



HAL
open science

Macroscopic softening in granular materials from a mesoscale perspective

Jiaying Liu, Antoine Wautier, Stéphane Bonelli, François Nicot, Félix Darve

► **To cite this version:**

Jiaying Liu, Antoine Wautier, Stéphane Bonelli, François Nicot, Félix Darve. Macroscopic softening in granular materials from a mesoscale perspective. *International Journal of Solids and Structures*, 2020, 193-194, pp.222-238. 10.1016/j.ijsolstr.2020.02.022 . hal-02946256

HAL Id: hal-02946256

<https://hal.inrae.fr/hal-02946256>

Submitted on 23 Sep 2020

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Macroscopic softening in granular materials from a mesoscale perspective

Jiaying Liu, Antoine Wautier, Stéphane Bonelli, François Nicot, Félix Darve

► **To cite this version:**

Jiaying Liu, Antoine Wautier, Stéphane Bonelli, François Nicot, Félix Darve. Macroscopic softening in granular materials from a mesoscale perspective. *International Journal of Solids and Structures*, Elsevier, 2020, 193-194, pp.222-238. 10.1016/j.ijsolstr.2020.02.022 . hal-02946256

HAL Id: hal-02946256

<https://hal.inrae.fr/hal-02946256>

Submitted on 23 Sep 2020

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Macroscopic softening in granular materials from a mesoscale perspective

Jiaying LIU^{a,c}, Antoine WAUTIER^{b,c,*}, Stéphane BONELLI^b, François NICOT^c, Félix DARVE^d

^aState Key Laboratory of Water Resources and Hydropower Engineering Science, Wuhan University, Wuhan 430072, China

^bINRAE, Aix-Marseille University, UR RECOVER, 3275 Rte Cézanne, CS 40061, 13182 Aix-en-Provence Cedex 5, France.

^cUniversité Grenoble Alpes, INRAE, UR ETGR, 2 rue de la Papeterie-BP 76, F-38402 St-Martin-d'Hères, France.

^dUniversité Grenoble Alpes, CNRS, G-INP, Laboratoire 3SR UMR5521, F-38000 Grenoble, France

Abstract

Stress-softening is one of the significant features experienced by cohesive-frictional granular materials subjected to deviatoric loading. This paper focuses on mesoscopic evolutions of the dense granular assembly during a typical drained biaxial test conducted by DEM, and proposes mesoscopically-based framework to interpret both hardening and softening mechanisms. In this context, force chains play a fundamental role as they form the strong contact phase in granular materials. Their geometrical and mechanical characteristics, as well as the surrounding structures, are defined and analyzed in terms of force chain bending evolution, local dilatancy, rotation and non coaxiality between the principal stress and the geometrical orientation of force chains. By distinguishing two zones inside and outside shear band, force chain rotations are shown to be of opposite sign, which may contribute to the observed macroscopic softening as one of the origin of the structural softening.

Keywords: DEM, granular materials, softening, mesomechanics, force chains, strain localization, rotation

1. Introduction

When going down to the microscale granular materials may appear deceptively simple but at the macroscale, the huge number of internal degrees of freedom results in very complex behaviors (Suiker et al., 2001; Roux, 2000; Kruyt, 2010; Tordesillas et al., 2016). It is widely accepted that the macroscopic mechanical responses are due to the combination of local contact mechanics and the geometrical arrangement of the granular assembly. Strain softening is maybe one of the most

*Corresponding author

Email address: antoine.wautier@inrae.fr (Antoine WAUTIER)

7 puzzling features in cohesive-frictional granular media. Opposite to strain hardening, strain softening
8 corresponds in plasticity theory to negative values for the hardening modulus. Being able to capture
9 accurately this feature has been one of the key issues in constitutive modeling of geomaterials for
10 decades. Two kinds of softening can be distinguished depending on the loading conditions (Sterpi,
11 1999): the “material softening” which is an intrinsic material property and the “structural softening”
12 for which the decrease in the shear resistance is related to the loss of homogeneity due to strain local-
13 ization. Drained triaxial tests are often used to characterize strain softening experimentally. Contrary
14 to the undrained triaxial test stress reduction observed during this test is partly driven by the boundary
15 conditions. If no loss of homogeneity is observed, the experimental test directly characterizes the
16 material softening as a consequence of the change in the plastic behaviors from strain hardening to
17 strain softening. Otherwise, the test characterizes a structural softening as the sample is composed
18 of two zones: the shear band domain where the material experiences locally material softening (Zhu
19 et al., 2016a) and the rest of the sample where the plasticity is hardly not activated. The mathematic
20 descriptions of the classical stress-strain relationship including softening phase have been mentioned
21 in many constitutive models (Lade, 1977; Sterpi, 1999), and typically for non-cohesive granular soils,
22 state-dependent models have been suggested (Been and Jefferies, 1985; Wan and Guo, 1998; Li and
23 Dafalias, 2000; Sun et al., 2017). However, we do mention that while structural softening takes place
24 within a given material specimen, the notion of constitutive behavior disappears on that specimen
25 scale.

26 Recently, perspectives at the micro- and mesoscale have been opened with the introduction of
27 efficient simulation tools (e.g. DEM, Discrete Element Method) and laboratory imaging techniques
28 (e.g., X-Ray Computed Tomography, Digital Image Correlation and Photoelastic stress analysis). The
29 micro- and mesoscale information can help understand the underlying mechanisms behind macro-
30 scopic observations and incorporate more physics in constitutive modeling. The microscopic scale
31 investigations focus on individual particle kinematics and contact dynamics, in some cases particle
32 breakage is considered (Ma et al., 2014, 2017; Yin et al., 2016; Zhou et al., 2015); while at the meso-
33 scopic scale, structural features are accounted for with clusters of a few particles such as force chains
34 and grain loops (in 2D) (Tordesillas et al., 2010; Zhu et al., 2016b). These two types of mesostructures
35 can stand as the dual characteristics of granular contact systems (Radjai et al., 1996, 1998). Meso-
36 scopic investigations have succeeded in explaining significant mechanisms in granular materials, such
37 as failure modes (e.g., Zhu et al. (2016a)), instability (e.g., Rechenmacher et al. (2011); Wautier et al.
38 (2018)) and shear band forming (e.g., Tordesillas (2007)). As a result, mesostructure-based consti-

39 tutive models have been proposed as a convenient way to homogenize the mechanical behavior of
40 granular materials (Nicot and Darve, 2011; Xiong et al., 2017).

41 The manuscript attempts to show the extent to which mesoscale analysis can address the macro-
42 scopic softening in granular materials. In previous contributions (Tordesillas and Muthuswamy, 2009;
43 Zhu et al., 2016a), the force chain bending was focused on, which was regarded as the local failure
44 of the mesostructure (Tordesillas and Muthuswamy, 2009; Nicot et al., 2017). Walker and Tordesil-
45 las (2010); Zhu et al. (2016b) claimed that the development of force chain bending is related to the
46 characteristic point (the switch between contractive and dilative behaviors before the stress peak) of a
47 biaxial test for dense granular assembly. At the same time, the fraction of sliding contacts decreases
48 and contact sliding localizes within some subdomains (Liu et al., 2018), and a non-affine deformation
49 mode is identified (Ma et al., 2018).

50 Internal structures become unstable before the macroscopic limit state is reached. It is therefore
51 necessary to describe and define the softening at the mesoscale as an indication of prefailure mech-
52 anism for the bulk. To this respect, the mechanical and geometrical evolutions of mesostructures
53 should be significant to the softening occurrence in granular materials, and interactions between force
54 chains and 2D loops mentioned by Zhu et al. (2016b); Tordesillas et al. (2010), is somehow thought
55 to influence the hardening/softening transition.

56 In this paper, the structural softening accompanied by shear banding is emphasized by mainly
57 focusing on dense granular materials subjected to drained tests. Investigations at the micro- and meso-
58 levels were carried out, and the hardening and softening phase mechanisms are explored in terms of
59 mesoscopic stress, strain and fabric evolutions. In particular, we analyze how the force chains and
60 the surrounding loops control the mechanical responses at the mesoscopic scale. It should be noted
61 that when softening occurs and one shear band forms, mesoscopic characteristics are investigated
62 separately inside and outside shear band.

63 This paper is organized as follows. In Section 2 two numerical samples are prepared and subjected
64 to drained biaxial tests. Thanks to the use of grain loop and force chain analysis, the respective
65 micro to macro links between grain displacements and strain, and also between contact forces and
66 stress are reviewed and discussed. Section 3 provides a comprehensive study on the mesoscopic
67 stress, fabric and topology exchanges, which are consistent with macroscopic stress-strain responses.
68 Finally, Section 4 focuses on the strain softening induced by the structural change (shear band). The
69 rotations of force chain fabric and principal stresses are found, and the failure mechanism of force
70 chains is discussed.

