]).

Alternatively, Richard et al. [205] have considered statistical mechanics approaches to describe the dynamics of powder compaction and their seeming correspondence with glass formers. More significantly, methods for continuum modeling of granular materials in terms of grain-scale mechanism by referring to orientational distribution of contacts have been proposed (see [206, 207]). Along these lines, the scientists have recently advanced a GMA for continuum modeling which considers Piola's ansatz for micro-macro kinematic identification [63, 160, 177, 208–212] and grain-pair elastic-damage-plastic interactions to find the elastic energy density and dissipation potential at the macro-scale [7–10, 107].

2.3 Granular Micromechanics Approach based damage-elasto-plastic micromechanical continuum model

Examining complex materials plays a prominent role in novel continuum modeling approaches by establishing a stress-strain response according to the loading path and ex-

hibiting exotic behaviors [213]. The continuum modeling of granular materials, which entails a detailed and comprehensive effort in engineering and scientific research, serves as a powerful tool for examination. The continuum framework for granular materials simplifies complex particle interactions and provides a well-developed theoretical method, leveraging practical approaches to describe macroscopic properties such as stress, strain, and density. Typical experimental results of classical loading scenarios can be targeted and replicated through new continuum models. Significant attempts have been made in deriving energy and variational methods and aimed at understanding mechanical behavior (see a limited selection of works for readers interested in continuum modeling for deformable solids [81, 150, 151, 214]). Advanced computational techniques beyond classical elasticity theory are necessitated to accurately predict the behavior of complex multi-scale structures (see for example strain-gradient theory [159, 161, 162, 215, 216]). Higher-gradient theories [103, 169, 217] generalize classical elasticity to elucidate geometric and size-dependent effects. Further, the refinement of generalized elasticity theories by incorporating higher-order models enhance geometric nonlinearity, finite strain measures, and microstructural scales using Lagrangian and Eulerian representations [99, 102, 212, 218, 219]. The potential of new mathematical models based on variational methods is discussed, and the validation scenarios are presented using different techniques, such as those applied to pantographic metamaterial [157, 179, 220, 221], granular motif [222], bone remodeling [91], and masonry [94–96].

Establishing continuous models for granular materials to investigate complex assemblies of particles requires a strong effort and a thorough understanding of the relevant phenomena. A GMA framework effectively characterizes granular materials and has been successfully applied in elastic [223], damage [108, 224], and elasto-plastic-damage models [7–10, 107]. In parallel, a GMA is designated to characterize the behavior of granular materials (see the exemplified works for granular motif [62, 87, 88, 222]). In this context, continuum models addressing effective grain-pair interactions are built upon GMA principles. This continuum description is kinematically associated with granular micromechanics via Piola’s ansatz (see, for example, homogenizing micro-models for metamaterials [210, 211]). At the microscale, the material behavior is characterized by two grains connected through spring elements in both the normal and shear directions, and these springs can experience damage and plasticity. At the macroscale, the mechanical behavior of the granular material results from the evolution of damage and plasticity of numerous grain-pairs interacting in various spatial directions. Homogenization is the schema of exploring the macroscopic response from the behavior of individual grain-pairs at the microscale by integrating the contributions of grain-pairs over all orientations. By integrating effective grain-scale relationships, a GMA reveals average macro-scale behaviors across all

orientations. In the proposed framework, no representative volume element is utilized. The continuum model detects grain-pair and kinematic variables from the micro-macro relationship regarding elastic and dissipation potential functionals. To achieve the desired behaviors in the stress-strain response and the coupled damage and plasticity with respect to these energies, this thesis expands upon previous studies and integrates them into a new energy functional [7–10, 107, 224, 225]. These effective energies, defined by damage-elasto-plastic spring elements, explore grain-scale interactions in normal and tangential directions, where the normal component aligns with the vector connecting the grains, and the tangential component is perpendicular to this direction. Homogenized energy functionals are adopted, and a hemi-variational principle is utilized to derive the Karush-Kuhn-Tucker (KKT) conditions via governing equations (see [224, 226, 227] for the application of a hemi-variational principle). Additionally, KKT conditions govern the evolution of irreversible phenomena related to damage and plasticity across all grain-pair orientations. In the proposed model, two dissipation mechanisms: damage and plasticity have been incorporated. Damage (or loss of stiffness) is the cumulative effect of grain-scale mechanisms that includes the loss of lateral support or confinement within the granular assembly, the collapse or buckling of particle chains and clusters due to particle rotation, rolling or grain sliding. Damage is, therefore, not treated as simply the result of loss of contacts between grains, but as a more complex phenomenon in which the micromechanical response weakens in particular orientations due to a change of microstructure that could also include loss of contacts. Further, grain-pair sliding and separation are the genesis of plasticity, which is characterized by the effective accumulation of irreversible deformations. These two coupled phenomena comprehensively describe the rate-independent dissipative mechanisms governing the behavior of granular materials. A series of numerical simulations has successfully demonstrated this model's efficacy in both homogeneous and non-homogeneous deformations [224, 226–229].

This thesis aims to extend a GMA continuum model to address the critical state and one-dimensional compression concerning grain-scale interactions, integrating new elastic energy and dissipation potential within the constitutive model. For instance, Placidi et al. [225] demonstrated the flexibility of this model by exhibiting the experimental results with numerical simulations using a granular micromechanics-based model for Ultra High Performance Fiber-Reinforced Concrete (UHP-FRC). Yilmaz et al. [7–10] investigated the emergence of critical state and the one-dimensional compression response by applying a GMA with appropriately formulated effective grain-scale elastic energy and dissipation potential functionals. To demonstrate a GMA's capability in identifying micro-macro interactions at the grain-scale, the critical state and one-dimensional compression concepts are first examined on a 2D model.

Emergence of critical state in granular materials

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Novel continuum modeling approaches, developed for complex materials, consist of the description of a continuum which comprises all the complex interactions occurring among the structural components constituting the material. However, modeling these complex media presents significant challenges and requires an in-depth understanding of the relevant phenomena. To address these challenges, the significance of energy and variational

methods have been increasingly recognized due to their foundational nature for development of mechanical theories [82]. Among these methods, the continuum model presented by dell’Isola et al. [177] illustrates the potential of variational techniques to systematically introduce new mathematical models robustly. Researchers have validated this model in numerous studies, demonstrating its versatility [178, 181, 230, 231]. Furthermore, similar approaches have been successfully adapted to model elasticity, damage, and elasto-plasticity in various classes of granular materials within the context of a Granular Micromechanics Approach (GMA) [63, 222, 223, 226, 227].

The mechanical response of granular materials, exemplified by frictional grain interactions, is characterized by a critical state in which deformation occurs without change of material volume or stresses when subjected to large shear deformation. The content presented in this chapter builds upon and partially incorporates material previously published in the following works:

1. Yilmaz et al. (2024), *Emergence of critical state in granular materials using a variationally-based damage-elasto-plastic micromechanical continuum model*.
DOI: 10.1002/nag.3795
2. Yilmaz et al. (2025), *A parametric study on a granular micromechanics continuum-based hemivariational approach: unraveling the emergence of critical states in granular materials*.
DOI: 10.2140/memocs.2025.13.25

Building upon these works, this chapter explores the emergence of critical-state behavior in granular materials, leveraging the insights gained from a GMA-based continuum model.

3.1 Mathematical model

The present model is conceived by improving the framework presented by Placidi et al. [107, 228]. Compared to the works [107, 224, 226–228], a new type of dissipation energy potential is adapted to examine complex coupled nature of damage and plasticity at the grain-scale of frictional granular materials. To this end, the constitutive model is first introduced by identifying grain-pair relative displacements in terms of the continuum strain measure. The grain-pair elastic and dissipation potential energies are then

introduced and a hemi-variational principle is applied to derive the Karush-Kuhn-Tucker (KKT) conditions for all the grain-pairs. A hemi-variational framework allows for modeling of elasto-plastic-damage problem without requiring any additional assumptions, such as flow rule and plastic potentials. These KKT conditions characterize the evolution of irreversible phenomena of damage and plasticity at the grain-scale. Further, a GMA micro-macro identification is utilized to define the continuum constitutive relationships. The rest of this chapter will explain the mathematical model in depth.

3.1.1 Piola's ansatz and continuum deformation measure

As depicted in Fig. 3.1, in the discrete description, a set of N grains is considered in a 2D Euclidean space E^2 . The position of the i^{th} grain in the reference configuration is denoted by $\mathbf{X}_i$, and its position in the deformed configuration at time t is defined through placement function $\chi_i(t)$ as follows

$$\mathbf{x}_i = \chi_i(t) = \mathbf{X}_i + \mathbf{u}_i(t), \quad i = 1, \dots, N, \quad (3.1)$$

where $\mathbf{u}_i(t)$ is the displacement vector of the i^{th} grain. Besides, in the continuum description, a continuous body $\mathcal{B}$ in E^2 containing very large (infinitely many) number of grains is considered (Fig. 3.1). The position of a material point in $\mathcal{B}$ is denoted by $\mathbf{X}$ in the reference configuration, and its position in the deformed configuration at time t is defined through placement function $\chi(\mathbf{X}, t)$ as follows

$$\mathbf{x} = \chi(\mathbf{X}, t) = \mathbf{X} + \mathbf{u}(\mathbf{X}, t), \quad (3.2)$$

where $\mathbf{u}(\mathbf{X}, t)$ is the displacement vector. Through Piola's ansatz in [210], the relationship between discrete and continuum configurations is set up to explore a connection between the placement function of N grains χ_i within the discrete description and the placement function χ for the continuous body $\mathcal{B}$:

$$\chi(\mathbf{X}_i, t) = \chi_i(t), \quad i = 1, 2, \dots, N. \quad (3.3)$$

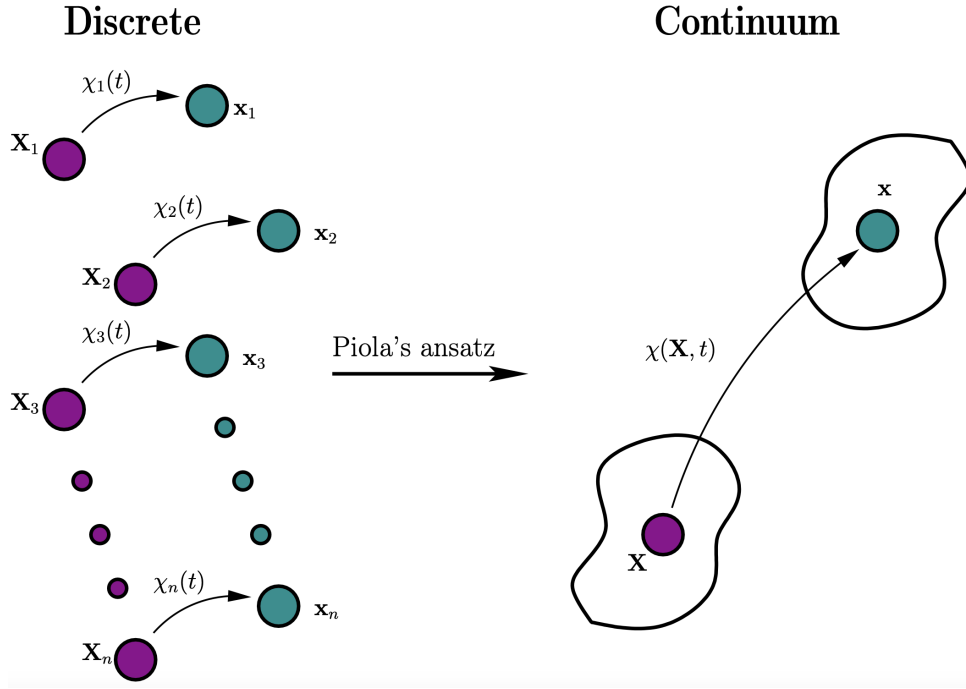


Figure 3.1: Description of discrete and continuum mechanics.

Let us consider two adjacent grains, n and p , located at $\mathbf{X}_n$ and $\mathbf{X}_p$ in the reference configuration, respectively. The relative position vector in the reference configuration (position of grain n with respect to grain p) is expressed by

$$\mathbf{X}_n - \mathbf{X}_p = L \hat{\mathbf{c}}, \quad (3.4)$$

where $\hat{\mathbf{c}}$ is a unit vector directed from grain p to grain n , and L is the distance between the two grains. By Piola's ansatz, their positions in the deformed configuration are given by $\mathbf{x}_n = \chi(\mathbf{X}_n, t)$ and $\mathbf{x}_p = \chi(\mathbf{X}_p, t)$, respectively. Then, the relative position vector in the deformed configuration is expressed by

$$\mathbf{x}_n - \mathbf{x}_p = \chi(\mathbf{X}_n, t) - \chi(\mathbf{X}_p, t). \quad (3.5)$$

Following the works of Placidi et al. [107, 227, 228], an objective relative displacement $\mathbf{u}^{np}$ is defined as follows

$$\mathbf{u}^{np} = \mathbf{F}^T(\mathbf{x}_n - \mathbf{x}_p) - (\mathbf{X}_n - \mathbf{X}_p), \quad (3.6)$$

where $\mathbf{F}$ is the deformation gradient, $\mathbf{F} = \nabla \chi$. Assuming the grains have similar defor-

mation, the Taylor's series expansion of placement $\chi(\mathbf{X}_n, t)$ around $\mathbf{X} = \mathbf{X}_p$ provides

$$\mathbf{x}_n = \chi(\mathbf{X}_n, t) \cong \mathbf{X}_p + L \mathbf{F} \hat{\mathbf{c}}, \quad (3.7)$$

where this expansion is ended at the first order only for the sake of simplicity and where the deformation gradient is expressed in terms of the gradient of the placement function χ evaluated at the position $\mathbf{X} = \mathbf{X}_p$ as follows

$$\mathbf{F} = \nabla \chi|_{\mathbf{X}=\mathbf{X}_p}. \quad (3.8)$$

For the sake of clarity, index notation is used in the rest of the text unless otherwise specified. Then, the objective relative displacement may be rewritten as follows

$$u_i^{np} = 2L G_{ij} \hat{c}_j, \quad (3.9)$$

where $\mathbf{G}$ is the Green – St-Venant tensor, expressed by

$$G_{ij} = \frac{1}{2} (F_{ai} F_{aj} - \delta_{ij}). \quad (3.10)$$

In the current work, only cases with homogeneous deformation are considered; consequently, the gradient of the Green–St. Venant strain ($G_{ij,h} = 0$), which becomes critically important for nonhomogeneous deformations [232], is not included. It is worth to note that this condition makes the simplification of ending the Taylor series expansion in Eq. 3.7 at first order not only a natural one but also without any practical consequences on the level of result approximations.

The normal displacement (a scalar quantity) is introduced by the half projection of the objective relative displacement vector on the unit vector $\hat{\mathbf{c}}$ as follows

$$u_\eta = \frac{1}{2} u_i^{np} \hat{c}_i, \quad (3.11)$$

and the tangent displacement vector u_{τ_i} by the projection of the objective relative displacement on the unit vector orthogonal to $\hat{\mathbf{c}}$ and its square u_τ^2 are determined as shown below

$$u_{\tau_i} = u_i^{np} - u_j^{np} \hat{c}_j \hat{c}_i, \quad u_\tau^2 = u_{\tau_i} u_{\tau_i}. \quad (3.12)$$

Then, by inserting Eq. 3.9 into Eqs. 3.11 and 3.12, the normal displacement, its square,

and the square of the norm of the tangent displacement vector are respectively given by

$$u_\eta = LG_{ij}\hat{c}_i\hat{c}_j, \quad (3.13)$$

$$(u_\eta)^2 = L^2G_{ij}G_{ab}\hat{c}_i\hat{c}_j\hat{c}_a\hat{c}_b, \quad (3.14)$$

$$u_\tau^2 = 4L^2G_{ij}G_{ab}(\delta_{ia}\hat{c}_j\hat{c}_b - \hat{c}_i\hat{c}_j\hat{c}_a\hat{c}_b). \quad (3.15)$$

These grain-pair variables represent two independent scalar invariants formed using the vectors u_i^{np} and $\hat{c}_i$. The first (i.e., the normal displacement) scalar invariant can be positive or negative, and the second (i.e., the squared tangential displacement) can only be positive. The elasto-plastic decomposition of those irreducible scalar invariants in Eq. 3.15 takes this comment on their signs into account. In particular, the aim is to respect the rule that the elastic and plastic parts of a positive quantity should always be positive and that of a general one does not have a prescribed sign.

The normal displacement u_η is decomposed into elastic and plastic parts as follows

$$u_\eta = u_\eta^{el} + u_\eta^{pl}, \quad (3.16)$$

and the square of its elastic part is given by

$$(u_\eta^{el})^2 = (u_\eta - u_\eta^{pl})^2 = L^2G_{ij}G_{ab}\hat{c}_i\hat{c}_j\hat{c}_a\hat{c}_b + (u_\eta^{pl})^2 - 2Lu_\eta^{pl}G_{ij}\hat{c}_i\hat{c}_j. \quad (3.17)$$

The square of plastic tangential displacement is defined only by u_τ^{2pl} , and the square of elastic tangent displacement is introduced via

$$u_\tau^{2el} = |u_\tau^2 - u_\tau^{2pl}|, \quad (3.18)$$

where u_η^{el} and u_η^{pl} are the normal elastic and plastic displacements, and u_τ^{2el} and u_τ^{2pl} are the squared elastic and plastic tangential displacements. Eq. 3.17 is an additive elasto-plastic decomposition for the normal displacement given in Eq. 3.16. Eq. 3.18 guarantees that the squared elastic tangential displacement u_τ^{2el} is positive even when the squared plastic part u_τ^{2pl} becomes larger than the square of the tangential displacement u_τ^2 , i.e. when $u_\tau^{2pl} > u_\tau^2$. This situation arises during unloading process when the squared tangential plastic displacement u_τ^{2pl} does not decrease, as can be seen by definition, and the square of the tangential displacement u_τ^2 decreases and reaches values less than the squared tangential plastic displacement u_τ^{2pl} , leading to a reverse elastic loading in the tangential direction.

Further, it is notable that the plastic normal displacement u_η^{pl} does not have a prescribed sign, and it is decomposed into two positive quantities, λ_η^t and λ_η^c , which represent the accumulated positive plastic variables for tension and compression in the normal direction, respectively. The normal plastic displacement u_η^{pl} (which can be either positive or negative) is calculated by subtracting the compression plastic variable from the tension plastic variable as given in Eq. 3.19. Further, the squared tangential plastic displacement u_τ^{2pl} is assumed to correspond to its positive accumulation λ_τ^2 as given in Eq. 3.19.

$$u_\eta^{pl} = \lambda_\eta^t - \lambda_\eta^c, \quad u_\tau^{2pl} = \lambda_\tau^2. \quad (3.19)$$

3.1.2 Elastic energy

An elastic energy U^{np} associated with a generic grain-pair interaction (grains n and p) is first discussed at the discrete level. To do this, the recoverable elastic parts of the normal and tangential components of the objective total grain-grain relative displacement given in Eqs. 3.17 and 3.18 are combined in a quadratic form as follows

$$U^{np} = \frac{1}{2}k_{\eta D} (u_\eta^{el})^2 + \frac{1}{2}k_{\tau D} u_\tau^{2el}, \quad (3.20)$$

where the damaged normal stiffness $k_{\eta D}$ in Eq. 3.20, varies with the elastic normal displacement u_η^{el} under tension and compression as follows

$$k_{\eta D} = \tilde{k}_{\eta D}(u_\eta^{el}) = \frac{1}{2} (k_{\eta D}^t + k_{\eta D}^c) + \frac{1}{\pi} (k_{\eta D}^t - k_{\eta D}^c) \arctan \left(\frac{u_\eta^{el}}{\alpha} \right), \quad (3.21)$$

where α is a regularization parameter for the tension-compression transition. In the limit of this regularization parameter α to zero, the damaged normal stiffness is found as follows

$$\lim_{\alpha \rightarrow 0} k_{\eta D} = \Theta(u_\eta^{el})k_{\eta D}^t + \Theta(-u_\eta^{el})k_{\eta D}^c, \quad (3.22)$$

where the function $\Theta(x)$ interprets the role of Heaviside function where α goes to 0. The sign of u_η^{el} determines whether the current state is tension or compression. Importantly, as illustrated in Fig. 3.2, it is evident that $k_\eta^t \ll k_\eta^c$. As α approaches zero, an abrupt transition between tension and compression is achieved based on the properties of the Heaviside function. It should be noted that the value of α should be much smaller than u_η^{el} . The damage phenomenon is characterized by the normal D_η and the tangential D_τ damage variables. The interpretations regarding the damage quantities are clearly revealed according to Eq. 3.23. The damaged stiffness (and the corresponding elastic

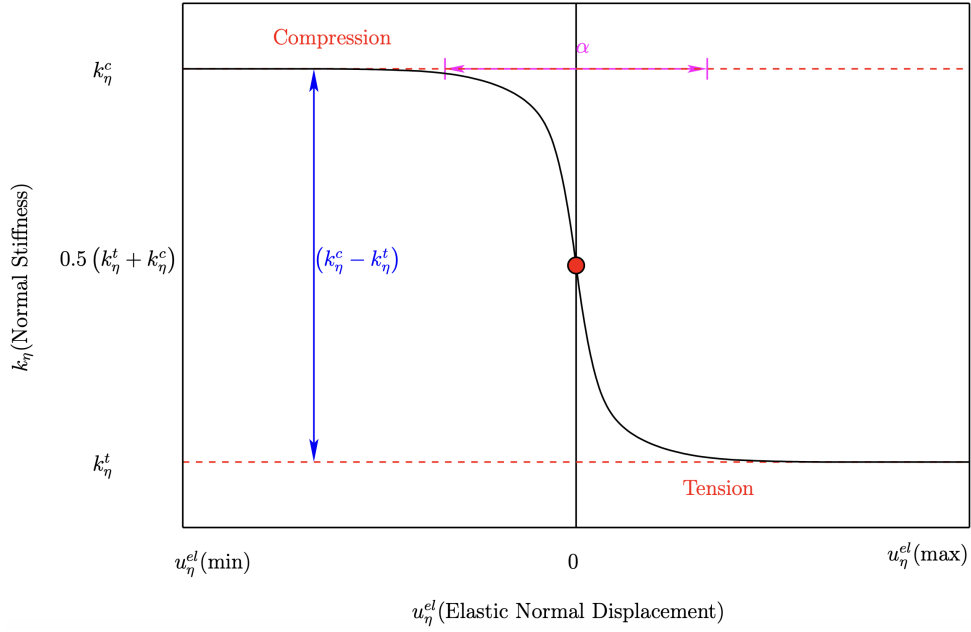


Figure 3.2: Normal stiffness k_η under tension and compression as a function of the elastic normal displacement u_η^{el} .

energy described in Eq. 3.20) approaches zero when the damage quantities approach the unity values.

For computations, the value of α should be much smaller than u_η^{el} . The damaged tension ($k_{\eta D}^t$) and compression ($k_{\eta D}^c$) normal stiffness, in which $k_{\eta D}^t \ll k_{\eta D}^c$, and the damaged tangential stiffness $k_{\tau D}$, are described in Eq. 3.23. Misra and Yang [233] modeled cohesive materials using pseudo-bonds, which inspired the consideration of asymmetry in grain-scale normal stiffness between tension and compression. In addition, Misra and Placidi [98] investigated the emergence of bimodulus (tension–compression asymmetric) behavior by attaining different values not only for the normal stiffness as it is here done in Eq. 3.21 but also for the tangential stiffness, for which a representation similar to Eq. 3.21 can be done. The damaged tension $k_{\eta D}^t$ and compression $k_{\eta D}^c$ normal stiffness and the damaged tangent $k_{\tau D}$ stiffness are defined as follows

$$k_{\eta D}^t = k_\eta^t(1 - D_\eta), \quad k_{\eta D}^c = k_\eta^c(1 - D_\eta), \quad k_{\tau D} = k_\tau(1 - D_\tau). \quad (3.23)$$

Indeed, k_η^t , k_η^c , and k_τ are the non-damaged normal stiffness, respectively, in tension, in compression, and the non damaged tangential stiffness. The damage phenomenon is characterized by two variables, normal damage parameter D_η and tangential damage parameter D_τ . The expressions 3.21 and 3.22 make clear the following interpretations of the damage quantities. If damage quantities approach the unity value, the damaged

stiffness goes to zero as well as the corresponding elastic energy in Eq. 3.20. In a given specimen of frictional granular material, all the possible M grain-pair interactions are considered. The total elastic energy is assumed to be the sum of the elastic energy U^{np} for all such pairs as follows

$$U_M = \sum_{np=1}^M U^{np}. \quad (3.24)$$

To obtain an elastic energy density in the continuum description, the simple homogenization rule discussed in Barchiesi et al. [223] is adopted,

$$U_M \xrightarrow{M \rightarrow \infty} U = \int_{\mathcal{S}} \left[\frac{1}{2} k_{\eta D} (u_{\eta}^{el})^2 + \frac{1}{2} k_{\tau D} u_{\tau}^{2el} \right] d\ell, \quad (3.25)$$

where all the grain-pairs are characterized by their direction $\hat{\mathbf{c}}$. The region $\mathcal{S}$ is the unit circle to which $\hat{\mathbf{c}}$ belongs, and $d\ell$ is the infinitesimal element $d\theta$ according to Fig. 3.3. In other words, the orientation $\theta \in [0, 2\pi]$ in an orthonormal frame of reference $(O, \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2)$ defines the unit vector, $\hat{\mathbf{c}} = \cos \theta \hat{\mathbf{e}}_1 + \sin \theta \hat{\mathbf{e}}_2$, with respect to the polar representation. Therefore, stiffnesses and damage parameters depend on the orientation in the continuum description: $k_{\eta} = \tilde{k}_{\eta}(\theta)$, $k_{\tau} = \tilde{k}_{\tau}(\theta)$, $D_{\eta} = \tilde{D}_{\eta}(\theta)$, and $D_{\tau} = \tilde{D}_{\tau}(\theta)$.

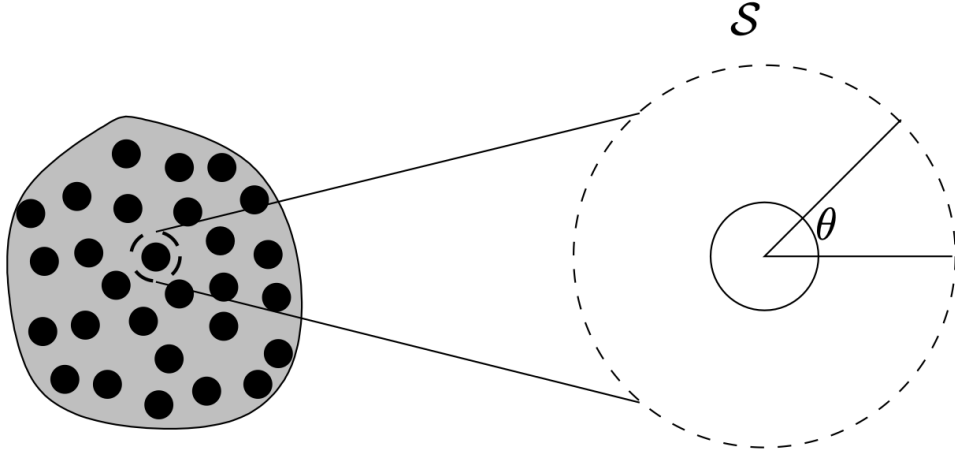


Figure 3.3: Orientation based grain-pair interaction.

Overall, the continuum elastic energy density can be written in the following form by using Eqs. 3.15 and 3.17 as follows

$$U = \frac{1}{2} \mathbb{C}_{ijab} G_{ij} G_{ab} + \mathbb{P}_{ij} G_{ij}, \quad (3.26)$$

where $\mathbb{C}_{ijab}$ and $\mathbb{P}_{ij}$ elastic stiffness tensors given by

$$\begin{aligned} \mathbb{C}_{ijab} = & L^2 \int_{\mathcal{S}} k_{\eta}(1 - D_{\eta}) \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b d\ell \\ & + L^2 \int_{\mathcal{S}} k_{\tau}(1 - D_{\tau}) ((\delta_{ia} \hat{c}_j \hat{c}_b + \delta_{ib} \hat{c}_j \hat{c}_a + \delta_{ja} \hat{c}_i \hat{c}_b + \delta_{jb} \hat{c}_i \hat{c}_a) - 4 \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b) d\ell, \end{aligned} \quad (3.27)$$

and

$$\mathbb{P}_{ij} = -L \int_{\mathcal{S}} k_{\eta}(1 - D_{\eta}) u_{\eta}^{pl} \hat{c}_i \hat{c}_j d\ell. \quad (3.28)$$

Notably, the second-order tensor $\mathbb{P}_{ij}$ which is referred to as pre-stress tensor has the normal plastic relative displacement component in its definition. For interested readers, the work of [177, 227] is referred on the details of adapted homogenization approach.

3.1.3 Dissipation energy potential

Two dissipation phenomena are considered as damage and plasticity in the proposed model. Damage indicates the cumulative effects arising from grain-scale mechanisms, and therefore introduces the collapse or buckling of particle chains and clusters due to particle rotation and rolling or grain sliding, and the loss of lateral support or confinement within the granular assembly. The proposed continuum model interprets damage as a loss of stiffness rather than the creation or loss of contacts between grains. Further, plasticity is characterized by the effective accumulation of irreversible deformations and essentially driven by grain-pair sliding and separation along with the considered orientations. Subsequently, these two coupled phenomena provide a comprehensive description of the rate-independent dissipative mechanisms governing the behavior of granular materials. Six fundamental kinematic variables (one vectorial and five scalar variables), u_{η} , u_{τ}^2 , D_{η} , D_{τ} , λ_{η}^t , and λ_{η}^c , representing damage and plasticity, respectively, for a generic grain-pair, are utilized to model dissipation energy potential. Here, λ_{η}^t and λ_{η}^c are the tension and compression plastic variables, respectively. The reason for the additive decomposition in Eq. 3.19 will be clear in Subsection 3.1.4. The total dissipation energy potential W can be decomposed into two parts

$$W = W_D + W_{pl}, \quad (3.29)$$

where W_D represents dissipated energy potential due to damage while W_{pl} represents dissipated energy potential due to plastic behavior. The term W_D can be further decomposed into its normal and tangential parts as follows

$$W_D = W_D^\eta + W_D^\tau, \quad (3.30)$$

where

$$W_D^\eta = \frac{1}{2} k_\eta^c (B_\eta)^2 \left[-D_\eta + \frac{2}{\pi} \tan \left(\frac{\pi}{2} D_\eta \right) \right] + \frac{1}{2} k_\eta^t (B_\eta)^2 \left[2 + (D_\eta - 1) (2 - 2\log(1 - D_\eta) + (\log(1 - D_\eta))^2) \right], \quad (3.31)$$

and

$$W_D^\tau = \frac{1}{2} k_\tau (B_\tau)^2 \left[2 + (D_\tau - 1) (2 - 2\log(1 - D_\tau) + (\log(1 - D_\tau))^2) \right]. \quad (3.32)$$

The choice for the functional forms in Eqs. 3.31 and 3.32 will be discussed in Subsection 3.1.4. It is worthwhile to note here that in the limit of damage variable going to unity, the dissipation energy potentials tend to infinity. This makes such an occurrence impossible and the numerical computation more stable. It is also evident that B_η^c and B_η^t are two characteristic displacements that correlate normal damage dissipation in compression and tension, respectively. It is reasonable to expect that $B_\eta^t \ll B_\eta^c$ for lightly-cohesive granular materials. In fact, damage rapidly progresses to its limit in tension with significantly lower elastic relative displacement. In addition, B_η and B_τ are the characteristic displacements associated with the normal and tangent damage variables, respectively, expressed as follows

$$B_\eta = \tilde{B}_\eta(u_\eta^{el}) = \frac{1}{2} (B_\eta^t + B_\eta^c) + \frac{1}{\pi} (B_\eta^t - B_\eta^c) \arctan \left(\frac{u_\eta^{el}}{\alpha} \right), \quad (3.33)$$

$$B_\tau = \tilde{B}_\tau(u_\tau^{el}) = \frac{1}{2} (B_{\tau 0} + \alpha_1 B_{\tau 0}) + \frac{1}{\pi} (B_{\tau 0} - \alpha_1 B_{\tau 0}) \arctan \left(\frac{u_\tau^{el}}{\alpha} \right), \quad (3.34)$$

here, α_1 introduces an additional constitutive parameter and regularizes the amount of characteristic damage displacements in tension. Here in Fig. 3.4, the distinction between tension and compression states are illustrated for the characteristic displacement B_τ , and the interpretation of parameters α and α_1 are made explicit. Besides, α_1 is introduced in order to model (with $\alpha_1 > 1$) a Coulomb-type frictional effect by ensuring that the characteristic tangential damage displacement B_τ depends upon the elastic normal displacement. In this way, the compression (i.e. with $u_\eta^{el} < -\alpha$) damage characteristic

displacement is $B_\tau = \alpha_1 B_{\tau 0}$, which is higher than that in tension (i.e. with $u_\eta^{el} \gg \alpha$) given as $B_\tau = B_{\tau 0}$, thus inducing a normal loading dependent frictional threshold for a given grain-pair direction. Further, the characteristic tangential damage displacement B_τ is explicitly controlled by $B_{\tau 0}$.

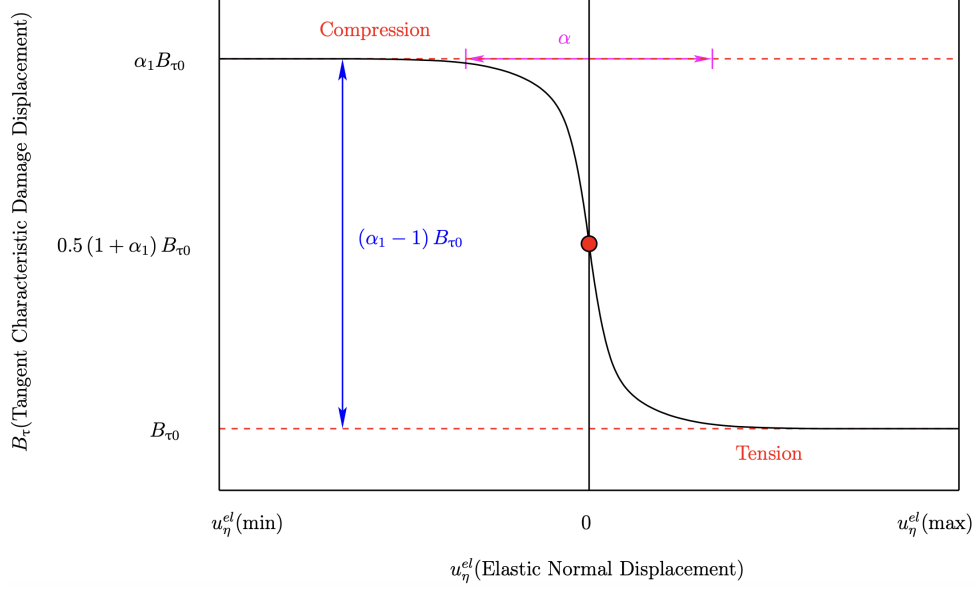


Figure 3.4: Characteristic tangential damage displacement B_τ under tension and compression depending on elastic normal displacement u_η^{el} .

The dissipation energy potential due to the normal component of plastic behavior is introduced as follows

$$W_{pl} = W_{pl}^\eta = (1 - D_\eta) (\sigma_\eta^t \lambda_\eta^t + \sigma_\eta^c \lambda_\eta^c + \sigma_{\eta\eta}^c (\lambda_\eta^c)^2), \quad (3.35)$$

where the yielding conditions of the damage-elasto-plastic behavior in tension and compression are determined by the constitutive parameters σ_η^t and σ_η^c , respectively, and the plastic hardening behavior is characterized by the term $\sigma_{\eta\eta}^c$. The physical interpretation of the constitutive parameters introduced in the dissipation energy potential, will be discussed further in Subsection 3.1.4. Here, it must be remarked that the tangential component of the plastic dissipation potential W_{pl} is not considered in this chapter. Moreover, the dissipation potential energy for plastic component W_{pl} is different than that proposed by Placidi et al. [107]. A new type of dissipation energy potential is adapted for plasticity phenomenon to model critical state simulations. It is finally worth noting that, in the proposed approach, the energy formalism is the main ingredient of the model, and it can be distinguished that all terms being positive. The formalism does not explicitly enforce consistency with the second law of thermodynamics. From a mathematical perspective,

the framework imposes no restrictions, and the total energy functional is a positive function. Moreover, the elastic potential is defined as a quadratic function (see Eq. 3.20) and positive definite. Dissipation potential can be distinguished into damage and plastic components. The damage dissipation potential W_D (see Eqs. 3.31 and 3.32) is always an increasing function with respect to damage and, because damage itself is an increasing function of time, W_D is also an increasing function of time. While the plastic dissipation potential W_{pl} (see Eq. 3.35) is positive definite and zero at the initial state, W_{pl} does not consistently exhibit an increasing behavior. This characteristic arises from its dependence on $1 - D_\eta$, but maintains overall thermodynamic admissibility by remaining positive throughout the simulations.

3.1.4 Hemi-variational formulation: governing equations and Karush-Kuhn-Tucker conditions

Let us consider a monotonously increasing time sequence $t_i \in \{t_i\}_{i=0,\dots,F}$ where $t_i \in \mathbb{R}$ and $F \in \mathbb{N}$. Neglecting kinetic energy, the action functional of the system is expressed by

$$\mathcal{E} = \int_{t_0}^{t_F} \left\{ \int_{\mathcal{B}} (U + W) d\Omega - U^{\text{ext}} \right\} dt, \quad (3.36)$$

where U^{ext} is the external energy

$$U^{\text{ext}} = \int_{\mathcal{B}} \mathbf{b}^{\text{ext}} \cdot \mathbf{u} d\Omega + \int_{\partial_t \mathcal{B}} \mathbf{t}^{\text{ext}} \cdot \mathbf{u} d\ell, \quad (3.37)$$

where $\mathbf{b}^{\text{ext}}$ and $\mathbf{t}^{\text{ext}}$ are the external forces distributed, respectively, on the domain $\mathcal{B}$ and of the part $\partial_t \mathcal{B}$ of the boundary $\partial \mathcal{B}$ on which Neuman conditions are imposed.