71 2. Biaxial test and granular mesostructures

72 In this section, the basic macroscopic stress-strain relationships of biaxial tests are recalled for
73 grain assemblies with two densities. Mesostructure definitions are introduced and a particular care
74 is paid to locally define the strain and stress indicators able to account for macroscopic observations.
75 Contrary to other coarse graining approaches, the use of mesostructures is central in our approach to
76 bridge the gap between micro and macro scales.

77 2.1. Numerical set up and macroscopic responses

78 Biaxial tests are carried out numerically with the use of the open-source DEM software YADE
79 (Šmilauer et al., 2015). The granular assemblies are generated within a rectangular box of aspect
80 ratio 1.5 (shown in Figure 1), containing a single layer of 20,000 spheres with a uniform distribution
81 of diameters ($d_{50} = 0.008$ m and $d_{\max}/d_{\min} = 2$). Dense and loose specimens are compressed to an
82 isotropic desired confining state of 4 kN/m, with initial parameters listed in Table 1. During the
83 preparation of dense and loose samples, different friction angles ϕ (2° for the dense and 35° for the
84 loose) are set to reach a large density gap between them. When biaxial conditions are met under
85 loading process, ϕ is set to 35° for both the samples. In Table 1, n is the 2D porosity of the assembly,
86 Z_m is the initial coordination number, k_n and k_t are the normal and tangential stiffness of the contact
87 model, $d_s = 2R_1R_2/(R_1 + R_2)$ is the harmonic average of the radii of the particles in contact and ϕ
88 is the contact friction angle between spheres. To accelerate the simulations, the numerical damping
89 coefficient is set to 0.25 (see details in Šmilauer et al. (2015) for its definition).

Table 1: Initial isotropic states and loading parameters of dense and loose specimen.

Specimen	n	Z_m	k_n/d_s	k_t/k_n	ϕ
Dense	0.161	4.01	300 MPa	0.5	35°
Loose	0.207	3.06	300 MPa	0.5	35°

90 Typical macro stress-strain relations are shown in Figure 2. For the dense sample, the deviatoric
91 stress ($q = \sigma_1 - \sigma_2$ where σ_1 and σ_2 are the major and minor principal stresses) demonstrates a peak
92 for $\varepsilon_{22} = 0.014$. Before this point, the stress state of the assembly is in the hardening regime while
93 after that the sample stress state is in the softening regime¹. The volumetric strain evolution of the

¹As recalled in the introduction, the distinction between the hardening and softening regimes can be read directly on the stress strain curve for drained biaxial test.

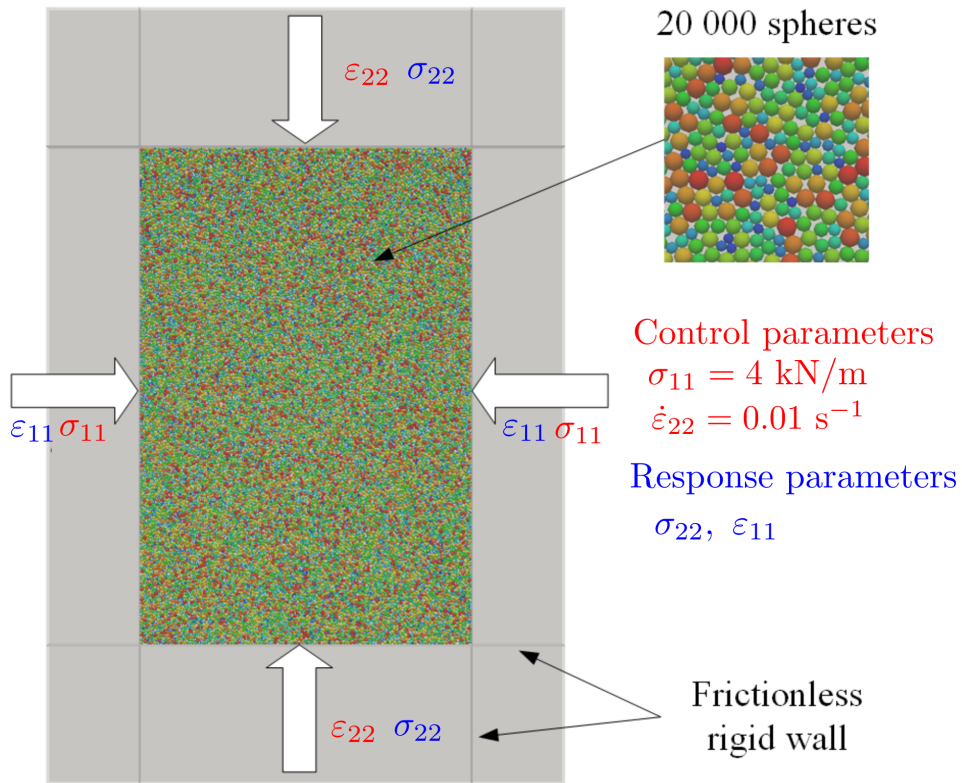


Figure 1: DEM specimen for biaxial tests.

94 dense sample also shows a characteristic point around $\epsilon_{22} = 0.01$, which corresponds to the transition
 95 from contractancy to dilatancy (characteristic point). As a result, 3 stages can be identified in Figure
 96 2(a):

- 97 - Stage I — hardening phase with shear contractancy;
- 98 - Stage II — hardening phase with shear dilatancy;
- 99 - Stage III — softening phase with shear dilatancy.

100 For the loose specimen, neither softening nor dilative characteristics are observed.

101 2.2. Contact based loop and local strain definition

102 For 2D granular materials, the contact network can be used to provide a partition of the material
 103 domain into polygonal shapes forming grain loops (Kuhn, 1999; Kruyt and Rothenburg, 1996; Satake,
 104 1992). The loops play an important role in volumetric and anisotropic evolutions, as they contain
 105 deformable pores. An example of the 2D loop tessellation is given in Figure 3. The larger the loop
 106 valence (the number of particles within the given loop), the larger its deformability. A number of

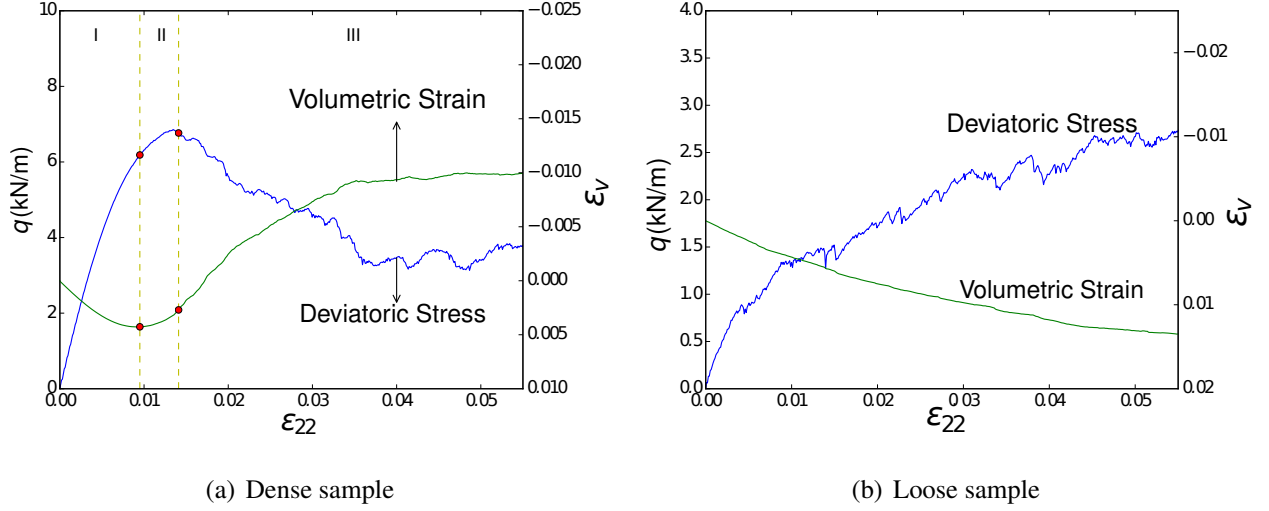


Figure 2: Macro stress strain relations during the biaxial loading for the dense (a) and loose (b) specimens.

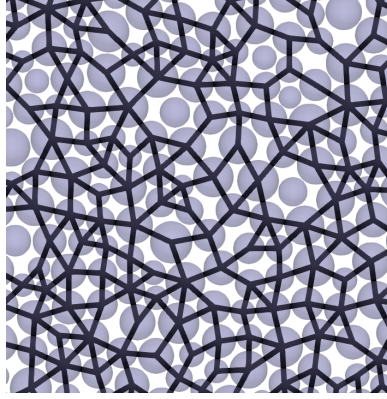


Figure 3: An example of 2D loop tessellation in granular materials

107 studies were conducted to describe the topological compositions (Zhu et al., 2016a,b; Tordesillas
 108 et al., 2010) and mechanical characteristics (Kuhn, 1999; Nguyen et al., 2012) of 2D loops.