A motion is defined as a displacement family $\mathbf{u}(\mathbf{X}, t_i)$ defined for each time $t = t_0, t_1, \dots, t_F$. For a specific time t , the set AM_t of kinematically admissible displacements is determined, and the associated space of kinematically admissible variations is designated as the set AV_t , i.e. $\delta \mathbf{u}(\mathbf{X}, t_i) \in AV_t$. The kinematically admissible displacement is constrained, e.g., by some imposed Dirichlet boundary conditions on a part $\partial_{\mathbf{u}} \mathcal{B}$, of the boundary $\partial \mathcal{B}$ such that $\partial \mathcal{B} = \partial_{\mathbf{u}} \mathcal{B} \cup \partial_t \mathcal{B}$,

$$\mathbf{u} = \bar{\mathbf{u}} \quad \forall \mathbf{X} \in \partial_{\mathbf{u}} \mathcal{B}. \quad (3.38)$$

Since damage and plasticity are irreversible kinematic quantities, their admissible variation are only positive, i.e.,

$$(\delta D_\eta, \delta D_\tau, \delta \lambda_\eta^t, \delta \lambda_\eta^c) \in \mathbb{R}^+ \times \mathbb{R}^+ \times \mathbb{R}^+ \times \mathbb{R}^+. \quad (3.39)$$

The first variation of the action functional (Eq. 3.36) is defined as

$$\begin{aligned} \delta \mathcal{E} = & \mathcal{E}(u_\eta + \delta u_\eta, u_\tau^2 + \delta u_\tau^2, \lambda_\eta^t + \delta \lambda_\eta^t, \lambda_\eta^c + \delta \lambda_\eta^c, D_\eta + \delta D_\eta, D_\tau + \delta D_\tau) \\ & - \mathcal{E}(u_\eta, u_\tau^2, \lambda_\eta^t, \lambda_\eta^c, D_\eta, D_\tau). \end{aligned} \quad (3.40)$$

The increments in kinematic quantities are calculated based upon the solution of the deformation process,

$$\begin{aligned} (\Delta u_\eta, \Delta u_\tau^2, \Delta \lambda_\eta^t, \Delta \lambda_\eta^c, \Delta D_\eta, \Delta D_\tau)_{t_i} = & (u_\eta, u_\tau^2, \lambda_\eta^t, \lambda_\eta^c, D_\eta, D_\tau)_{t_i} \\ & - (u_\eta, u_\tau^2, \lambda_\eta^t, \lambda_\eta^c, D_\eta, D_\tau)_{t_{i-1}}, \end{aligned} \quad (3.41)$$

where t_i is the current time and t_{i-1} is the previous time. Then, the increment in total energy is defined in the same manner:

$$\begin{aligned} \Delta \mathcal{E} = & \mathcal{E}(u_\eta + \Delta u_\eta, u_\tau^2 + \Delta u_\tau^2, \lambda_\eta^t + \Delta \lambda_\eta^t, \lambda_\eta^c + \Delta \lambda_\eta^c, D_\eta + \Delta D_\eta, D_\tau + \Delta D_\tau) \\ & - \mathcal{E}(u_\eta, u_\tau^2, \lambda_\eta^t, \lambda_\eta^c, D_\eta, D_\tau). \end{aligned} \quad (3.42)$$

Now, a hemi-variational principle is expressed as follows [224]

$$\Delta \mathcal{E} \leq \delta \mathcal{E} \quad \forall (\delta \mathbf{u}) \in AV_t, \quad (\delta D_\eta, \delta D_\tau, \delta \lambda_\eta^t, \delta \lambda_\eta^c) \in \mathbb{R}^+ \times \mathbb{R}^+ \times \mathbb{R}^+ \times \mathbb{R}^+, \quad (3.43)$$

The application of the mentioned hemi-variational approach along with the traditional variational approach leads to the following governing equations, constitutive relations and boundary conditions

$$\operatorname{div}(\mathbf{S}) + \mathbf{b}^{\text{ext}} = 0 \quad \forall \mathbf{X} \in \mathcal{B}, \quad (3.44)$$

$$\mathbf{S} = \mathbf{C} \mathbf{G} + \mathbf{P} \quad \forall \mathbf{X} \in \mathcal{B}, \quad (3.45)$$

$$\mathbf{S} \mathbf{n} = \mathbf{t}^{\text{ext}} \quad \forall \mathbf{X} \in \partial_t \mathcal{B}, \quad (3.46)$$

where the vector $\mathbf{n}$ is the outward unit normal vector to domain boundary, and the elastic

energy per unit area in Eq. 3.26 forms the stress tensor $\mathbf{S}$ as follows

$$\mathbb{S}_{ij} = \frac{\partial U}{\partial G_{ij}} = \mathbb{C}_{ijab}G_{ab} + \mathbb{P}_{ij}. \quad (3.47)$$

Finally, Karush-Kuhn-Tucker (KKT) type conditions are derived corresponding to the 4 irreversible kinematic descriptors

$$\left\{ -\frac{1}{2}k_\eta(u_\eta - \lambda_\eta^t + \lambda_\eta^c)^2 + \frac{1}{2}k_\eta^c(B_\eta)^2 \left[\tan\left(\frac{\pi}{2}D_\eta\right) \right]^2 + \frac{1}{2}k_\eta^t(B_\eta)^2(\log(1 - D_\eta))^2 - \sigma_\eta^t\lambda_\eta^t - \sigma_\eta^c\lambda_\eta^c - \sigma_{\eta\eta}^c(\lambda_\eta^c)^2 \right\} \Delta D_\eta = 0, \quad (3.48)$$

$$\left\{ -\frac{1}{2}k_\tau u_\tau^2 + \frac{1}{2}k_\tau(B_\tau)^2(\log(1 - D_\tau))^2 \right\} \Delta D_\tau = 0, \quad (3.49)$$

$$\left\{ -k_\eta(1 - D_\eta)(u_\eta - \lambda_\eta^t + \lambda_\eta^c) + (1 - D_\eta)\sigma_\eta^t \right\} \Delta \lambda_\eta^t = 0, \quad (3.50)$$

$$\left\{ k_\eta(1 - D_\eta)(u_\eta - \lambda_\eta^t + \lambda_\eta^c) + (1 - D_\eta)(\sigma_\eta^c + 2\sigma_{\eta\eta}^c\lambda_\eta^c) \right\} \Delta \lambda_\eta^c = 0. \quad (3.51)$$

The KKT conditions can be written in a compact form as follows

$$\{D_\eta - \tilde{D}_\eta(u_\eta, \lambda_\eta^t, \lambda_\eta^c)\} \Delta D_\eta = 0, \quad (3.52)$$

$$\{D_\tau - \tilde{D}_\tau(u_\tau^{el}, u_\tau^2)\} \Delta D_\tau = 0, \quad (3.53)$$

$$\{\lambda_\eta^t - \tilde{\lambda}_\eta^t(u_\eta, \lambda_\eta^c)\} \Delta \lambda_\eta^t = 0, \quad (3.54)$$

$$\{\lambda_\eta^c - \tilde{\lambda}_\eta^c(u_\eta, \lambda_\eta^t)\} \Delta \lambda_\eta^c = 0, \quad (3.55)$$

where $\tilde{D}_\eta$, $\tilde{D}_\tau$, $\tilde{\lambda}_\eta^t$, and $\tilde{\lambda}_\eta^c$ are the threshold functions defined by

$$\tilde{D}_\eta(u_\eta, \lambda_\eta^t, \lambda_\eta^c) = \begin{cases} 1 - \exp\left(-\frac{\sqrt{(u_\eta - \lambda_\eta^t + \lambda_\eta^c)^2 + 2\frac{\sigma_\eta^t \lambda_\eta^t + \sigma_\eta^c \lambda_\eta^c + \sigma_{\eta\eta}^c (\lambda_\eta^c)^2}{k_\eta}}}{B_\eta}\right), & u_\eta^{el} = u_\eta - \lambda_\eta^t + \lambda_\eta^c \geq 0, \\ \frac{2}{\pi} \arctan\left(\frac{\sqrt{(u_\eta - \lambda_\eta^t + \lambda_\eta^c)^2 + 2\frac{\sigma_\eta^t \lambda_\eta^t + \sigma_\eta^c \lambda_\eta^c + \sigma_{\eta\eta}^c (\lambda_\eta^c)^2}{k_\eta}}}{B_\eta}\right), & u_\eta^{el} = u_\eta - \lambda_\eta^t + \lambda_\eta^c < 0, \end{cases} \quad (3.56)$$

$$\tilde{D}_\tau(u_\eta^{el}, u_\tau^2) = 1 - \exp\left(-\frac{u_\tau^2}{\tilde{B}_\tau(u_\eta^{el})}\right) = 1 - \exp\left(-\frac{u_\tau^2}{B_\tau}\right), \quad (3.57)$$

$$\tilde{\lambda}_\eta^t(u_\eta, \lambda_\eta^c) = u_\eta + \lambda_\eta^c - \frac{\sigma_\eta^t}{k_\eta^t}, \quad (3.58)$$

$$\tilde{\lambda}_\eta^c(u_\eta, \lambda_\eta^t) = \frac{(\lambda_\eta^t - u_\eta) k_\eta^c - \sigma_\eta^c}{k_\eta^c + 2\sigma_{\eta\eta}^c}. \quad (3.59)$$

In the homogeneous deformation case investigated in this thesis, $\mathbf{G}$ is constant with respect to $\mathbf{X} \in \mathcal{B}$ and $\mathbf{b}^{\text{ext}}$ is null. Thus, $\mathbf{C}$ and $\mathbf{P}$ are independent of $\mathbf{X} \in \mathcal{B}$, and Eq. 3.44 is automatically satisfied. Some observations are made regarding the KKT conditions. It should be noted that the forms of KKT conditions given in Eqs. 3.56-3.59 are achieved by solving respectively the equations coming from setting to zero the curled parentheses in Eqs. 3.48-3.51. It is observed that Eq. 3.56 is decomposed into two parts, the first for tension and the second for compression. The notion of tension and compression is defined with the sign of the elastic part u_η^{el} of the normal displacement. At the beginning of the deformation history, the presumed normal damage $\tilde{D}_\eta$, as well as the normal damage itself, is null. Besides, in the limit of the infinite elastic part or the normal displacement, the normal damage $\tilde{D}_\eta$ tends asymptotically to one. In the absence of plastic deformation (i.e. with $\lambda_\eta^t = \lambda_\eta^c = 0$), Eqs. 3.56 yield the perceptible interpretations for both B_η^t and B_η^c : that is they provide, respectively, the order of magnitude of the values of the normal displacement for which is a non negligible normal damage. In the same way, Eq. 3.57 gives the interpretation of B_τ as the order of magnitude of the value of the modulus of the tangent displacement for which is a non negligible tangent damage. Further, Eq. 3.58 gives the interpretation of σ_η^t . In particular, the ratio σ_η^t/k_η^t gives the value of the normal displacement necessary to achieve plastic tensile normal displacement. An analogous interpretation in the case $\sigma_{\eta\eta}^c = 0$ is attributed to $\sigma_\eta^c = 0$ for the compression case. Finally, $\sigma_{\eta\eta}^c$ is a hardening parameter because it reduces the magnitude of plastic compression displacement.

3.2 Numerical results and discussion

3.2.1 Implementation of the algorithm

The numerical simulation of biaxial tests are performed in two stages (see Fig. 3.5) assuming that specimen in such tests experience homogeneous deformations such that Eq. 3.44 degenerates to the solution of Eq. 3.45. Stage 1, also referred to as confining stage, consists of isotropic compression up to a pre-determined confining stress $\bar{\mathbb{S}}$. In the proposed model, the stress tensor is defined in Eq. 3.45, and the strain components, G_{11} and G_{22} , are equally increased in modulus to reach $G_{11} = G_{22} = -\bar{G}$ in a stepwise manner until the confining stress, $\bar{\mathbb{S}} = -\mathbb{S}_{11} = -\mathbb{S}_{22}$, is reached. Then, in Stage 2 (shearing stage), strain $G_{22} = -\bar{G} - G$ in 2-direction (vertical direction in Fig. 3.5) is increased in modulus (i.e. with $G > 0$) and in a stepwise manner while in the 1-direction (horizontal direction in Fig. 3.5) stress is fixed to confining stress $\mathbb{S}_{11} = -\bar{\mathbb{S}}$.

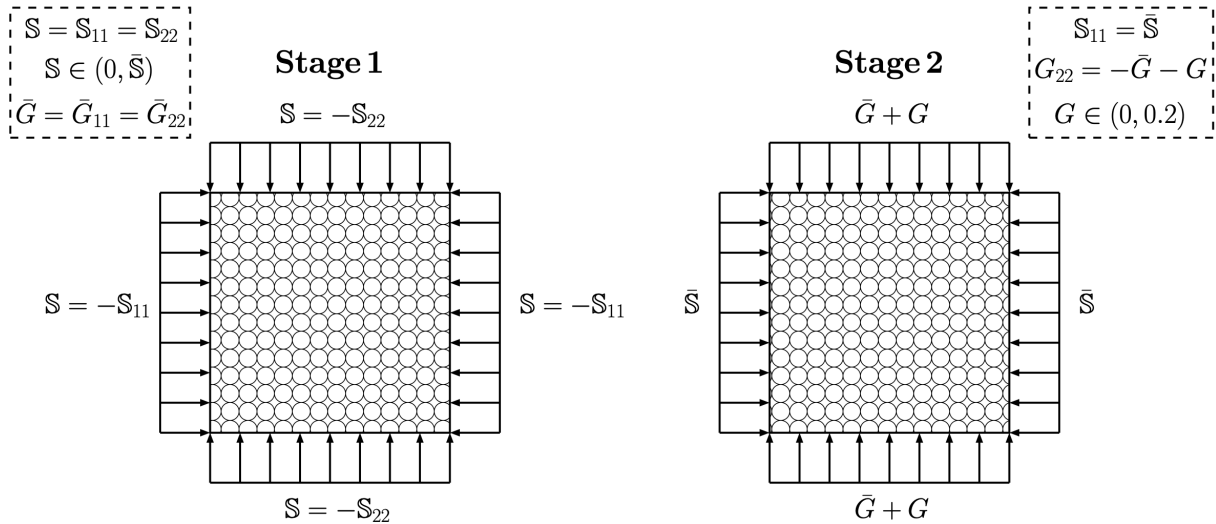


Figure 3.5: Implementation of Stage 1 and Stage 2 on the homogeneous square model. In Stage 1, $\mathbb{S}$ is increasing from 0 to $\bar{\mathbb{S}}$, and the strain $\bar{G}$ is reached. In Stage 2 strain, G is increasing from the null value.

The stiffness ($\mathbb{C}_{ijab}$) and pre-stress ($\mathbb{P}_{ij}$) tensors at the beginning of each loading step are computed, according to Eqs. 3.27 and 3.28, by integrating over the orientation space using trapezoidal rule. These tensors are determined based upon the damage and plastic variables that are determined for each discretized orientation by using the Karush-Kuhn-Tucker conditions from Eqs. 3.52-3.55 as described in the previous section. During Stage 2, to keep the stress fixed to the confining stress in the horizontal direction, Eq. 3.45 with

$\bar{G}_{12} = 0$ and $\mathbb{S}_{11} = -\bar{\mathbb{S}}$ is utilized to determine the strain component G_{11} for each loading step as follows

$$G_{11} = -\frac{\bar{\mathbb{S}} + \mathbb{P}_{11} + \mathbb{C}_{1122}G_{22}}{\mathbb{C}_{1111}}. \quad (3.60)$$

where the strain component $G_{22} = -\bar{G} - G$ is the updated strain for the current loading step and externally prescribed. The strain in the current step is then utilized to update the damage parameters and plastic multipliers according to the Karush-Kuhn-Tucker conditions for use in the subsequent step. As is typical in experimental soil mechanics literature, the linearized approximation of volumetric strain,

$$G_V = \det(\mathbf{F}) - 1 \simeq G_{11} + G_{22}, \quad (3.61)$$

G_V is utilized as the measure of material volume change, and the stress ratio $\mathbb{S}_{22}/\mathbb{S}_{11}$ is also defined.

Overall, the code outline for the emergence of the critical state is presented by following the described evolution process of damage and plasticity variables, as demonstrated in Algorithm 1. It is worth noting that, in the proposed approach, while calculating the strain G_{11} , the value for the current time step is determined using the elastic stiffness parameters $\mathbb{P}_{11}$, $\mathbb{C}_{1111}$, and $\mathbb{C}_{1122}$ obtained from the previous time step. This formulation, as presented in Eq. 3.60, is intended to serve as a numerically explicit scheme, where the strain evolution is directly computed without requiring iterative solutions. Algorithm 1 illustrates this process clearly and shows how the next time step values are obtained based on the previous time step. This approach simplifies this process by employing an analytical expression for the strain. This reduces computational complexity and provides consistency according to the strain-controlled loading path given in the model.

3.2.2 Numerical experiments

3.2.2.1 Parameter identification for different initial density states

For the investigation about the emergence of critical state, material parameters for five different specimens of initial density states for performing the numerical simulations were first identified. The material properties were adapted in such a way that different dilatancy/compaction characteristics are achieved such that 5 specimens are categorized from

for each step do

The strain components G_{11} and G_{22} are calculated with respect to confining stress $\bar{S}$ in Stage 1,

- $D_\eta(t_0, \theta) = 0$, $D_\tau(t_0, \theta) = 0$, $\lambda_\eta^t(t_0, \theta) = 0$, $\lambda_\eta^c(t_0, \theta) = 0 \forall \theta$ at $t_0 = 0$,
- $D_\eta(t_{i-1}, \theta) = D_\eta$, $D_\tau(t_{i-1}, \theta) = D_\tau$, $\lambda_\eta^t(t_{i-1}, \theta) = \lambda_\eta^t$, $\lambda_\eta^c(t_{i-1}, \theta) = \lambda_\eta^c$ from previous step,

for all orientations (θ) do

Compute $\tilde{D}_\eta$, $\tilde{D}_\tau$, $\tilde{\lambda}_\eta^t$, and $\tilde{\lambda}_\eta^c$ by using threshold functions with D_η , D_τ , λ_η^t , and λ_η^c , respectively, in the current time,

if $\tilde{D}_\eta > D_\eta$, $\tilde{D}_\tau > D_\tau$, $\tilde{\lambda}_\eta^t > \lambda_\eta^t$, $\tilde{\lambda}_\eta^c > \lambda_\eta^c$ **then**

 Set $D_\eta(t_i, \theta) = \tilde{D}_\eta$, $D_\tau(t_i, \theta) = \tilde{D}_\tau$, $\lambda_\eta^t(t_i, \theta) = \tilde{\lambda}_\eta^t$, $\lambda_\eta^c(t_i, \theta) = \tilde{\lambda}_\eta^c$

else

 Set $D_\eta(t_i, \theta) = D_\eta$, $D_\tau(t_i, \theta) = D_\tau$, $\lambda_\eta^t(t_i, \theta) = \lambda_\eta^t$, $\lambda_\eta^c(t_i, \theta) = \lambda_\eta^c$

end

Damage and plastic variables are calculated for current step t_i .

end

- The stiffness tensors $\mathbb{C}_{ijab}$ and $\mathbb{P}_{ij}$ are computed by utilizing damage and plastic variables at each step.
- Stage 1 is performed up to the stress limit $\bar{S} = -S_{11} = -S_{22}$.
- In Stage 2, the strain component G_{22} is increased while the stress component $S_{11} = -\bar{S}$ remains constant.

end

Algorithm 1: Code outline for the evolution of damage and plasticity phenomena.

dense (Specimen 1) to loose (Specimen 5) frictional granular media. As the first step, the shear modulus G_{2D} is related to the microscale stiffness parameters, presented, e.g., in Barchiesi et al. [223]

$$G_{2D} = \frac{L^2}{8} (k_\eta^c + 4k_\tau), \quad k_\tau = 0.1k_\eta^c. \quad (3.62)$$

The experimental dependence of the shear modulus G_{emp} upon porosity in such granular materials is proposed in Chang et al. [234] and simplified in this thesis as follows

$$G_{2D} = G_{\text{emp}} = \frac{A}{(e - 0.2)^{1.8}}, \quad (3.63)$$

where $e = V_V/V_S$ is the initial void ratio defined in terms of the void volume V_V and solid

volume V_S . In Eq. 3.63, the material-specific constant A is initially set as outlined in Table 3.1. Additionally, the initial void ratio e (see Table 3.2) was assigned to Specimens 1 through 5. The shear modulus G_{2D} was calculated using the material constant A and the initial void ratio e via Eq. 3.63. By exploiting Eqs. 3.62 and 3.63, along with the correlation between k_η^c and k_τ (see Table 3.1), the corresponding k_η^c values were determined for each specimen as follows

$$k_\eta^c = \frac{8G_{2D}}{L^2} - 4k_\tau. \quad (3.64)$$

The material constant A , the stiffness parameters k_η^t and k_τ , the normal characteristic damage displacement B_η^t in tension, the plastic yielding parameter σ_η^t in tension, the inter-granular interaction distance L , and the constitutive parameters α and α_1 were individually defined for each specimen. Table 3.1 lists the fixed simulation parameters.

Table 3.1: The fixed parameters for all specimens.

A (J/m ²)	k_η^t (J/m ⁴)	k_τ (J/m ⁴)	B_η^t (m)	σ_η^t (J/m ³)	L (m)	α (m)	α_1
1.4×10^6	$0.1k_\eta^c$	$0.1k_\eta^c$	$0.1B_\eta^c$	0	0.01	5×10^{-10}	10

In addition to these fixed parameters, the initial void ratio e , the shear modulus G_{2D} , the damage characteristic displacements B_η^c and $B_{\tau 0}$, and the plasticity constitutive parameters σ_η^c and $\sigma_{\eta\eta}^c$ were illustrated based on specific assumptions that differentiate the behavior of each specimen in Table 3.2.

Table 3.2: The simulation parameters varied from the densest specimen (Specimen 1) to the loosest specimen (Specimen 5).

Specimen	e	G_{2D} (J/m ²) [see Eq. 3.63]	B_η^c (m)	$B_{\tau 0}$ (m)	σ_η^c (J/m ³)	$\sigma_{\eta\eta}^c$ (J/m ⁴)
1	0.5	1.22×10^7	$5.0 \times 10^{-3}L$	$0.24B_\eta^c$	$0.06k_\eta^cL$	$0.28k_\eta^c$
2	0.6	7.0×10^6	$7.6 \times 10^{-3}L$	$0.24B_\eta^c$	$0.07k_\eta^cL$	$0.45k_\eta^c$
3	0.7	4.55×10^6	$1.05 \times 10^{-2}L$	$0.20B_\eta^c$	$0.23k_\eta^cL$	0
4	1.0	2.1×10^6	$2.2 \times 10^{-2}L$	$0.20B_\eta^c$	$0.50k_\eta^cL$	0
5	1.2	1.45×10^6	$3.1 \times 10^{-2}L$	$0.20B_\eta^c$	$0.72k_\eta^cL$	0

3.2.2.2 Effects of initial density states and confining stress on failure state

A set of numerical simulations of biaxial tests were performed for 5 specimens utilizing the parameters in Table 3.2 for confining stress $\bar{S}$ ranging from 70 kN/m to 130 kN/m. In Fig. 3.6, the model predictions in loading stage 2 (shearing stage) are provided for the densest (Specimen 1) and loosest (Specimen 5) specimens, in terms of the principal stress ratio ($\bar{S}_{22}/\bar{S}_{11}$) and volumetric strain, $G_V = G_{11} + G_{22}$, as functions of the imposed strain component $G = -G_{22} - \bar{G}$. The results are shown for seven different confining stress values, namely $\bar{S} = 70, 80, 90, 100, 110, 120$, and 130 kN/m. For the densest specimen (Specimen 1), the principal stress ratio for all confining stresses show a significant peak with remarkable post peak softening asymptoting to a residual principal stress ratio. For the loosest specimen (Specimen 5), the principal stress ratio over the same strain shows a gradual softening with defined peak only for the case of high confinement followed asymptote to a residual principal stress ratio. It is also remarkable that for the loose specimen the peak value is achieved at a significantly larger strain compared to the dense specimen. For both, dense and loose specimens, higher principal stress ratio values are obtained for lower confining stress values. The predicted principal stress ratio and axial strain behavior is reminiscent of typical frictional granular material response observed in experiments [235]. Similarly, the predicted volume change behavior of the dense and loose specimens show the typical contractive (i.e. with $G_V < 0$), dilative (i.e. with $G_V > 0$), and asymptotic (i.e. with large G) behavior observed in experiments. For the dense specimen (see Fig. 3.6b), a small contraction is predicted followed by a characteristic zero volume change point, de-densification and eventual volume dilation, particularly for lower confining stress. For the loose specimen (see Fig. 3.6d), volumetric strain shows a contractive behavior at high confinement. At low confinement, a zero volume change point is predicted after initial contraction followed by de-densification. From these results, it can be observed that the model predicts the expected dilative (for densest specimen) and contractive (for loosest specimen) behaviors depending on confining stress. Overall, the predictions compare qualitatively very well the experimental measurements presented in the literature (such as by Lee and Seed [235]) for different initial density states and confining stresses.

Furthermore, for dense (Specimen 1), mid-dense (Specimen 3), and loose (Specimen 5) specimens in Fig. 3.7a, volumetric strain at failure $G_V = G_{VF}$ is given as a function of void ratio (e) for all the considered confining stresses. Here, the volumetric strain at failure G_{VF} is calculated for the strain (G) when the maximum principal stress ratio is reached (see Fig. 3.6). Also, in Fig. 3.7b, volumetric strain at failure is given as a function

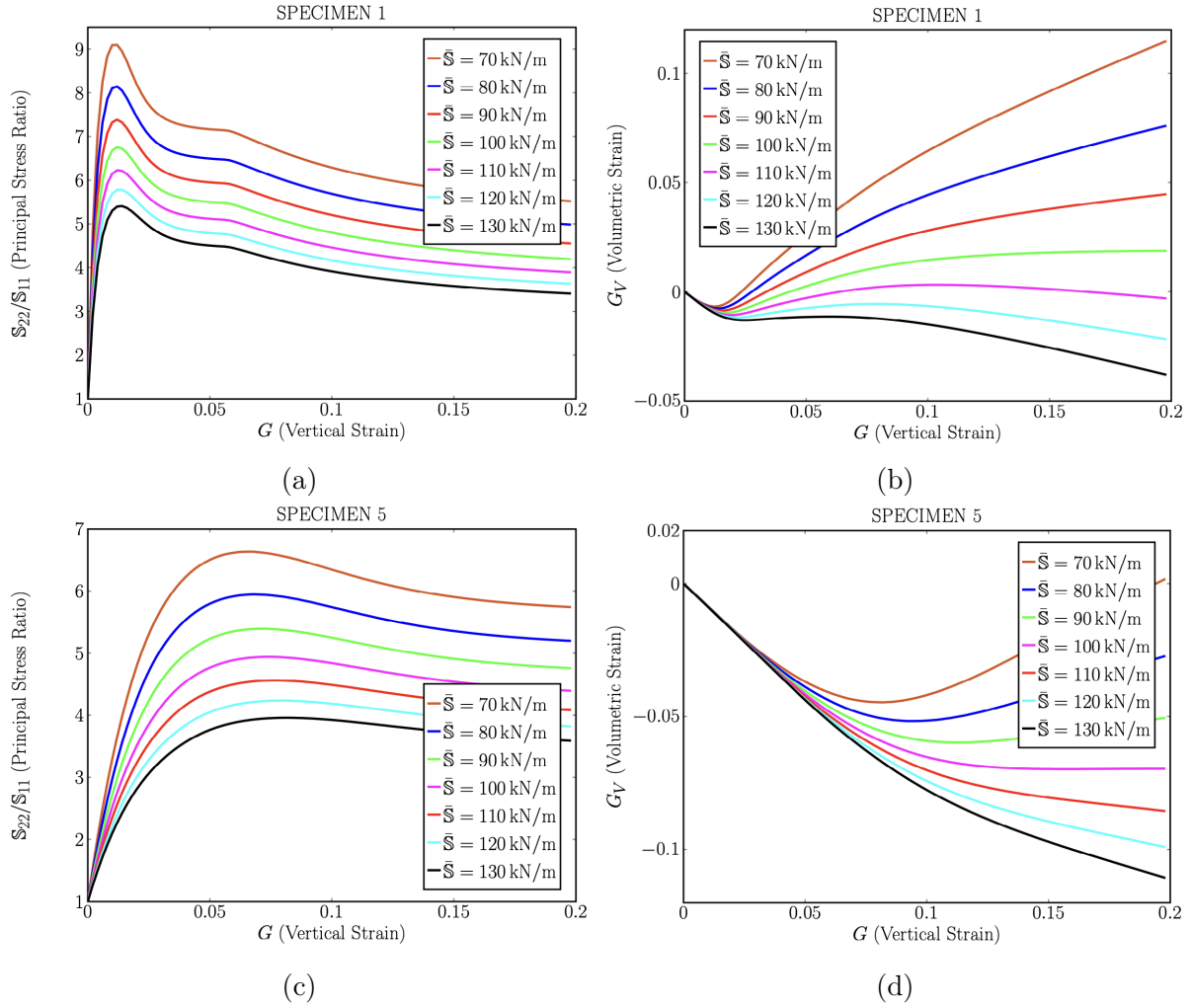


Figure 3.6: The differences of principal stress ratio $\bar{S}_{22}/\bar{S}_{11}$ (a, c) and volumetric strain G_V (b, d) for dense (Specimen 1) and loose (Specimen 5) specimens at different confining stresses in Stage 2.

of confining stress ($\bar{S}$) for dense, mid-dense, and loose specimens.

The volumetric strain values given in Fig. 3.7a were computed for 3 different specimens, namely Specimen 1, 3, and 5 with the corresponding values of e as defined in Table 3.2. Since void ratio decreases from loose to dense specimen, volumetric strain values decrease with increasing void ratio values. Importantly, for the dense specimen, similar volumetric strain values (around -1×10^{-2}) are predicted for all the considered confining stresses, compared to those obtained for specimens with low void ratio. These observations agree qualitatively with experimental measurements [235] on different density sands subjected to conventional triaxial compression.

In Fig. 3.7b, to gain further insight into the effects of confining stresses at failure

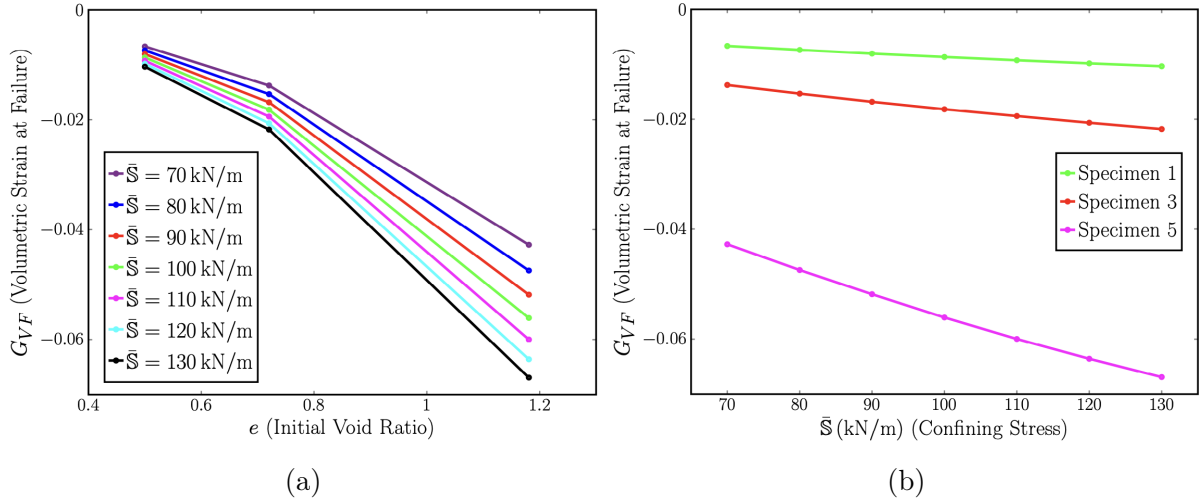


Figure 3.7: (a) Volumetric strain at failure G_{VF} with respect to void ratio e for different confining stresses $\bar{S}$. (b) Volumetric strain at failure G_{VF} for 70, 80, 90, 100, 110, 120 and 130 (kN/m) confining stresses $\bar{S}$.

based on the work of Lee and Seed [235], volumetric strain at failure is given as a function of confining stress for dense (Specimen 1), mid-dense (Specimen 3) and loose (Specimen 5) specimens. The predicted responses qualitatively agree with the experimental observations that volumetric strain at failure decreases with increasing confining stress and that the rate of volumetric strain decrease is larger for less dense specimens.

3.2.2.3 Emergence of critical state

It is clear from the predictions in Figs. 3.6 and 3.7 that the model is able to replicate salient features of the behavior of frictional granular materials deformed under biaxial shear. It has been particularly observed that the model predicts critical state conditions for the set of parameters in Table 3.2 for all 5 specimens of initial void ratios under a confining stress of $\bar{S} = 100$ kN/m. Figs. 3.8a and 3.8b give the predicted principal stress ratio and volumetric strain, respectively, as a function of the vertical strain G for all 5 specimens. It can be observed that the predicted principal stress ratio and the volumetric strain reach a constant value at large deformations for all the specimens. The indication is that, under biaxial loading, the material arrives to the condition in which the deformation can proceed without change of stress or volume, so that the classical critical state condition is achieved. Let us define hardening (or softening) as the deformation phase when an increase (or decrease) of stress ratio and dilative (or contractive) behavior occur as the situation for which, for large deformation, $G_V > 0$ (or $G_V < 0$). Thus, it should be remarked that hardening, softening and dilative behaviors are observed for

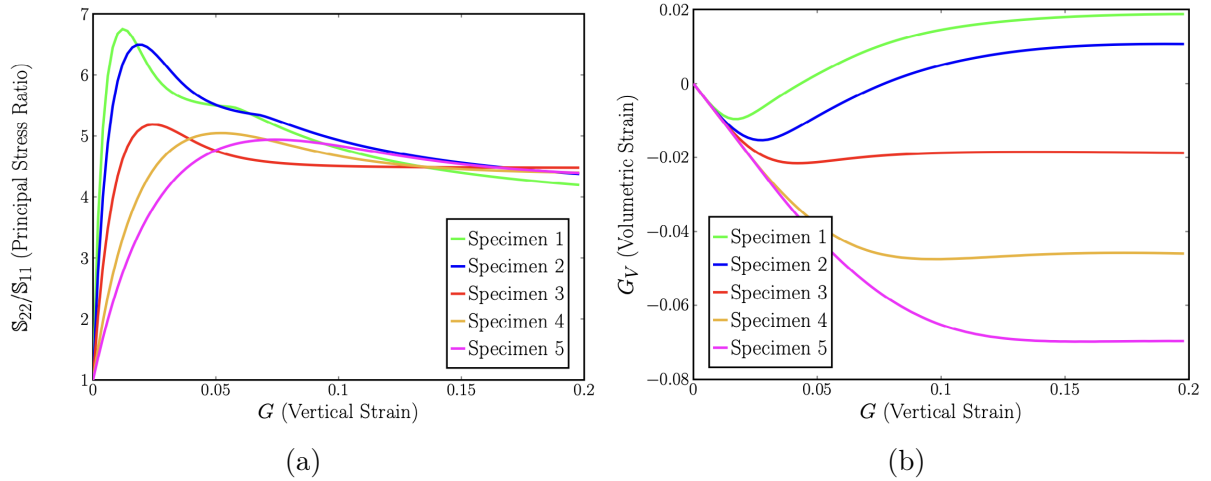


Figure 3.8: Critical state for principal stress ratio S_{22}/S_{11} (a) and volumetric strain G_V (b) for $\bar{S}=100$ kN/m.

dense specimens (Specimen 1 and 2) while hardening, softening, and contractive behaviors are observed for mid-dense and loose specimens (Specimen 3, 4, and 5).

To elucidate the coupled damage and plastic behavior occurring during the simulations, polar plots are provided in Figs. 3.9-3.12 for damage and plasticity variables. As the damage and plastic behavior is orientation dependent emanating from the grain-pair interaction, polar plots show how these irreversible quantities evolve in all orientations during the simulations.

In Figs. 3.9 and 3.10, the evolution of the normal and tangential damage variables (D_η and D_τ) are presented, respectively, for all 5 specimens. The provided polar plots are given for Stage 1 and selected ranges of axial strain G in Stage 2 of loading. The first stage is in the column i), and the second stage is given for 4 different vertical strain intervals in the columns ii), iii), iv), and v) as shown in Figs. 3.9 and 3.10. Each polar plot was prepared by dividing the corresponding strain interval into 10 equal steps. The normal and tangential damage terms evolve due to the KKT conditions given in Eqs. 3.56 and 3.57. In Stage 1, as the confining stress is applied equally from both sides, the normal damage evolution is the same in all orientations (circular shape of the polar plots), and higher normal damage values are obtained in loose specimens (Specimen 4 and 5). This growth in damage is not unexpected, since some amount of grain rearrangement occurs during the confinement process. However, in frictional granular systems, this grain rearrangement is accompanied by stiffening due to elastic nonlinearity of grain contact interactions and potential growth in contact density. In this thesis, these nonlinear effects have been deliberately ignored to keep the formulation simple. Notably, the assumed

elastic energy is quadratic, and the above nonlinear stiffening effects are not considered. However, by including higher order power of u_η^{el} in elastic energy Eq. 3.25 such stiffening effects can be incorporated at the cost of additional parameters (it is expected to pursue in near future). In Stage 1, under equi-biaxial loading, tangential damage does not evolve.

In Stage 2, for dense specimens (Specimen 1 and 2), the predicted normal and tangential damage grow rapidly in the low strain range ($0 < G_{22} < 0.04$) compared to those predicted for the loose specimens (Specimen 4 and 5). The damage growth then slows and saturates at larger strains. This damage growth pattern is expected as the dense material undergoes a more rapid loss of stiffness arriving to the peak strength at a lower strain compared to the loose material. It is remarkable here that damage in a GMA represents loss of stiffness, which in granular system can be interpreted as a measure of loss of structure in given direction. This loss of structure and stiffness can involve a host of grain-scale mechanisms, including collapse/buckling of particle chains accompanied by particle rotation/rolling or grain sliding. The normal and tangential damage variable is the effective representation of the consequences of these mechanism in a given direction of the grain-pair orientation space. The mechanisms are in general complex and difficult to delineate, however from a mechanistic viewpoint normal damage is representative of buckling/collapse of chains and clusters, while the tangential damage represents the loss of lateral support or confinement to these structure in grain neighborhoods.

It is further observed that the normal damage growth is larger in the vertical direction along the direction of principal strain increase. Under the same loading, the tangential damage increase is larger in band of orientations inclined to the principal strain direction. Let us analyze the first part of Stage 2, represented in the second column of polar plots of Fig. 3.10. For Specimen 5, a standard flower-shape, where the most damaged orientations are at 45° with respect to the horizontal and vertical directions, is observed. The reason is that the tangential damage has a maximum value in that orientations. For Specimen 4, the same flower-shape polar plot is observed but with higher value for damage. The reason is that the characteristic damage tangential displacement B_τ for a somewhat denser Specimen 4 is lower than that of Specimen 5 and, because of Eq. 3.57, the tangential damage is higher. At the beginning of Stage 2 and for both Specimens 4 and 5, every orientations are in compression. Therefore, the characteristic damage displacement B_τ from Eq. 3.34, is the same for every orientations. This is not the case for Specimen 3, where in the neighborhood of horizontal orientations the elastic part of the normal displacement is, because of Poisson's effect, positive and the characteristic damage tangential displacement B_τ passes, because of Eq. 3.34, from $B_{\tau 0}(1 + \alpha_1)$ to $B_{\tau 0}(1 - \alpha_1)$. This drop of characteristic damage tangential displacement, regularized by the parameter α , makes

these orientations most tangentially damaged. This is true except for a tiny region in the space of orientations around the horizontal one, where the plastic displacement in tension (see Fig. 3.11) takes the role to decrease the elastic part of the normal displacement. The same tendency, but more pronounced, is observed in Specimen 1 and 2. By increasing the imposed strain normal damage reaches near unity for a large band of the compressed vertical directions. The horizontal directions are in tension and, because of the fact that the characteristic damage normal displacement in tension is much smaller than that in compression, then it is expected an increase of normal damage in the horizontal directions. However, this is not visible because the plastic tensile displacement evolves due to the assumption that $\sigma_\eta^t = 0$ (which ensures that any tensile displacement is a plastic one). The width of orientation band and rate of growth depends upon the normal elastic displacement in those orientations. In the orientations that experience tensile displacement, the tangential damage grows faster in contrast to the orientations experiencing compressive displacements. As the deformation proceeds beyond peak in the stress-strain response ($G_{22} > 0.04$ see Fig. 3.8a), the damage growth slows and saturates to its maximum value at the critical state of the deformation history ($G_{22} > 0.12$).

The growth of normal damage (or the loss of stiffness) in the major principal stress direction appears to contradict the apparent gain in the number of contacts along this direction often observed in experiments with rod assemblies and other granular assemblies, and in discrete simulations [58, 236]. However, the contact number increase is likely to be modulated by the evolution of contact deformation energies which are clearly just sufficient to support the given load that reach a peak value and in the critical state a constant value. It is also noteworthy that the normal damage in the horizontal direction does not change after Stage 1 for each specimen, which is a significant contributor to material elastic anisotropy, such that if the elastic response of the system is probed at a given stage (i.e. given axial strain G_{22}), the response will not only be anisotropic (in this case cross-anisotropic) but also the degree of anisotropy will depend upon the material initial density state.

Figs. 3.11 and 3.12 give the polar plots of the directional evolution of the tension and compression plastic multipliers (λ_η^t and λ_η^c), respectively. These plastic multipliers are representative of the cumulative irrecoverable grain-pair displacements in a given orientation. In the current formulation, effective irrecoverable grain-pair displacements are considered only through the normal component of displacement. These are formulated to represent the effective accumulation of plastic deformation resulting from grain-pair sliding and separation in the considered orientation. The polar plots are given only for Stage 2 dividing into 5 strain intervals as, expectedly, no plastic evolution was observed during

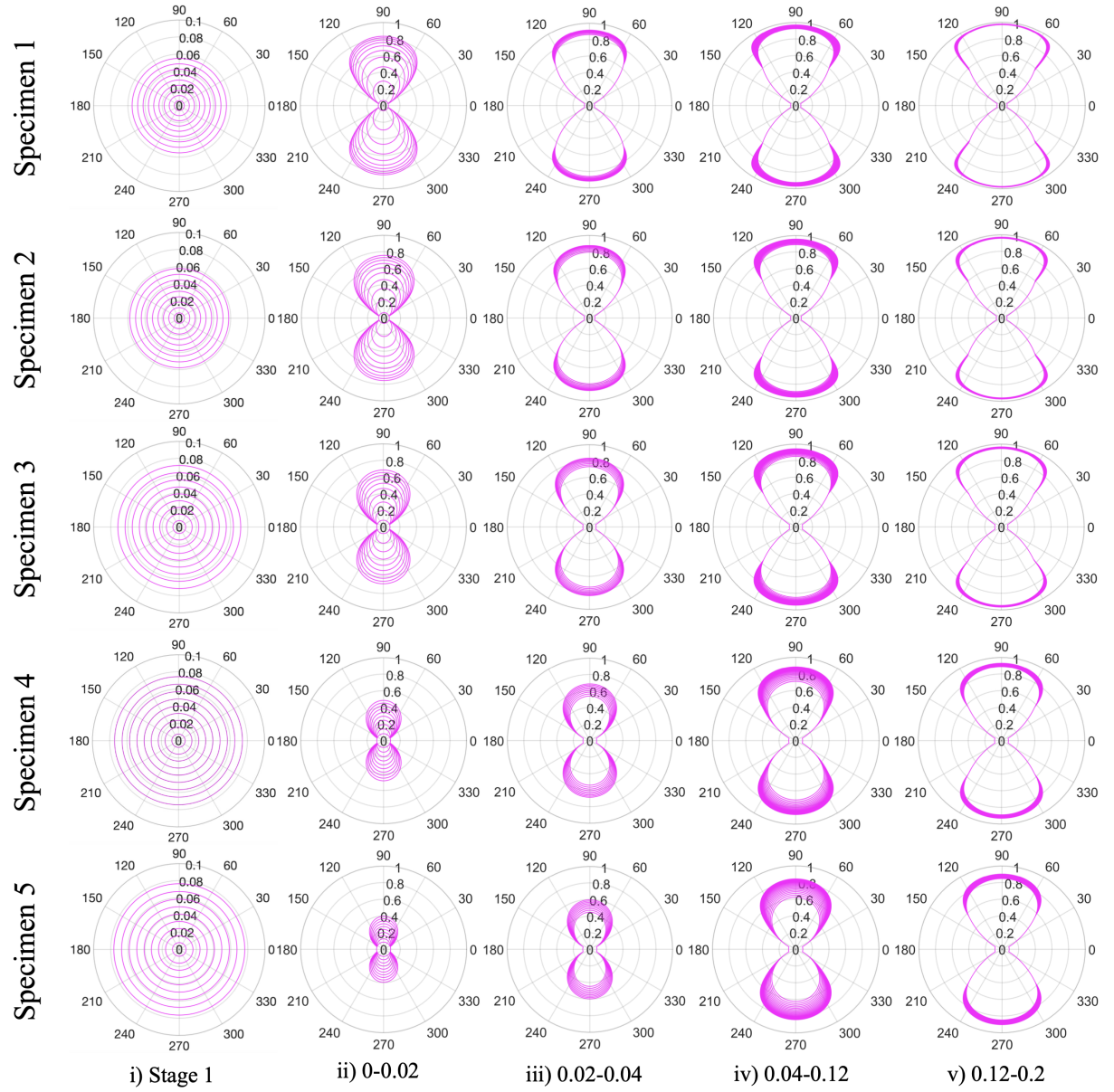


Figure 3.9: Normal damage D_η polar plots from dense to loose specimens at Stages 1 and 2 for different strain intervals.

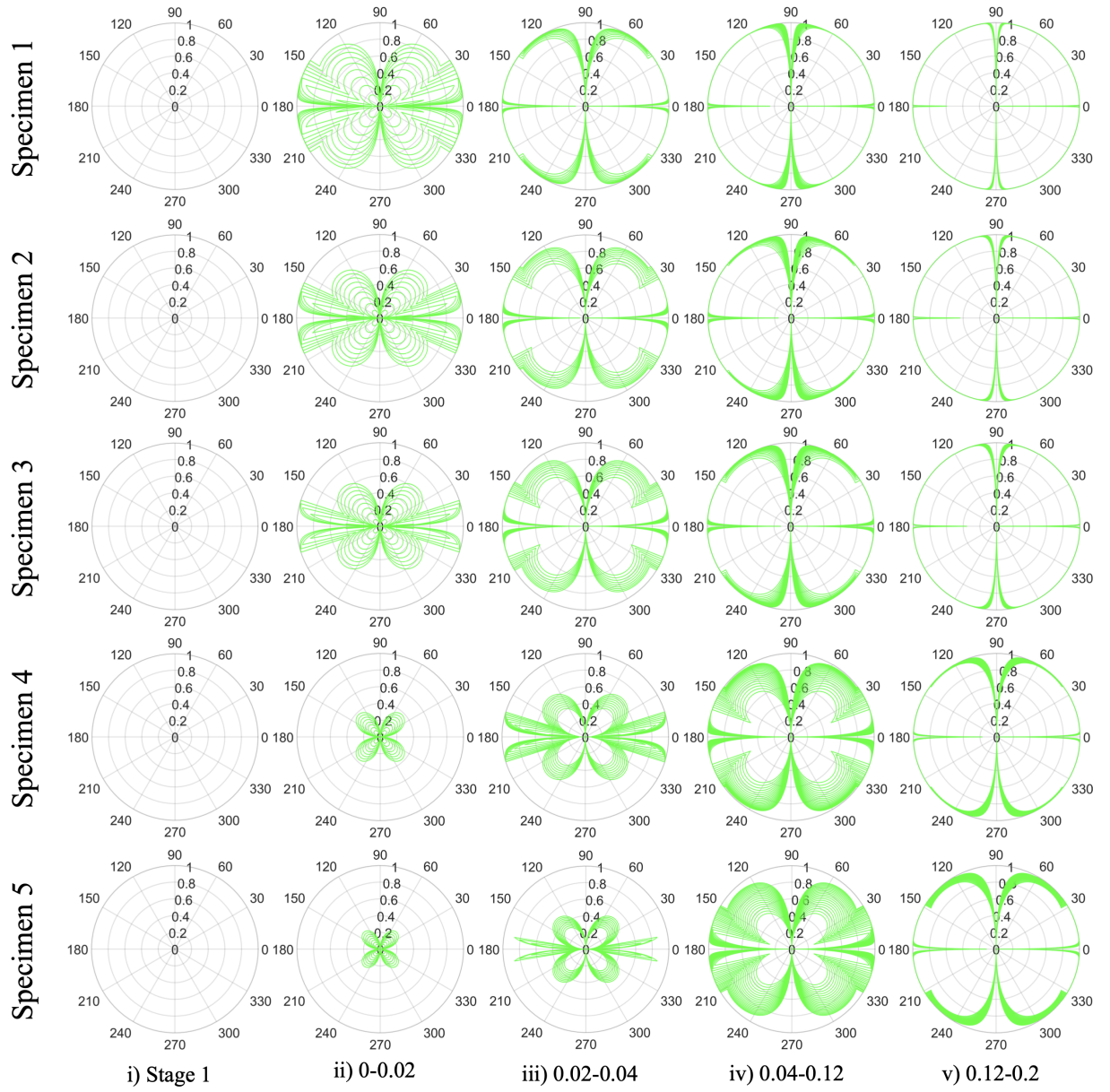


Figure 3.10: Tangential damage D_τ polar plots from dense to loose specimens at Stages 1 and 2 for different strain intervals.

Stage 1 due to the current simplified formulations of plastic dissipation energy potentials, such that the threshold values are not reached to trigger the KKT conditions (see Eqs. 3.58 and 3.59) related to plastic multipliers. Also, the evolution of the compression plastic multiplier (see Fig. 3.12) is given only for dense specimens (Specimen 1 and 2) as no evolution occurs for the mid-dense and loose specimens (Specimen 3, 4, and 5) during the simulations. For all the specimens, while the evolution of the tension plastic multiplier is dominant in the horizontal direction, the evolution of the compression plastic multiplier is dominant in the vertical direction.

In the horizontal direction, there is an effective tension as the lateral strain G_{11} evolves in response to the applied axial compression and constant lateral stress. As a result, tension plastic multiplier λ_η^t evolves as shown in Fig. 3.11. To achieve dilatational behavior in the simulations, the tension plastic yielding parameter σ_η^t is fixed to zero, and in this way, the softening behavior commences early during Stage 2 for all the specimens. Also, for mid-dense and loose specimens (Specimen 3, 4, and 5), as the plastic compression yielding parameter σ_η^c is high, the compression plastic multiplier λ_η^c does not evolve leading to the establishment of the critical state. In other words, the contractive behavior of these specimens is over and the critical state is achieved as the compression plastic multiplier does not progress during the simulations. Remarkably, the hardening parameter $\sigma_{\eta\eta}^c$ controls the evolution of compression plastic multiplier to reach the critical state for dense specimens (Specimen 1 and 2). In fact, after the softening behavior (see Fig. 3.8), the hardening parameter allows adjustment of the volumetric strain. It is remarkable, as seen from the results in Fig. 3.8, that the proposed model is able to successfully predict the emergence of critical state in frictional granular materials. Overall, the interplay between directional damage growth (loss of stiffness) and evolution of irrecoverable deformation is responsible for the nonlinear evolution of Poisson's effect and anisotropy that leads to the non-monotonic volume change behavior of granular materials.

To investigate the evolution of elastic anisotropy, the eigenvalues λ_1 and λ_2 of the elastic stiffness tensor $\mathbb{C}_{ijab}$ are considered. For the given loading conditions, these distinct eigenvalues evolve with loading, and the matrix representation are provided below

$$\begin{Bmatrix} \mathbb{S}_{11} \\ \mathbb{S}_{22} \end{Bmatrix} = \begin{pmatrix} \mathbb{C}_{1111} & \mathbb{C}_{1122} \\ \mathbb{C}_{2211} & \mathbb{C}_{2222} \end{pmatrix} \begin{Bmatrix} G_{11} \\ G_{22} \end{Bmatrix},$$

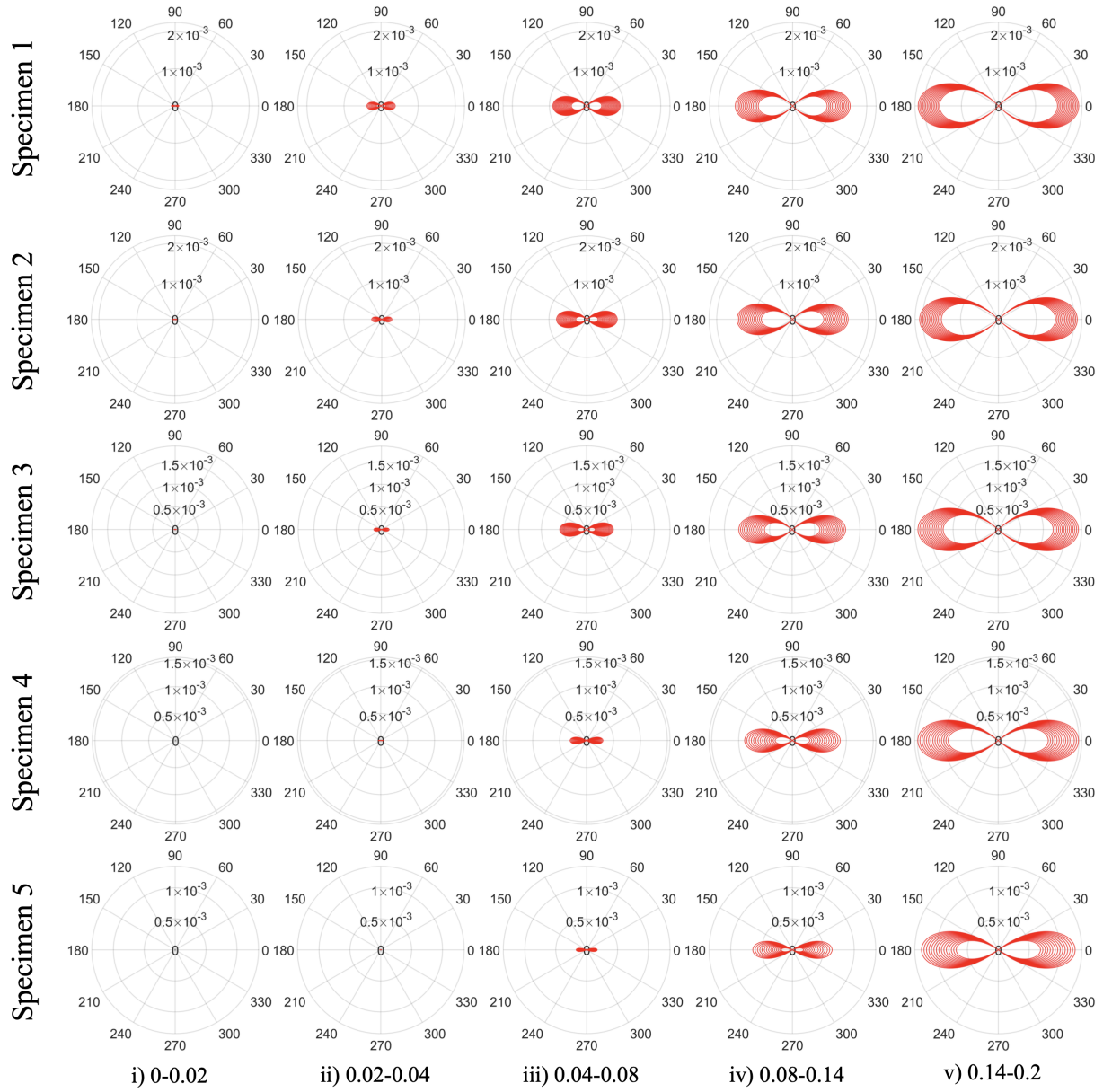


Figure 3.11: Tension λ_{η}^t plastic multiplier polar plots from dense to loose specimens at vertical strain for different strain intervals of Stage 2.

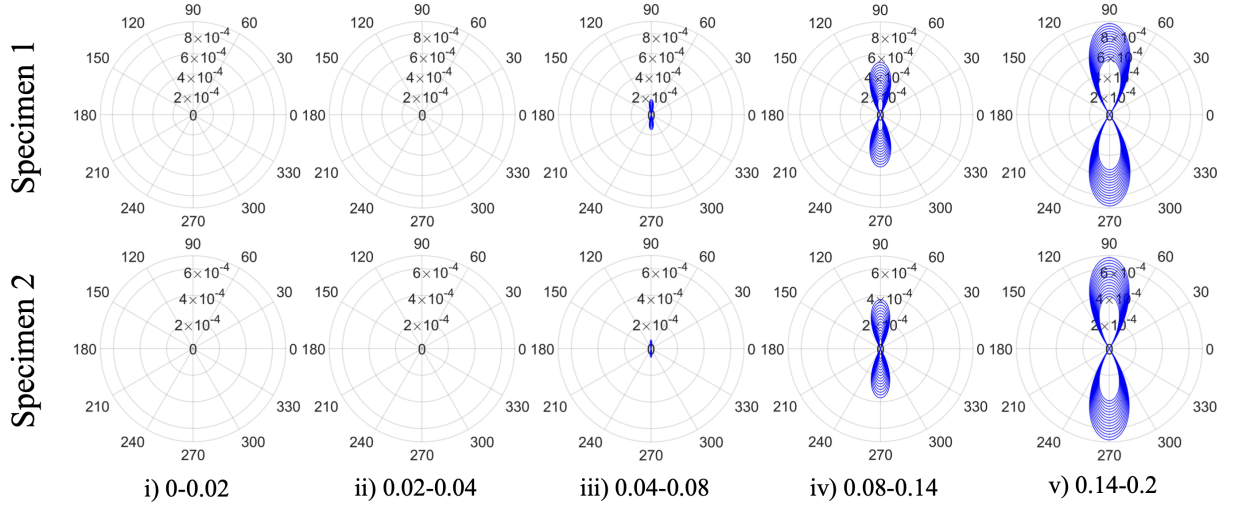


Figure 3.12: Compression λ_η^c plastic multiplier polar plots for dense specimens only at vertical strain for different strain intervals of Stage 2.

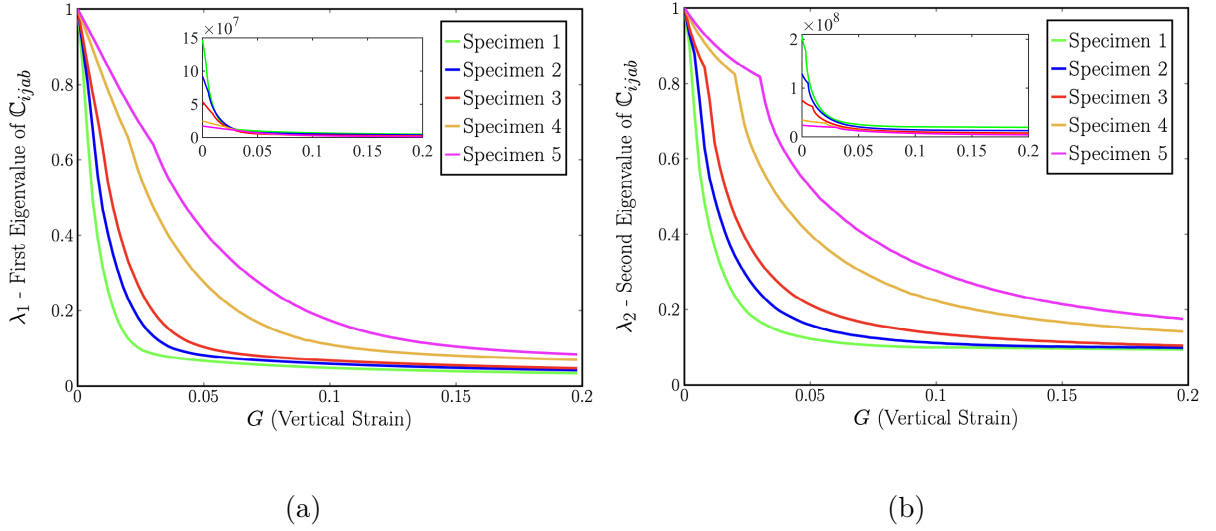


Figure 3.13: Normalized first λ_1 (a) and second λ_2 (b) eigenvalues of the elastic stiffness tensor.

and the determinant of 2×2 matrix is found by

$$\begin{vmatrix} \mathbb{C}_{1111} - \lambda & \mathbb{C}_{1122} \\ \mathbb{C}_{1122} & \mathbb{C}_{2222} - \lambda \end{vmatrix}.$$

Fig. 3.13 gives the normalized eigenvalues (normalized with their initial value at $G = 0$) plotted against axial strain G . The inset gives the actual values over the complete loading. As expected the dense specimens have higher initial stiffness as indicated by the larger eigenvalues, however the loss of stiffness for these specimens is also faster as shown by the damage growth described earlier. After the vertical strain value exceeds 5×10^{-2} , change in the eigenvalues is significantly small. What is remarkable is that the evolution of the two eigenvalues are at different rates indicating the growth of anisotropy.

3.3 A parametric study for unraveling the emergence of critical state

This section presents a parametric study to explore the response of a numerical model for 3 specimens, referred to as dense (Specimen 1), mid-dense (Specimen 3), and loose (Specimen 5) in Subsection 3.2.2, with different initial density states by investigating the emergence of the critical state in granular materials. Within the numerical framework presented in Section 3.1, the constitutive relations are established based on multiple parameters. The simulation parameters, which are defined in distinctive assumptions, are determined using non-dimensionalization coefficients (as shown in Tables 3.1 for the fixed parameters of all specimens and 3.2) to ensure consistent units of measure across the compression constitutive parameters. These assumptions aim to capture the idealized critical state behavior regarding deformation evolution. The damage and plasticity evolution is also analyzed to demonstrate how gradual variations in compression parameters contribute to achieving the idealized critical state behavior.

A set of parametric studies are conducted on a granular micromechanics continuum model by systematically adjusting the material constitutive parameters of each specimen. During the simulations, one material constitutive parameter is varied while others remain constant. These simulations focus on the principal stress ratio ($\mathbb{S}_{22}/\mathbb{S}_{11}$) and volumetric strain ($G_V = G_{11} + G_{22}$). The model predictions in loading Stage 2 (shearing stage) are presented with respect to the imposed strain component $G = -G_{22} - \bar{G}$. The predictive accuracy insights gained from these parametric studies contribute to more reliable model

predictions in future attempts. The numerical analyses focus on compression k_η^c normal stiffness, characteristic compression B_η^c normal displacement, compression σ_η^c plastic yielding and hardening $\sigma_{\eta\eta}^c$ parameters. Notably, in Stage 1 (confining stage), the confining stress $\bar{S}$ is set to 100 kN/m for all simulations.

The initial void ratio e , the shear modulus G_{2D} , the compression normal stiffness k_η^c , the damage characteristic displacements B_η^c and $B_{\tau 0}$, and the plasticity constitutive parameters σ_η^c and $\sigma_{\eta\eta}^c$ are individually assumed and listed for 3 specimens in Table 3.3.

Table 3.3: The simulation parameters for dense, mid-dense, and loose specimens.

Specimen	e	G_{2D} (J/m ²) [see Eq. 3.63]	k_η^c (J/m ⁴) [see Eq. 3.64]
Dense	$\bar{e}_D = 0.5$	$\bar{G}_{2D_D} = 1.22 \times 10^7$	$\bar{k}_{\eta_D}^c = 7.0 \times 10^{11}$
Mid-dense	$\bar{e}_M = 0.7$	$\bar{G}_{2D_M} = 4.55 \times 10^6$	$\bar{k}_{\eta_M}^c = 2.6 \times 10^{11}$
Loose	$\bar{e}_L = 1.2$	$\bar{G}_{2D_L} = 1.45 \times 10^6$	$\bar{k}_{\eta_L}^c = 8.3 \times 10^{10}$
B_η^c (m)	$B_{\tau 0}$ (m)	σ_η^c (J/m ³)	$\sigma_{\eta\eta}^c$ (J/m ⁴)
$\bar{B}_{\eta_D}^c = 5.0 \times 10^{-3}L$	$0.24B_\eta^c$	$\bar{\sigma}_{\eta_D}^c = 0.06k_\eta^c L$	$\bar{\sigma}_{\eta\eta_D}^c = 0.28k_\eta^c$
$\bar{B}_{\eta_M}^c = 1.05 \times 10^{-2}L$	$0.20B_\eta^c$	$\bar{\sigma}_{\eta_M}^c = 0.23k_\eta^c L$	0
$\bar{B}_{\eta_L}^c = 3.1 \times 10^{-2}L$	$0.20B_\eta^c$	$\bar{\sigma}_{\eta_L}^c = 0.72k_\eta^c L$	0

Variations are applied solely to the non-dimensionalization coefficients for the parameters $\bar{k}_\eta^c$, $\bar{B}_\eta^c$, $\bar{\sigma}_\eta^c$, and $\bar{\sigma}_{\eta\eta}^c$ (see Table 3.3), as employed in [7, 8]. Further, the material parameters $\bar{e}$, $\bar{G}_{2D}$, $\bar{k}_\eta^c$, $\bar{B}_\eta^c$, $\bar{\sigma}_\eta^c$, and $\bar{\sigma}_{\eta\eta}^c$ are listed with their index notations for each specimen.

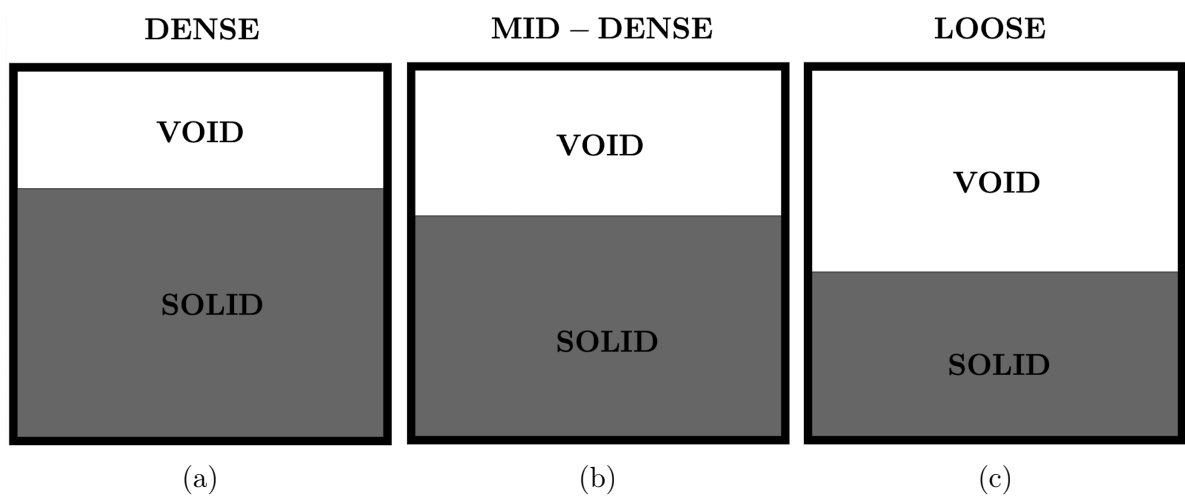


Figure 3.14: Schematic representation of dense ($e = 0.5$), mid-dense ($e = 0.7$), and loose ($e = 1.2$) specimens from (a) to (c), respectively, comparing the solid particles arrangement and voids in relation to the initial void ratio.

Fig. 3.14 provides a comparative visualization of square specimens referred to as dense, mid-dense, and loose and shows the particle arrangement associated initial void ratio. Each specimen is depicted to highlight the sectional distribution of solid particles and voids. In dense specimen (see Fig. 3.14a), the particle arrangement has a high solid density and minimal void space with a low initial void ratio. While mid-dense specimen in Fig. 3.14b exhibits a packing composition less intense than dense specimen with a medium initial void ratio regarding the solid particles, loose specimen in Fig. 3.14c has significantly larger void spaces and a higher initial void ratio compared to the other specimens.

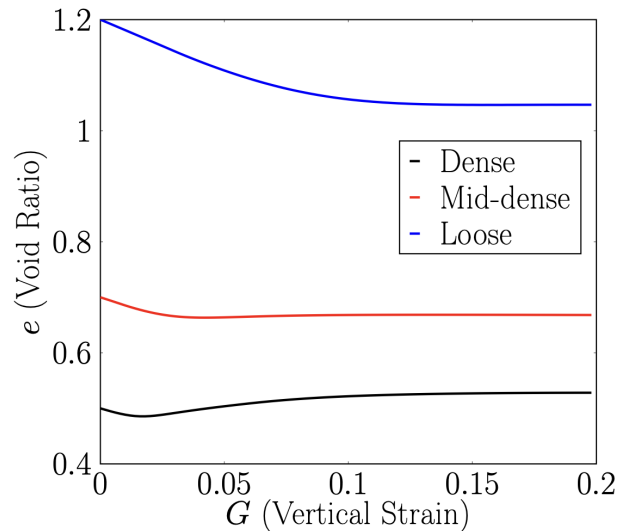


Figure 3.15: Tendency of void ratios for all specimens.

In these simulations, the initial void ratios of the specimens were chosen to differ significantly from each other. In Fig. 3.15, while the tendency of the void ratios to converge within a restricted range is evident, the results do not fully align with the experimental observation that critical void ratios become identical not depending on their initial values. This could be a limitation inherent in the simulation. Further investigation into void ratio behavior through a comprehensive parameter analysis is necessary. Acknowledging the importance of this aspect, future work aims to replicate one-dimensional compression simulations that more closely reflect experimental findings by adjusting the initial packing configurations and boundary conditions to more effectively capture the stress-strain relations observed in experimental applications.

3.3.1 Parametric study on compression k_η^c normal stiffness parameter

Firstly, the compression k_η^c normal stiffness parameter was utilized in the numerical simulations. In Fig. 3.16, the predicted principal stress ratio and volumetric strain behaviors are presented for three different specimens. In each simulation, only the values of $\bar{k}_{\eta_D}^c$, $\bar{k}_{\eta_M}^c$, and $\bar{k}_{\eta_L}^c$ for the dense, mid-dense, and loose specimens, respectively, were increased or decreased by multiplying with a non-dimensionalization coefficient. It is noteworthy to remark that all parameters related to the compression k_η^c normal stiffness parameter in Tables 3.1 and 3.3 were updated automatically. Further, an increase in the compression normal stiffness triggers an increase in the shear modulus (G_{2D}) at the same rate, as seen in Eq. 3.62, which leads to a decrease in the initial void ratio (e), according to the relationship between shear modulus and initial void ratio in Eq. 3.63. Thus, the stiffening behavior of the material can be observed by correlating the changes in compression normal stiffness with the initial void ratio. Notably, as given in Eq. 3.63, the initial void ratios do not change at the same rate as the non-dimensionalization coefficients of the compression normal stiffness parameter. The initial void ratio ranges from $e \in (0.47, 0.54)$ for dense, $e \in (0.67, 0.79)$ for mid-dense, and $e \in (1.09, 1.31)$ for loose specimens, depending on the highest and lowest compression normal stiffness values. For a dense specimen, the principal stress ratio for all varied compression $\bar{k}_{\eta_D}^c$ normal stiffness parameters (see Fig. 3.16a) exhibits a significant peak, subsequently followed by remarkable post-peak softening that asymptotically approaches a residual principal stress ratio over the same vertical strain, and a small contraction is predicted around a characteristic zero volume change point, followed by de-densification and eventual volume dilation at different vertical strains, particularly at high compression normal stiffness parameters (see Fig. 3.16b).

For a mid-dense specimen, the principal stress ratio in Fig. 3.16c serves moderate softening with a distinct peak for all cases of compression $\bar{k}_{\eta_M}^c$ normal stiffness, followed by no change in principal stress ratio. Regarding the volumetric strain, Fig. 3.16d shows a contractive response at low compression normal stiffness. Similarly, for a loose specimen, the principal stress ratio in Fig. 3.16e illustrates gradual softening with a defined peak only at high compression $\bar{k}_{\eta_L}^c$ normal stiffness, followed by an asymptotic decrease in the residual principal stress ratio, while the volumetric strain presents a contractive behavior across all compression normal stiffness parameters in Fig. 3.16f. A proportional increase in the stiffness value is predicted when the compression normal stiffness is increased, since the elastic stiffness tensors are derived via Eqs. 3.27 and 3.28.