109 Under certain assumptions, strain definitions based on these local loops can be proposed (Kuhn,
 110 1999; Bagi, 1996; Li and Yu, 2009; Dedecker et al., 2000; Wang et al., 2007; Cambou et al., 2013).
 111 In this paper, a simple 2D definition is adopted by assuming uniform deformation within each loop L :

$$\varepsilon_{ij} = \frac{1}{|L|} \int_L \frac{u_{i,j} + u_{j,i}}{2} dS \quad (1)$$

112 where $|L|$ is the area of the loop domain L and $u_{i,j} = \frac{\partial u_i}{\partial x_j}$ is the gradient of displacement field within
 113 L . The definition of 3D loops is however a difficult task because of void connectivity and the notion
 114 of loop has to be replaced by grain clusters (containing grains and internal pores) for instance.
 115

116 For an enclosed system, the integration can be changed to the loop boundary ∂L :

$$\varepsilon_{ij} = \frac{1}{|L|} \int_{\partial L} \frac{u_i n_j + u_j n_i}{2} dl \quad (2)$$

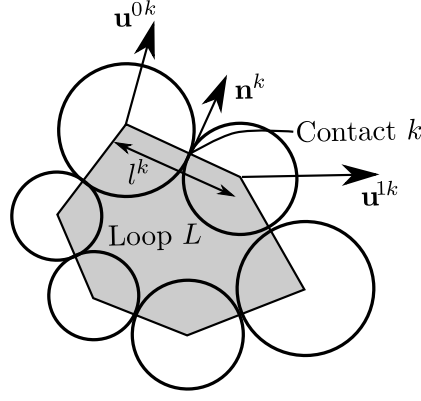


Figure 4: Mesostrain definition of a loop domain L .

117 in which \mathbf{n} is the outer normal to ∂L . At the microscale, the notion of continuous displacement
 118 field is meaningless and only grain displacements are known. By assuming a linear interpolation of
 119 the displacement along the loop edges, the incremental strain tensor is eventually defined as (see for
 120 example [Bonelli et al. \(2012\)](#)):

$$\varepsilon_{ij} = \frac{1}{|L|} \sum_{k=1}^c \frac{1}{2} l^k \left(n_j^k \frac{u_i^{1k} + u_i^{0k}}{2} + n_i^k \frac{u_j^{1k} + u_j^{0k}}{2} \right) \quad (3)$$

121 where \mathbf{u}^{1k} and \mathbf{u}^{0k} are the incremental displacement of the vertice of k^{th} edge. The notations used
 122 in Equation (3) are summarized in Figure 4. In this definition, grain rotations are not taken into
 123 account, and the incremental displacement field is interpolated only based on the discrete incremental
 124 displacements of grain centers. If grain rotations are considered as the second-order terms of local
 125 strain, Equation 3 has to be changed as in [Kruyt et al. \(2014\)](#) for instance. But as shown in the
 126 cited paper, the contribution of rotations to the average displacement gradient is negligible for dense
 127 granular assemblies.

128 The spatial distributions of the incremental deviatoric strain for $\varepsilon_{22} = 0.03$ are shown in Figure
 129 5, for both dense and loose specimens. Patterns of diffuse failure (loose specimen) and localized
 130 failure (dense specimen) are evident, as exhibited in previous studies ([Sibille et al., 2015](#); [Zhu et al.,](#)
 131 [2016a](#)). Similar to the biaxial simulation in [Liu et al. \(2018\)](#), shear bands with an “X” shape firstly
 132 appear in the dense assembly at the stress peak, and then evolves to a diagonal persistent one as
 133 shown in Figure 5(a). This evident loss of homogeneity shall induce macroscopic strain softening.
 134 Since the domains inside and outside the shear band belongs to different stress states, we investigate
 135 their micro- and mesoscopic features individually during Stage III in the following sections. For a
 136 quantitative definition of the shear band domain, the reader can refer to [Liu et al. \(2018\)](#).

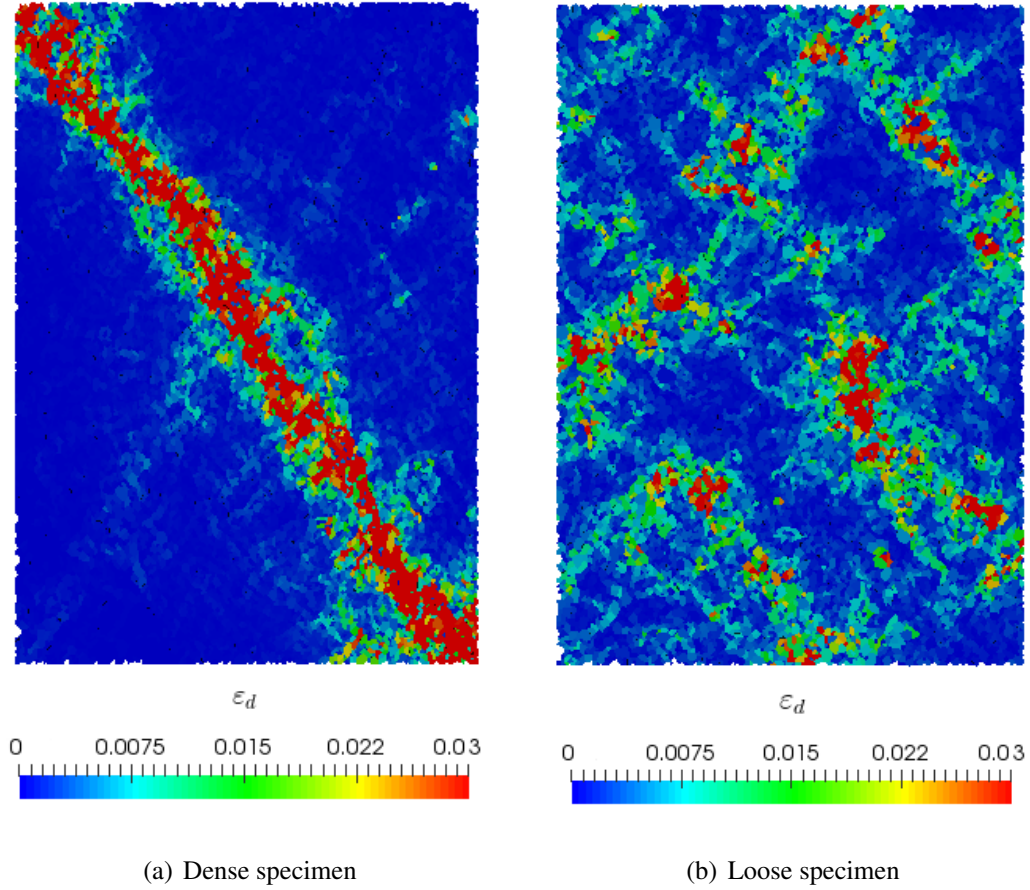


Figure 5: Spatial distributions of incremental deviatoric strains ε_d for dense (a) and loose (b) specimens during biaxial tests at $\varepsilon_{22} = 0.03$. Local incremental strains are computed with macroscopic strain increments $d\varepsilon_{22} = 10^{-3}$.

137 2.3. Force chains as stress transmission paths

138 As recalled in the introduction, the force chain concept provides a relevant mesoscopic scale to
 139 account for the macroscopic mechanical behavior of granular materials (Zhu et al., 2016a; Zhang
 140 et al., 2017; Wautier et al., 2017; Tordesillas et al., 2010). The definition of a force chain used
 141 throughout this paper is similar to the one proposed by Peters et al. (2005). It is illustrated in Figure
 142 6(a) and briefly reviewed here:

- 143 - The particles belonging to a force chain have a larger major principal stress than the mean major
 144 principal stress ($\sigma_1 \geq \langle \sigma_1 \rangle$).
- 145 - The major principal stress direction of chained particles is aligned with the geometrical direc-
 146 tion of contact (less than 45° deviation).
- 147 - A force chain contains at least 3 contacting particles.