3.3.2 Parametric study on characteristic compression B_η^c normal displacement

Secondly, the characteristic compression B_η^c normal displacement is adopted for the parametric studies, and the principal stress ratio and volumetric strain responses are shown depending on the parameters $\bar{B}_{\eta_D}^c$, $\bar{B}_{\eta_M}^c$, and $\bar{B}_{\eta_L}^c$ with respect to the dense, mid-dense, and loose specimens, respectively, in Fig. 3.17. In the threshold functions (see Eqs. 3.56 and 3.57), the evolution equations of normal and tangential damage were also derived based on characteristic damage displacements. Moreover, the characteristic tension normal B_η^t and tangent $B_{\tau 0}$ displacements are provided in terms of the characteristic compression normal displacement in Tables 3.1 and 3.3, respectively. As observed in Figs. 3.9 and 3.10, the damage evolution in a dense specimen progresses faster than in a loose specimen with respect to low the characteristic compression normal displacement (see Table 3.2 for the amount of B_η^c parameter of all specimens). During all simulations, only $\bar{B}_\eta^c$ values of the specimens were multiplied with non-dimensionalization coefficients. For a dense specimen, a significant peak is observed in the principal stress ratio (see Fig. 3.17a) at different strain values, followed by remarkable post-peak softening and an asymptotic decrease. After the softening behavior occurs up to the same certain strain in volumetric strain, volume dilation occurs at high the characteristic compression $\bar{B}_{\eta_D}^c$ normal displacement parameters (see Fig. 3.17b). After a peak is observed in the principal stress ratio, softening and no change in the stress are observed in a mid-dense specimen (see Fig. 3.17c), while volumetric strain (see Fig. 3.17d) exhibits dilative behavior at high the characteristic compression $\bar{B}_{\eta_M}^c$ normal displacement. In a loose specimen, the peak in the principal stress ratio disappears at low the characteristic $\bar{B}_{\eta_L}^c$ compression normal displacement (see Fig. 3.17e), and a contractive response raises at all the characteristic

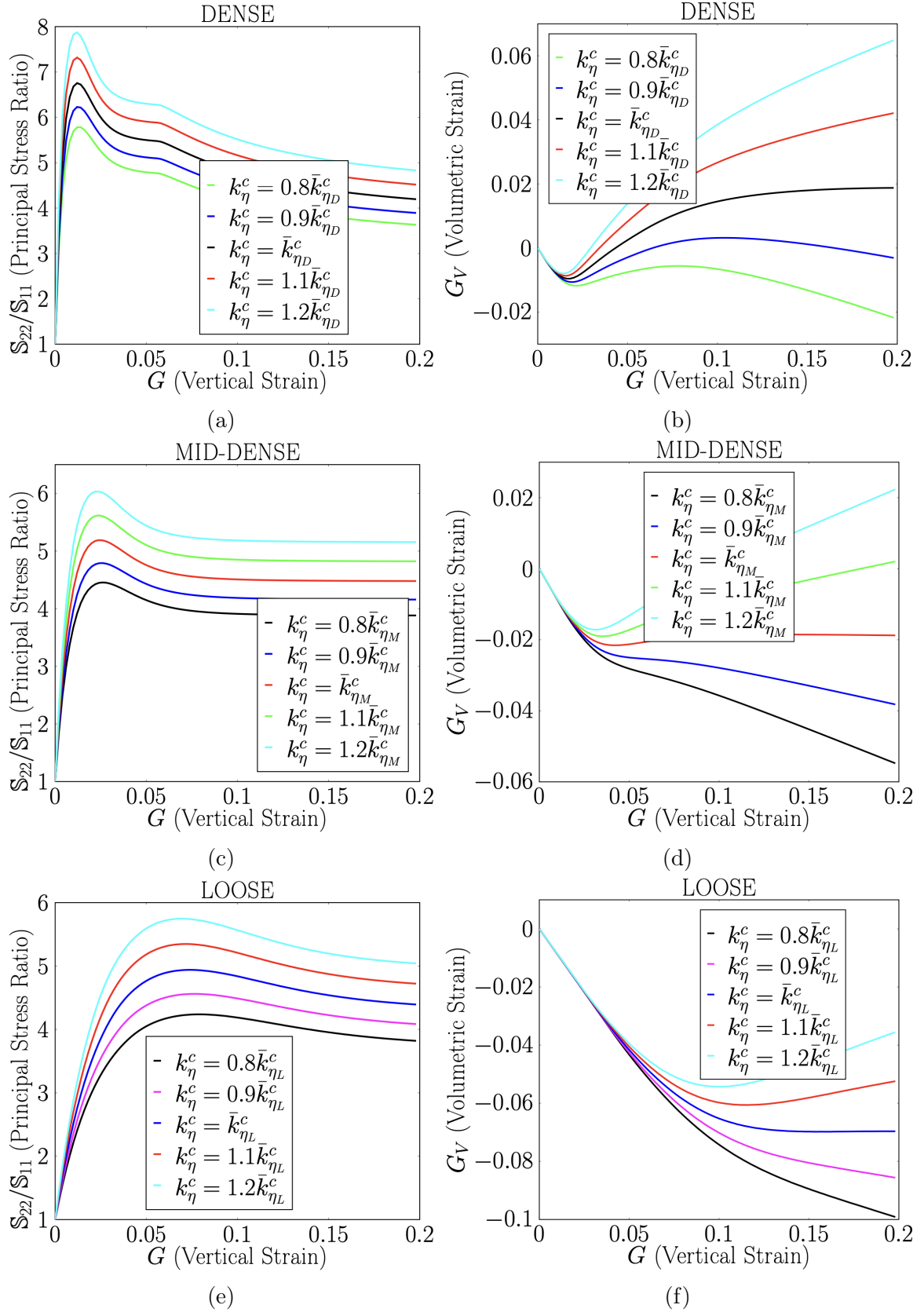


Figure 3.16: Parametric analysis by changing compression $\bar{k}_\eta^c$ normal stiffness for all specimens in terms of principal stress ratio S_{22}/S_{11} (a, c, e) and volumetric strain G_V (b, d, f).

compression normal displacement parameters (see Fig. 3.17f). The characteristic compression normal displacement plays a vital role in determining the elastic stiffness tensors in Eqs. 3.27 and 3.28 and material strength properties because it regulates damage evolution.

According to the first two parametric studies based on the compression k_η^c normal stiffness and characteristic compression B_η^c normal displacement, there are both similarities and differences in the volumetric strain and principal stress ratio behaviors. Softening behavior after the significant peak was commonly observed for the principal stress ratio at high values. Volumetric strain exhibited dilative behavior at high and contractive behavior at low values of these constitutive parameters. When the compression normal stiffness is varied, the peak in the principal stress ratio occurs at the same strain in all specimens (see Figs. 3.16a, 3.16c, and 3.16e), while the volumetric strain differs across different strains in Figs. 3.16b, 3.16d, and 3.16f. Conversely, for characteristic compression normal displacement, the principal stress ratio peaks at different strain values for each specimen in Figs. 3.17a, 3.17c, and 3.17e, but the volumetric strain starts from the same strain value and then shows either dilative or contractive behavior as demonstrated in Figs. 3.17b, 3.17d, and 3.17f.

3.3.3 Parametric study on compression σ_η^c plastic yielding parameter

Thirdly, the compression σ_η^c plastic yielding parameter is obtained by the multiplying of compression k_η^c normal stiffness and the inter-granular distance L in terms of catching the same unit of measure. The principal stress ratio and volumetric strain were examined in relation to $\bar{\sigma}_{\eta D}^c$, $\bar{\sigma}_{\eta M}^c$, and $\bar{\sigma}_{\eta L}^c$ values of dense, mid-dense, and loose specimens, respectively, for all specimens as shown in Fig. 3.18. The compression plastic yielding parameter plays a crucial role in determining the strain at which the evolution of compression λ_η^c plastic multipliers can start and how much their quantities increase. During the numerical simulations, only the non-dimensionalization coefficient belonging to compression plastic yielding parameter was varied. In fact, this was done to examine how affected the behavior of numerical model by either accelerating or delaying the evolution of compression plastic multipliers. For a dense specimen, the significant peak of principal stress ratio occurs at the same strain for all multiplied compression $\bar{\sigma}_{\eta D}^c$ plastic yielding parameter parameters, while the post-peak occurs at different strains depending on the evolution of compression plastic multipliers, resulting in an asymptotic decline, as seen in Fig. 3.18a. After the

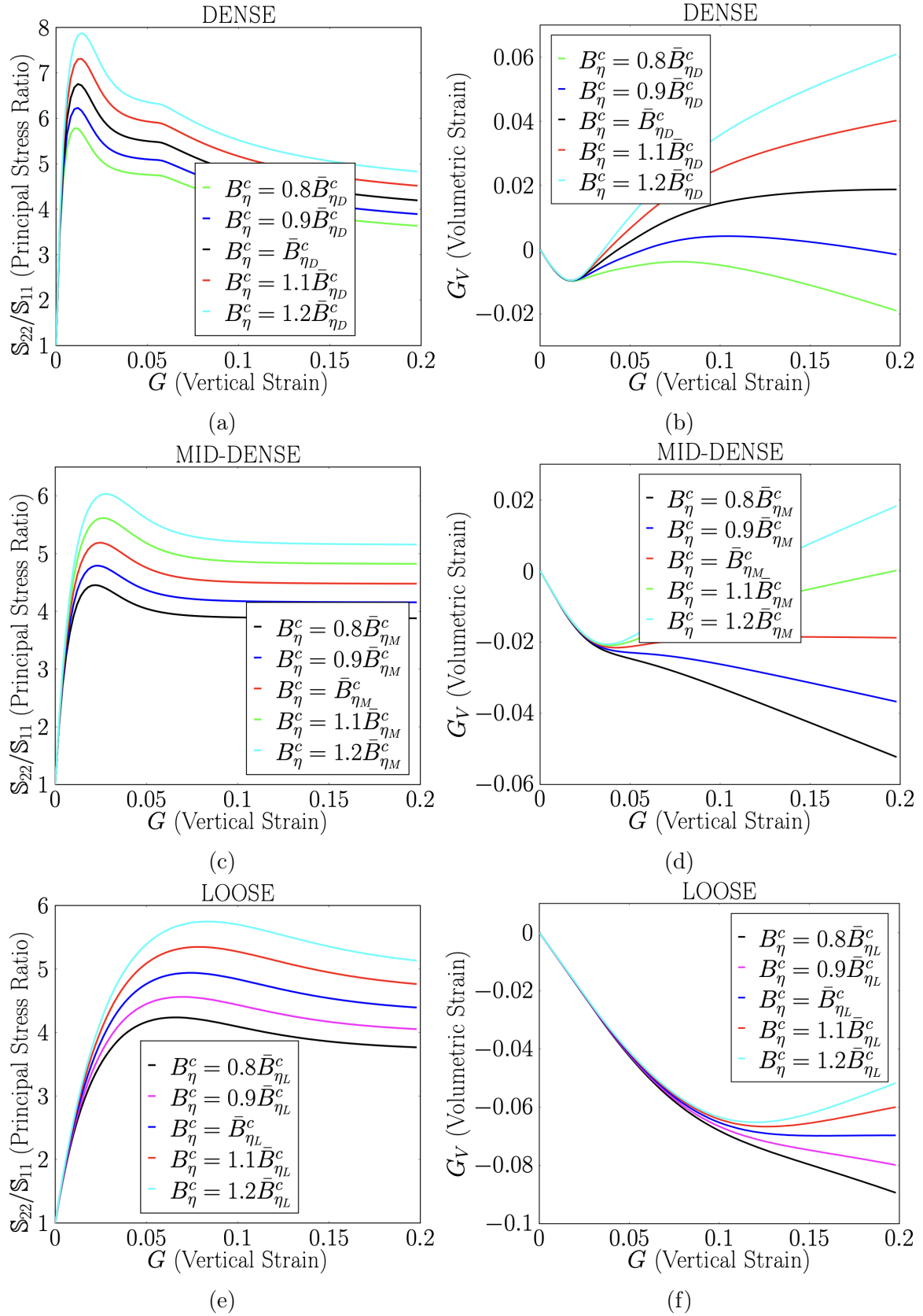


Figure 3.17: Parametric analysis by changing compression $\bar{B}_\eta^c$ characteristic normal displacement for all specimens in terms of principal stress ratio $\mathbb{S}_{22}/\mathbb{S}_{11}$ (a, c, e) and volumetric strain G_V (b, d, f).

softening and subsequent hardening behaviors arise at volumetric strain up to a certain strain, dilative behavior is observed for high compression plastic yielding parameter in Fig. 3.18b. In more detail, with the postponed evolution of λ_η^c , the strain component G_{11} becomes more dominant than the other strain component G_{22} , and there is an increase in volumetric strain. Upon reaching the classical critical state response, the evolution of compression plastic multipliers was not observed in the mid-dense and loose specimens. Therefore, in these specimens, the compression $\bar{\sigma}_{\eta_M}^c$ and $\bar{\sigma}_{\eta_L}^c$ plastic yielding parameters were reduced, and the compression plastic multipliers evolved, allowing the remaining analyses to be completed. In both specimens, the principal stress ratio in Figs. 3.18c and 3.18e decreased asymptotically at lower strains, while contractive behavior occurred with the strain component G_{22} becoming more dominant in volumetric strain (see Figs. 3.18d and 3.18f). From these simulations, it appears that the evolution of compression plastic multipliers affects the second-order tensor $\mathbb{P}_{ij}$ given in Eq. 3.28, causing changes in both the stress component S_{22} and the strain component G_{11} in Eq. 3.60.

3.3.4 Parametric study on hardening $\sigma_{\eta\eta}^c$ parameter

Finally, the parametric analysis was accomplished varying the hardening parameter $\sigma_{\eta\eta}^c$, which is associated with the compression k_η^c normal stiffness (having the same unit of measure) and a non-dimensionalization coefficient. Only the principal stress ratio and volumetric strain for a dense specimen are presented based the hardening parameter $\bar{\sigma}_{\eta\eta_D}^c$ in Fig. 3.19. Depending on whether the hardening parameter is increased or decreased, the quantities of compression plastic multipliers are adjusted following Eq. 3.59. For a dense specimen, a significant peak in the principal stress ratio was observed at the same strain, followed by a change at the same strain where the subsequent post-peak occurred for all hardening parameter values in Fig. 3.19a. At high hardening parameter, the evolution of compression plastic multipliers decelerates, and both the principal stress ratio and volumetric strain increase, resulting in dilative behavior (see Fig. 3.19b). Conversely, at low hardening parameter, the evolution of compression plastic multipliers accelerates, causing the principal stress ratio to decrease asymptotically. While the volumetric strain still exhibits dilative behavior, the amount tends to decrease compared to the preceding work's outcomes. These studies indicate that the evolution of compression plastic multipliers affects the second-order tensor $\mathbb{P}_{ij}$ in Eq. 3.28, impacting both the stress component S_{22} in Eq. 3.45 and the strain component G_{11} in Eq 3.60.

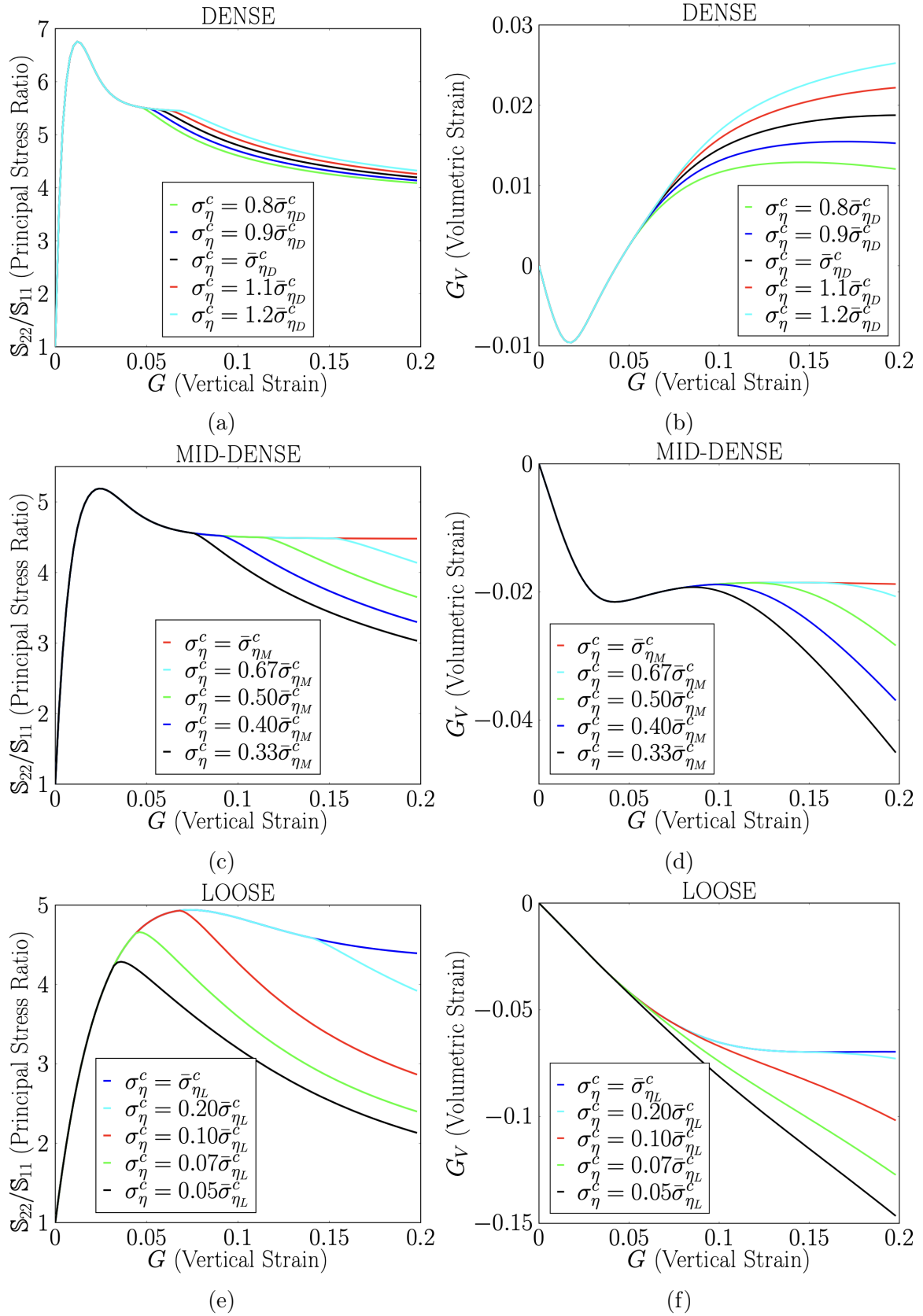


Figure 3.18: Parametric analysis by compression $\bar{\sigma}_\eta^c$ plastic yielding parameter for all specimens in terms of principal stress ratio S_{22}/S_{11} (a, c, e) and volumetric strain G_V (b, d, f).

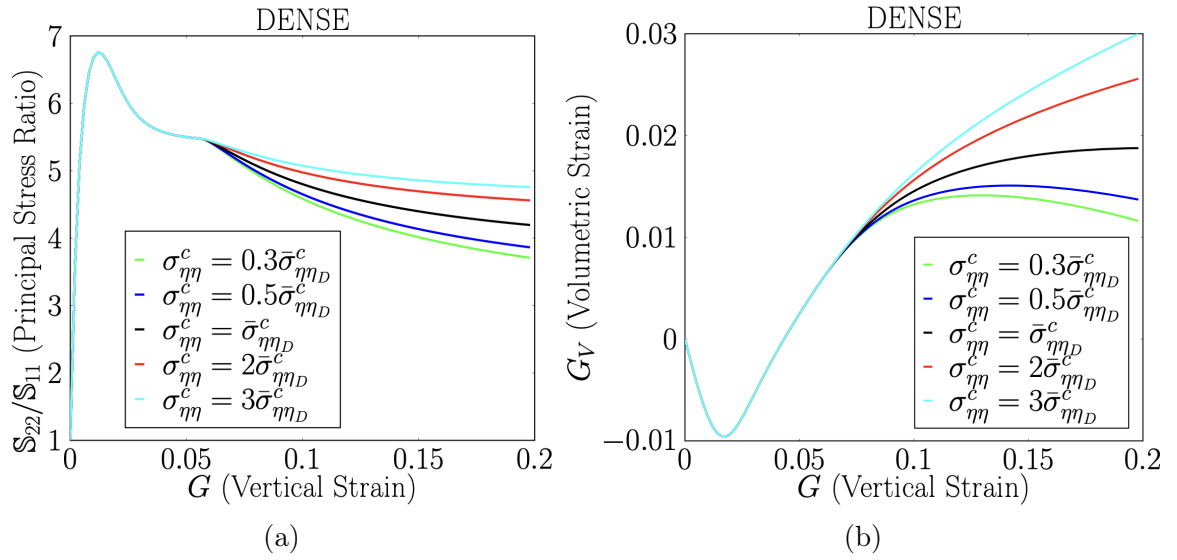


Figure 3.19: Parametric analysis by hardening $\bar{\sigma}_{\eta\eta}^c$ parameter for dense specimen in terms of principal stress ratio S_{22}/S_{11} (a) and volumetric strain G_V (b).

Granular micromechanics-based modeling of one-dimensional compression in granular materials

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During one-dimensional compression of elasto-frictional granular materials, a stiffer assembly is created while accruing irrecoverable deformations. While compaction leads to a transition from a loose to dense state, the mechanical energy required for the transition is influenced by the grain-pair contacts. The core thrust of these works is to address the concept of one-dimensional compression by exploiting grain-scale mechanisms. These mechanisms are activated extending the framework of elastic and dissipation potential energy functionals in GMA-based continuum mechanics. The energy terms are developed from the damage-elasto-plastic springs, which represent effective grain-pair interactions in both the normal and tangential directions. The resultant continuum theory was applied to investigate the macroscopic behavior during the loading–unloading cycle of one-dimensional compression. Since such compression experiments are analyzed as a single continuum material point in terms of strain and the measured reaction is interpreted as stress, the simulation here assumes homogeneous deformations. The results highlight the elastic hardening behavior and the evolution of damage and plasticity, which are crucial factors affecting the behavior of granular materials. The first study aims to quantitatively validate the experimental findings for three different specimen types, also referred to as dense, mid-dense, and loose, by comparing them with simulation results. Additionally, this first work of chapter draws upon material presented by Yilmaz et al. (2025), *Exploring One-Dimensional Uniaxial Compression through a Granular Micromechanics Model* (DOI: 10.14356/kona.2026014). In this context, the chapter further demonstrates the numerical model’s capability to capture the behavior of granular materials subjected

to one-dimensional compression. The second work focuses on analyzing how irreversible behavior and anisotropy evolve, with particular attention to tangential plasticity in the extended GMA framework presented by Yilmaz et al. (2026), *Geometrical and Material Nonlinear Effects in Granular Micromechanics: Effects of Grain-Pair Tangential Plasticity and Induced Anisotropy* (DOI: 10.1007/s00161-026-01476-2).

4.1 Exploring one-dimensional uniaxial compression through a granular micromechanics model

4.1.1 Mathematical model

The emergence of elastic hardening behavior is desired to reflect the stiffer material properties exhibited by granular materials under one-dimensional compression. Therefore, new terms have been added to the elastic and normal damage and plastic dissipation potential functionals regarding Eqs. 3.20, 3.31 and 3.35, respectively, in a granular micromechanics model presented in this chapter. By introducing a third term, as a quartic term with respect to the elastic normal displacement u_η^{el} and the duffing stiffness $k_{\eta\eta}$, to the elastic energy density the model aims to capture the elastic hardening behavior to replicate the experimental observations. The details of these modifications in the mathematical model are provided in the remainder of this section.

4.1.1.1 Elastic energy

Let U^{np} denote the total elastic energy associated with the effective grain-pair interaction between two contacting grains, n and p , for whom the line connecting their centroids is aligned in the direction $\hat{\mathbf{c}}$. U^{np} can be expressed as follows in terms of the normal and tangential decomposition of the objective total relative displacement between the grains,

$$U^{np} = \frac{1}{2}k_{\eta D} (u_\eta^{el})^2 + \frac{1}{4}k_{\eta\eta D} (u_\eta^{el})^4 + \frac{1}{2}k_{\tau D} u_\tau^{2el}, \quad (4.1)$$

where the quartic power of the elastic normal displacement is expressed as follows

$$\begin{aligned} (u_\eta^{el})^4 = (u_\eta - u_\eta^{pl})^4 = & L^4 G_{ij} G_{ab} G_{cd} G_{ef} \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b \hat{c}_c \hat{c}_d \hat{c}_e \hat{c}_f - 4L^3 G_{ij} G_{ab} G_{cd} \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b \hat{c}_c \hat{c}_d (u_\eta^{pl}) \\ & + 6L^2 G_{ij} G_{ab} \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b (u_\eta^{pl})^2 - 4L G_{ij} \hat{c}_i \hat{c}_j (u_\eta^{pl})^3 + (u_\eta^{pl})^4. \end{aligned} \quad (4.2)$$

The first and third terms in Eq. 4.1 are the standard ones already investigated in [7, 8, 107, 223–225, 227, 228] and related to the geometrical nonlinear behavior. The second term is of different nature because it is quartic with respect to the elastic normal displacement u_η^{el} . It therefore corresponds not anymore to a linear standard spring but to a cubic (duffing) non-standard spring. The reason for such a new term is connected to the necessity of investigating the high strain level of those uniaxial compression tests it is aimed to model in this study. The inclusion of quartic terms is inspired by their ability to capture nonlinear behaviors that traditional quadratic models often overlook. These quartic terms account for stiffening interaction between particles that become significant at higher strains. Further, quartic terms help to model the softening and stiffening phenomena observed in granular materials. This aspect is crucial for accurately representing the stress-strain response in experiments. Inspired by the work of Misra and Yang [233], which derived incremental stiffnesses at the grain-scale under tension and compression for cohesive materials through pseudo-bonds, the quartic term with duffing stiffness ($k_{\eta\eta}$), which has not yet been presented in the literature, were particularly determined to elucidate the potential enhancement of the stress-strain relationship. In Eq. 4.1, $k_{\eta D}$ symbolizes the damaged normal stiffness (different in tension and in compression) while $k_{\eta\eta D}$ indicates the damaged duffing stiffness:

$$k_{\eta\eta D} = \frac{k_{nn} k_{\eta D}}{L^2}, \quad k_{\eta\eta D} = k_{\eta\eta} (1 - D_\eta), \quad (4.3)$$

where k_{nn} is a non-dimensional material constant indicating the weight of the new duffing contribution. The damaged tension $k_{\eta D}^t$ and compression $k_{\eta D}^c$ normal stiffness and the damaged tangent $k_{\tau D}$ stiffness are reduced by two damage variables as given in Eq 3.23. In particular, k_η^t and k_η^c refer to the non-damaged normal stiffness, respectively, in tension and compression, and k_τ denotes the non-damaged tangential stiffness. The sign of u_η^{el} declares whether the current direction $\hat{\mathbf{c}}$ (or np pair) is characterized by tension or compression.

Let us consider that within a specimen composed of frictional granular material, there are possible M grain-pair interactions. The total elastic energy is found by the sum of the elastic energy U^{np} over all such pairs. In line with the simple homogenization rule (see selected works that also include a brief review about the details of adapted homogenization

approach [63, 223]), a revised form of Eq. 3.25 for an elastic energy density is assumed with respect to the definition of the continuum as follows

$$U_M \xrightarrow{M \rightarrow \infty} U = \int_S \left[\frac{1}{2} k_{\eta D} (u_{\eta}^{el})^2 + \frac{1}{4} k_{\eta\eta D} (u_{\eta}^{el})^4 + \frac{1}{2} k_{\tau D} u_{\tau}^{2el} \right] d\ell, \quad (4.4)$$

where the continuum model has been defined in Subsection 3.1.2. Indeed, stiffnesses and damage parameters depend on the orientation in the continuum description: $k_{\eta} = \tilde{k}_{\eta}(\theta)$, $k_{\eta\eta} = \tilde{k}_{\eta\eta}(\theta)$, $k_{\tau} = \tilde{k}_{\tau}(\theta)$, $D_{\eta} = \tilde{D}_{\eta}(\theta)$, and $D_{\tau} = \tilde{D}_{\tau}(\theta)$.

The continuum elastic energy density can be formulated utilizing Eqs. 3.13-3.18 in the following form:

$$U = \frac{1}{2} \mathbb{C}_{ijab} G_{ij} G_{ab} + \frac{1}{3} \mathbb{L}_{ijabcd} G_{ij} G_{ab} G_{cd} + \frac{1}{4} \mathbb{N}_{ijabcdef} G_{ij} G_{ab} G_{cd} G_{ef} + \mathbb{P}_{ij} G_{ij}, \quad (4.5)$$

where $\mathbb{C}_{ijab}$ (4th-order), $\mathbb{L}_{ijabcd}$ (6th-order), $\mathbb{N}_{ijabcdef}$ (8th-order), and $\mathbb{P}_{ij}$ (2nd-order) are elastic stiffness tensors identified as follows

$$\begin{aligned} \mathbb{C}_{ijab} = & L^2 \int_S k_{\eta} (1 - D_{\eta}) \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b d\ell + L^2 \int_S 3k_{\eta\eta} (1 - D_{\eta}) \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b (u_{\eta}^{pl})^2 d\ell \\ & + L^2 \int_S k_{\tau} (1 - D_{\tau}) ((\delta_{ia} \hat{c}_j \hat{c}_b + \delta_{ib} \hat{c}_j \hat{c}_a + \delta_{ja} \hat{c}_i \hat{c}_b + \delta_{jb} \hat{c}_i \hat{c}_a) - 4\hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b) d\ell, \end{aligned} \quad (4.6)$$

$$\mathbb{L}_{ijabcd} = -L^3 \int_S 3k_{\eta\eta} (1 - D_{\eta}) \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b \hat{c}_c \hat{c}_d (u_{\eta}^{pl}) d\ell, \quad (4.7)$$

$$\mathbb{N}_{ijabcdef} = L^4 \int_S k_{\eta\eta} (1 - D_{\eta}) \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b \hat{c}_c \hat{c}_d \hat{c}_e \hat{c}_f d\ell, \quad (4.8)$$

$$\mathbb{P}_{ij} = -L \int_S k_{\eta} (1 - D_{\eta}) \hat{c}_i \hat{c}_j (u_{\eta}^{pl}) d\ell - L \int_S k_{\eta\eta} (1 - D_{\eta}) \hat{c}_i \hat{c}_j (u_{\eta}^{pl})^3 d\ell. \quad (4.9)$$

$\mathbb{C}_{ijab}$, $\mathbb{L}_{ijabcd}$, $\mathbb{N}_{ijabcdef}$, and $\mathbb{P}_{ij}$ comprise different powers of the normal plastic relative displacement u_{η}^{pl} . Notably, these stiffness tensors are obtained by integrating over all considered orientations employing the trapezoidal rule. Unlike previous studies by Placidi et al. [107, 227, 228], the effects of the normal plastic relative displacement u_{η}^{pl} are seen both in $\mathbb{P}_{ij}$, also referred to as pre-stress tensor, and in other higher-order stiffness tensors. Additionally, a duffing stiffness $k_{\eta\eta}$ injects the nonlinear effects in all the other elastic stiffness tensors. Finally, in Eqs. 4.6-4.9, the increase in damage makes a loss of stiffness. This loss can be explained as a decrease not only in the buckling and crumbling of chains and clusters from normal damage but also in the side support and enclosure of these structures within grain neighborhoods from tangent damage.

4.1.1.2 Dissipation energy potential

This approach utilizes the six fundamental scalar kinematic variables (one vectorial and five scalar variables) to determine dissipation energy potential considering a generic grain-pair: u_η and u_τ^2 (normal and squared tangential displacements), as well as D_η , D_τ , λ_η^t , and λ_η^c (describing damage and plasticity), as discussed in Section 3.1.3. The total dissipation energy potential W can be divided into damage and plastic parts as given in Eq. 3.30. While the tangential component of damage dissipation potential W_D^τ is expressed as given in Eq. 3.32, the normal component W_D^η is defined based on the revised form of Eq. 3.31 as follows

$$W_D^\eta = \frac{1}{2}k_\eta(B_\eta)^2 \left[-D_\eta + \frac{2}{\pi} \tan \left(\frac{\pi}{2} D_\eta \right) \right]. \quad (4.10)$$

W_{pl} reports the dissipated energy potential due to the normal component of plastic behavior and is expressed via

$$W_{pl} = W_{pl}^\eta = (1 - D_\eta)^2 \left(\sigma_\eta^t \lambda_\eta^t + \sigma_\eta^c \lambda_\eta^c + \sigma_{\eta\eta}^t (\lambda_\eta^t)^2 + \sigma_{\eta\eta}^c (\lambda_\eta^c)^2 + \sigma_{\eta\eta}^{tc} \lambda_\eta^t \lambda_\eta^c \right), \quad (4.11)$$

where the plasticity yielding conditions are governed for the coupled damage-elasto-plastic behavior under tension and compression by the constitutive parameters σ_η^t and σ_η^c , respectively. The parameters $\sigma_{\eta\eta}^t$ and $\sigma_{\eta\eta}^c$ characterize the plastic softening/hardening behavior in tension and compression (see the citation [237] as an initial guide for the linear hardening phenomena by modeling elasto-plastic spring), $\sigma_{\eta\eta}^{tc}$ introduces the coupling between the evolution of plastic deformations. It is worth emphasizing that the tangential component of the plastic dissipation potential W_{pl} was not considered in the first work on one-dimensional compression, whereas in the present study, W_{pl} differs from previous formulations [107, 224], and a coupling term is introduced for the first time in the dissipation potential. In the following Subsection 4.1.1.3, the relevance and effects of these constitutive parameters indicated in the dissipation energy potential during one-dimensional compression will be revealed with regard to irreversible quantities. A new type of dissipation energy potential is presented for the evolution of irreversible phenomena to introduce the concept of one-dimensional uniaxial compression.

4.1.1.3 Hemi-variational formulation: governing equations and Karush-Kuhn-Tucker conditions

In the light of traditional variational approach (see Section 3.1.4), the constitutive relations are presented in relation to the application of the mentioned hemi-variational approach for the stress tensor $\mathbf{S}$ as follows

$$\mathbf{S} = \mathbf{C}\mathbf{G} + \mathbf{L}\mathbf{G}^2 + \mathbf{N}\mathbf{G}^3 + \mathbf{P} \quad \forall \mathbf{X} \in \mathcal{B}. \quad (4.12)$$

Further, the following Karush-Kuhn-Tucker (KKT)-type conditions are derived as written below

$$\left\{ -\frac{1}{2}k_\eta (u_\eta - \lambda_\eta^t + \lambda_\eta^c)^2 - \frac{1}{4}k_{\eta\eta} (u_\eta - \lambda_\eta^t + \lambda_\eta^c)^4 + \frac{1}{2}k_\eta (B_\eta)^2 \left[\tan \left(\frac{\pi}{2} \tilde{D}_\eta \right) \right]^2 - 2(1 - \tilde{D}_\eta) \left(\sigma_\eta^t \lambda_\eta^t + \sigma_\eta^c \lambda_\eta^c + \sigma_{\eta\eta}^t (\lambda_\eta^t)^2 + \sigma_{\eta\eta}^c (\lambda_\eta^c)^2 + \sigma_{\eta\eta}^{tc} \lambda_\eta^t \lambda_\eta^c \right) \right\} \Delta D_\eta = 0, \quad (4.13)$$

$$\left\{ -\frac{1}{2}k_\tau u_\tau^2 + \frac{1}{2}k_\tau (B_\tau)^2 \left(\log(1 - \tilde{D}_\tau) \right)^2 \right\} \Delta D_\tau = 0, \quad (4.14)$$

$$\left\{ -k_\eta (u_\eta - \tilde{\lambda}_\eta^t + \lambda_\eta^c) - k_{\eta\eta} (u_\eta - \tilde{\lambda}_\eta^t + \lambda_\eta^c)^3 + (1 - D_\eta) \left(\sigma_\eta^t + 2\sigma_{\eta\eta}^t \tilde{\lambda}_\eta^t + \sigma_{\eta\eta}^{tc} \lambda_\eta^c \right) \right\} \Delta \lambda_\eta^t = 0, \quad (4.15)$$

$$\left\{ k_\eta (u_\eta - \lambda_\eta^t + \tilde{\lambda}_\eta^c) + k_{\eta\eta} (u_\eta - \lambda_\eta^t + \tilde{\lambda}_\eta^c)^3 + (1 - D_\eta) \left(\sigma_\eta^c + 2\sigma_{\eta\eta}^c \tilde{\lambda}_\eta^c + \sigma_{\eta\eta}^{tc} \lambda_\eta^t \right) \right\} \Delta \lambda_\eta^c = 0. \quad (4.16)$$

The KKT-type conditions can be described concisely in relation to the four irreversible kinematic descriptors as follows

$$\{D_\eta - \tilde{D}_\eta(u_\eta, \lambda_\eta^t, \lambda_\eta^c)\} \Delta D_\eta = 0, \quad (4.17)$$

$$\{D_\tau - \tilde{D}_\tau(u_\tau^{el}, u_\tau^2)\} \Delta D_\tau = 0, \quad (4.18)$$

$$\{\lambda_\eta^t - \tilde{\lambda}_\eta^t(u_\eta, D_\eta, \lambda_\eta^c)\} \Delta \lambda_\eta^t = 0, \quad (4.19)$$

$$\{\lambda_\eta^c - \tilde{\lambda}_\eta^c(u_\eta, D_\eta, \lambda_\eta^t)\} \Delta \lambda_\eta^c = 0, \quad (4.20)$$

where $\tilde{D}_\tau$ is the threshold function expressed via

$$\tilde{D}_\tau(u_\eta^{el}, u_\tau^2) = 1 - \exp\left(-\frac{u_\tau^2}{\tilde{B}_\tau(u_\eta^{el})}\right) = 1 - \exp\left(-\frac{u_\tau^2}{B_\tau}\right). \quad (4.21)$$

In Eqs. 4.13-4.16, the threshold functions are obtained by setting the equations in the curly braces to zero. However, due to the quartic power of the elastic normal displacement u_η^{el} , nonlinear equations arise from the first variation of the elastic energy equation (see Eq. 4.1) with respect to irreversible quantities. $\tilde{D}_\eta$, $\tilde{\lambda}_\eta^t$, and $\tilde{\lambda}_\eta^c$ are updated using the irreversible quantities from the previous time step as initial guesses in Eqs. 4.17, 4.19, and 4.20, respectively. To find the real variables, the single root for each variable is calculated by iteratively solving the nonlinear equations until a certain tolerance of 10^{-10} is reached. Notably, the $\tilde{D}_\tau$ threshold function in Eq. 4.14 is derived analytically as given in Eq. 4.21. It is important to underline that the evolution of damage and plasticity depends on the distinction between tension and compression conditions for normal stiffness in Eq. 3.21 and characteristic damage displacements in Eqs. 3.33 and 3.34. At the beginning of the deformation history, $\tilde{D}_\eta$, $\tilde{D}_\tau$, $\tilde{\lambda}_\eta^t$, and $\tilde{\lambda}_\eta^c$ are null and evolve over time. Additionally, damage and plasticity do not decrease over time; their evolution continues if and only if the threshold value of the current time step is higher than that of the previous time step. Otherwise, these variables remain constant, fixed at the previous time step. At the limits where the elastic normal displacement or the normal displacement goes to infinity, normal and tangent damage asymptotically increase towards one. However, having the damage variables reach a value of one is not desired, as this would nullify the elastic stiffnesses, as clearly seen in Eqs. 4.6-4.9. In Eqs. 4.13, 4.15, and 4.16, the predicted behavior of these irreversible quantities under loading-unloading, including both D_η and the coupling term $\sigma_{\eta\eta}^{tc}$ between plasticity evolution, will be examined in the next section. Remarkably, the coupling term plays a crucial role with loading-unloading history under one-dimensional compression by activating the effects of plasticity evolution on each other when $\sigma_{\eta\eta}^{tc} \neq 0$. Furthermore, the softening parameter $\sigma_{\eta\eta}^t$ for tension and hardening parameter $\sigma_{\eta\eta}^c$ for compression regularize the growth in plasticity. Finally, it should be noted that the orientation-dependent evolution of the irreversible quantities is the same for all grains considered, regardless of which grain is selected from the material.