148 According to this definition, elementary parts of force chains are composed of groups of three
 149 aligned and heavily stressed contacting particles. Such elementary structures, referred to as “3-p

150 groups” hereafter, are the simplest mesostructures that can be defined to investigate the stress trans-
 151 mission in granular materials [Tordesillas and Muthuswamy \(2009\)](#)². Attached to each 3-p group,
 152 a stress tensor can be defined in quasi-static conditions in the sense of Love-Weber formula ([Love,](#)
 153 [1927](#); [Weber, 1966](#); [Bagi, 1996](#); [Maeda et al., 2001](#); [Nguyen et al., 2012](#)). By assuming the existence
 154 of a micro-stress field, a mesoscopic stress tensor can be defined by averaging this micro-stress over
 155 a given domain Ω_{3-p} containing the entire 3-p group. If the frontier $\partial\Omega_{3-p}$ of the domain is chosen
 156 such that i) it contains only contact points c_p attached to the 3-p group and ii) at each contact point
 157 c_p , the outward normal \mathbf{n} to Ω_{3-p} equals the contact normal, then the meso-stress $\sigma_{\Omega_{3-p}}$ reads

$$\sigma_{\Omega_{3-p}} = \frac{1}{|\Omega_{3-p}|} \int_{\Omega_{3-p}} \sigma \, dS = \frac{1}{|\Omega_{3-p}|} \int_{\partial\Omega_{3-p}} (\sigma \cdot \mathbf{n}) \otimes \mathbf{x} \, dl = \frac{1}{|\Omega_{3-p}|} \sum_p \sum_{c_p} \mathbf{F}_{c_p} \otimes \mathbf{x}_{c_p} \quad (4)$$

158 where \mathbf{x}_{c_p} is the vector position of contact c_p belonging to particle p and $|\Omega_{3-p}|$ is the area of domain
 159 Ω_{3-p} . Note that Equation 4 remains valid in 3D by replacing dS and dl with dV and dS respectively.
 160 In the above formula, a strong underlying hypothesis is implicitly introduced by imposing locally
 161 the mechanical equilibrium ($\text{div } \sigma = 0$ and $\sum_{c_p} \mathbf{F}_{c_p} = 0$). Under this condition, the summations in
 162 Equation 4 can be applied to all the contacts included in Ω_{3-p} and not limited to the contacts located
 163 on the boundary $\partial\Omega_{3-p}$.

164 In the meso-stress definition given in Equation (4), the domain Ω_{3-p} has not been specified. As
 165 illustrated in Figure 6(b), two particular domains can be considered as:

- 166 - the domain Ω_{3-p}^{\min} composed of the three grains only (dark domain in Figure 6(b));
- 167 - the domain Ω_{3-p}^{\max} composed of the three grains and the inner area of the surrounding loops (light
 168 and dark domain in Figure 6(b)).

169 These two domains correspond to the minimal and maximal surface respectively which fulfill the
 170 two properties of Ω_{3-p} Equation (4). By construction, these two domains give different levels of
 171 information in order to describe the stress at the mesoscale:

- 172 - $\sigma_{\Omega_{3-p}^{\min}}$ corresponds to the mean stress tensor inside 3-p groups (only for the solid phase) and
 173 provides information about the intensity of the contact forces;

²Note that “3-p groups” are considered here instead of the whole force chains for the two following reasons needed for the analyses shown in Section 4: i) these mesostructures are sufficiently simple to be characterized by a single geometric parameter and ii) these mesostructures have better chances to be persistent between to strain increments such that incremental quantities can be defined.

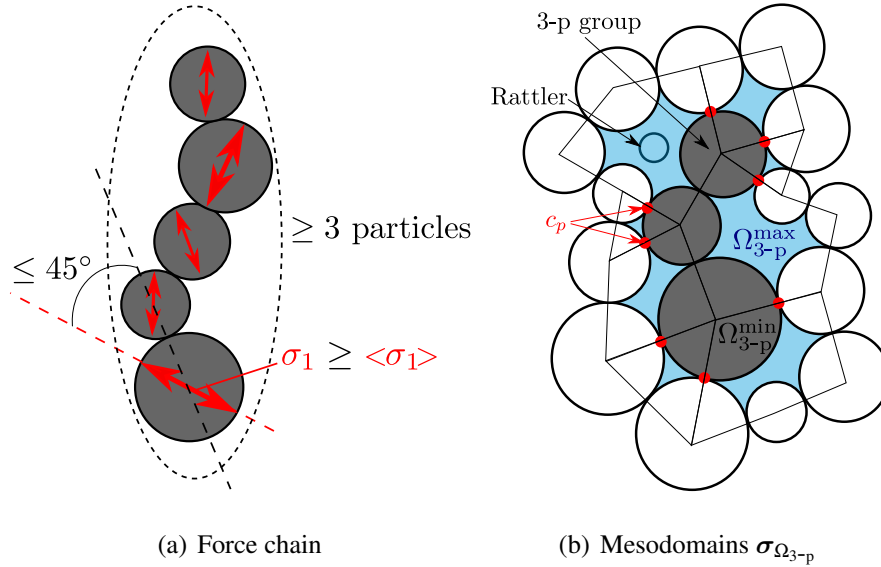


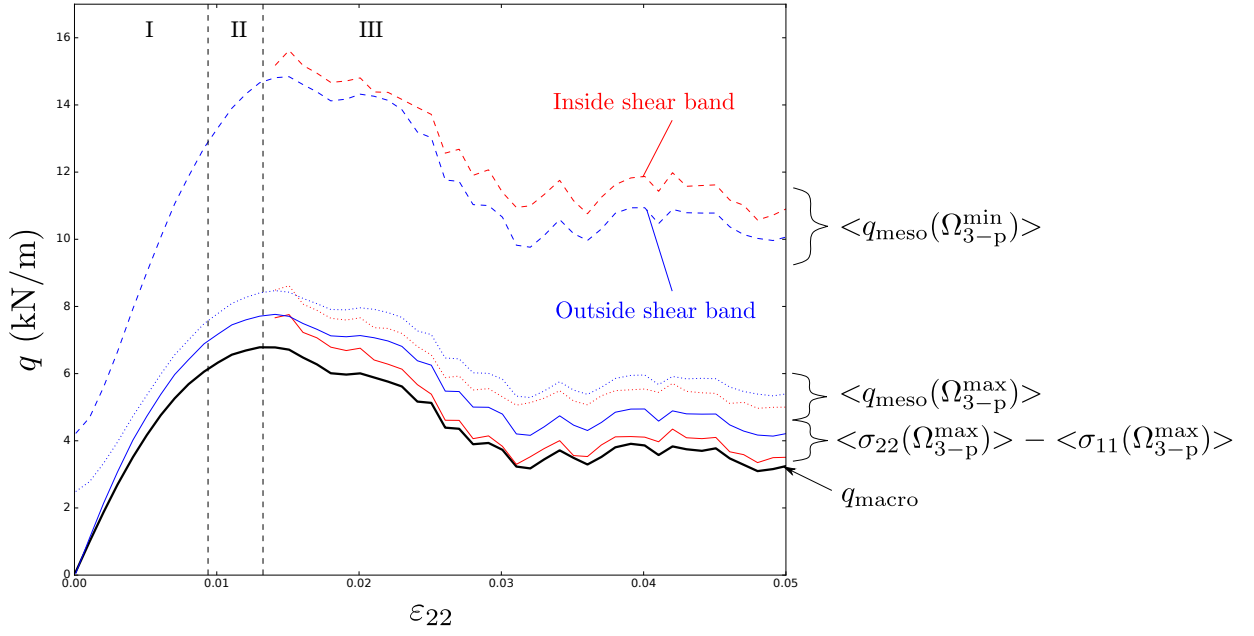
Figure 6: Definition of (a) a force chain according to Peters et al. (2005) and (b) the two mesodomains $\sigma_{\Omega_{3-p}^{\min}}$ (3-p group in grey) and $\sigma_{\Omega_{3-p}^{\max}}$ (3-p group in grey and pore space in light blue). Contact points c_p involved in Equation (4) are shown as red dots.

174 - $\sigma_{\Omega_{3-p}^{\max}}$ takes into account the void phase in the stress averaging process and accounts for the
 175 local porosity around force chains.

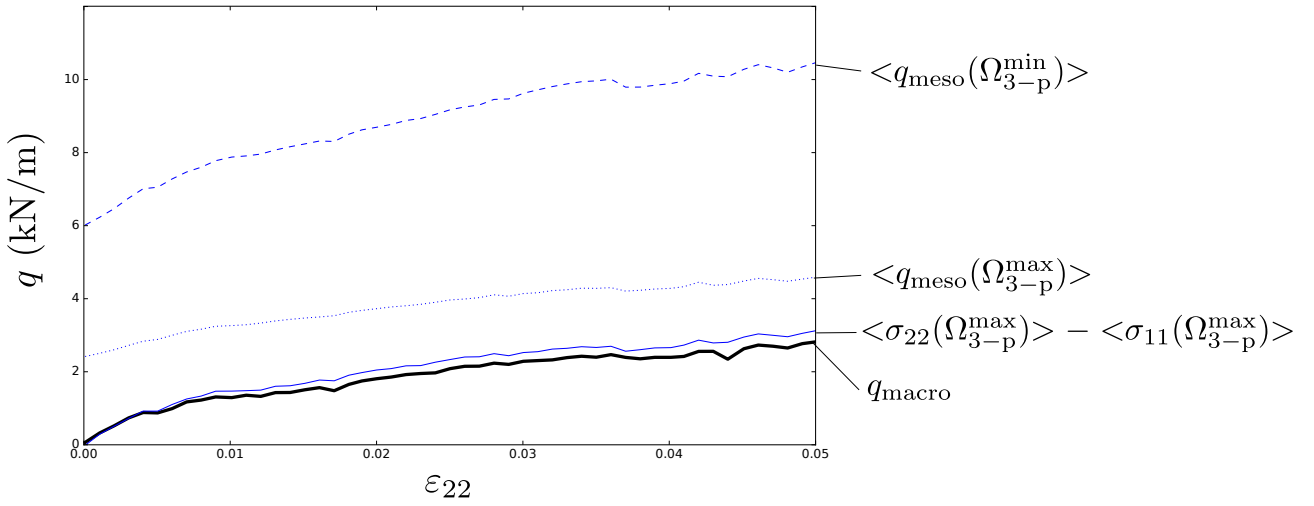
176 In Figure 7, the strain evolution of the mean deviatoric stresses (over all 3-p groups) computed
 177 for Ω_{3-p}^{\min} and Ω_{3-p}^{\max} are shown for the biaxial test presented in Section 2.1 and compared to the macro-
 178 scopic deviatoric stress shown in Figure 2. For the dense case, as a shear band appears after the stress
 179 peak, averaged mesoscopic stresses are computed separately inside and outside the shear band.