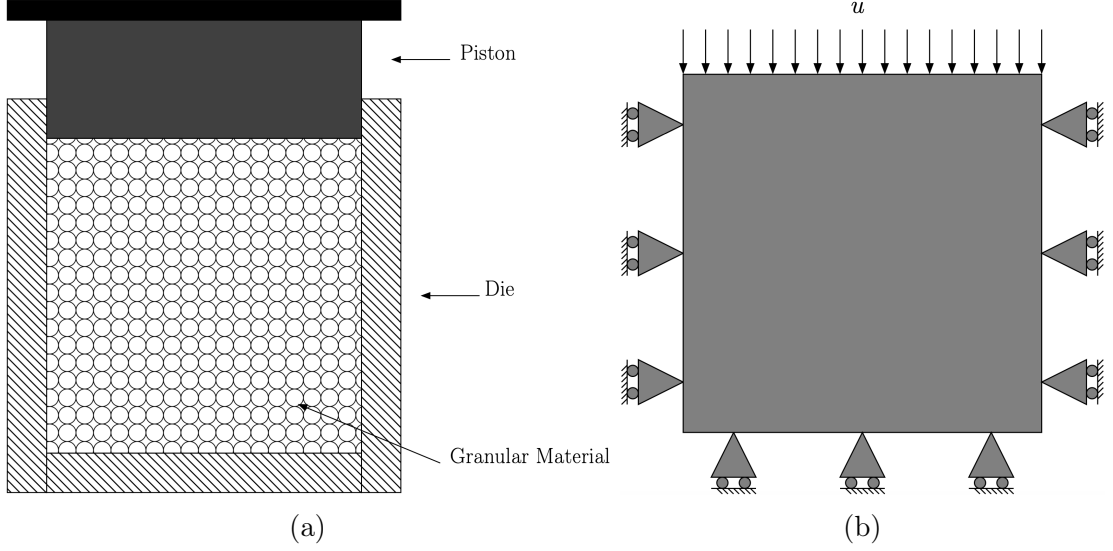


Figure 4.1: (a) Schematic illustration of one-dimensional compression of granular materials. (b) Boundary condition of one-dimensional compression.

4.1.2 Results and discussion

4.1.2.1 One-dimensional compression loading condition

As depicted in Fig. 4.1a, one-dimensional compression consists of compressing granular material contained within a die (or oedometer) with a piston plunging in the axial direction. The material is completely confined within rigid boundaries on all the other sides, including the lateral sides. The boundary conditions are schematically shown in Fig. 4.1b, in which the roller support both in the 1-direction (2 side boundaries) and the bottom boundary of the specimen represent the rigid boundaries while the axial compression is represented by displacement $\bar{u}$ in 2-direction (top boundary).

The numerical simulations are performed for a square specimen with an edge length of S by subjecting to loading-unloading cycles. In the loading stage, the compressive displacement is first increased in the vertical direction to reach the maximum imposed displacement denoted by $\mathbf{u}$. Subsequently, in the unloading process the displacement is decreased, introduced as $u_2 = \mathbf{u} - \bar{u}$ till the axial stress $\mathbb{S}_{22}$ reduces to zero. In this simulation, the lateral strain G_{11} and the shear strain G_{12} (or G_{21}) are zero while the vertical strain $G_{22} = -G$ ($G > 0$) is calculated based on the displacement field according to Eq. 3.10 as follows

$$u_1 = 0, u_2 = \frac{\bar{u}}{S} X_2, \quad \Rightarrow \quad \mathbf{F} = \begin{pmatrix} 1 & 0 \\ 0 & 1 + \frac{\bar{u}}{S} \end{pmatrix}, \quad \Rightarrow \quad \mathbf{G} = \begin{pmatrix} 0 & 0 \\ 0 & \frac{1}{2} \left(\frac{\bar{u}}{S} \right)^2 + \frac{\bar{u}}{S} \end{pmatrix}. \quad (4.22)$$

Based on the numerical solution of Eqs. 4.13, 4.15, and 4.16 and the analytical solution of Eq. 4.21, the evolution of damage and plasticity phenomena are found. Further, the elastic stiffness tensors, $\mathbb{C}_{ijab}$ (4th-order), $\mathbb{L}_{ijklcd}$ (6th-order), $\mathbb{N}_{ijklcdef}$ (8th-order), and $\mathbb{P}_{ij}$ (2nd-order), are calculated by utilizing Eqs. 4.6-4.9. The vertical stress $\mathbb{S}_{22}$ and the lateral stress $\mathbb{S}_{11}$ are defined in Eq. 3.45 based on the updated strain G_{22} by changing the compressive displacement $\bar{u}$ (see Eq. 4.22).

4.1.2.2 Dependence of parameter on initial density state and material type

The mechanical response under uniaxial compression test is simulated for three granular material specimen derived from glass beads, Toyoura sand and Masado sand as described by Wu et al. [238]. Since a 2D theoretical formulation is utilized, an equivalence needs to be established with 3D axisymmetric experimental measurements, such that the stresses in 2D, which have a unit of measure of force per unit length, can be properly mapped to the experimental stress with a unit of measure of force per unit area. For this equivalence, it is considered that a 2D model has a pseudo thickness, $\mathfrak{t}$, related to the cross-section area of typically cylindrical samples, such that the unit of measure remain consistent in the following manner:

$$\mathfrak{t} = \sqrt{\pi r^2}, \quad \frac{\mathbb{S}_{22}}{\mathfrak{t}} = \sigma_{22} \text{ (MPa)}, \quad (4.23)$$

where r is the radius (typically 25.7 mm) of the specimen used in the experiments.

The model parameters can be determined by exploiting the relationship of material elastic modulus and the void ratio e , as well as the identification of elastic modulus in terms of the microscale stiffness parameters given by Barchiesi et al. [223]. As the reference material for parameter identification, the experimental measurements for Toyoura sand are considered presented by Wu et al. [238]. In these experiments, the initial void ratio of the specimen is close to 0.62 (which can also be considered as a mid-dense sand). It is reasonable to estimate that the shear modulus at the unloaded state or at the initial incipient loading is extremely low as is easily observable from the initial part of stress-strain curves of granular materials under compression (see for example Fig. 4 of [238]).

For the numerical calculations, an initial nominal shear modulus of 230 Pa is estimated, such that the 2D shear modulus is $G_{2D} = 5.1 \times 10^3 (\text{J/m}^2)$. For these experimental values of initial void ratio and 2D shear modulus, the material-specific constant A is found to be $985 (\text{J/m}^2)$. Consequently, the normal stiffness k_η^c can be identified from Eq. 3.64.

For further discussion, the 2D shear modulus and the normal compression stiffness for the reference Toyoura sand (mid-dense) specimen are symbolized with $\bar{G}_{2D}$ and $\bar{k}_\eta^c$, respectively, as given in Table 4.1. To define the material properties for the glass beads specimen (which behaved as a dense granular packing) and Masado sand specimen (which behaved as a loose granular packing), the material stiffness parameter of a Toyoura sand specimen $\bar{k}_\eta^c$ were multiplied 1.6 and 0.6, respectively. Given the initial 2D shear modulus, either the initial void ratio or the material-specific constant A for these specimens can be calculated using Eqs. 3.62 and 3.63, respectively. It is indeed noteworthy that the packing stiffness behavior is affected both by the particle stiffness and the initial void ratio (initial density states) in a similar manner (high particle stiffness or higher initial density typically yield stiffer packing behavior). In these cases, carefully controlled studies are needed to find the relative influences of a myriad of characteristics of granular packing, including grain material types, grain surface characteristics, grain particle sizes, grain shapes and packing density.

Further, the compression characteristic damage displacement B_η^c is assigned using a trial and error approach through a fitting procedure. All the other model parameters are assumed to be same for all the three specimen. Table 4.1 gives the material-specific constant A , the shear modulus $\bar{G}_{2D}$, the stiffness $\bar{k}_\eta^c$, k_η^t , and k_τ , the characteristic damage displacements B_η^c , B_η^t , and $B_{\tau 0}$, the plasticity constitutive parameters σ_η^t , σ_η^c , $\sigma_{\eta\eta}^t$, $\sigma_{\eta\eta}^c$, and $\sigma_{\eta\eta}^{tc}$, the side length of a square specimen S , the average intergranular distance L , the regularization factors α and α_1 , and the duffing stiffness coefficient k_{nn} .

Table 4.1: The simulation parameters for all specimens.

A (J/m ²)	$\bar{G}_{2D}$ (J/m ²) [see Eq. 3.63]	$\bar{k}_\eta^c$ (J/m ⁴)	k_η^t (J/m ⁴)	k_τ (J/m ⁴)	B_η^c (m)
985	5.1×10^3	2.93×10^8	$0.1k_\eta^c$	$0.1k_\eta^c$	$6.08L$
B_η^t (m)	$B_{\tau 0}$ (m)	σ_η^t (J/m ³)	σ_η^c (J/m ³)	$\sigma_{\eta\eta}^t$ (J/m ⁴)	$\sigma_{\eta\eta}^c$ (J/m ⁴)
$0.1B_\eta^c$	$0.1B_\eta^c$	0	$0.34k_\eta^c L$	$4.55k_\eta^c$	$227.27k_\eta^c$
$\sigma_{\eta\eta}^{tc}$ (J/m ⁴)	S (m)	L (m)	α (m)	α_1	k_{nn}
$-2.27k_\eta^c$	0.1	0.01	2.5×10^{-5}	10	5.0×10^4

In Table 4.1, the non-dimensionalization is utilized to simplify the simulation system by reducing the number of independent parameters. Non-dimensionalization provides the way of material identification by rescaling the key characteristic parameters. This technique is utilized via the stiffness parameter k_η^c , the compression characteristic damage displacement B_η^c , and intergranular distance L in the numerical simulations as depicted in Table 4.1.

4.1.2.3 One-dimensional compression : comparison with experimental results

To demonstrate the model performance and its capability to replicate the macroscopic behavior in one-dimensional compression of granular materials, a set of numerical simulations of uniaxial test was performed for the three specimens discussed in the previous section. In Fig. 4.2, the model calculations and the experimental results (from Fig. 9 of [238]) are plotted for comparison. The experiments were performed in a cyclic manner to reach a maximum stress σ_{22} of 22.5 MPa with subsequent unloading to zero stress.

Fig. 4.2 illustrates that glass beads specimen achieves the maximum stress at a lower strain exhibiting a dense packing behavior. In contrast, Masado sand specimen exhibits a loose packing behavior requiring a considerably higher strain to reach the same maximum stress level. In granular materials, the observed stiffening behavior can be attributed to two mechanisms, one related to the stiffening of the grain-pair contact due to compression and the other related to the increased number of grain contacts due to rearrangement process during loading stage. At the beginning of the loading history (or at very low strain), the stiffening response rate is slow for all cases. The GMA response in the region where the stress is close to zero can indeed be justified by the occurrence of plastic deformations while elastic deformations are negligible. For the glass beads specimen, a significant stiffening is observed with maximum curvature at relatively low strain ($G = 0.02 - 0.03$) followed by a considerably steep slope of the stress-strain response at higher strains ($G > 0.05$). The steep stress-strain response indicates limited densification of glass bead packing, which is also attested by the relatively small change of void ratio reported in the experimental data (see Fig. 3 of [238]). The Masado sand, which is considered a soft material, undergoes large deformation for the same stress-level. Clearly, in this case the rearrangement of particles accompanied by collapse of granular structures as well as particle fragmentation play an important role. In this case, two significant points need to be considered. Firstly, the large deformation suffered by the specimen requires that finite deformation measures are used for describing the behavior as utilized in this chapter. Secondly, and importantly, this granular material experiences both considerable

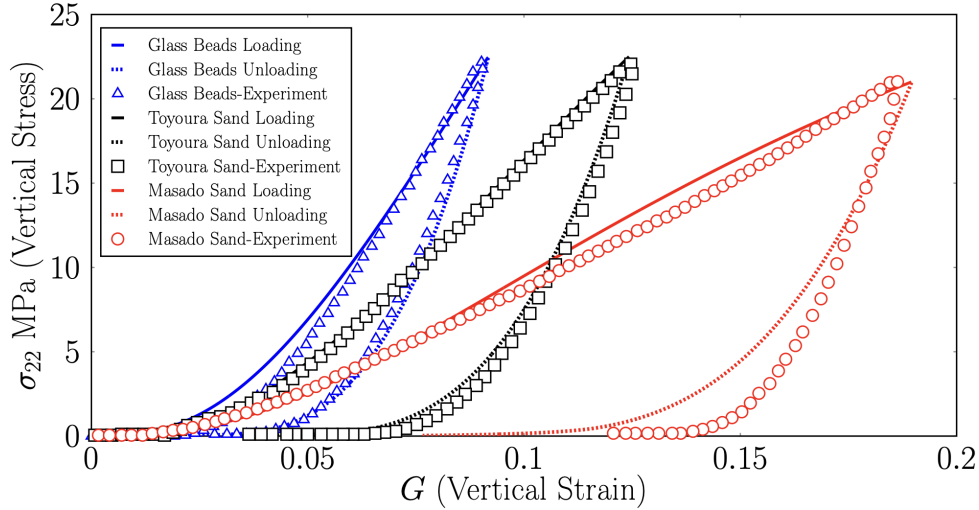


Figure 4.2: Vertical stress σ_{22} with respect to vertical strain G for three different specimens by replicating the experimental observations based on the numerical simulations under first loading-unloading until reaching a maximum stress 22.5 MPa.

damage (defined as combined effects of grain-scale mechanisms, such as collapse/buckling of particle chains and loss of lateral support or confinement of grain neighborhoods) and plasticity (defined as the effective accumulation of plastic deformation resulting from grain breakage and grain-pair sliding and separation). It is interesting to observe that in this case the stiffening effect is considerably gradual in comparison to both the glass beads packing and Toyoura sand. The accumulation of damage, with likely loss of stiffness, and plasticity for the 3 specimen is visible from the unloading behavior. Clearly, for the case of glass beads specimen, the proportion of dissipated energy is likely to be higher due to plasticity mechanism than the loss of stiffness due to damage mechanism. For the case of Toyoura and Masado sands, both mechanisms appear to contribute with plasticity being dominant. The close agreement of the model results and the experiments over the loading-unloading cycle is encouraging, given that only normal stiffness k_{η}^c was varied for the 3 specimen and all the other model parameters adjusted according to the prescription in Table 4.1. The prediction, therefore, point to a nearly universal scaling with respect to the model parameters exhibited by granular materials of different material types (or packing density).

Fig. 4.3 shows the void ratio e plotted against the logarithmically scaled vertical stress σ_{22} based upon model calculations and experimental observations (see Fig. 3 of [238]). The model predictions provide an encouraging agreement with the experimental observations. It is seen that the glass beads show the least change in void ratio while the Masado sand have the largest change. The rapid decrease in void ratio at high stresses

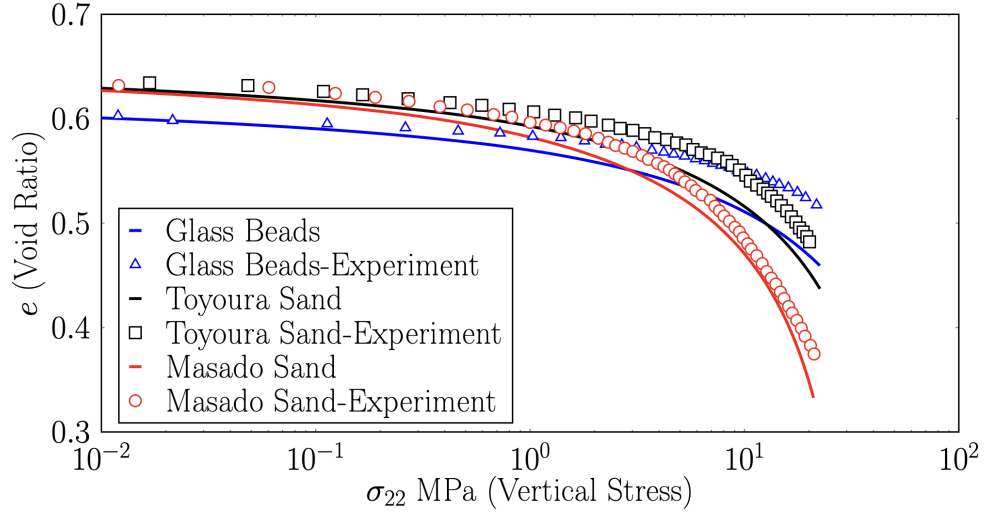


Figure 4.3: Void ratio e with respect to vertical stress σ_{22} for the glass beads, Toyoura sand, and Masado sand specimens based on the numerical simulations under loading until reaching a maximum stress 22.5 MPa.

is typically indicative of grain crushing. This particularly true for Masado sand whose particle strength is known to be relatively low [25] compared to that of glass beads and Toyoura sand. In Fig. 4.4, the relationship between the volumetric strain, $G_V = G_{11} + G_{22}$, and the vertical stress (based on Fig. 4 of [238]) is given on a logarithmic scale for the three materials. Again, a good agreement is achieved between the prediction and experimental observations of the volume compaction behavior of the three materials. It is worthwhile to reiterate that only one model parameter is varied to obtain the predictions for the three materials.

In Fig. 4.5, the relationship between the vertical and lateral stresses through the evolution of coefficient, $K_0 = \sigma_{11}/\sigma_{22}$, is investigated, as the three materials undergo the loading-unloading cycle. During the loading phase, the lateral coefficient, which starts at around 0.15, under very low stress, exhibits a gradual but slight increase as the vertical stress rises. At the maximum stress, the coefficient K_0 for soft (loose) material is higher than that for stiff (dense) material. In particular, the largest increase in K_0 value is observed for the Masado sand specimen. Under the boundary conditions shown in Fig. 4.1, an increase in the vertical stress inevitably causes an increase in lateral stress for all specimens due to particle rearrangement and crushing and corresponds to the propensity to expand in the 1-direction. During the unloading stage, the lateral coefficient continues to increase gradually with unloading until the low stress ranges where a rapid increase is predicted. The model predicted K_0 behavior follows the typical experimental observations

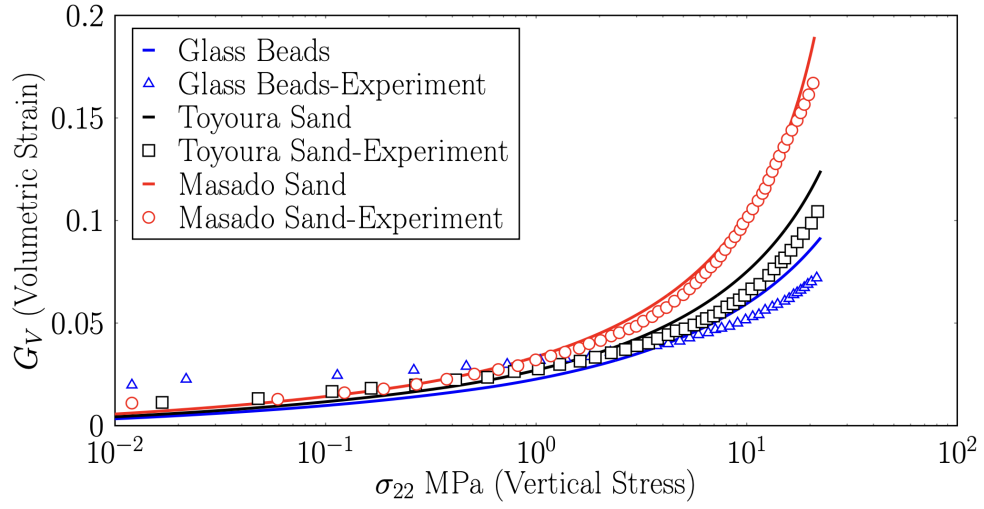


Figure 4.4: Volumetric strain G_V with respect to vertical stress σ_{22} for the glass beads, Toyoura sand, and Masado sand specimens based on the numerical simulations under loading until reaching a maximum stress 22.5 MPa.

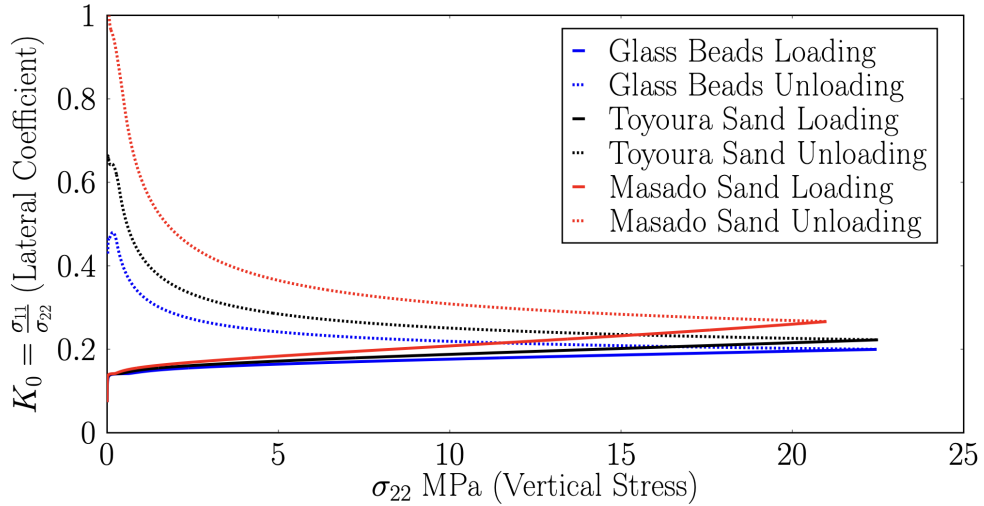


Figure 4.5: Lateral coefficient K_0 with respect to vertical stress σ_{22} for the glass beads, Toyoura sand, and Masado sand specimens based on the numerical simulations under first loading-unloading until reaching a maximum stress 22.5 MPa.

for granular materials in both loading and unloading. However, it is noted that the present model somewhat under predicts the rapid increase that is experimentally observed for the 3 materials (see Fig. 15 of [238]). Such discrepancy can possibly be remedied by further refinement of the grain-pair elastic energy functional to include higher-order dependence on tangential displacement as well as inclusion of plastic dissipation potential due to tangential displacement. It is also notable that the present energy-based approach is distinct from previous approaches that typically invoke macroscale phenomenological concepts, such as Mohr-Coulomb frictional models, with ad hoc modifications to explain such loading-unloading K_0 behavior. In this work, the predicted K_0 behavior emerges from microscale assumptions of elastic deformation energy and dissipation potential.

Figs. 4.6 and 4.7, further elaborate the predictive capacity of the present approach. Fig. 4.6 gives the axial loading-unloading behavior for the three granular materials with unloading performed from different loading-levels. Fig. 4.7 gives the corresponding lateral stress versus axial stress behavior. There are two observations that are visible for all the three materials. Firstly, the materials stiffen as the loading-level is raised, however, the stiffening rate is highest for glass beads, then Toyoura sand followed by Masado sand. It is also noted that in Fig. 4.6c, at the large loading-level, there is a tendency for stiffening to slowdown, and likely transition to softening. Such transition to softening has been observed at large loading-levels in classical experiments [239]. Secondly, the dissipated energy, as indicated by the area of the loading-unloading loop, increases with loading-level, however, the dissipation is the highest for Masado sand followed by Toyoura sand and glass bead. It is clear that not only glass bead particles have higher stiffness and failure strength than the 2 sands, but also, the packing density of almost monodispersed glass beads is high. At the same time it is likely, that the particles stiffness/strength as well as the packing density of more polydispersed sands is lower. The model parameters used in the prediction reflect the particle and the packing characteristics. The consequence of these characteristics is the different stiffening behavior as well energy dissipation predicted for the three granular materials. It is remarkable that the predicted results are confirmed by the experimental observations both for the vertical stress-strain response in Fig. 4.6 and lateral stress versus vertical stress response Fig. 4.7 (see also Figs. 6-8 of [238]).

4.1.2.4 One-dimensional compression : parametric study

The nearly universal scaling observed in comparison of model predictions with experiments is exploited to perform a suite of parametric study under one loading-unloading cycles

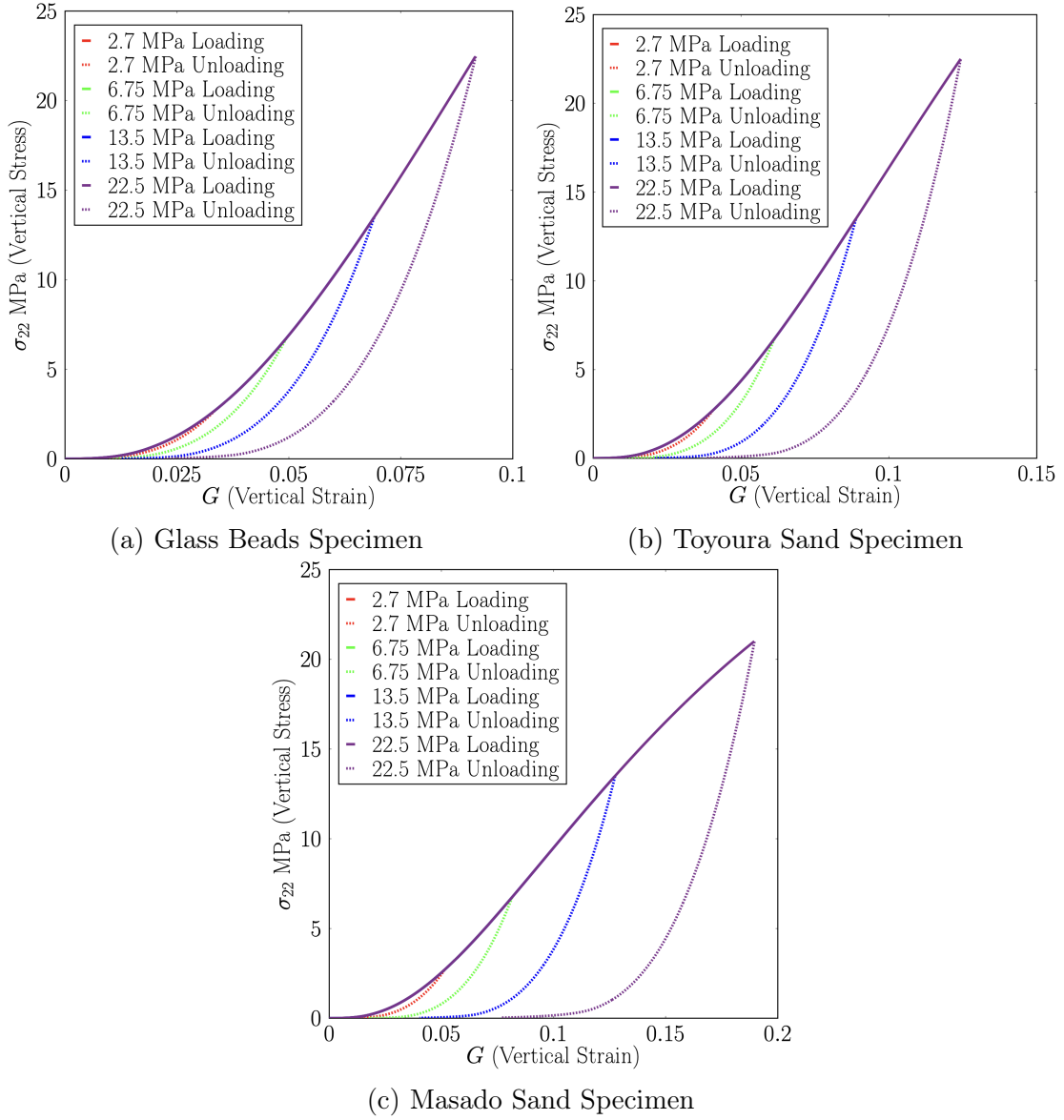


Figure 4.6: Vertical stress σ_{22} with respect to vertical strain G for glass beads (a), Toyoura sand (b) and Masado sand (c) specimens based on the numerical simulations under first loading-unloading until reaching different maximum stresses.

as well as under repeated loading-unloading cycles. In these parametric studies, the behavior of lateral stress is also examined during one-dimensional compression as well as micro-scale quantities including the directional evolution of grain-pair elastic energy and the grain-pair dissipation parameters of damage and plasticity. These parametric studies are interpreted as that for specimen of three different density states following from the discussion in previous section related to experimental behavior.

4.1.2.4.1 Scaling in loading-unloading cycle for one-dimensional compression

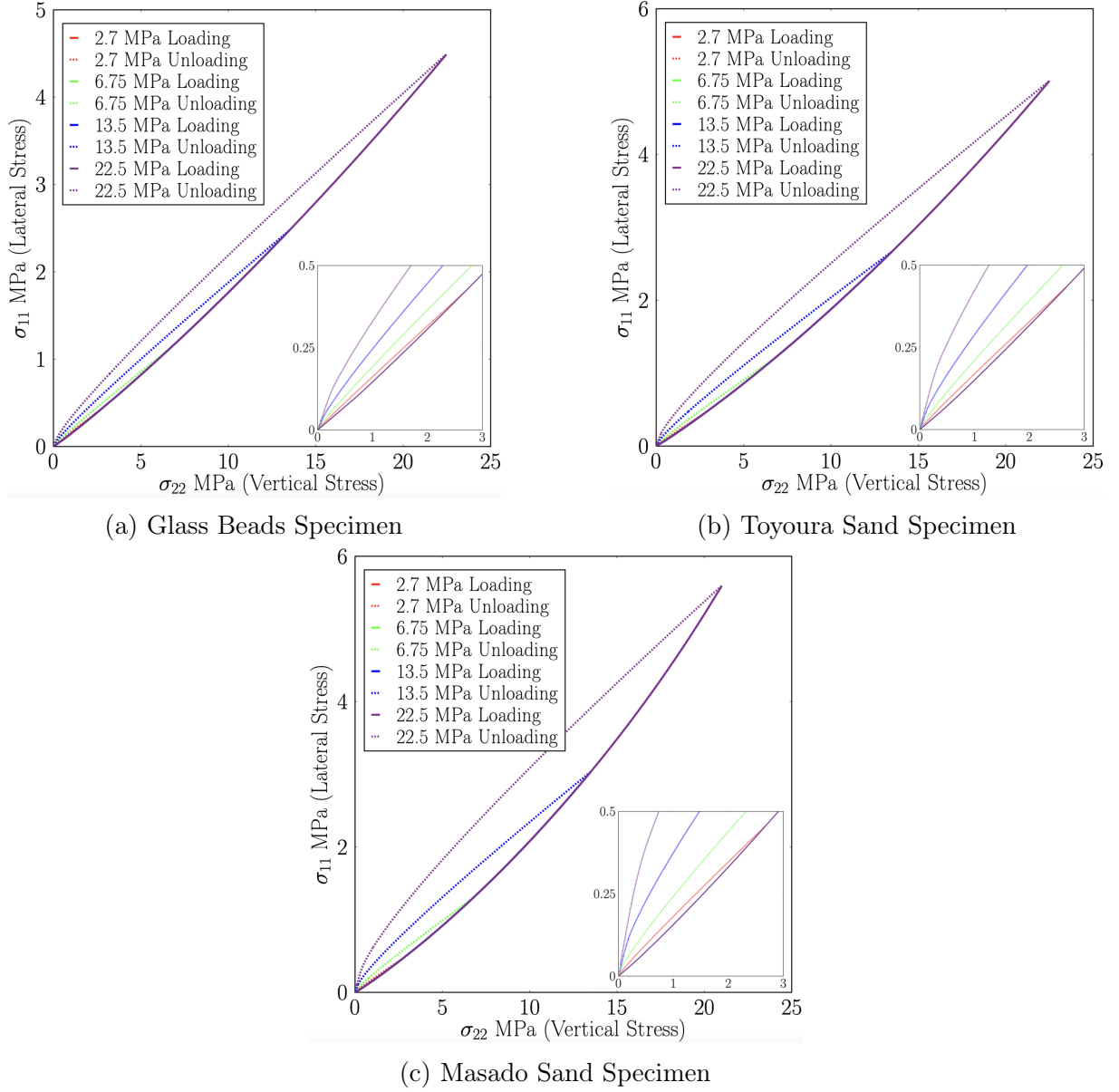


Figure 4.7: Lateral stress σ_{11} with respect to vertical stress σ_{22} for glass beads (a), Toyoura sand (b) and Masado sand (c) specimens based on the numerical simulations under first loading-unloading until reaching different maximum stresses.

Fig. 4.8a plots the vertical stress $\mathbb{S}_{22}$ against the vertical strain G responses for three specimen (denoted as dense, mid-dense and loose) under loading-unloading cycles. During the simulations, a maximum displacement of $\bar{u} \simeq 0.01$ m is applied along the vertical direction, until a strain $G = 0.1$ was achieved. As expected, the loose specimen has the lowest resistance at the same compaction as compared to the dense specimen. As it has been noted, the compaction behavior can be scaled by either considering the particle stiffness or the initial void ratio (initial density states). Indeed, the three density states considered here have been realized by simply changing the stiffness k_η^c . Fig. 4.8b presents the normalized vertical stress $\bar{\mathbb{S}}_{22}(= \mathbb{S}_{22}/k_\eta^c L^2)$ versus the vertical strain G behavior where

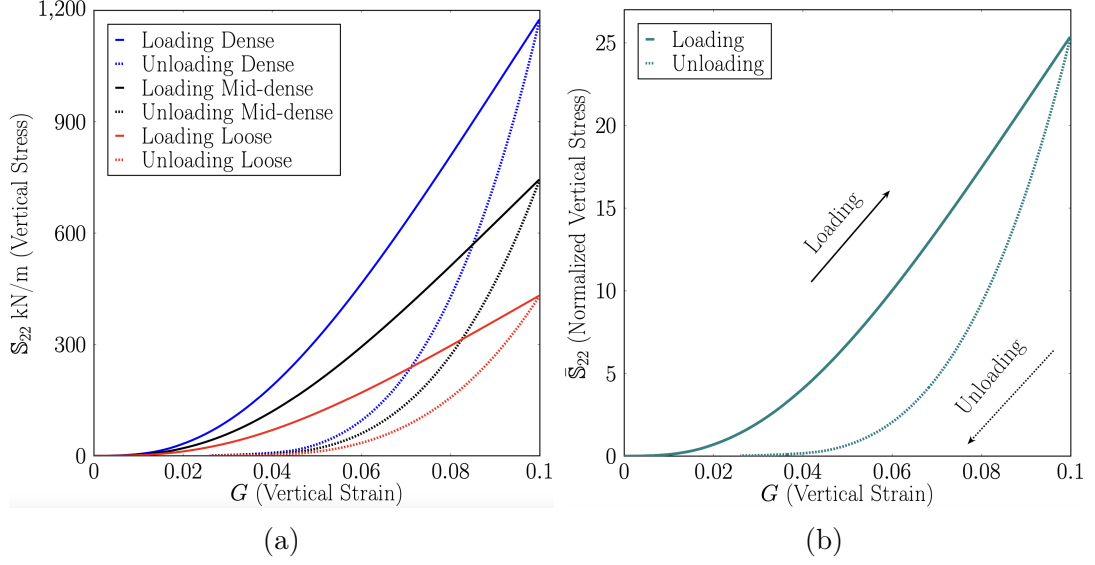


Figure 4.8: (a) Vertical stress S_{22} versus vertical strain G obtained from the numerical simulations for dense, mid-dense, and loose specimens at maximum strain ($G=0.1$) under first loading-unloading. (b) Normalized vertical stress $\bar{S}_{22}$ versus vertical strain G obtained from the numerical simulations for dense, mid-dense, and loose specimens by dividing $k_{\eta}^c L^2$ at maximum strain ($G=0.1$) under first loading-unloading.

the vertical stress normalization is obtained by dividing the stress values by the product of material stiffness (k_{η}^c) and squared intergranular distance (L), i.e. $k_{\eta}^c L^2$, resulting in a non-dimensional quantity in terms of the unit of measure. It can be observed that all the curves merge into one, suggesting the nearly universal scaling for one-dimensional compression is possible. It is specifically noteworthy that the model parameters can be categorized into equivalence class based on the stiffness k_{η}^c and intergranular distance to explain the scaling. Further, it is notable that the stiffness k_{η}^c represents not only the stiffness of a grain-pair isolated from the assembly, but also the effect of the neighboring grain packing (see also the discussion in [127]). In this sense, the model parameters in the presented approach represent the effect of the neighboring grain packing on the grain-pair behavior. Such an effective grain-pair representation is, therefore, different from that used in a discrete model of granular materials.