180 In Figure 7, the qualitative trends observed at the macro and the meso scales are similar. For the
 181 dense specimen a stress peak followed by a softening regime is observed for both Ω_{3-p}^{\min} and Ω_{3-p}^{\max} .
 182 A better quantitative agreement between meso and macro data is achieved when voids around force
 183 chains are taken into account in the meso-stress computation. Indeed, $\sigma_{\Omega_{3-p}^{\max}}$ incorporates the porous
 184 nature of granular materials while $\sigma_{\Omega_{3-p}^{\min}}$ does not³. Ω_{3-p}^{\min} and Ω_{3-p}^{\max} corresponds indeed to two limit
 185 cases for the voids: only solid phase and the solid phase with maximum surrounding void area (see
 186 Figure 6(b)). The trend shown by the deviatoric stress computed for Ω_{3-p}^{\min} is very informative in the
 187 sense that the macro softening results not simply from an increase in the porosity around force chains
 188 but also from the decrease in the grain stresses.

³It should be underlined that the local porosity corresponding to Ω_{3-p}^{\max} is larger than the geometric porosity computed for the whole sample and corresponds to the notion of equivalent porosity (or void ratio) used in soil mechanics to account for the fraction of grain not involved in stress transmission.



(a) Dense case



(b) Loose case

Figure 7: Axial strain evolution of the mean deviatoric stresses computed for Ω_{3-p}^{\min} and Ω_{3-p}^{\max} compared to the macroscale data.

189 While comparing the mean deviatoric stress noted inside the shear band in Figure 7(a) to the one
 190 measured outside it should be noted that $\sigma_{\Omega_{3-p}^{\min}}^{\text{in}} > \sigma_{\Omega_{3-p}^{\min}}^{\text{out}}$ while $\sigma_{\Omega_{3-p}^{\max}}^{\text{in}} < \sigma_{\Omega_{3-p}^{\max}}^{\text{out}}$. This can be physically
 191 interpreted as follows:

- 192 - 3-p group density is smaller inside the shear band which results in stress concentration ($\sigma_{\Omega_{3-p}^{\min}}^{\text{in}} >$
 193 $\sigma_{\Omega_{3-p}^{\min}}^{\text{out}}$);
- 194 - In the meantime, local porosity around 3-p group inside the shear band is higher and counter
 195 balances the stress concentration in the solid phase ($\sigma_{\Omega_{3-p}^{\max}}^{\text{in}} < \sigma_{\Omega_{3-p}^{\max}}^{\text{out}}$).

196 In Figure 7, we can observe that the deviatoric meso-stress is non-zero at the initial state, which
 197 is due to the fact that the directional information is ignored in the deviatoric meso-stress averaging
 198 (q_{meso} is a scalar quantity). The overall average of meso-stresses can be accounted for by computing
 199 the deviatoric stress from the mean meso-stress tensor $\langle \sigma_{\Omega_{3-p}^{\max}} \rangle$ as $\langle \sigma_{22}^{\text{meso}} \rangle - \langle \sigma_{11}^{\text{meso}} \rangle$ in Figure
 200 7(a).

201 3. Mesoscopic evolutions: stress, fabric and topology

202 During the deviatoric loading, macroscopic stress-strain responses are shown in Figure 2. To
 203 reveal the underlying mechanisms of the typical Stages I, II and III from new mesoscopic perspec-
 204 tives, this section provides a comprehensive investigation in terms of meso-stress, meso-fabric and
 205 topological evolution.

206 3.1. Chained grain population and meso-stress evolutions

207 At the first stage of the deviatoric loading of the dense specimen (Stage I), a nearly elastic response
 208 with contractancy in volumetric strain is observed in Figure 2. The evolutions of the number of
 209 chained particles (the set of particles composing force chains) given in Figure 8 characterize the
 210 adaptability of the contact network to the evolving external loading.

211 In Figure 8, the number of force chain particles increases up to the characteristic point (Stage I) in
 212 the dense sample. After the characteristic point (Stages II and III, especially for Stage III), the number
 213 of chained particles decreases until reaching a constant value. For the dense specimen, the increasing
 214 number of chained particles seems to enhance the strength, as the deviatoric stress increases until
 215 Stage II. However, if we consider the loose sample in Figure 8, a weak hardening is accompanied
 216 with a decrease in the number of chained particles. This counter intuitive trend may be explained by
 217 looking at force chain spatial distributions in Figure 9. As the biaxial loading starts, both the loose

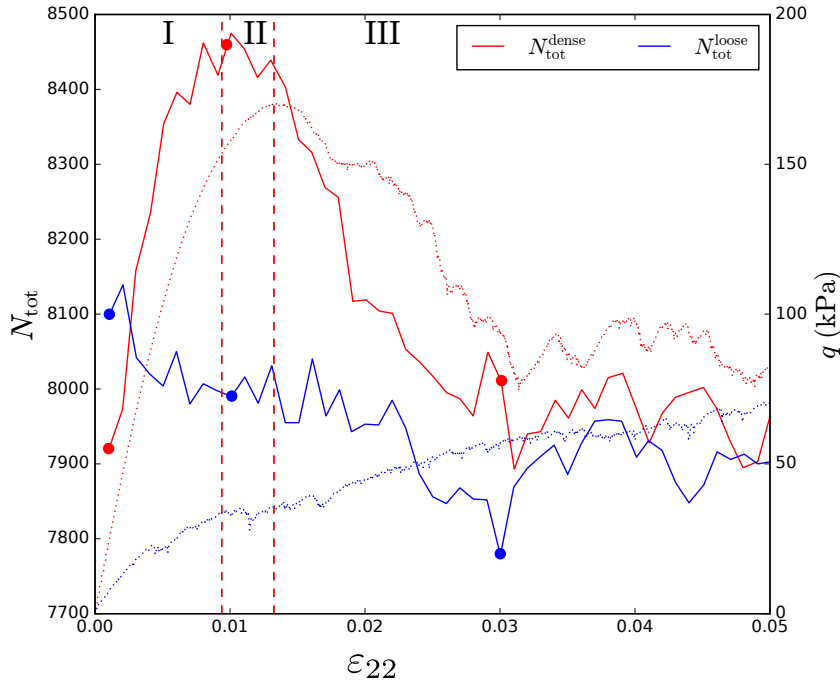


Figure 8: Evolutions of the number of chained particles during biaxial tests for the dense (red) and loose (blue) specimens. The stress-strain macroscopic responses are recalled in dots and the three identified stages for the dense sample are shown with vertical dashed lines. The spatial distributions of chained particles corresponding to the six dot points are given in Figure 9

218 and dense samples lose horizontal force chains. Thanks to the lateral support of the weak phase,
 219 longer and more aligned force chains in the vertical direction are found in the dense sample than in
 220 the loose sample (see Figure 9). As a result, the mesoscopic origin of the stress hardening observed
 221 in the loose sample corresponds only to the load bearing capacity of preexisting short force chains in
 222 the vertical direction while in the dense sample it corresponds to the increase in both the number of
 223 chained particles and in the length of force chains as well.

224 During Stage II for the dense sample, no more particles are recruited to build new force chains
 225 but the macroscopic deviatoric stress does not stop rising, which may be due to the fact that at the
 226 characteristic point, the existing strong contact network is not yet used at the maximum bearing
 227 capacity. As a result, stress concentration within 3-p groups should be observed after the characteristic
 228 point.