Fig. 4.9 presents the corresponding lateral stress S_{11} versus the vertical stress S_{22} for the three cases. The lateral stress results from the tendency of specimens to dilate laterally due to positive Poisson's effect and the confining lateral boundary conditions as the vertical stress is increased. It is notable that the vertical stress, typically, increases at a faster rate than the lateral stress, although with a minor slowdown. Upon unloading, the rate at which the vertical stress decreases is typically faster, such that the lateral stress near complete unloading is higher than the vertical stress, which also agrees with classical

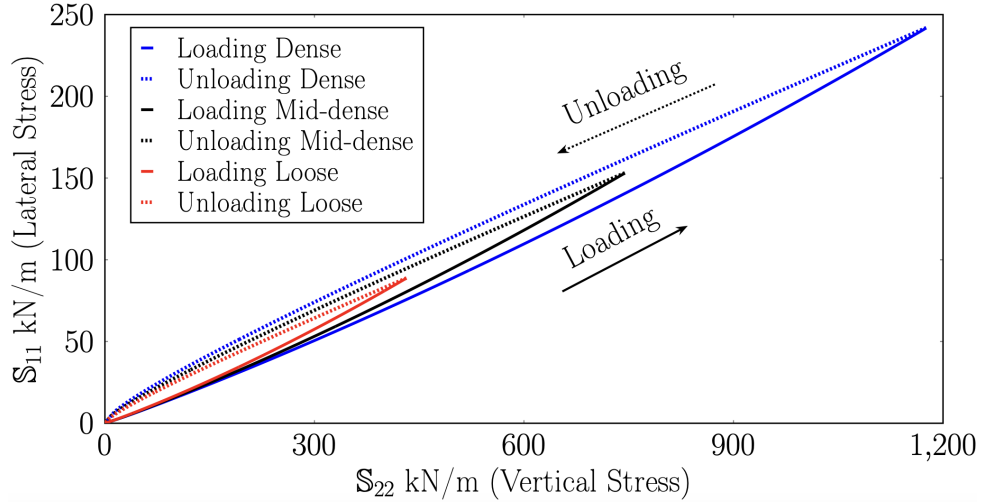


Figure 4.9: Lateral stress S_{11} versus vertical stress S_{22} obtained from the numerical simulations for dense, mid-dense, and loose specimens under first loading-unloading until reaching a maximum strain ($G=0.1$).

experimental observations [239]. It is also observed that the resulting lateral to vertical stress ratio (also known as coefficient of later pressure $K_0 = \sigma_{11}/\sigma_{22}$) can become larger than 1 during unloading. It is notable that the rate of change of vertical and lateral stress is determined by the directional evolution of damage and plasticity that will be examined in detail in a later section.

4.1.2.4.2 Repeated loading-unloading under one-dimensional compression

In Fig. 4.10, the stress-strain response is given for a mid-dense specimen in one-dimensional compression for repeated loading-unloading over 2-cycles: 1st Loading, 1st Unloading, 2nd Loading, and 2nd Unloading. Under one-dimensional compression, the material suffers a majority of damage and plasticity during the 1st load-unload cycle. During the 2nd loading, the initial behavior is softer compared to the 1st loading. However, the stiffening proceeds rapidly until the original stress-strain curve is intercepted, beyond which the response follows the virgin or 1st loading curve as is widely observed in experiments for granular geomaterials (see for example [240]). It is encouraging to observe that the 2nd unload curve follows the 1st unload curve as is typically observed. Finally, as expected, it can be observed that the energy dissipation in the 2nd loading-unloading cycle, reckoned as the area of the load-unload loop, is considerably smaller than the 1st cycle or virgin loading as the material undergoes less damage/plastic evolution.

4.1.2.4.3 Directional evolution of elastic energy, damage and plasticity

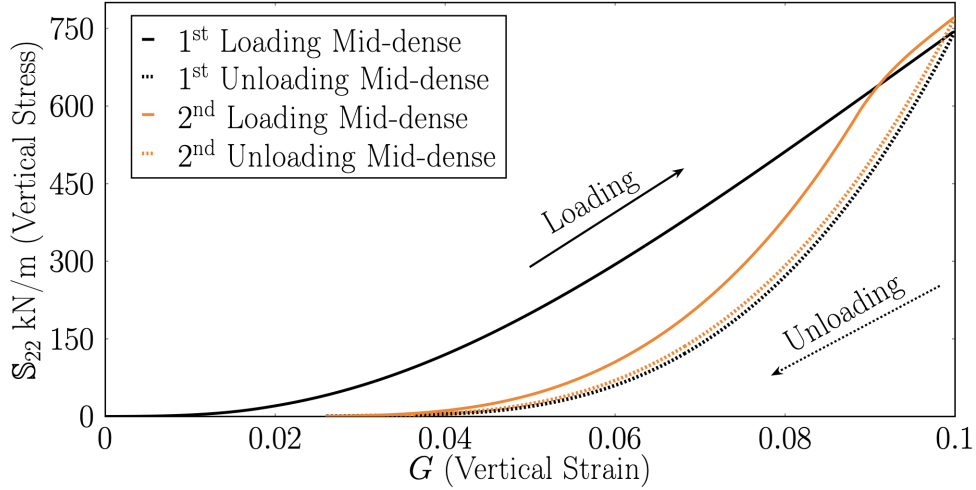


Figure 4.10: Vertical stress S_{22} versus vertical strain G obtained from the numerical simulations for a mid-dense specimen at maximum strain ($G=0.1$) under two cyclic loading-unloading.

A key aspect of the presented model based upon granular micromechanics is that the discrete nature of granular materials get accounted by the effective behavior of the grain-pair. Thus the evolution of elastic energy, damage and plasticity of grain-pairs oriented in various spatial directions can reveal important insights to the emerging macroscale response of the granular material. In Fig. 4.11, the polar plots of elastic energy evolution of effective grain-pairs oriented in different directions for the simulations are given in the previous section. The loading-unloading-reloading stages were divided into four different vertical strain intervals in columns (i), (ii), (iii), and (iv). Further, for each polar plot, 10 equal steps within its vertical strain range are considered. It is observed that the elastic energy exhibits a gradual increase in all directions during 1st loading with the larger increase, as expected, in grain-pairs oriented closer to the direction of loading (vertical or 2-direction). Since the grain-pair elastic energy includes a quartic dependency upon grain-pair normal displacement, an anisotropic stiffening in the loading direction evolves which is reflected in the directional distribution of elastic energy. Clearly, the direction of larger grain-pair energy results implies a higher elastic stiffness in that direction. In this sense, GMA provides the advantage of directly connecting the microscale stiffening to the emergent macroscale stiffening of the granular material.

During unloading, a part of the stored elastic energy is recovered as seen by the reduction of elastic energy in the vertical direction (neighboring orientation of 90°) as seen in row 2 of Fig. 4.11 in which the unloading proceeds from right to left. It is interesting to note that the vertical directions unload faster as opposed to almost uniform rate of increase in all directions during loading. This phenomena is particularly visible during

unloading at strains below 0.05. Such elastic energy evolution for the effective grain-pairs is influenced by the assumed dissipation behavior for tangential direction, which is only due to damage. In particular, for grain-pair orientations inclined with respect to the principal loading direction (vicinity of 45° , 135° , 225° , and 315° , respectively), the elastic displacement, especially in tangential direction, reduces at a slower rate. Consequently, elastic energy reduction in these inclined directions is more gradual. In the subsequent load-unload cycle, a similar phenomena repeated, however, with nuanced variation that is influenced both by the directional evolution of damage and plastic displacements, which are depicted in Figs. 4.12-4.15. It can be observed that during loading, the normal damage (Fig. 4.12) and plastic multiplier (Fig. 4.14) evolve faster in the direction of principal loading (neighboring orientation of 90°). The result is that the normal stiffness in these directions is reduced. In addition, the elastic displacement in these direction reduces at a faster rate during unloading and grows at a slower rate during the 2nd loading. As a consequence, the elastic energy elastic energy evolution takes a flat 8 shape as seen in the 3rd row of Fig. 4.11.

It is further notable that the directional evolution of damage and plasticity leads to an induction of anisotropy as the loading progresses. The anisotropy development is also influenced by the quartic dependence of effective grain-pair elastic energy upon the elastic normal displacement u_η^{el} with the duffing stiffness $k_{\eta\eta}$ in Eq. 4.31. Undoubtedly, the directional evolution of microscale elastic energy, damage and plasticity as illustrated by the polar plots play an important role in understanding hardening/softening behavior, loading-unloading path dependency, and deformation mechanisms.

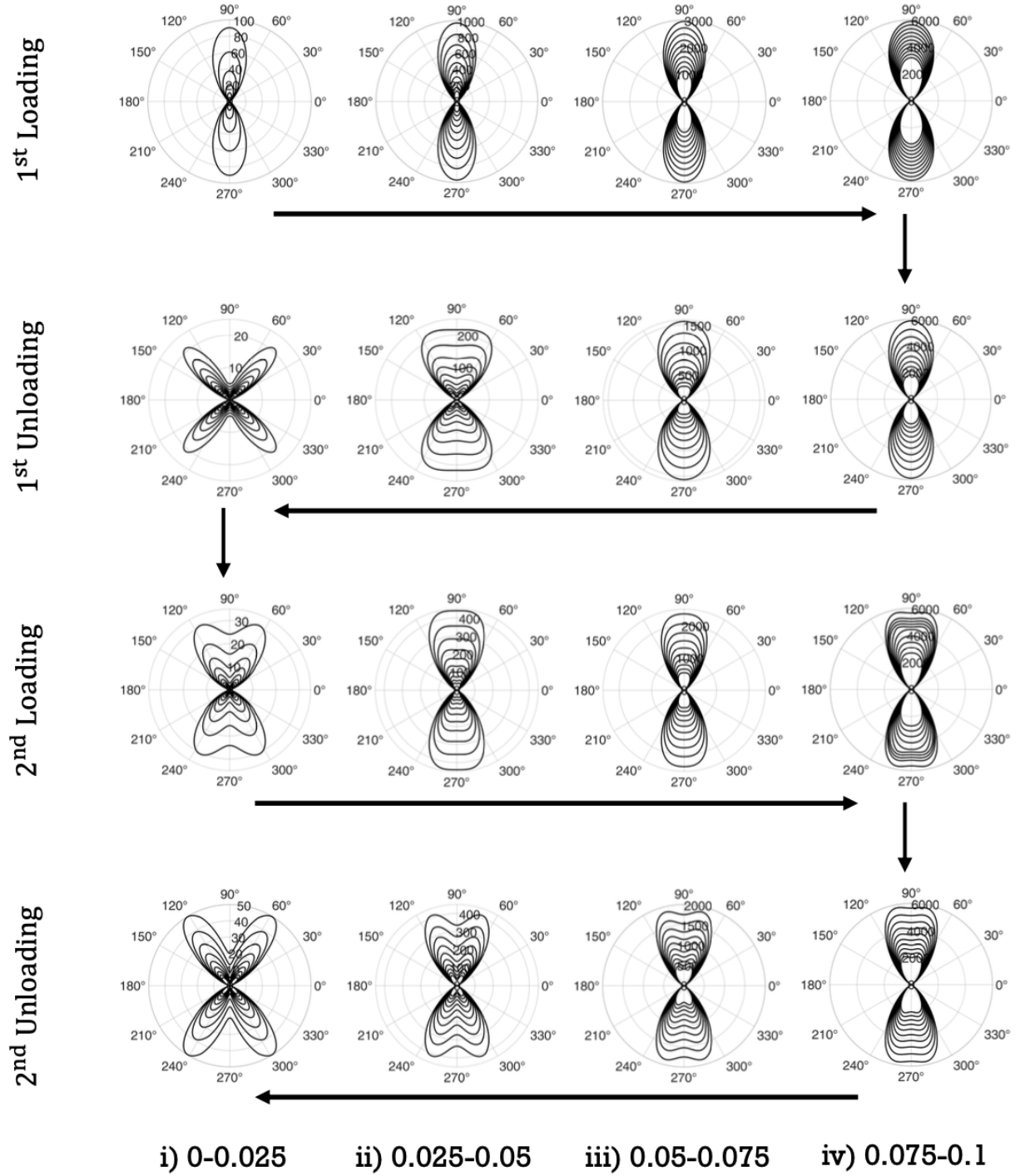


Figure 4.11: Elastic energy U polar plots for a mid-dense specimen under cyclic loading-unloading in one-dimensional compression at different strain intervals.

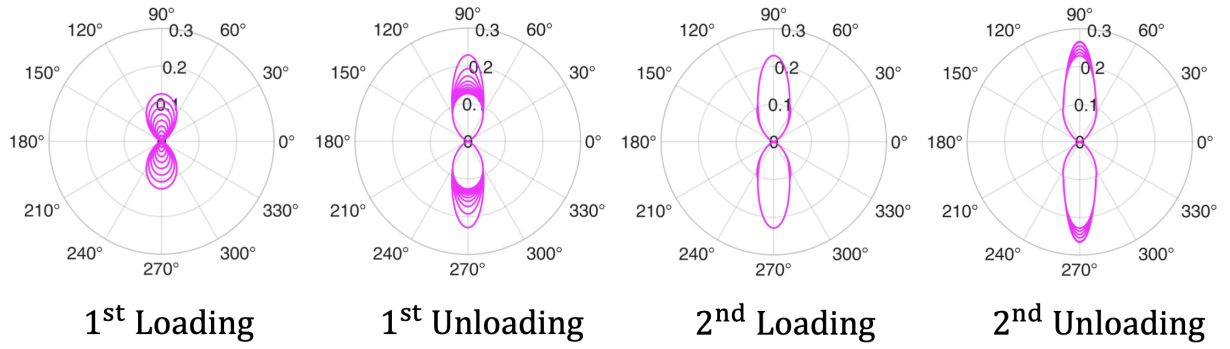


Figure 4.12: Normal damage D_η polar plots for a mid-dense specimen under cyclic loading-unloading in one-dimensional compression.

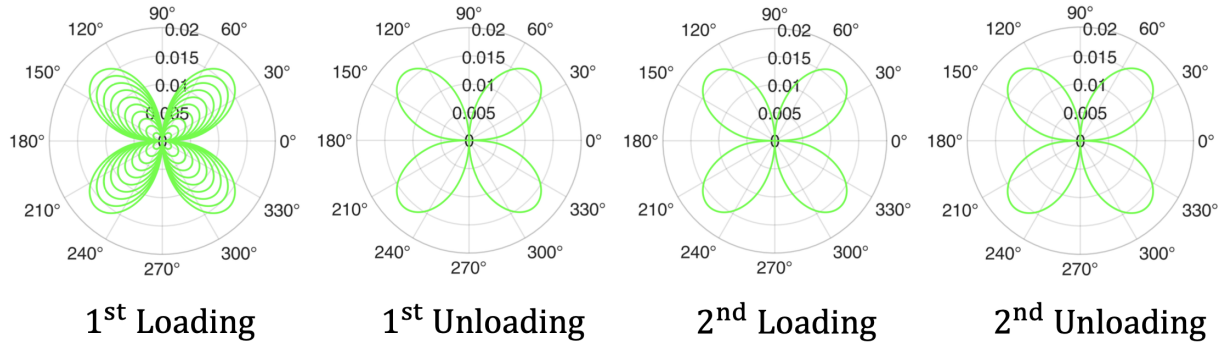


Figure 4.13: Tangential damage D_τ polar plots for a mid-dense specimen under cyclic loading-unloading in one-dimensional compression.

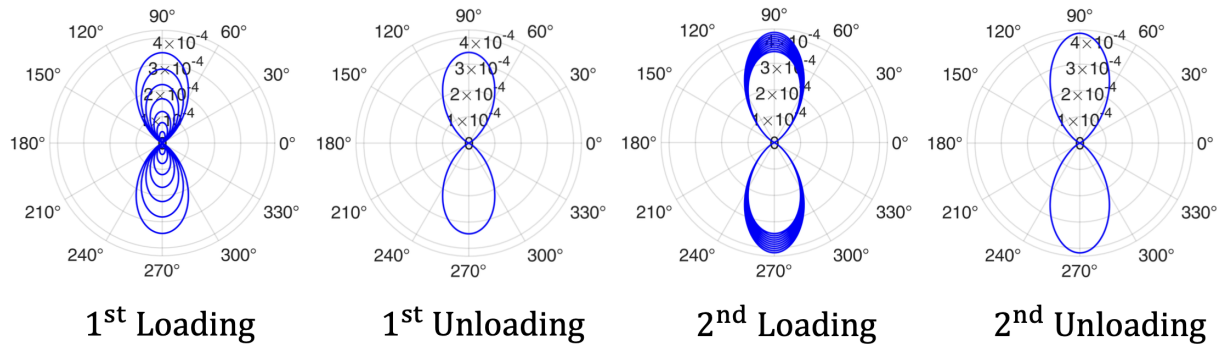


Figure 4.14: Compression λ_η^c plastic multiplier polar plots for a mid-dense specimen under cyclic loading-unloading in one-dimensional compression.

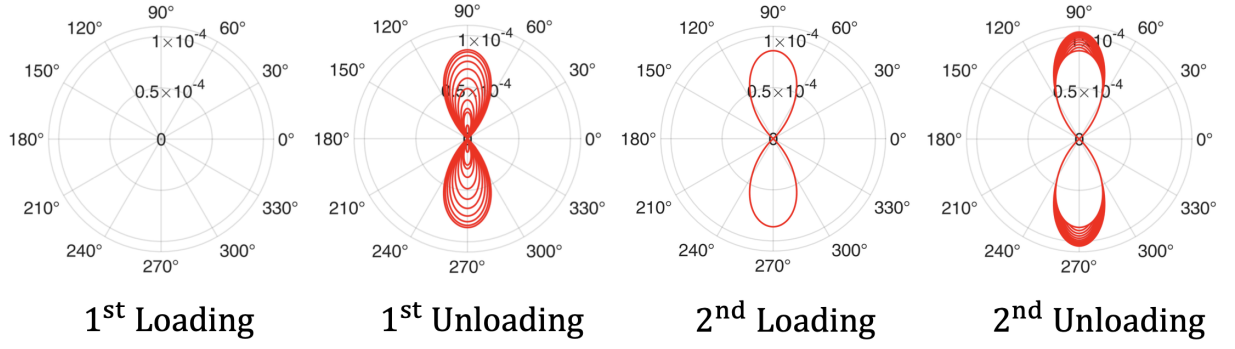


Figure 4.15: Tension λ_η^t plastic multiplier polar plots for a mid-dense specimen under cyclic loading-unloading in one-dimensional compression.

4.2 Geometrical and material nonlinear effects in granular micromechanics: effects of grain-pair tangential plasticity and induced anisotropy

4.2.1 Mathematical model

In this section, an extended GMA is used by redefining the grain-pair elastic energy and dissipative potential functionals. The elastic potential is expressed in the framework of complete functions of quadratic and quartic (duffing) terms in both normal and tangential relative displacements regarding Eq. 4.1. The dissipation potential includes the tangential plastic dissipation and a coupling mechanism between tensile and compression normal plastic multipliers. To better capture the granular material nonlinearity, the newly introduced terms encourage, the newly introduced terms enhance the model's ability to represent key micromechanical mechanisms such as grain rearrangement, sliding, rotation, densification and strain localization within the continuum framework.

4.2.1.1 Elastic energy

The elastic energy U^{np} represents the effective elastic grain-pair interaction between adjacent grains n and p associated with those grain-pairs aligned with the direction $\hat{\mathbf{c}}$. The formulation of grain-pair elastic energy is new because it differs from that of previous works [7–10] by introducing a general quartic function of elastic relative displacements.

In particular, a coupling between normal and tangential elastic displacement is included,

$$U^{np} = \frac{1}{2}k_{\eta D} (u_{\eta}^{el})^2 + \frac{1}{4}k_{\eta\eta D} (u_{\eta}^{el})^4 + \frac{1}{2}k_{\tau D} u_{\tau}^{2el} + \frac{1}{4}k_{\tau\tau D} (u_{\tau}^{2el})^2 + k_{\eta\tau D} (u_{\eta}^{el})^2 u_{\tau}^{2el}. \quad (4.24)$$

Although the first and third addends were included in earlier works for describing only geometrical non-linear elastic behavior [7, 8, 107, 224], it is notable that even the third term is now modified to include tangential plasticity. Further, quartic terms are included in the second, fourth and fifth terms. These quartic terms introduce material nonlinearity in addition to the geometrical nonlinearity (present due to the choice of Green-Lagrange strain). For example, Hertzian contact can be approximated using these even-order terms. Since the squared elastic tangential displacement is defined using its absolute value (see Eq. 3.18), the elastic energy density in Eq. 4.24 always remains positive. The insertion of tangential quartic term (i.e., the fourth one in Eq. 4.24) and coupling between normal and tangential term (i.e., the fifth one in Eq. 4.24) in the postulated elastic energy density serves two purposes: (i) capturing the nonlinear shear stiffening that contacting grain-pairs with rough surfaces experience under compression and (ii) extending the model's ability to predict the evolution of squared tangential plasticity, as well as the interdependence of two plastic variables.

The damaged normal stiffness $k_{\eta D}$ in Eq. 4.24, varies with the elastic normal displacement u_{η}^{el} under tension and compression as expressed in Eq. 3.21. Stiffness parameters $k_{\eta\eta D}$, defined as the normal component of the damaged (quartic) duffing stiffness as shown in Eq. 4.3. As mentioned earlier, two new energy terms have been introduced in this chapter, and the corresponding damaged (quartic) duffing stiffness $k_{\tau\tau D}$ and the damaged coupling stiffness $k_{\eta\tau D}$ are defined using the damage variables as follows

$$k_{\tau\tau D} = \frac{k_{tt}k_{\tau D}}{L^2}, \quad k_{\eta\tau} = \frac{k_{nt} (k_{\eta}k_{\tau})^{1/2}}{L^2}, \quad (4.25)$$

where k_{nn} , k_{tt} and k_{nt} represent the normal, tangential, and coupling non-dimensional material constants, respectively, characterizing the influence of the new (quartic) duffing contributions. The representation in Eq. 4.25 is of interest because the tension-compression asymmetry prescribed in Eq. 3.21 is automatically transferred to other corresponding stiffness components. It is observed, for example, that with the inclusion of the quartic term the equivalent normal stiffness (i.e. the coefficient of the square of the normal elastic displacement u_{η}^{el}) increases with increasing the normal elastic displacement u_{η}^{el} . Notably, this increase is expected to be different in tension, where the damage will evolve more rapidly, compared to that in compression, such that an elastic hardening behavior may result. It is possible that the quartic term could overpredict or underpredict too much

stiffening phenomena. Additionally, the effect of confinement on critical state behavior can be investigated, including the need for exhaust work.

As a consequence of this contribution, the emergent potential energy interaction behavior is, as can be seen in Fig. 4.17, of a molecular-type, such as Lennard-Jones type, with an asymptotic plateau as the grain-pair distance increases under tension and a stiffening response as the grain-pair is compressed. The insertion of Eq. 3.21 and of the last expression of Eq. 3.23 into the last equation of Eq. 4.25 induces the definition of $k_{\eta\tau}$,

$$k_{\eta\tau D} = k_{\eta\tau} ((1 - D_\eta)(1 - D_\tau))^{1/2} \text{sign}(u_\eta^{el}). \quad (4.26)$$

Insertion of the last expression of Eq. 3.23 into the first equation of Eq. 4.25 induce the definition of $k_{\tau\tau}$,

$$k_{\tau\tau D} = k_{\tau\tau}(1 - D_\tau). \quad (4.27)$$

Here, by utilizing the simple homogenization approach, such as that considered in [223], the elastic energy density is derived as deined in Subsection 3.1.2 as follows

$$\begin{aligned} U_M \xrightarrow{M \rightarrow \infty} U = \int_S \left[\frac{1}{2} k_{\eta D} (u_\eta^{el})^2 + \frac{1}{4} k_{\eta\eta D} (u_\eta^{el})^4 + \frac{1}{2} k_{\tau D} u_\tau^{2el} \right. \\ \left. + \frac{1}{4} k_{\tau\tau D} (u_\tau^{2el})^2 + k_{\eta\tau D} (u_\eta^{el})^2 u_\tau^{2el} \right] d\theta. \end{aligned} \quad (4.28)$$

Within this continuum framework, stiffness and damage parameters are orientation-dependent, represented by functions of θ , i.e., $k_\eta = \tilde{k}_\eta(\theta)$, $k_{\eta\eta} = \tilde{k}_{\eta\eta}(\theta)$, $k_\tau = \tilde{k}_\tau(\theta)$, $k_{\tau\tau} = \tilde{k}_{\tau\tau}(\theta)$, $k_{\eta\tau} = \tilde{k}_{\eta\tau}(\theta)$, $D_\eta = \tilde{D}_\eta(\theta)$ and $D_\tau = \tilde{D}_\tau(\theta)$.

Consequently, the quartic powers of both the elastic normal and the elastic tangential displacements are expressed, respectively, by

$$\begin{aligned} (u_\eta^{el})^4 = (u_\eta - u_\eta^{pl})^4 = L^4 G_{ij} G_{ab} G_{cd} G_{ef} \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b \hat{c}_c \hat{c}_d \hat{c}_e \hat{c}_f - 4L^3 G_{ij} G_{ab} G_{cd} \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b \hat{c}_c \hat{c}_d u_\eta^{pl} \\ + 6L^2 G_{ij} G_{ab} \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b (u_\eta^{pl})^2 - 4L G_{ij} \hat{c}_i \hat{c}_j (u_\eta^{pl})^3 + (u_\eta^{pl})^4, \end{aligned} \quad (4.29)$$

and

$$\begin{aligned} (u_\tau^{2el})^2 = 16L^4 G_{ij} G_{ab} G_{cd} G_{ef} (\delta_{ia} \hat{c}_j \hat{c}_b - \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b) (\delta_{ce} \hat{c}_d \hat{c}_f - \hat{c}_c \hat{c}_d \hat{c}_e \hat{c}_f) \\ - 2 (4L^2 G_{ij} G_{ab} (\delta_{ia} \hat{c}_j \hat{c}_b - \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b)) \lambda_\tau^2 + (\lambda_\tau^2)^2. \end{aligned} \quad (4.30)$$

Finally, by substituting the elastic displacements in Eqs. 3.17 and 3.18 with Eqs. 4.29

and 4.30 into the elastic energy density in Eq. 4.28, the fully expanded form of the elastic energy is found via

$$\begin{aligned}
 U = & \int_S \left[\frac{1}{2} k_\eta (1 - D_\eta) \left(L^2 G_{ij} G_{ab} \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b - 2 L G_{ij} \hat{c}_i \hat{c}_j (u_\eta^{pl}) + (u_\eta^{pl})^2 \right) \right. \\
 & + \frac{1}{4} k_{\eta\eta} (1 - D_\eta) \left(L^4 G_{ij} G_{ab} G_{cd} G_{ef} \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b \hat{c}_c \hat{c}_d \hat{c}_e \hat{c}_f - 4 L^3 G_{ij} G_{ab} G_{cd} \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b \hat{c}_c \hat{c}_d (u_\eta^{pl}) \right. \\
 & + 6 L^2 G_{ij} G_{ab} \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b (u_\eta^{pl})^2 - 4 L G_{ij} \hat{c}_i \hat{c}_j (u_\eta^{pl})^3 + (u_\eta^{pl})^4 \left. \right) \\
 & + \frac{1}{2} k_\tau (1 - D_\tau) \left(|4 L^2 G_{ij} G_{ab} (\delta_{ia} \hat{c}_j \hat{c}_b - \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b) - \lambda_\tau^2| \right) \\
 & + \frac{1}{4} k_{\tau\tau} (1 - D_\tau) \left(16 L^4 G_{ij} G_{ab} G_{cd} G_{ef} (\delta_{ia} \hat{c}_j \hat{c}_b - \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b) (\delta_{ce} \hat{c}_d \hat{c}_f - \hat{c}_c \hat{c}_d \hat{c}_e \hat{c}_f) \right. \\
 & - 2 (4 L^2 G_{ij} G_{ab} (\delta_{ia} \hat{c}_j \hat{c}_b - \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b)) \lambda_\tau^2 + (\lambda_\tau^2)^2 \left. \right) \\
 & + k_{\eta\tau} ((1 - D_\eta)(1 - D_\tau))^{1/2} \text{sign}(u_\eta^{el}) (L^2 G_{ij} G_{ab} \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b |4 L^2 G_{ij} G_{ab} (\delta_{ia} \hat{c}_j \hat{c}_b - \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b) - \lambda_\tau^2| \\
 & - 2 L u_\eta^{pl} G_{ij} \hat{c}_i \hat{c}_j |4 L^2 G_{ij} G_{ab} (\delta_{ia} \hat{c}_j \hat{c}_b - \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b) - \lambda_\tau^2| \\
 & + (u_\eta^{pl})^2 |4 L^2 G_{ij} G_{ab} (\delta_{ia} \hat{c}_j \hat{c}_b - \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b) - \lambda_\tau^2| \left. \right] d\ell, \tag{4.31}
 \end{aligned}$$

where $\mathbb{C}_{ijab}$ (4th-order), $\mathbb{L}_{ijklcd}$ (6th-order), $\mathbb{N}_{ijklcdef}$ (8th-order) and $\mathbb{P}_{ij}$ (2nd-order) are elastic stiffness tensors and defined as follows

$$\begin{aligned}
 \mathbb{C}_{ijab} = & L^2 \int_S k_\eta (1 - D_\eta) \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b d\ell + L^2 \int_S 3 k_{\eta\eta} (1 - D_\eta) \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b (u_\eta^{pl})^2 d\ell \\
 & + L^2 \int_S k_\tau (1 - D_\tau) ((\delta_{ia} \hat{c}_j \hat{c}_b + \delta_{ib} \hat{c}_j \hat{c}_a + \delta_{ja} \hat{c}_i \hat{c}_b + \delta_{jb} \hat{c}_i \hat{c}_a) - 4 \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b) \text{sign}(u_\tau^{2el}) d\ell \\
 & - L^2 \int_S k_{\tau\tau} (1 - D_\tau) ((\delta_{ia} \hat{c}_j \hat{c}_b + \delta_{ib} \hat{c}_j \hat{c}_a + \delta_{ja} \hat{c}_i \hat{c}_b + \delta_{jb} \hat{c}_i \hat{c}_a) - 4 \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b) \lambda_\tau^2 d\ell \\
 & + L^2 \int_S 8 k_{\eta\tau} ((1 - D_\eta)(1 - D_\tau))^{1/2} \text{sign}(u_\eta^{el}) (\delta_{ia} \hat{c}_j \hat{c}_b - \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b) (u_\eta^{pl})^2 \text{sign}(u_\tau^{2el}) d\ell \\
 & - L^2 \int_S 2 k_{\eta\tau} ((1 - D_\eta)(1 - D_\tau))^{1/2} \text{sign}(u_\eta^{el}) \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b \lambda_\tau^2 \text{sign}(u_\tau^{2el}) d\ell, \tag{4.32}
 \end{aligned}$$

$$\begin{aligned}
 \mathbb{L}_{ijklcd} = & -L^3 \int_S 3 k_{\eta\eta} (1 - D_\eta) \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b \hat{c}_c \hat{c}_d (u_\eta^{pl}) d\ell \\
 & - L^3 \int_S 24 k_{\eta\tau} ((1 - D_\eta)(1 - D_\tau))^{1/2} \text{sign}(u_\eta^{el}) \hat{c}_i \hat{c}_j (\delta_{ac} \hat{c}_b \hat{c}_d - \hat{c}_a \hat{c}_b \hat{c}_c \hat{c}_d) (u_\eta^{pl}) \text{sign}(u_\tau^{2el}) d\ell, \tag{4.33}
 \end{aligned}$$

$$\begin{aligned}
 N_{ijklmnpq} = & L^4 \int_S k_{\eta\eta}(1 - D_\eta) \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b \hat{c}_c \hat{c}_d \hat{c}_e \hat{c}_f d\ell \\
 & + L^4 \int_S 16k_{\tau\tau}(1 - D_\tau)(\delta_{ia} \hat{c}_j \hat{c}_b - \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b)(\delta_{ce} \hat{c}_d \hat{c}_f - \hat{c}_c \hat{c}_d \hat{c}_e \hat{c}_f) d\ell \\
 & + L^4 \int_S 16k_{\eta\tau}((1 - D_\eta)(1 - D_\tau))^{1/2} \text{sign}(u_\eta^{el}) \hat{c}_i \hat{c}_j \hat{c}_a \hat{c}_b (\delta_{ce} \hat{c}_d \hat{c}_f - \hat{c}_c \hat{c}_d \hat{c}_e \hat{c}_f) \text{sign}(u_\tau^{2el}) d\ell,
 \end{aligned} \tag{4.34}$$

$$\begin{aligned}
 P_{ij} = & -L \int_S k_\eta(1 - D_\eta) \hat{c}_i \hat{c}_j (u_\eta^{pl}) d\ell - L \int_S k_{\eta\eta}(1 - D_\eta) \hat{c}_i \hat{c}_j (u_\eta^{pl})^3 d\ell \\
 & + L \int_S 2k_{\eta\tau}((1 - D_\eta)(1 - D_\tau))^{1/2} \text{sign}(u_\eta^{el}) \hat{c}_i \hat{c}_j (u_\eta^{pl}) \lambda_\tau^2 \text{sign}(u_\tau^{2el}) d\ell.
 \end{aligned} \tag{4.35}$$

The fully expanded form of the elastic energy is obtained in Eq. 4.28, or, in compact form,

$$U = \frac{1}{2} \mathbb{C}_{ijab} G_{ij} G_{ab} + \frac{1}{3} \mathbb{L}_{ijklmn} G_{ij} G_{ab} G_{cd} + \frac{1}{4} N_{ijklmnop} G_{ij} G_{ab} G_{cd} G_{ef} + P_{ij} G_{ij}, \tag{4.36}$$

where, the elastic stiffness tensors $\mathbb{C}_{ijab}$, $\mathbb{L}_{ijklmn}$, $N_{ijklmnop}$ and P_{ij} are given in Eqs. 4.32-4.35. As shown in the earlier work [9], the effects of plastic normal displacement appear not only in P_{ij} (also called the pre-stress tensor) but also in all the other higher-order stiffness tensors. Along with that, the effect of squared tangential plasticity is observed in all elastic stiffness tensors due to the quartic and coupling terms of elastic tangential relative displacement. It is remarkable that large plastic deformation (high λ_τ^2 and/or high u_η^{pl}) induce stiffness changes also for small deformation as seen from Eq. 4.32. The stiffness tensors are calculated by integrating over all orientations using the trapezoidal rule. As seen in Eqs. 4.32-4.35, an increase in both damage variables leads to a loss of stiffness. This effect results not only from the buckling and fragmentation of chains and clusters leading to normal damage (loss of normal stiffness) but also from the reduction in lateral support and confinement within grain neighborhoods leading to tangential damage (loss of tangential stiffness).

4.2.1.2 Dissipation potential

The five fundamental scalar kinematic variables are used for the damage and plasticity descriptors (D_η , D_τ , λ_η^t , λ_η^c and λ_τ^2) to compute the dissipation potential of a generic grain-pair. The evolution of these descriptors is driven by dissipation mechanisms, that are quantitatively represented into a dissipation potential. The total dissipation potential W is decomposed into damage and plasticity contributions, as described in Subsection 3.1.3. The damage dissipation potential W_D has already been introduced in the previous sections, and its normal and shear components are given in Eqs. 4.10 and 3.32, respectively. The dissipation energy potential W_{pl} caused by plastic variables is also decomposed as introduced in the previous sections as follows

$$W_{pl} = W_{pl}^\eta + W_{pl}^\tau, \quad (4.37)$$

where the normal component has already been expressed in Eq. 4.11, and the tangential component is described as given below

$$W_{pl}^\tau = (1 - D_\tau)^2 (\sigma_{\tau\tau} \lambda_\tau^2). \quad (4.38)$$

It is important to note that the plastic dissipation potential W_{pl} is different from earlier studies [7, 8, 107, 224]. In this work, beyond the coupling term given in Eq. 4.11 originally introduced and explained its role in the previous section (see [9]), a new term, the tangential plastic dissipation potential W_{pl}^τ , is introduced to govern the evolution of tangential plasticity. In addition, the tangential plasticity yielding condition is governed by the new constitutive parameter $\sigma_{\tau\tau}$. The significance and effects of each model parameter on the evolution of damage and plastic variables depending on the loading path will be discussed in the following sections of this chapter.

4.2.1.3 Hemi-variational formulation: Governing equations and Karush-Kuhn-Tucker conditions

The (action) energy functional $\mathcal{E}$ is defined in terms of the kinematic descriptors (the placement χ and the damage and plastic descriptors $\mathfrak{e} = (D_\eta, D_\tau, \lambda_\eta^t, \lambda_\eta^c, \lambda_\tau^2)$) as expressed in Subsection 3.1.4. A first variation of the action energy functional from Eq. 3.36 with regard to the six fundamental kinematic quantities is built via Eq. 3.39. The hemi-variational principle reported in this subsection drives the evolution of all the kinematic descriptors, including the irreversible ones and it is comprehensively explained in earlier

studies (for interested readers, see [7–10]). The first set of Euler-Lagrange equations are those related to the displacement bilateral kinematic descriptor $\mathbf{u}$. It is easy to represent such a set of equations in terms of balance relation as given in Eq. 3.44, constitutive relation as shown in Eq. 4.39 and, boundary conditions as given in Eq. 3.46 along with Eq. 3.38,

$$\mathbf{S} = \mathbf{C}\mathbf{G} + \mathbf{L}\mathbf{G}^2 + \mathbf{N}\mathbf{G}^3 + \mathbf{P} \quad \forall \mathbf{X} \in \mathcal{B}, \quad (4.39)$$

where $\mathbf{G}^2 = \mathbf{G} \otimes \mathbf{G}$ and $\mathbf{G}^3 = \mathbf{G} \otimes \mathbf{G} \otimes \mathbf{G}$ are the noted tensor products. Further, the outward unit vector $\mathbf{n}$ is normal to the boundary of the domain. The elastic energy per unit area in Eq. 4.36 is used to evaluate the stress tensor $\mathbf{S}$

$$\mathbb{S}_{ij} = \frac{\partial U}{\partial G_{ij}} = \mathbb{C}_{ijab}G_{ab} + \mathbb{L}_{ijabcd}G_{ab}G_{cd} + \mathbb{N}_{ijabcdef}G_{ab}G_{cd}G_{ef} + \mathbb{P}_{ij}, \quad (4.40)$$

where $\mathbf{G}$ is a homogeneous strain with respect to $\mathbf{X} \in \mathcal{B}$ leading to null strain gradient terms and an immediate satisfaction of Eq. 3.44. The second set of Euler-Lagrange equations is related to the monolateral damage and plastic descriptors (collectively denoted as entropic variables). The following Karush-Kuhn-Tucker (KKT)-type conditions for five

kinematic variables are derived as written below

$$\begin{aligned} \mathcal{A}_{D_\eta}(u_\eta, u_\tau^2, \mathbf{e}) &= -\frac{1}{2}k_\eta(u_\eta^{el})^2 - \frac{1}{4}k_{\eta\eta}(u_\eta^{el})^4 \\ &- \frac{k_{\eta\tau}(1 - D_\tau)\text{sign}(u_\eta^{el})}{2((1 - D_\eta)(1 - D_\tau))^{1/2}} (u_\eta^{el})^2 |u_\tau^{2el}| + \frac{1}{2}k_\eta(B_\eta)^2 \tan^2\left(\frac{\pi}{2}D_\eta\right) \\ &- 2(1 - D_\eta) (\sigma_\eta^t \lambda_\eta^t + \sigma_\eta^c \lambda_\eta^c + \sigma_{\eta\eta}^t (\lambda_\eta^t)^2 + \sigma_{\eta\eta}^c (\lambda_\eta^c)^2 + \sigma_{\eta\eta}^{tc} \lambda_\eta^t \lambda_\eta^c), \end{aligned} \quad (4.41)$$

$$\begin{aligned} \mathcal{A}_{D_\tau}(u_\eta, u_\tau^2, \mathbf{e}) &= -\frac{1}{2}k_\tau |u_\tau^{2el}| - \frac{1}{4}k_{\tau\tau} (u_\tau^{2el})^2 \\ &- \frac{k_{\eta\tau}(1 - D_\eta)\text{sign}(u_\eta^{el})}{2((1 - D_\eta)(1 - D_\tau))^{1/2}} (u_\eta^{el})^2 |u_\tau^{2el}| \\ &+ \frac{1}{2}k_\tau(B_\tau)^2 (\log(1 - D_\tau))^2 - 2(1 - D_\tau) (\sigma_{\tau\tau} \lambda_\tau^2), \end{aligned} \quad (4.42)$$

$$\begin{aligned} \mathcal{A}_{\lambda_\eta^t}(u_\eta, u_\tau^2, \mathbf{e}) &= -k_\eta(1 - D_\eta)u_\eta^{el} - k_{\eta\eta}(1 - D_\eta)(u_\eta^{el})^3 \\ &- 2k_{\eta\tau}((1 - D_\eta)(1 - D_\tau))^{1/2}\text{sign}(u_\eta^{el})u_\eta^{el}|u_\tau^{2el}| \\ &+ (1 - D_\eta)^2(\sigma_\eta^t + 2\sigma_{\eta\eta}^t \lambda_\eta^t + \sigma_{\eta\eta}^{tc} \lambda_\eta^c), \end{aligned} \quad (4.43)$$

$$\begin{aligned} \mathcal{A}_{\lambda_\eta^c}(u_\eta, u_\tau^2, \mathbf{e}) &= k_\eta(1 - D_\eta)u_\eta^{el} + k_{\eta\eta}(1 - D_\eta)(u_\eta^{el})^3 \\ &+ 2k_{\eta\tau}((1 - D_\eta)(1 - D_\tau))^{1/2}\text{sign}(u_\eta^{el})u_\eta^{el}|u_\tau^{2el}| \\ &+ (1 - D_\eta)^2(\sigma_\eta^c + 2\sigma_{\eta\eta}^c \lambda_\eta^c + \sigma_{\eta\eta}^{tc} \lambda_\eta^t), \end{aligned} \quad (4.44)$$

$$\begin{aligned} \mathcal{A}_{\lambda_\tau^2}(u_\eta, u_\tau^2, \mathbf{e}) &= -k_\tau(1 - D_\tau)\text{sign}(u_\tau^{2el}) - k_{\tau\tau}(1 - D_\tau)u_\tau^{2el} \\ &- 2k_{\eta\tau}((1 - D_\eta)(1 - D_\tau))^{1/2}\text{sign}(u_\eta^{el}) (u_\eta^{el})^2 \text{sign}(u_\tau^{2el}) + 2(1 - D_\tau)^2 \sigma_{\tau\tau}. \end{aligned} \quad (4.45)$$

Due to the monolaterality expressed on the right-hand side of Eq. 3.43, they are derived from the hemi-variational principle in Eq. 3.43 in terms of the following KKT type conditions

$$\mathcal{A}_{D_\eta}(u_\eta, u_\tau^2, \mathbf{e}) \Delta D_\eta = 0, \quad (4.46)$$

$$\mathcal{A}_{D_\tau}(u_\eta, u_\tau^2, \mathbf{e}) \Delta D_\tau = 0, \quad (4.47)$$

$$\mathcal{A}_{\lambda_\eta^t}(u_\eta, u_\tau^2, \mathbf{e}) \Delta \lambda_\eta^t = 0, \quad (4.48)$$

$$\mathcal{A}_{\lambda_\eta^c}(u_\eta, u_\tau^2, \mathbf{e}) \Delta \lambda_\eta^c = 0, \quad (4.49)$$

$$\mathcal{A}_{\lambda_\tau^2}(u_\eta, u_\tau^2, \mathbf{e}) \Delta \lambda_\tau^2 = 0, \quad (4.50)$$

where the explicit forms of the functions $\mathcal{A}_{D_\eta}$, $\mathcal{A}_{D_\tau}$, $\mathcal{A}_{\lambda_\eta^t}$, $\mathcal{A}_{\lambda_\eta^c}$ and $\mathcal{A}_{\lambda_\tau^2}$ are given in Eqs. 4.41-4.45, respectively, and represent implicit definitions of the corresponding tentative entropic variables. For the numerical simulations presented later in this chapter, an explicit scheme in which each of the KKT conditions are evaluated in the current loading

step utilizing the damage and plasticity descriptors from the previous step is used. The expressions in Eqs. 4.41-4.45 are therefore set to zero to determine the corresponding tentative entropic functions and numerical effort is needed to solve them. In other words, a root is found in the neighborhood of the corresponding entropic values at the previous time step reaching a tolerance of 10^{-10} . If a given tentative entropic value satisfies the entropic condition on the right-hand side of Eq. 3.43, then it is used as the corresponding entropic variable for the current time step. Otherwise, the KKT conditions are satisfied by assuming null increment for the entropic variable and therefore they take the value of the previous time step.

4.2.2 Results and discussion

4.2.2.1 The constitutive numerical setting

The methodology for the determination of the needed material parameters for the proposed model has been discussed in detail in the previous work [9], as given in Section 4.1. Following the discussed methodology, the material parameters used for the numerical example in this chapter are given in Table 4.2.

Table 4.2: The parameters for numerical example.

k_η^c (J/m ⁴)	k_η^t (J/m ⁴)	k_τ (J/m ⁴)	B_η^c (m)		B_η^t (m)	$B_{\tau 0}$ (m)
2.93×10^8	$0.1\,k_\eta^c$	$0.1\,k_\eta^c$	$6.08\,L$		$0.1\,B_\eta^c$	$0.1\,B_\eta^c$
σ_η^t (J/m ³)	σ_η^c (J/m ³)	$\sigma_{\eta\eta}^t$ (J/m ⁴)	$\sigma_{\eta\eta}^c$ (J/m ⁴)	$\sigma_{\eta\eta}^{tc}$ (J/m ⁴)	$\sigma_{\tau\tau}$ (J/m ⁴)	
0	$0.34\,k_\eta^c L$	$4.55\,k_\eta^c$	$227.27\,k_\eta^c$	$-2.27\,k_\eta^c$	$0.45\,k_\eta^c$	
k_{nn}		k_{tt}	k_{nt}	S (m)	L (m)	α (m)
5×10^4		5×10^3	10^3	10 L	0.01	2.5×10^{-5}
						α_1
						10

Table 4.2 lists the microscale stiffness k_η^c , k_η^t and k_τ , the characteristic damage displacements B_η^c , B_η^t and $B_{\tau 0}$, the plasticity constitutive parameters σ_η^t , σ_η^c , $\sigma_{\eta\eta}^t$, $\sigma_{\eta\eta}^c$, $\sigma_{\eta\eta}^{tc}$ and $\sigma_{\tau\tau}$, the duffing stiffness coefficients k_{nn} , k_{tt} and k_{nt} , the size of square specimen S considered for the numerical example, the intergranular distance L , the regularization factor α and the constitutive factor α_1 . Further, in Table 4.2, a non-dimensionalization is adopted with respect to the characteristic inter-granular distance, L , and normal stiffness in compression k_η^c . The aim of non-dimensionalization is to decrease the number of

independent parameters. Thus, all other stiffness parameters are expressed in the terms of k_η^c . Consequently, the ratios of tension to compression and tangential to compression stiffness are assigned with a non-dimensional pre-factor number. In addition, the damage characteristic displacements appear as a multiple of the characteristic inter-granular distance, L , implying that the loss of stiffness represents a meso-scale mechanism. It is also clear that the loss of normal stiffness under compression occurs at a larger compression damage characteristic displacement B_η^c , in contrast to those in tension $B_\eta^t = 0.1B_\eta^c$ and tangential $B_{\tau 0} = 0.1B_\eta^c$. Further, the non-dimensional parameter $\alpha_1 = 10$ makes the tangential damage characteristic displacement in compression again equal to B_η^c . Plasticity parameter σ_η^c has the same unit of measure as that of the product $k_\eta^c L$, and therefore, it is given in terms of this factor. No threshold for tension is needed for the plastic activation, and therefore, σ_η^t is set equal to zero. The plastic hardening/softening parameters have the same unit of measure of k_η^c , and therefore, they are given in terms of it. Finally, the duffing stiffness parameters are non-dimensional numbers as noted in Eq. 4.25. To ensure the positive definiteness of the elastic energy (see Eq. 4.24) at least at the initial stage when no damage is considered, the relationships between the duffing stiffness coefficients are established as follows

$$(k_{\eta\tau})^2 \leq \frac{1}{4}(k_{\eta\eta}k_{\tau\tau}) = \frac{1}{4} \frac{k_{nn}k_{tt}(k_\eta k_\tau)}{L^4}, \quad (k_{nt})^2 \leq \frac{1}{4}k_{nn}k_{tt}. \quad (4.51)$$

The inequality shown on the left-hand side ensures the positive definiteness of the quartic part of Eq. 4.24, incorporating the normal (k_{nn}) and tangential (k_{tt}) duffing stiffness coefficients defined in Eq. 4.25. On the right-hand side of Eq. 4.51, the same inequality is presented, incorporating the coupling duffing stiffness coefficient k_{nt} defined in Eq. 4.25. Further, to ensure that the dissipation potential in Eq. 4.11 is also positive definite, the following conditions are applied: $\sigma_{\eta\eta}^t > 0$, $\sigma_{\eta\eta}^c > 0$ and $4\sigma_{\eta\eta}^t\sigma_{\eta\eta}^c - (\sigma_{\eta\eta}^{tc})^2 > 0$. This is not a necessary condition, since the plastic multipliers are positive by definition, and the reported Hessian condition is valid for general variables and it should be properly generalized. Assigning the plasticity constitutive parameter parallels the relationship provided for the duffing stiffness coefficients as given in the second expression of Eq. 4.51. The positive definiteness of the dissipation potential in Eq. 4.11 is always satisfied, and the above sentence is referred to a part of dissipation.

4.2.3 An evidence of the numerical approximation

To evaluate the accuracy of the explicit numerical calculations used in this example,

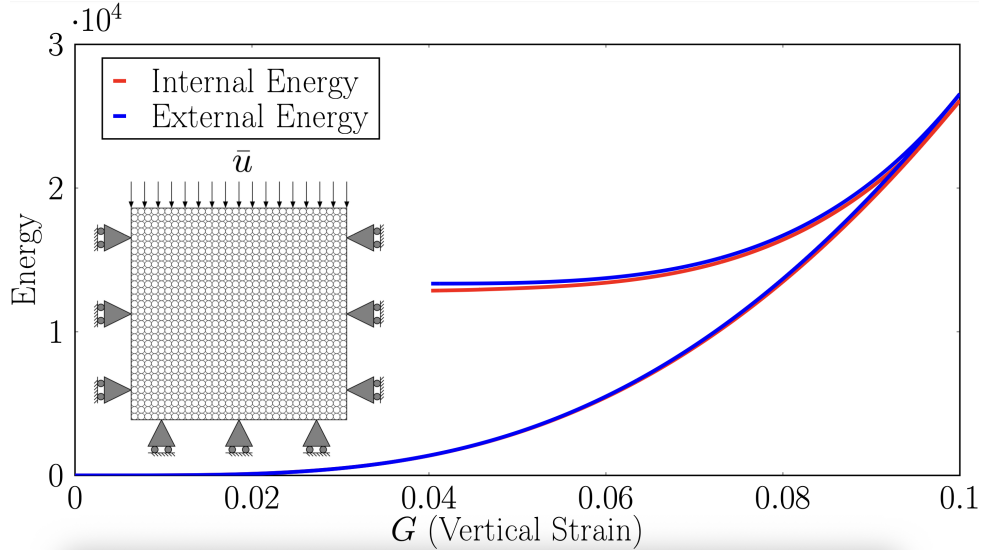


Figure 4.16: Comparison between internal and external energies plotted against vertical strain G up to the maximum strain ($G=0.1$) under uniaxial compression showing a negligible small difference caused by computational error.

the difference between the internal and external energies is considered. In Fig. 4.16 the model calculations are shown in terms of internal and external energies based upon Eq. 3.36 and are plotted for the one-dimensional compressive loading and unloading described in Subsubsection 4.1.2.1. The internal energy represents the summation of elastic energy and dissipation potential over all orientations at each time step integrated over the domain. The external energy is evaluated from the reaction distributed along the top boundary on which the displacement is prescribed (see Fig. 4.18a). Note that the vertical boundaries have prescribed zero horizontal displacements and zero vertical force, and the bottom horizontal boundary has zero vertical displacement and zero horizontal force, and therefore, do not contribute to the external energy. It is notable that only a small difference arises between the external and internal energies indicating that the numerical procedure is reasonable.

4.2.3.1 Molecular-type elastic energy response

Fig. 4.17 shows six curves described in the legend. Dotted curves are related to compression loading and successive unloading. Full curves are related to tension loading and successive unloading. For each of the six curves, a new virgin sample is used so that all entropic descriptors are initially reset to zero.

For the elastic energy of all the loading parts of the six curves (see Fig. 4.17 where

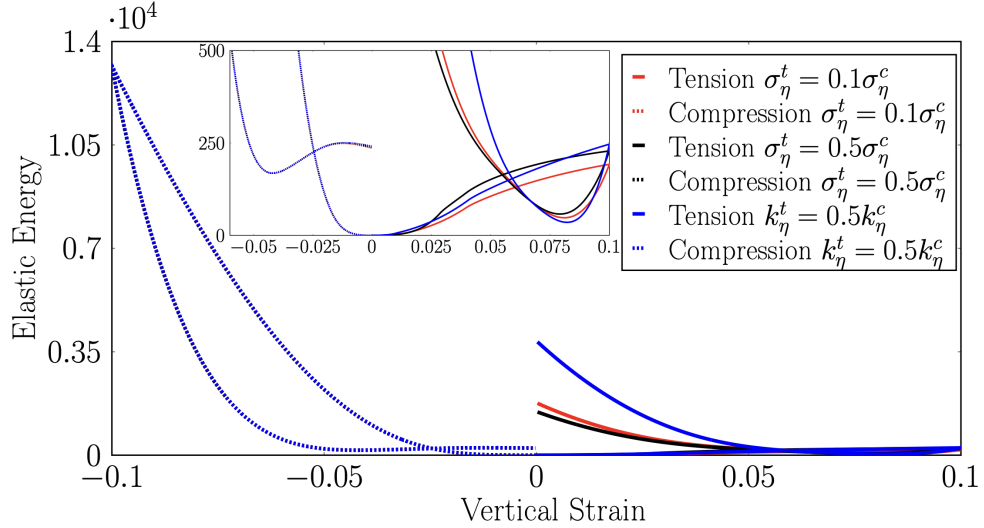


Figure 4.17: Elastic energy dependence on loading showing a molecular-type behavior in which the elastic energy increases rapidly in compression and reaches a plateau at large tension. Repeated cyclic loading has the effect of translating the energy well along the loading axis. Note that the blue and the black dashed curves are coincident in loading-unloading compression cycle. Also, the parameter σ_η^t is the same for the blue and the black curves.

the inset gives a zoomed view near the energy minima), an apparent molecular-type, such as Lennard-Jones type, energy behavior emerges in which the elastic energy rises rapidly under compression and under tension the emergent response depends upon the parameter σ_η^t , that is this figure (and only in this figure) different from that prescribed in Table 4.2. For the case of elasto-frictional granular materials, where $\sigma_\eta^t = 0$, the elastic energy in tension vanishes. However, for the case of elasto-frictional-cohesive systems, where $\sigma_\eta^t > 0$, elastic energy increases with tension reaching an inflection that tends to an asymptote at large tensile deformation, akin to the molecular potential. An apparent molecular-type elastic energy response has been defined. The reason is that it is mainly due to the damage-plastic irreversible phenomena. In fact, it is interesting to observe that under unloading condition the elastic energy paths are not at all the same of the loading ones. Besides, the effect of translating the energy well along the loading axis can be observed in Fig. 4.17, where the minimum of the elastic energy under cyclic compression shifts left, establishing a new equilibrium configuration. Similarly, under cyclic tension, the minima shifts right. This shift is the result of dissipation which in a GMA model has a complex coupled damage-plastic mechanism due to the grain-scale processes the material experiences under macroscale deformation.

4.2.3.2 The stress-strain response

In the results of this subsection, a one-dimensional compression test is examined under repeated loading-unloading over 2-cycles, where the sequence is 1st loading, 1st unloading, 2nd loading and 2nd unloading. Fig. 4.18 gives the model predictions. The vertical S_{22} and lateral S_{11} stresses are calculated in Eq. 4.39 as a function of the updated strain tensor $\mathbf{G}$ based upon increasing/decreasing applied displacement $\bar{u}$, as given in Eq. 4.22.

Fig. 4.18a presents the vertical stress S_{22} plotted against the vertical strain G under the repeated loading cycles. At the initial stage of loading, the stiffening mechanism progresses gradually until the end of the first loading. An evidence for such a stiffening is that the tangent of this curve increases with G . Past the steep stiffening ($G = 0.02 - 0.03$) during the 1st loading, the material exhibits a more gradual stiffening stress-strain behavior ($G > 0.04$), reflecting a competition between the stiffening of grain-pairs under compression—including a possible increase in grain contacts due to particle rearrangement, modeled via the quartic term in the grain-pair elastic energy—and damage-related softening.

During the first unloading, the path is different. The reason is that the damage and plastic descriptors have evolved, and the material exhibits a softening due to the accumulation of damage during the first loading stage. The first unloading is stopped when the vertical component of the stress tensor, S_{22} , becomes close to zero. As expected, such an event occurs at a non-null strain level. This is expected since the plastic deformation has evolved during the first loading stage, and therefore, a load-free configuration is, according to the representation of Eq. 4.40, different from the initial one because of the evolution of the pre-stress $\mathbb{P}$. The second loading path is slightly different with respect to the first unloading one. In particular, the second loading is stiffer than the first unloading due to the microscale mechanism that predicate stiffening in the direction of external loading (to be discussed in detail later in Section 4.2.3.3). The second loading stage is terminated at the same strain level in which the 1st loading stage is stopped. A higher value of the final stress is observed compared to 1st loading.

In Fig. 4.18b, the lateral stress S_{11} versus the vertical strain G is shown. The lateral stress evolves as the specimen tends to expand laterally due to an increase in the vertical deformation because of the positive Poisson's effect. Similar to the behavior in the vertical direction, the lateral response stiffens rapidly at low vertical strain. It is worth to note that, at the end of first unloading (when such an end was chosen under the condition

to have null vertical stress), the horizontal stress is non-zero. This is a characteristics of granular materials, which can be called locked stress, that emerges from plasticity in grain interactions leading to macroscale material plasticity which implies that additional tensile deformation is needed in the vertical direction to achieve stress free horizontal direction. A similar effect of grain-scale plasticity can be observed in Fig. 4.18c, which gives the evolution of lateral stress S_{11} plotted against the vertical stress S_{22} . During loading a nearly linear evolution is observed, agreeing with the classical constant lateral earth pressure coefficient $K_0 = S_{11}/S_{22}$, under loading. On the other hand, during unloading the vertical stress decreases at increasingly greater rate than the horizontal stress. As a consequence, the lateral earth pressure coefficient $K_0 = S_{11}/S_{22}$ increases during unloading with a particular rapidity when approaching complete unloading (zero stress) in the vertical direction. This behavior of the lateral earth pressure coefficient K_0 , is well known in the soil mechanics literature (see for example the discussion in [9, 241]).

4.2.3.3 Evolution of microscale damage and plasticity

Since a GMA based models consider the link between the macroscale response and grain (micro)-scale phenomena, it is instructive to examine the orientation-dependent evolution of microscale damage and plasticity of effective grain-pairs and its relationship to the emergent response. Figs. 4.19-4.23 present polar plots for damage and plastic variables during each loading-unloading stages. These variables are computed using the KKT conditions given in Eqs. 4.46-4.50. Each polar plot is given at 10 equal intervals of corresponding strain.

Fig. 4.19 gives the directional evolution of normal damage D_η during the repeated uniaxial loading-unloading. The normal damage is associated with the loss of normal stiffness (see Eq. 4.25) due to the combined effects of grain-scale mechanisms that include the collapse or buckling of particle chains. Since the granular material is confined on the lateral sides, the normal damage does not grow in the horizontal orientations around in the neighborhood of 0° and 180° . In both unloading processes, since the threshold is not reached in Eq. 4.41, there is no growth of normal damage. During the second loading, the normal damage only slightly increases and reaches its maximum value. It is also noteworthy that the magnitude of damage growth is relatively low reaching a maximum of 0.12.

In Fig. 4.20, the polar plots for the tangential damage D_τ are given based on the

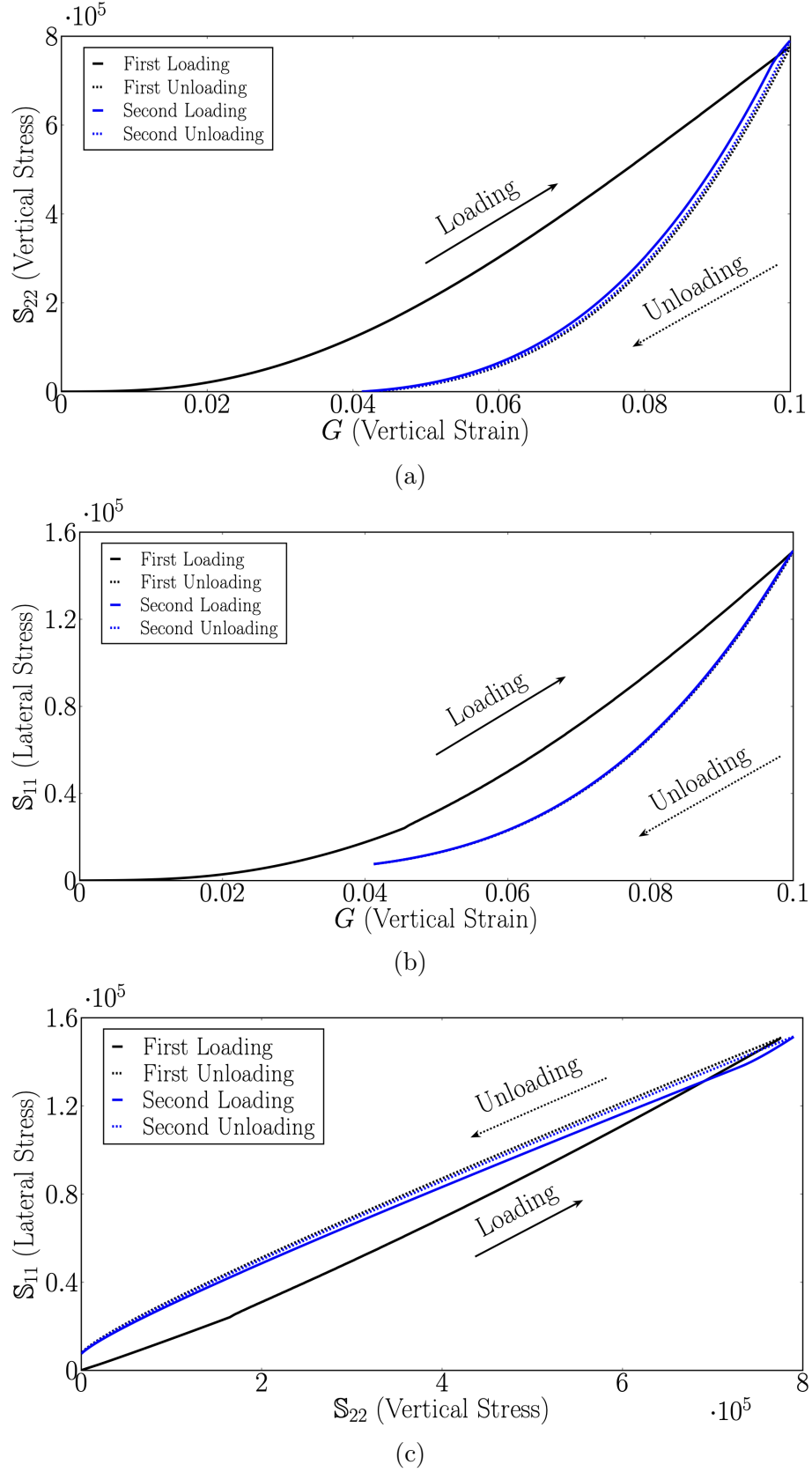


Figure 4.18: Stress-strain behavior during the numerical simulation at maximum strain ($G=0.1$) under two cyclic loading-unloading; (a) vertical stress S_{22} versus vertical strain G , (b) lateral stress S_{11} versus vertical strain G and (c) lateral stress S_{11} versus vertical stress S_{22} .

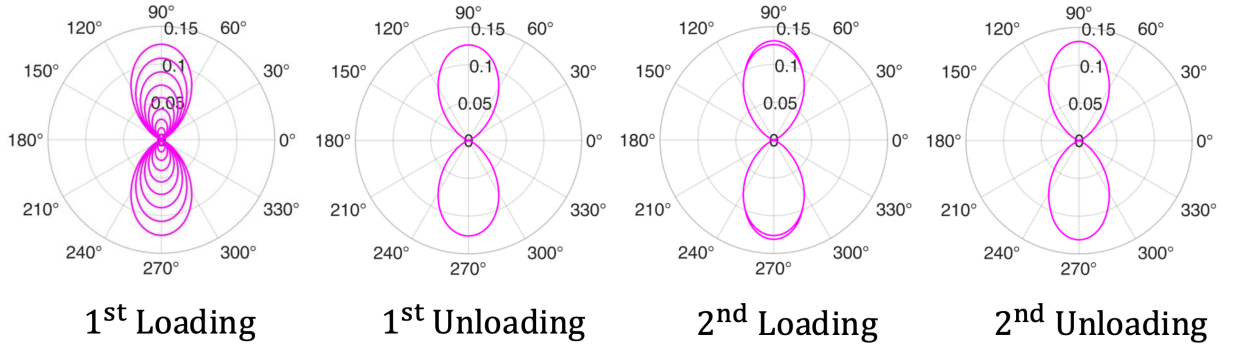


Figure 4.19: Normal damage D_η polar plots under cyclic loading-unloading in one-dimensional compression.

directional evolution. The growth in tangential damage is governed by Eq. 4.42. The growth is observed to be dominant in the directions oblique to the compression direction (with growth developing in the neighborhood of 45° , 135° , 225° and 315° where tangential displacement is larger). Interestingly, a non-intuitive growth of tangential damage is observed during the end of 1st unloading. Since damage is a monolateral variable, it is usually not expected to grow during macroscale unloading. However, due to tangential plasticity, reverse elastic tangential loading commences as indicated in Section 3.1.1. To elaborate further, the squared elastic tangential displacement u_τ^{2el} drives the evolution of tangential damage. During the first loading it has reached a certain value due to both u_τ^2 and λ_τ^2 evolution. At the end of the first loading they reach both a maximum value. During the first unloading, however, only u_τ^2 decreases its value and λ_τ^2 , because of irreversibility, remains constant. Thus, at the end of the first unloading, u_τ^2 reaches zero and λ_τ^2 remains at its maximum value. As a consequence also u_τ^{2el} reaches the maximum value of λ_τ^2 . In this case, this last maximum value is larger than that reached by u_τ^{2el} at the end of the first loading. As a consequence at the end of the first unloading the squared elastic tangential displacement u_τ^{2el} increases its value and this leads to a tangential damage evolution. It is noted, however, that the magnitude of damage growth is relatively low reaching a maximum of 0.07. In subsequent loading and unloading stages, the damage threshold is never exceeded. As a consequence, there is no evolution during the second loading-unloading stages. Finally, it is noted that the growth of both damage mechanisms is influenced by the rearrangement of particles along with particle rotation/rolling or grain sliding. Grain crushing, while a coupled damage-plasticity phenomena, could also lead to an increase in grain contact interactions triggering stiffening and evolution of anisotropy.

The polar plots for the normal compression λ_η^c and tension λ_η^t plastic multipliers are provided in Figs. 4.21 and 4.22, respectively. In GMA, these plastic variables represent

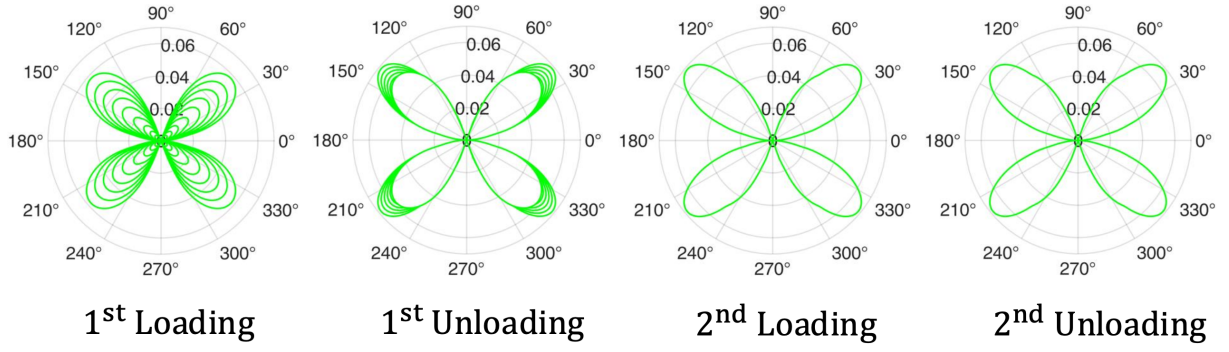


Figure 4.20: Tangential damage D_τ polar plots under cyclic loading-unloading in one-dimensional compression.

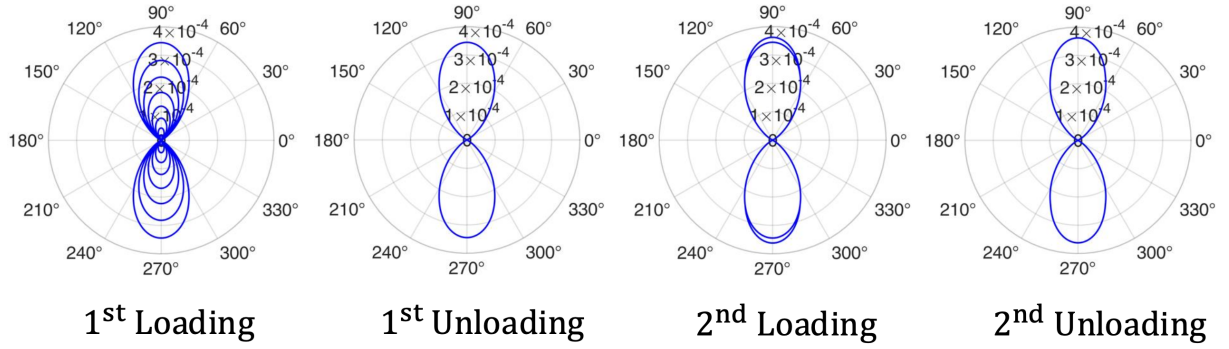


Figure 4.21: Compression λ_η^c plastic multiplier polar plots under cyclic loading-unloading in one-dimensional compression.

irrecoverable deformations due to grain-pair frictional sliding and separation in specific directions. The normal tension and compression plastic multipliers are computed based on Eqs. 4.43 and 4.44, respectively. Notably, the plastic variables grow in the direction of loading and its vicinity. The compression plastic multiplier, see Fig. 4.21, primarily grows during the first loading stage, with a smaller growth in the second loading phases. As expected, no growth happens in compression plastic multiplier during unloading. In contrast, the tension plastic multiplier grows, see Fig. 4.22, during the first and second unloading phases, although at a relatively slower rate. As discussed, the end of the first unloading has been prescribed when the vertical stress becomes zero. Thus, no positive elastic normal displacement in tension is expected at the end of the first unloading. However, plastic deformation is possible. Since, towards the end of unloading, some directions are still under elastic compression, contributing to compressive vertical stress, some other directions must compensate. As a consequence, they reach elastic tension, contributing to tensile vertical stress, leading to the evolution of plastic multipliers in tension.

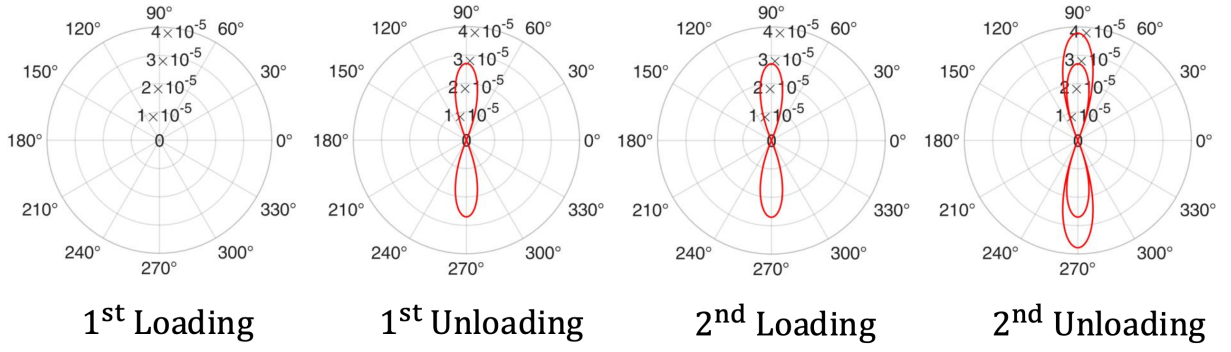


Figure 4.22: Tension λ_{η}^t plastic multiplier polar plots under cyclic loading-unloading in one-dimensional compression.

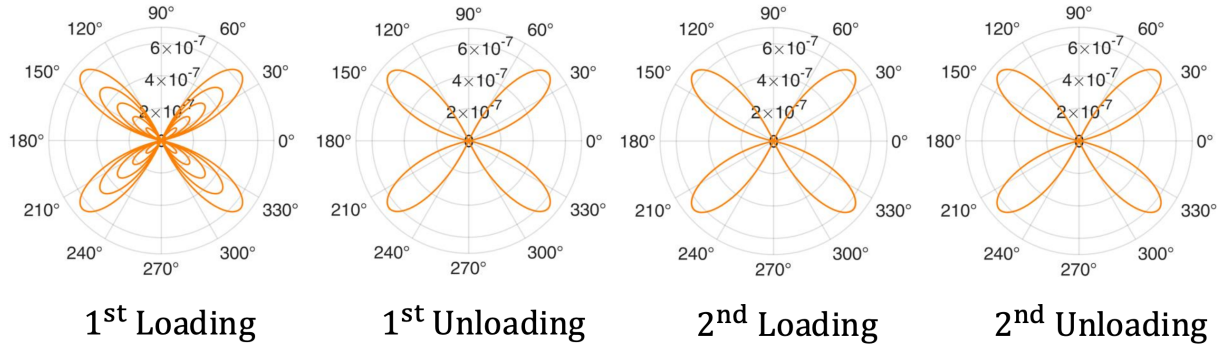


Figure 4.23: Squared tangential λ_{τ}^2 plastic multiplier polar plots under cyclic loading-unloading in one-dimensional compression.

Fig. 4.23 gives the polar plots for the squared tangential plastic multiplier λ_{τ}^2 under cyclic loading-unloading. By using Eq. 4.45, the growth of squared tangential plasticity is governed. During the simulation, the growth occurs only during the first loading phase in particular in the quadrant directions, i.e. 45° , 135° , 225° and 315° , and no evolution is observed in the rest of phases. It is worth again to note that at the end of the first unloading phase the elastic squared tangential damage grows and the squared tangential plasticity does not.

In fact, as seen in Fig. 4.18, the hysteresis loop occurs due to the accumulation of normal plastic deformation. The newly adapted squared tangential plastic term accumulates the lateral stress, and it does not reach zero at the strain value in which the vertical stress is zero (see Fig. 4.18b).