229 In Figure 10 the stress concentration phenomenon is quantified by rescaling the mesoscopic deviatoric
 230 stress q_{meso} derived from $\sigma_{\Omega_{3-p}}^{\text{max}}$ (as introduced in Section 2.3) with the macroscopic value q_{macro} .
 231 The evolutions of $q_{\text{meso}}/q_{\text{macro}}$ are given for three passing fractions (20%, 50% and 80%) of the cumu-

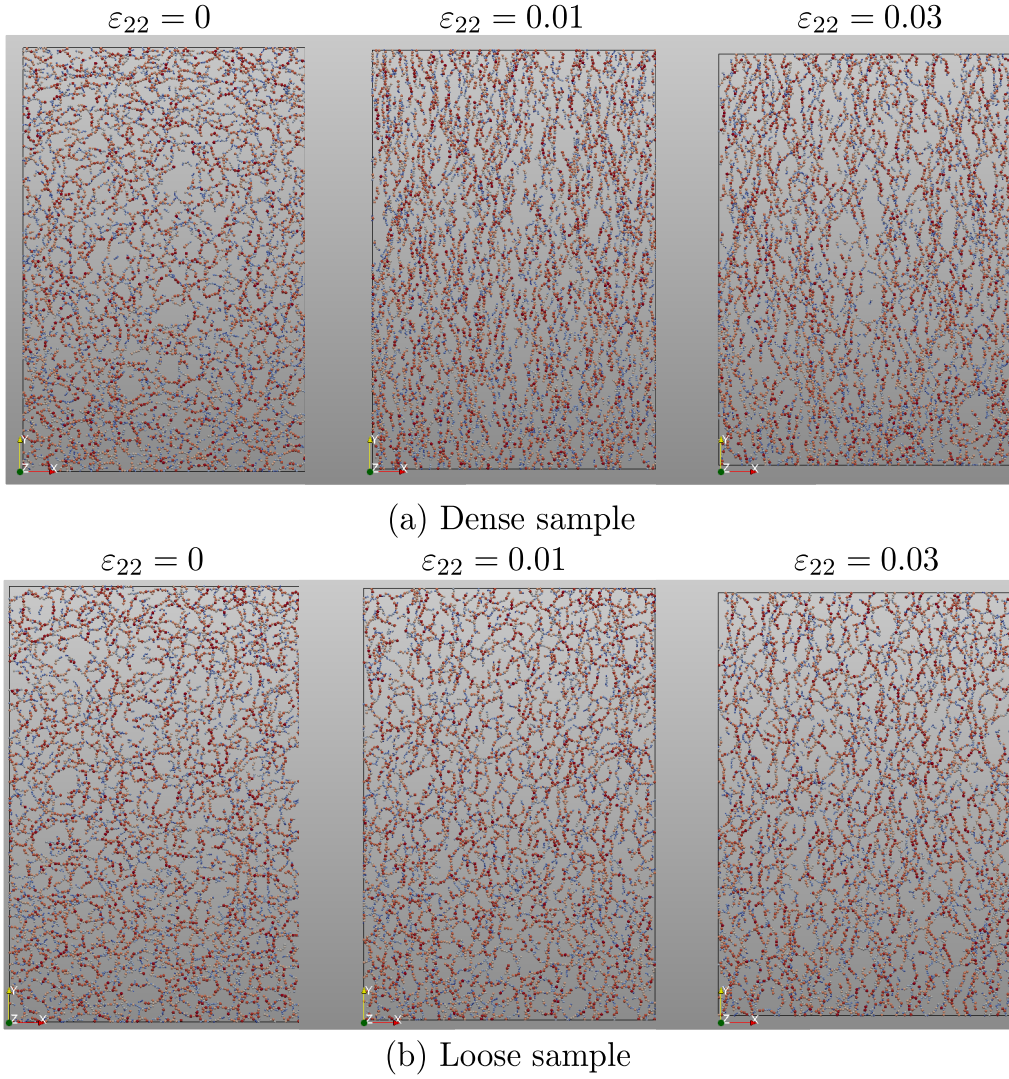


Figure 9: Spatial distributions of chained particles corresponding to the six dot points shown in Figure 8. Particles are colored according to their radius values.

relative distribution curves⁴: $(q_{\text{meso}}/q_{\text{macro}})_{50}$ (median value), $(q_{\text{meso}}/q_{\text{macro}})_{20}$ and $(q_{\text{meso}}/q_{\text{macro}})_{80}$.
 The statistical distribution of $q_{\text{meso}}/q_{\text{macro}}$ characterizes whether the macroscopic stress is evenly distributed on chained particles while the median value characterizes to which extent stress concentrates in force chains. If only few chained particles contribute to the macroscopic stress, $q_{\text{meso}}/q_{\text{macro}}$ is expected to be quite larger than 1; while if all the particles contribute evenly to the macroscopic stress, $q_{\text{meso}}/q_{\text{macro}}$ is expected to be around unity.

In Figure 10 the ratio $q_{\text{meso}}/q_{\text{macro}}$ decreases until $\varepsilon_{22} = 0.01$ (the hardening regime) before increasing again in stage II and III, which corresponds to stress concentration in force chains during the

⁴The cumulative distributions of $q_{\text{meso}}/q_{\text{macro}}$ are not shown here, but they experience similar shapes as the rotation distribution for 3-p groups (see in Section 4, Figure 20).

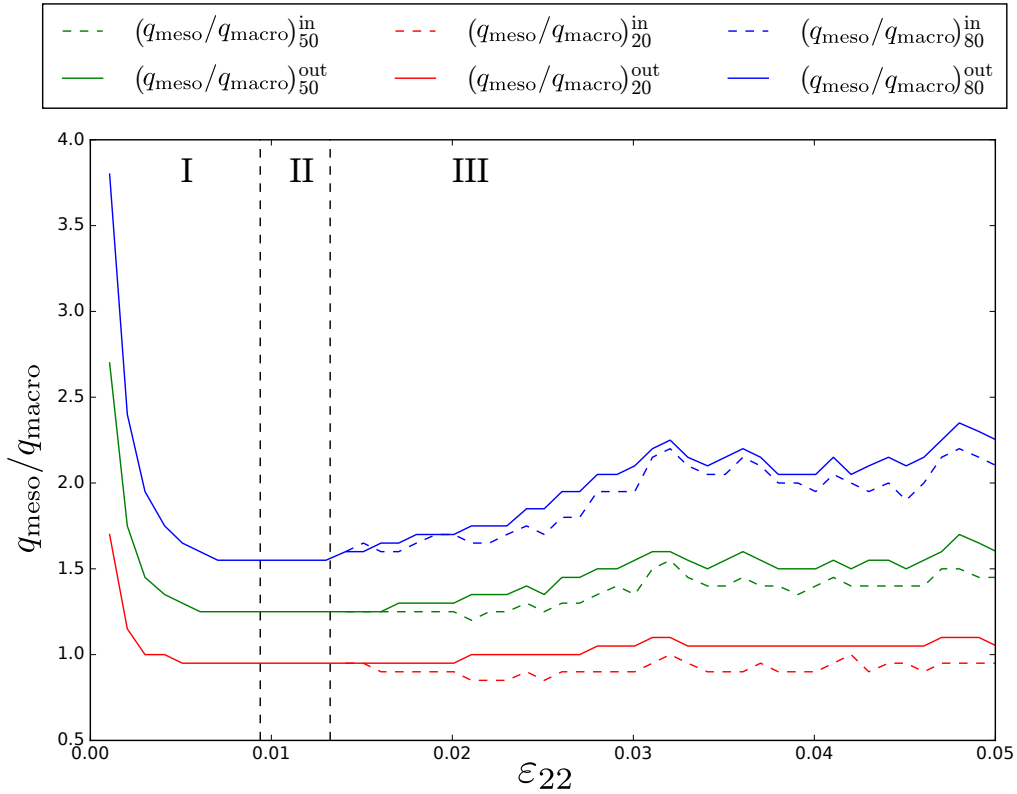


Figure 10: Evolution of the 20 % (lower), 50 % (middle) and 80 % (upper) passing fractions of the cumulative distribution of $q_{\text{meso}}/q_{\text{macro}}$ during biaxial loading for the dense specimen. After the stress peak, cumulative distributions are computed separately inside (dashed) and outside (solid) of the shear band. q_{meso} is computed based on $\sigma_{\Omega_{3-p}}^{\text{max}}$ (see Section 2.3)

240 softening regime. These observations are consistent with Figure 8 and 9 showing that the number of
 241 chained particles increases during Stage I (the macroscopic load is distributed among an increasing
 242 number of chained particles), and decreases in Stages II and III (the macroscopic load becomes more
 243 and more concentrated on the remaining 3-p groups as the number of chained particles decreases
 244 rapidly).

245 The stress concentration phenomenon is also consistent with the differences in deviatoric meso-
 246 stresses inside and outside the shear band observed in Figure 7(a). When the local porosity is not
 247 taken into account, the deviatoric meso-stress inside the shear band shows a higher magnitude.

248 3.2. Mesoscale fabric

249 At the contact level, the non-directional connectivity of a network can be assessed through the
 250 coordination number. For the whole contact system, $Z_c^{\text{tot}} = 2N_c/N_p$, where N_c is the total number
 251 of contacts within the overall system, and N_p is the total number of particles. Moreover, the con-
 252 tact system without rattlers (particles with no contact) should also be concerned, to better show the
 253 average transmission path of loaded particles. The coordination number disregarding the rattlers is

254 calculated as $Z_c^{nonFree} = 2N_c / (N_p - N_{free})$, where N_{free} denotes to the number of rattlers. In Figure
 255 11, coordination number for all contacts Z_c^{tot} and for the contact system without rattlers $Z_c^{nonFree}$ are
 256 shown, together with the volumetric strain evolution. The decreasing trend of coordination number
 257 is identified for all the three periods (I, II, III) for the dense specimen, while the loose specimen
 258 seems to gain more contacts during the loading process. A significant feature is that the coordination
 259 number drops during Stage I for the dense specimen despite the contractant behavior and an increase
 260 in the number of chained particles. As already shown by [Kruyt and Rothenburg \(2016\)](#), this can be
 261 explained by the anisotropy of the contact network which increases in the vertical direction during
 262 Stage I. The coordination number as a scalar information is not sufficient to describe or explain the
 hardening phase with contractancy in dense granular materials.

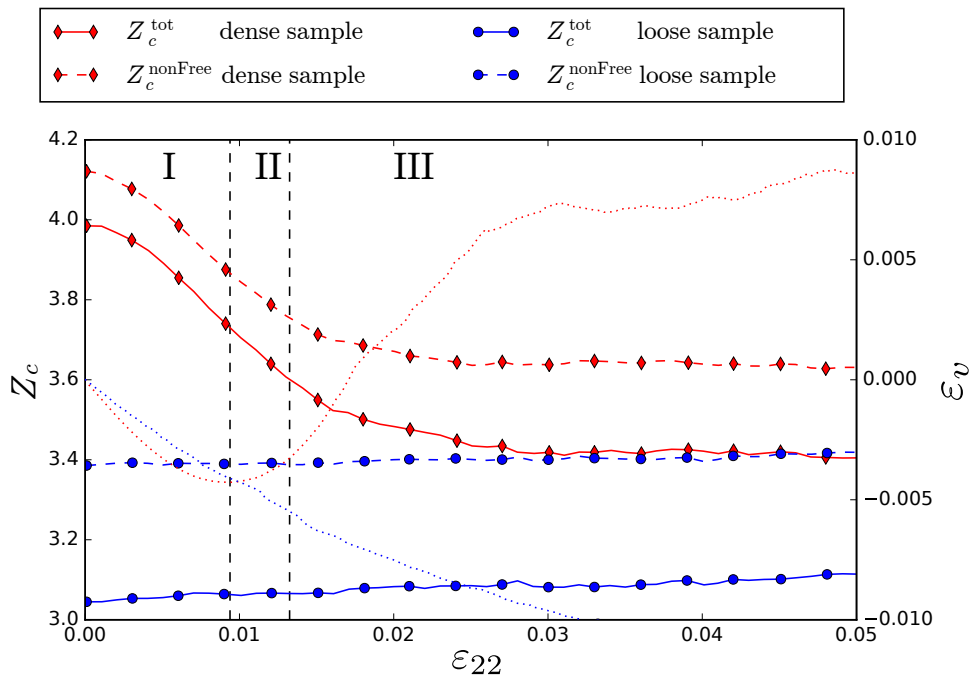


Figure 11: Mean coordination numbers computed for all particles (solid) and for non-rattlers (dashed) over the whole sample domain. The evolutions are given for the dense (red diamonds) and the loose (blue dots) specimens during the biaxial test. The volumetric strain curves are recalled in dotted lines.

263

264 Considering the contact orientation characteristics, the fabric tensor of granular contact system
 265 was introduced ([Oda, 1982](#); [Satake, 1982](#)) and widely applied in anisotropy analysis. The concept of
 266 fabric in granular materials is quite important for describing the statistical and geometrical informa-
 267 tion of the structure, and it has also been incorporated in some modified constitutive models ([Li and](#)
 268 [Dafalias, 2012](#); [Dafalias, 2016](#)). The contact-based anisotropy provides the complementary informa-
 269 tion to the global loss of contacts and force chain population evolution, for both the hardening and
 270 softening phases. As commonly used, the second-order fabric tensor \mathbf{F} within granular assembly is

271 averaged by contact normals within a system:

$$\mathbf{F} = \frac{1}{N_c} \sum_{c=1}^{N_c} \mathbf{n}^c \otimes \mathbf{n}^c \quad (5)$$

272 where the \mathbf{n}^c is the contact normal vector. Usually, this fabric tensor \mathbf{F} is analyzed on the whole con-
 273 tact system ($c \in [1, N_c]$) and is proved to be one of the contributions to the stress anisotropy (Rothen-
 274 burg and Bathurst, 1989; Li and Yu, 2013; Guo and Zhao, 2013). To distinguish the role of strong and
 275 weak contact systems, the anisotropy evolutions of different contact systems were shown in Guo and
 276 Zhao (2013). Particularly, for a single force chain k , the same formal expression as Equation 5 could
 277 also be adopted. The corresponding fabric tensor \mathbf{F}^k is then fully characterized in 2D by the major
 278 direction θ_k and eigen values F_{\pm}^k :

$$\tan(2\theta_k) = \frac{2F_{12}^k}{F_{11}^k - F_{22}^k} \quad (6)$$

279

$$F_{\pm}^k = \frac{1}{2}(F_{11}^k + F_{22}^k) \pm \sqrt{\left(\frac{1}{2}(F_{11}^k - F_{22}^k)\right)^2 + (F_{12}^k)^2} \quad (7)$$

280 For a given force chain k , the deviatoric invariant (second invariant of the deviatoric part of the fabric
 281 tensor) $D_k = F_{+}^k - F_{-}^k$ characterizes the recti-linearity of the mesostructure, while θ_k provides an
 282 estimation of the force chain orientation. By definition, $D_k \in [0, 1]$ with $D_k = 1$ corresponding to a
 283 perfectly straight force chain and $D_k = 0$ to a sort of ‘‘isotropic’’ force chain (very tortuous in other
 284 words). Figure 12 gives these two extreme conditions of force chain linearity. Usually, according to
 285 the definition of force chains given in Section 2.3, the maximum deviation angle for each 3-p group
 286 is 45° . This geometrical limit results in D_k larger than 0.5 in most cases.

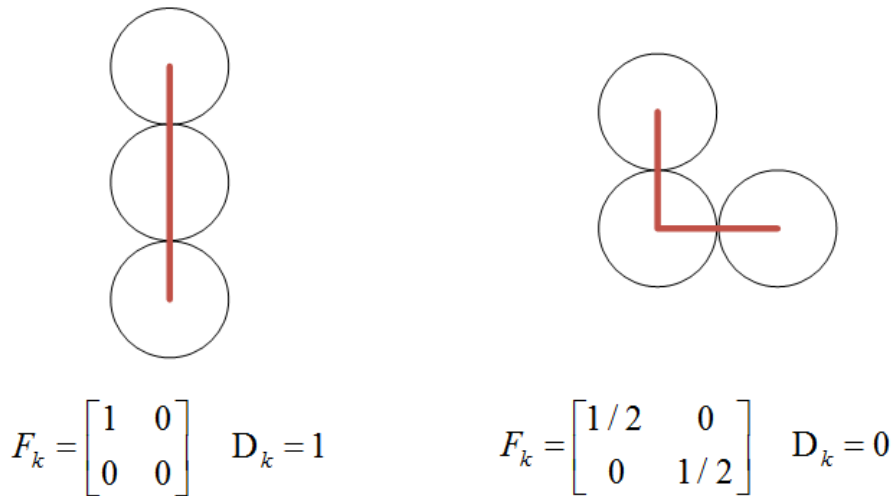


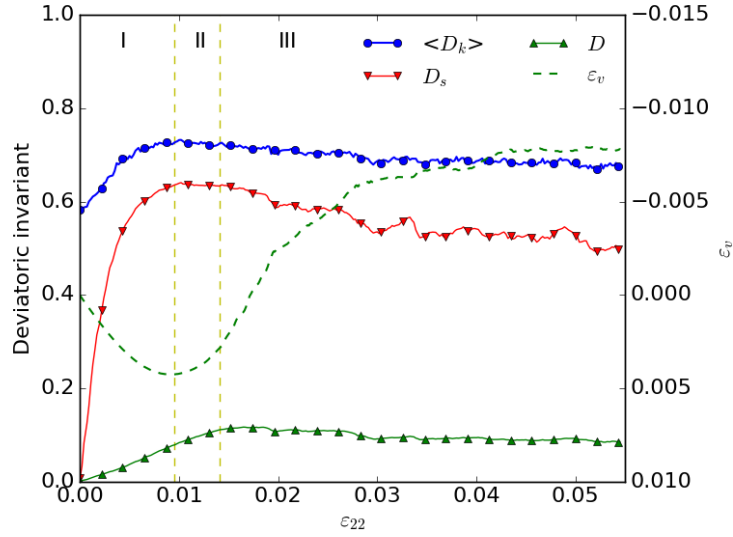
Figure 12: Extremal conditions of force chain linearity D_k .