4.2.3.4 Evolution of macroscale anisotropy

4.2.3.4.1 Definition of the equivalent damage-elasto-plastic stiffness tensor

To investigate the macroscale anisotropy, the changes in the macroscale elastic behavior are examined by applying very small probes in the axial (G_{11} and G_{22}) and tangential (G_{12}/G_{21}) directions at chosen specific loading steps during the first loading-unloading cycle of one-dimensional compression. To trace the evolution of anisotropy, these probes were applied at non-uniform strain intervals: at every time step until the vertical strain G reached 0.001, every 40 time steps until it reached 0.01, and then every 400 steps up to the end of the first unloading phase. The applied probe is chosen to be small such that no evolution of damage and plasticity occurs. Using the Taylor series expansion of Eq. 4.39 (given in Eq. 4.52), the equivalent damage-elasto-plastic stiffness tensor is defined as follows

$$\mathbf{S}(\mathbf{G} + \Delta \mathbf{G}) = \mathbf{S}(\mathbf{G}) + \left. \frac{\partial \mathbf{S}}{\partial \mathbf{G}} \right|_{\mathbf{G}} \Delta \mathbf{G}, \quad (4.52)$$

where $\tilde{\mathbf{C}} = \left. \frac{\partial \mathbf{S}}{\partial \mathbf{G}} \right|_{\mathbf{G}}$ is the 4th rank equivalent stiffness and obtained by solving the formula given below:

$$\Delta \mathbf{S} = \mathbf{S}(\mathbf{G} + \Delta \mathbf{G}) - \mathbf{S}(\mathbf{G}) = \tilde{\mathbf{C}} \Delta \mathbf{G}. \quad (4.53)$$

The eigenvalues [242, 243] and harmonic decomposition [244, 245] of the equivalent damage-elasto-plastic stiffness tensor are employed to investigate the evolution of material anisotropy during loading-unloading cycle.

4.2.3.4.2 Evolution of eigenvalues of equivalent damage-elasto-plastic stiffness tensor

In general, three eigenvalues (eigenstiffnes) of the 4th-order symmetric elastic stiffness tensor $\tilde{\mathbf{C}}$ can be obtained for every loading step. For isotropy, there are two independent eigenvalues representing pure shear and dilatation. In the transverse isotropy, there are three independent eigenvalues (λ_1 , λ_2 and λ_3) representing two isochoric (deviatoric and pure shear) and a dilatation mode, respectively [242]. Fig. 4.24 gives the evolution with loading of the normalized eigenvalues, in which the normalization is based upon the largest eigenvalue corresponding to dilatation mode. To indicate the magnitude of the

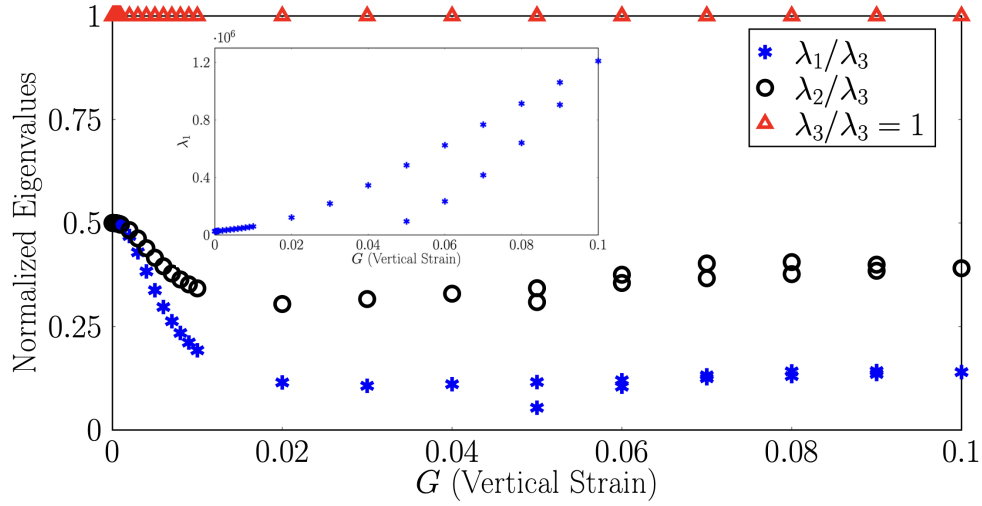


Figure 4.24: Normalized eigenvalues for quasi-deviatoric stress ratio λ_1 , pure shear λ_2 and quasi-dilatation λ_3 versus vertical strain G for investigating macroscale anisotropy at non-uniform time steps.

eigenstiffnesses, the inset in Fig. 4.24 gives the evolution of the largest eigenvalue. In the reference state, the material is isotropic, the dilatation eigenvalue λ_3 is exactly twice the shear eigenvalue. Under one-dimensional compression an anisotropy evolves in which the deviatoric eigenstiffness λ_1 exhibits a sharper decrease compared to pure shear λ_2 . Beyond strain level, $G < 0.02$, the evolution appears to slow down eventually reaching an asymptotic value at large strain. It is clear from the evolution of the eigenstiffnesses that the material will have a softer response under deviatoric deformation as compared to a pure shear deformation.

To show the evolution of relative stiffness in the deviatoric and pure shear deformation modes, the ratio of eigenvalues (λ_2/λ_1) versus the vertical strain G is given in Fig. 4.25. The inset presents the directional evolution of material anisotropy based on eigenvalues in the isochoric deformation space. Initially, when the material is isotropic, these eigenvalues are equal, and the inset in Fig. 4.24 is simply a circle. During loading, the ratio increases until the vertical strain reaches $G = 0.03$. However, at higher strain levels ($G > 0.07$), the ratio is constant at $\sqrt{3}$ and shows no further change. During unloading, both the eigenvalue ratio and the directional evolution of anisotropy exhibit a sharp increase. The implication is that the pure shear mode is significantly stiffer than the deviatoric mode in the unloaded state at the end of a load-unload cycle. Such a phenomenon can be interesting from an experimental viewpoint. The reason is that it is possible to conceive a small amplitude deviatoric and pure shear wave propagation through the specimen and during all the time range when it is subjected to a one-dimensional loading-unloading

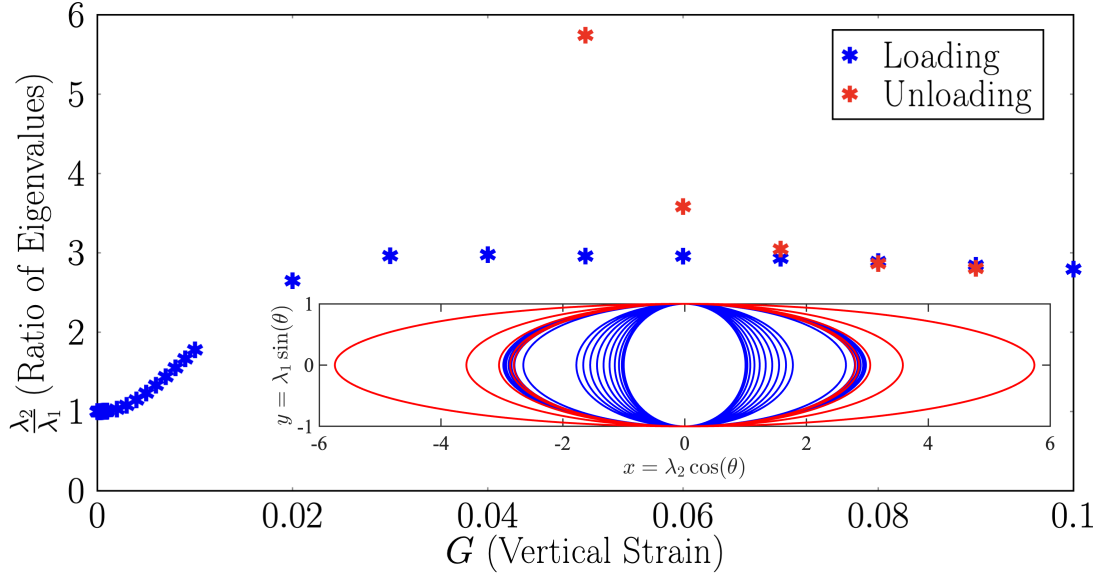


Figure 4.25: Ratio of eigenvalues λ_2/λ_1 between pure shear and quasi-deviatoric stress ratio versus vertical strain G and orientational evolution of macroscale anisotropy at non-uniform time steps. The inset presents the same results with the directional evolution of material anisotropy.

cycle.

4.2.3.4.3 Harmonic decomposition of equivalent damage-elasto-plastic stiffness tensor

It is instructive to also investigate the evolution of anisotropy through the harmonic decomposition of the equivalent damage-elasto-plastic stiffness tensor $\tilde{\mathbf{C}}$ using the methodology in [244, 245]. The macroscale anisotropy evolution is to compute the harmonic decompositions [244, 245] of the equivalent damage-elasto-plastic stiffness tensor $\tilde{\mathbf{C}}$, given by the parameters γ , $\mathbf{h}$, β and $\mathbf{H}$ as follows

$$\begin{aligned}
 \gamma &= \frac{1}{2} \mathbf{1} : \tilde{\mathbf{C}} : \mathbf{1} = \frac{1}{2} \delta_{ij} \tilde{\mathbf{C}}_{ijab} \delta_{ab}, \\
 \mathbf{h} &= \mathbf{1} : \tilde{\mathbf{C}} : \mathbf{J}, \quad \mathbb{h}_{ab} = \delta_{ij} \tilde{\mathbf{C}}_{ijcd} \mathbb{J}_{cdab}, \\
 \beta &= \frac{1}{2} \mathbf{1} : \text{Tr}_{13}(\mathbf{J} : \tilde{\mathbf{C}} : \mathbf{J}) = \frac{1}{2} \delta_{jk} \text{Tr}_{13}(\mathbb{J}_{ijab} \tilde{\mathbf{C}}_{abcd} \mathbb{J}_{cdhk}) = \frac{1}{2} \delta_{jk} \mathbb{J}_{ijab} \tilde{\mathbf{C}}_{abcd} \mathbb{J}_{cdik}, \\
 \mathbf{H} &= \mathbf{J} : \tilde{\mathbf{C}} : \mathbf{J} - \beta \mathbf{J}, \quad \mathbb{H}_{ijhk} = \mathbb{J}_{ijab} \tilde{\mathbf{C}}_{abcd} \mathbb{J}_{cdhk} - \beta \mathbb{J}_{ijhk}, \\
 \mathbf{J} &= \mathbf{II}^4 - \mathbf{K}, \quad \mathbb{J}_{ijab} = \frac{1}{2} (\delta_{ia} \delta_{jb} + \delta_{ib} \delta_{ja} - \delta_{ij} \delta_{ab}), \\
 \mathbf{II}^4_{ijab} &= \frac{1}{2} (\delta_{ia} \delta_{jb} + \delta_{ib} \delta_{ja}), \quad \mathbf{K} = \frac{1}{2} \mathbf{1} : \mathbf{1}, \quad \mathbb{K}_{ijab} = \frac{1}{2} \delta_{ij} \delta_{ab}.
 \end{aligned} \tag{4.54}$$

Here γ and β are scalars that give the isotropic part of the stiffness tensor, and $\mathbf{h}$ and $\mathbf{H}$ give the anisotropic part of the stiffness tensor. The projection operators are given by $\mathbf{J}$, $\mathbf{II}^4$ and $\mathbf{K}$. The above Eq. 4.54, can be further expressed in the following index form

$$\gamma = \frac{1}{2} \tilde{\mathbf{C}}_{ijjj}, \tag{4.55}$$

$$\mathbb{h}_{ab} = \tilde{\mathbf{C}}_{iiab} - \frac{1}{2} \tilde{\mathbf{C}}_{ijjj} \delta_{ab}, \tag{4.56}$$

$$\beta = \frac{1}{2} \tilde{\mathbf{C}}_{ijji} - \frac{1}{4} \tilde{\mathbf{C}}_{ijjj}, \tag{4.57}$$

$$\begin{aligned}
 \mathbb{H}_{ijab} &= \tilde{\mathbf{C}}_{ijab} - \frac{1}{2} \tilde{\mathbf{C}}_{ijcc} \delta_{ab} - \frac{1}{2} \tilde{\mathbf{C}}_{ccij} \delta_{ab} + \frac{1}{4} \tilde{\mathbf{C}}_{ccdd} \delta_{ij} \delta_{ab} \\
 &\quad - \frac{1}{2} \left(\frac{1}{2} \tilde{\mathbf{C}}_{cdcd} - \frac{1}{4} \tilde{\mathbf{C}}_{ccdd} \right) (\delta_{ia} \delta_{jb} + \delta_{ib} \delta_{ja} - \delta_{ij} \delta_{ab}).
 \end{aligned} \tag{4.58}$$

The scalar parameter γ represents the bulk modulus, second-rank tensorial parameter $\mathbf{h}$ represents the deviatoric modulus, and scalar β defines the generalized shear modulus. Further, to quantify, the material's shear response, the 4th-rank tensor $\mathbf{H}$ is also considered. For isotropic materials, the harmonic decomposition is given using Lamé parameters λ (Lamé's first parameter) and μ (shear modulus) as follows

$$A = D = 2\mu + \lambda, \quad B = \lambda, \quad C = \mu, \tag{4.59}$$

$$I_1 = \gamma = 2\mu + 2\lambda, \quad \mathbb{h}_{ab} = 0, \quad J_1 = \beta = 2\mu, \quad \mathbb{H}_{ijhk} = 0, \quad I_2 = J_2 = I_3 = 0, \tag{4.60}$$

where only the isotropic parameters γ and β are non-zero. In addition, invariants I_1 , J_1 , I_2 , J_2 and I_3 are defined in Eq. 4.61 as:

$$I_1 = \gamma, \quad J_1 = \beta, \quad I_2 = \mathbb{h}_{ab} \mathbb{h}_{ab}, \quad J_2 = \mathbb{H}_{ijab} \mathbb{H}_{ijab}, \quad I_3 = \mathbb{h}_{ij} \mathbb{H}_{ijab} \mathbb{h}_{ab}. \tag{4.61}$$

For this numerical example, the equivalent damage-elasto-plastic stiffness tensor $\tilde{\mathbf{C}}$ that evolves during one-dimensional loading is expressed in matrix form using the following symbolic representation:

$$\tilde{\mathbf{C}} = \begin{pmatrix} A & 0 & 0 & B \\ 0 & C & C & 0 \\ 0 & C & C & 0 \\ B & 0 & 0 & D \end{pmatrix}. \quad (4.62)$$

For this equivalent damage-elasto-plastic stiffness tensor $\tilde{\mathbf{C}}$, harmonic decomposition parameters and the invariants are as follows:

$$I_1 = \gamma = \frac{A+D}{2} + B, \quad J_1 = \beta = \frac{A+D}{4} - \frac{B}{2} + C, \quad (4.63)$$

$$\mathfrak{h}_{11} = -\mathfrak{h}_{22} = \frac{A-D}{2}, \quad \mathfrak{h}_{12} = \mathfrak{h}_{21} = 0 \quad \mathbb{H}_{1111} = \mathbb{H}_{2222} = \frac{A+D}{8} - \frac{B}{4} - \frac{C}{2}, \quad (4.64)$$

$$\mathbb{H}_{1122} = \mathbb{H}_{1212} = \mathbb{H}_{1221} = \mathbb{H}_{2112} = \mathbb{H}_{2121} = \mathbb{H}_{2211} = -\frac{A+D}{8} + \frac{B}{4} + \frac{C}{2}, \quad (4.65)$$

$$I_2 = \mathfrak{h}_{ab}\mathfrak{h}_{ab} = \frac{(A-D)^2}{2}, \quad J_2 = \mathbb{H}_{ijab}\mathbb{H}_{ijab} = 8 \left(\frac{A+D}{8} - \frac{B}{4} - \frac{C}{2} \right)^2,$$

$$I_3 = \mathfrak{h}_{ij}\mathbb{H}_{ijab}\mathfrak{h}_{ab} = (A-D)^2 \left(\frac{A+D}{8} - \frac{B}{4} - \frac{C}{2} \right). \quad (4.66)$$

The evolution of parameters γ , $\mathbf{h}$, β and $\mathbf{H}$, particularly their non-zero emergence of $\mathbf{h}$ and $\mathbf{H}$ during loading, can indicate the transition in anisotropy states, including possible emergence of certain exotic states [244]. Figs. 4.26, 4.27 and 4.28 provide the evolution of γ , $\mathbf{h}$, β and $\mathbf{H}$, and the invariants plotted against the applied vertical strain G . For isotropic materials, there are only two non-zero parameters, the bulk modulus γ and the shear modulus β . As expected for the initial state, which is assumed to be isotropic, these non-zero parameters are shown in the insets of Figs. 4.26 (see also Eq. 4.60), while all other parameters are zero. As the loading progresses, some components of the second-rank deviatoric modulus $\mathbf{h}$ and the fourth-rank generalized shear modulus $\mathbf{H}$ evolve to non-zero values as seen from Figs. 4.26 and 4.27. The material remains nearly isotropic at small strains ($G < 0.001$) as the invariants $I_2 = J_2 = I_3 \approx 0$ are negligibly small. As the loading progresses and damage and plasticity evolve, the emergent anisotropy maybe classified as that of type D_2 belonging to the set of orthotropic materials as the invariants $I_2 = J_2$ become significantly large. It is notable that the invariant J_2 is a non-monotonic function of loading, reducing after certain strain-level ($G \approx 0.05$) indicating a transition towards type D_4 belonging to the set of tetragonal materials. Upon unloading, all the parameters decrease in magnitude and it appears that at the unloaded state ($\mathbb{S}_{22} = 0$),

the material anisotropy is of type D_4 or of tetragonal material.

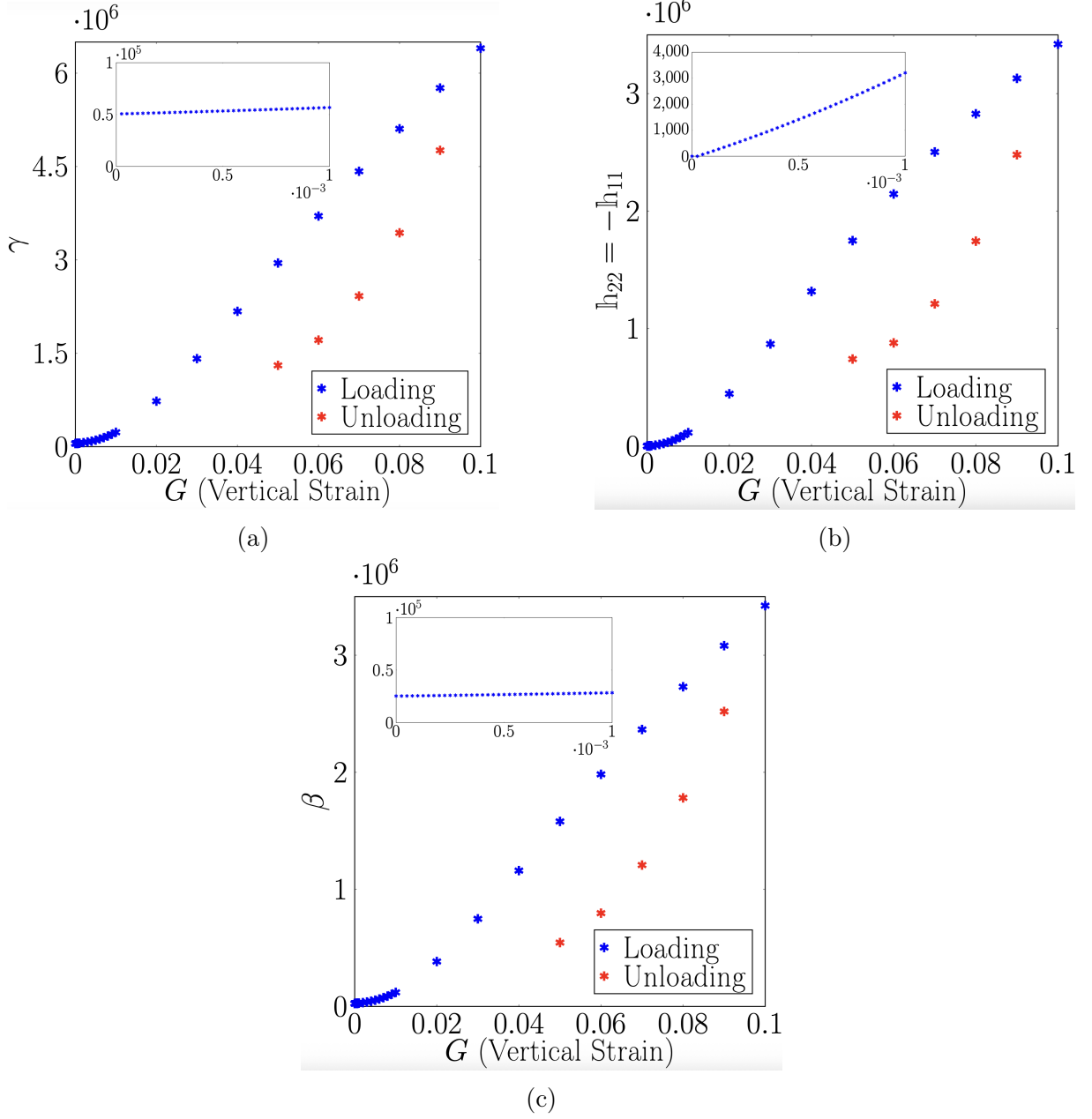


Figure 4.26: Evolution of the harmonic decomposition parameters plotted against vertical strain G at non-uniform time steps; (a) the bulk modulus γ , (b) the deviatoric modulus h and (c) the generalized shear modulus β .

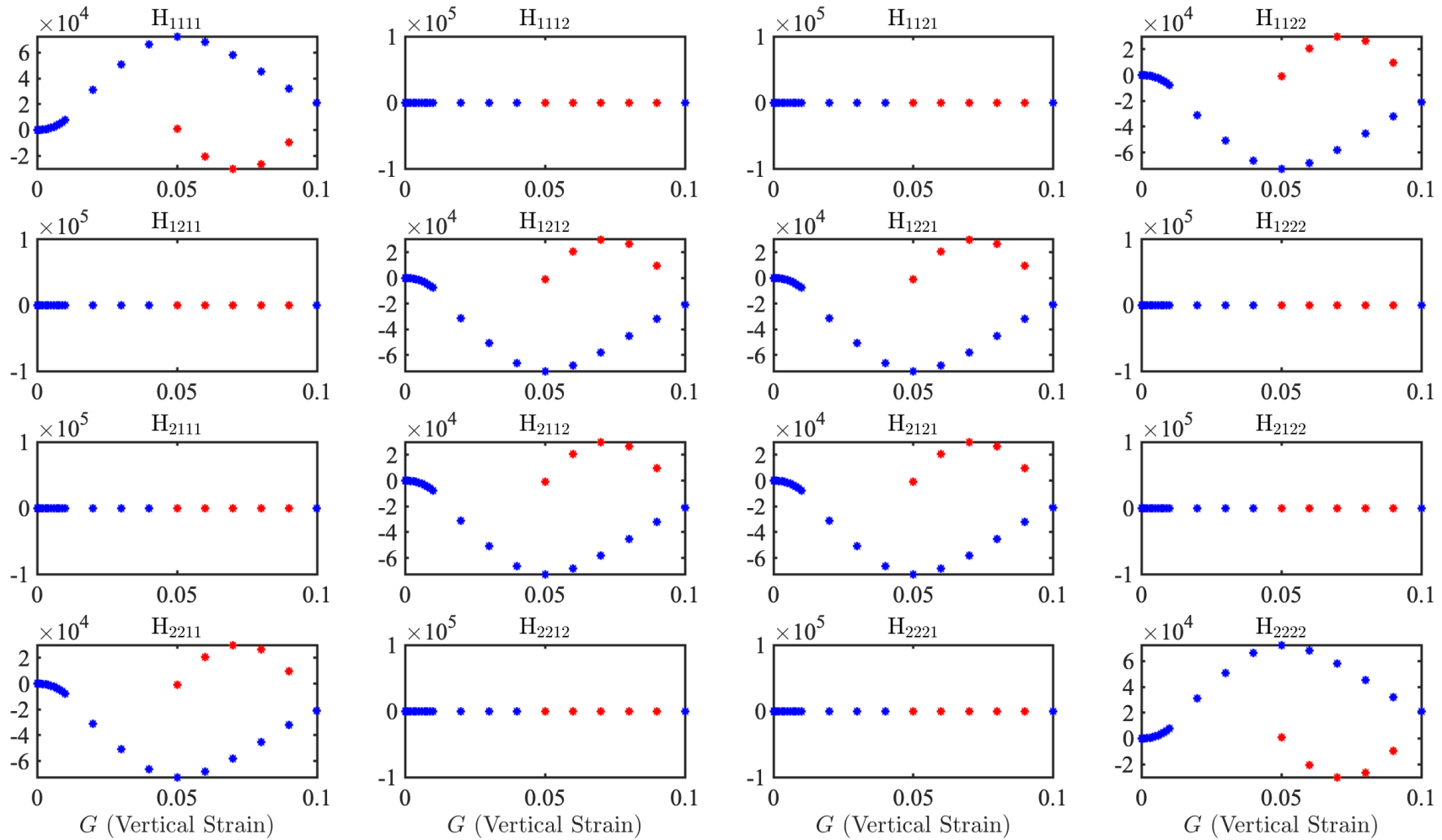


Figure 4.27: Evolution of 4th-order harmonic decomposition tensorial invariant $\mathbb{H}$ versus vertical strain G at non-uniform time steps, presenting $2^4 = 16 \mathbb{H}_{ijab}$ for 2D model.

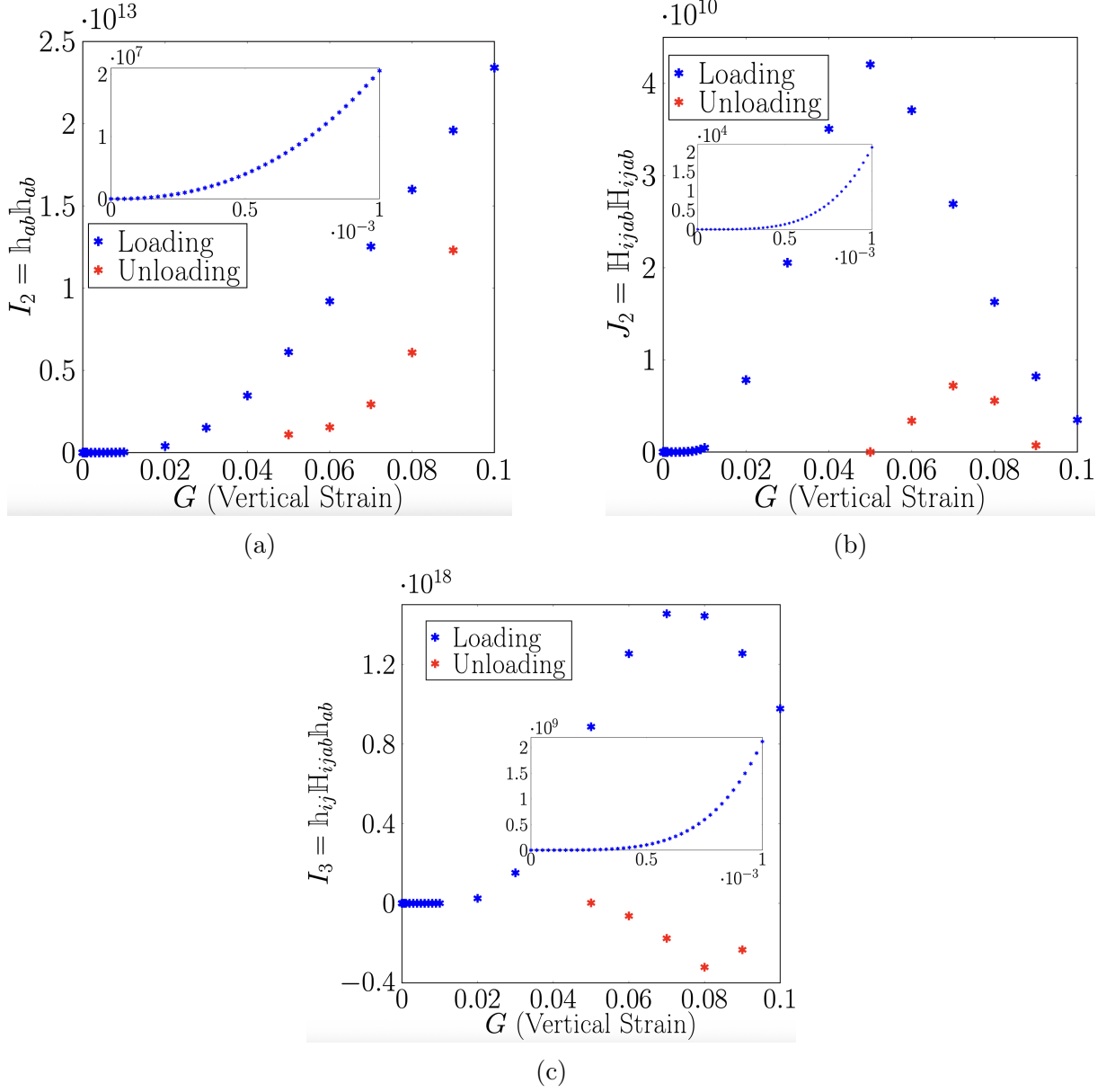


Figure 4.28: Evolution of the harmonic decomposition invariants plotted against vertical strain G at non-uniform time steps; (a) I_2 , (b) J_2 and (c) I_3 .

General conclusion and perspectives

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5.1 Conclusion

The results obtained in this thesis demonstrate that critical state in granular materials can be predicted by continuum models derived using a Granular Micromechanics Approach (GMA). Besides, this thesis is devoted for a parametric study to investigate the behavior of a numerical framework that examines the macro-scale critical state. These works focus on revealing stress and volumetric strain responses during simulations by varying characteristic compression constitutive parameters with non-dimensionalization coefficients (see [7, 8]). Further, other novel contribution of this thesis is to apply a GMA for developing a continuum model that replicate the experimental observations in one-dimensional compression according to constituent grain stiffness or different initial density states. It has been shown that the emergent macroscale behavior can be explored by utilizing properly conceived damage-elasto-plastic spring elements in the normal and tangential directions that represent the effective behavior of grain-pairs in a granular material. The energy functions represent an average response of a grain-pair embedded in a multitude of grains of a specimen subjected to boundary loading. In the presented approach, damage is defined as the loss of stiffness, structural integrity, and lateral support due to the interplay of microstructural mechanisms such as rotation/sliding of particles and compaction, while plasticity is defined as the cumulative irreversible displacements because of grain rearrangement, grain fracture and crushing, and buckling/collapse of particle chains. This approach is independent from classical macro-plasticity by focusing on micro-level plasticity. The elastic energy functionals and the dissipation potential of

the grain-pair damage-elasto-plastic spring elements have been modified from the previous works of [7–10, 107, 225].

A hemi-variational approach is employed to establish the Karush-Kuhn-Tucker (KKT)-type conditions that give the evolution equations for grain-pair damage and plasticity at the micro-scale. These kinematic irreversible quantities do not decrease over time and evolve regarding orientation-based growth depending on the loading path. However, these conditions do not directly apply at the macro-level, where classical macro-plasticity lacks an explicit criterion for the emergence of plastic behavior. Formal identification between a plasticity criterion and a flow-rule used in macro-plasticity is not directly incorporated or emergent in the proposed micro-level model. The current approach does not aim to derive macro-scale models such as a flow-rule or macro-level plasticity. Indeed, this model focuses on capturing the grain-scale mechanisms and their direct contributions to the material's overall response, offering a different perspective from traditional macro-plasticity formulations. For a continuum material point representative of a large number of grain contacts oriented in various directions, the overall constitutive behavior is obtained by integration over the grain-pair orientation space.

In the critical state concept, the predicted behavior using the derived model replicated the typical experimentally observed behavior of frictional granular materials. For example, dense specimens presented dilative behavior and loose specimens exhibited compressive behavior. Particularly, the peak stress (failure) of dense specimens appeared at small vertical strain values while the failure of loose specimens had large strain values. The strain where the stress peak occurs, and the lowest volume strain occurs may differ depending on which material parameter is changed. Poisson's effect demonstrates a non-linear response according to the evolution of directional damage growth (loss of stiffness) and irrecoverable deformation (plastic), which triggers anisotropic behavior in the volumetric strain.

The model was applied to simulate the one-dimensional compression response. The results were obtained not only as the stress-strain responses but also as polar plots of the effective grain-pair elastic energy and coupled damage and plasticity when subjected to uniaxial compressive displacement. The stiff and soft specimens were proportionally determined according to the material stiffness of a mid-dense specimen, their stress-strain responses varied at the same rate. The model was validated by comparison with typical experimental tests. Model results were in conformity with the initial linear behavior, evident curvature, secondary linear increase, and peak stress. The model was able to correctly predict the observed variation of void ratio and volume strain during loading. In

addition, lateral to axial stress ratio behavior under loading-unloading cycle, particularly the growth of this ratio under unloading, was replicated by the model results. A parametric study was performed which revealed that the one-dimensional compression behavior has nearly universal scaling for different constituent grain types or packing density. The results of parametric study were also used to investigate the directional evolution of elastic energy, damage and plasticity, during loading-unloading-reloading process.

The main focus of the second work of one-dimensional compression was on extending a GMA based elasto-damage-plasticity model for elasto-frictional granular materials. In particular, this work introduces additional terms in grain-pair elastic energy functional and dissipation potential to better capture the granular material nonlinearity. Such nonlinearity manifests its presence not only due to an increase of the equivalent stiffness under compression but also because of the coupling between normal and tangential elastic and dissipation mechanisms. The newly introduced terms profoundly modify the coupled elasto-damage-plasticity response predicted by the derived model.

The newly introduced material elastic nonlinearity is not only influenced by damage, which is expected by definition, but also it is coupled to plastic dissipation. Moreover, the introduction of these quartic terms in grain-pair elastic energy leads to the stiffening behavior under compression. Besides, the coupling of damage-plastic dissipation along with higher-order elastic energy results in the emergence of an apparent molecular-type, such as Lennard-Jones type, elastic energy landscape for the uniaxial loading response. In fact, the elastic energy rises rapidly on the one hand under compression. On the other hand, under tension, the elastic energy reaches an inflection that tends to an asymptote. This kind of potential is generally interpreted as that of elastic type and the connected loss of ellipticity has been considered in the literature [246–248]. The present work gives a framework in which the elastic positive definitive energy is maintained. As a result, the ellipticity properties are preserved. It has to be noted that the evidenced Lennard-Jones type potential energy is here induced by both damage and plastic non-reversible dissipation contributions and therefore it is not due to a purely elastic effect. Finally, eigenvalue and harmonic decomposition of the equivalent damage-elasto-plastic stiffness tensor are utilized to investigate the emergent macroscale anisotropy evolution. The anisotropy evolution analysis indicated the possible approach for experimental evaluation of loading induced anisotropy in elasto-frictional granular materials. Furthermore, it was found that the emergent elastic anisotropy can vary from isotropic to orthotropic to tetragonal with the evolution of damage and plasticity during loading-unloading cycle.

5.2 Perspectives

A key finding from the obtained results is that macroscale behavior emerges as a consequence of the evolution of grain-scale deformations involving described elastic and dissipative processes. It is remarkable that the present model based upon relatively simple grain-pair elastic energy and dissipative potential functions is able to predict these complex phenomena. A key aspect of the mechanical behavior of granular materials is the deformation mechanisms, illustrated by the orientation-dependent evolution of damage, referred to as loss of stiffness (also encompassing the breakage of particle chains and the loss of lateral confinement) and plasticity (defined as the effective accumulation of plastic deformation due to grain-pair sliding or rotation). To demonstrate the impacts of these irreversible grain-scale processes, polar plots for irreversible variables were analyzed. The coupling of directional damage growth (loss of stiffness) and evolution of irrecoverable (plastic) deformation was seen as responsible for the nonlinear evolution of Poisson's effect and anisotropy that leads to the non-monotonic volume change behavior of granular materials. As shown in Figs. 3.16-3.19, when different material parameters are adapted into the simulations, changes in the principal stress ratio and volumetric strain behavior of the specimens appear. It should be emphasized that the critical state may not be observed depending on changes in material parameters, since one behavior may tune to the typical response while the other might not conform to this classical concept. In fact, improperly defined material parameters in the model might cause behaviors that deviate from the desired response by significantly influencing the stress-strain relationship and deformation characteristics. Besides, the material can become correspondingly stiffer/looser due to the increase/decrease in the compression constitutive parameters, leading to more/less deformation evolution. These studies also provide the guidance for improving the predictions that a numerical model will provide for the future studies under various loading scenarios by refining the energy functions and properly assigning the constitutive parameters.

For further modifications, the path-dependent analysis can be simulated in the future works by implementing additional deformation mechanisms into the effective grain-pair elastic energy and dissipation potential. The model can be refined by incorporating newly introduced entropic terms and establishing coupling terms between normal and tangential irreversible quantities. The resultant GMA based model can be applied to unravel the behavior under homogeneous deformations or under non-homogeneous condition by implement into Finite Element (FE) analysis. Such FE implementations can be used to elucidate behavior of larger complex geo-structures in which critical state plays an important role, such as problems of slope failure, landslides and avalanches, in which shear

localization zone develops which is dominated by critical state behavior. Examples of the implementation of a GMA based models to investigate non-homogeneous and localized deformations have been presented in the works of Placidi et al. [107], Timofeev et al. [224], and Maksimov et al. [226]. For instance, further advancements can be made in understanding the mechanical behavior of granular materials under various loading conditions by combining findings in [7–10, 107, 224, 225].

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List of publications

- Michele De Angelo, Nurettin Yilmaz, M Erden Yildizdag, Anil Misra, François Hild, and Francesco dell’Isola. Identification and validation of constitutive parameters of a Hencky-type discrete model via experiments on millimetric pantographic unit cells. *International Journal of Non-Linear Mechanics*, 153:104419, 2023.
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