287 Similarly, the deviatoric invariants D and D_s corresponding to the overall fabric tensor F (con-
 288 sidering contacts within the whole sample) and to the fabric tensor F_s built only from the chained
 289 contacts can be defined. Figure 13(a) shows the evolutions of D , D_s and $\langle D_k \rangle$ (the average D_k
 290 over all force chains) during the biaxial loading, and Figure 13(b) gives the schematic drawing of the
 291 difference between D_s and D_k . $\langle D_k \rangle$ increases and reaches a maximum level at the end of Stage I,
 292 indicating that force chains become more and more linear during this period. At the same time, D_s
 293 rises from 0 to around 0.6 and D increases with a weaker trend. It is accepted that the strong contact
 294 system plays an important role in fabric anisotropy generation (Radjai et al., 1998; Guo and Zhao,
 295 2013), and the increase in force chain recti-linearity and force chain population during Stage I both
 296 reflect that fact. $\langle D_k \rangle$ and D_s reach their maximum levels around the characteristic point (dividing
 297 line between Stage I and II), while the overall fabric invariant D reaches its maximum even after the
 298 stress peak (at the beginning of Stage III). Indeed during Stage II, the overall anisotropy increases due
 299 to the weak contact phase. By combining these observations with stress concentration results from
 300 Figure 10, it can be inferred that:

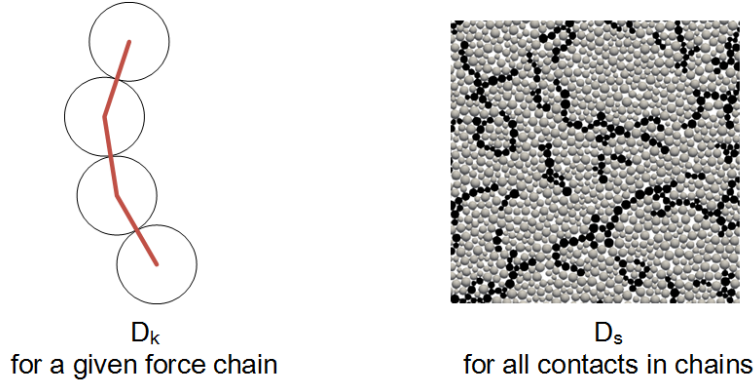
- 301 - The first stage of hardening is associated with a strong increase in fabric anisotropy and pro-
 302 portions of strong contact phase (force chains);
- 303 - The hardening with dilatancy (Stage II) corresponds to the beginning of load concentration and
 304 to the increase in weak contact anisotropy;
- 305 - During the softening phase, the mesoscopic fabric anisotropy related to the force chain recti-
 306 linearity decreases in general, leading to the axial stress reduction.

307 3.3. Topological and geometrical exchanges

308 Introduced in Section 2.3, 3-p groups are the elementary parts composing force chains responsible
 309 for stress transmission. Their geometric evolutions are strongly coupled with the deformability of the
 310 grain loops surrounding the force chains. These loops can change either in topology (coordination
 311 number) or in geometry (area). For a given loop, the change in topology can be divided in three
 312 categories: (a) keep the same particles and contacts, i.e, unchanged in topology, called “C-loop”;
 313 (b) lose one or several contacts and become larger, called “L-loop”; (c) create new contacts among
 314 the particle participants and get smaller cells, called “S-loop”. Possible topological exchanges of
 315 “L-loop”, “C-loop” and “S-loop” are illustrated in Figure 14.



(a)



(b)

Figure 13: Force chain linearity compared with the anisotropies of force chain network and the overall contact network. Quantities are computed over the whole sample domain. The evolution curves are shown in (a), and the sketches for how to calculate D_k and D_s are shown in (b).

316 Around each 3-p group, there exists dozens of loops which could be identified as “C-loop”, “S-
 317 loop” or “L-loop”. The average fractions of the three topological exchanges related to each 3-p
 318 group are plotted in Figure 15. The exchanges are defined incrementally for strain increments of
 319 0.1 %. From the beginning to the end, the set of “C-loop” around 3-p groups represents the largest
 320 population (over 90%). The set of “L-loop” represents a larger proportion than “S-loop” before the
 321 stress peak ($\epsilon_{22} = 0.014$), which is consistent with the decrease in coordination number shown in
 322 Figure 11. Therefore during the hardening phase, several contacts are opened to form larger loops,
 323 which contributes to fabric anisotropy. As the shear band forms after the stress peak, topological
 324 exchanges concentrate inside the shear band where the fraction of “C-loop” decreases significantly.

325 In Figure 15, “L-loop” represents a larger proportion than “S-loop” during the hardening phase

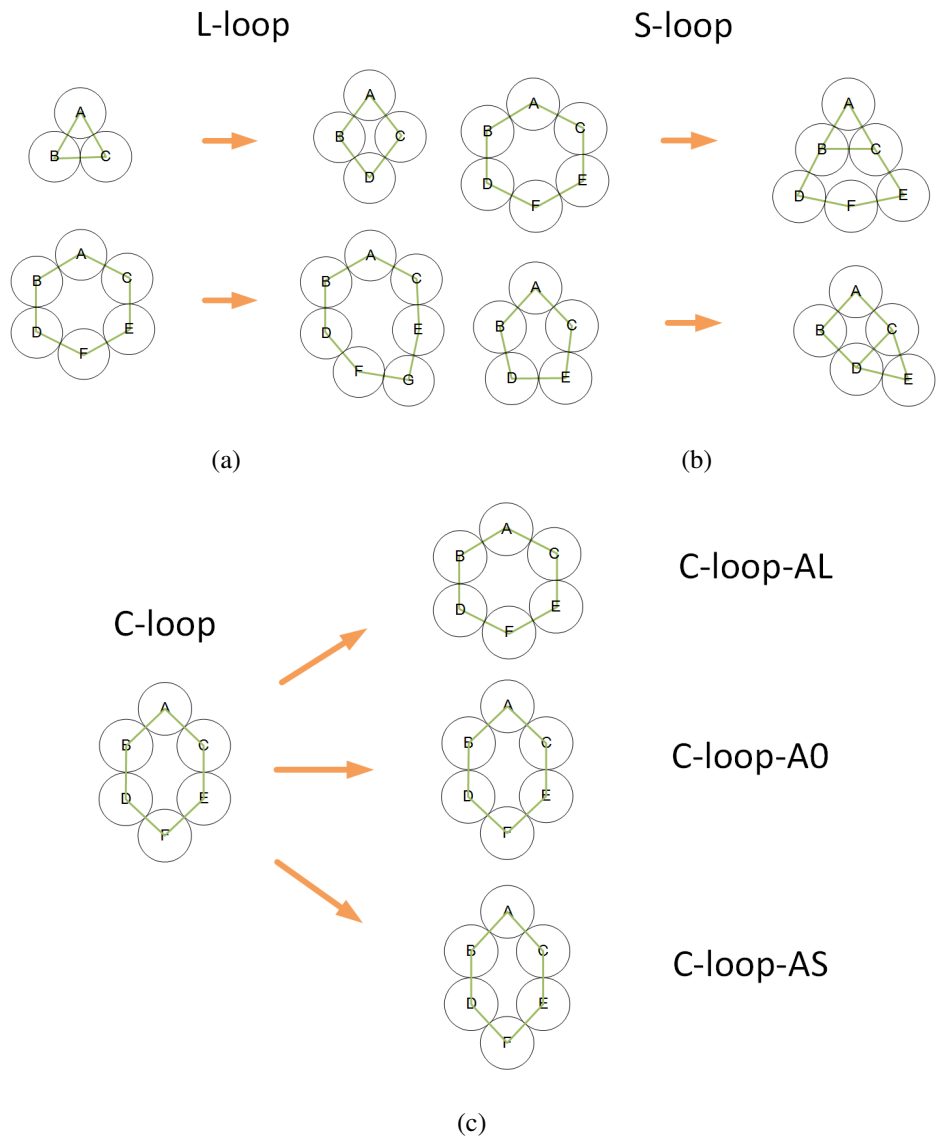


Figure 14: Possible changes for 2D loops between steps: (a) “L-loop”: loops will be enlarged in topology; (b) “S-loop”: loops will shrink in topology; “C-loop”: loops will keep the same topology, composed by “C-loop-AL” (larger area in next step), “C-loop-A0”(same area in next step) and “C-loop-AS”(smaller area in next step).

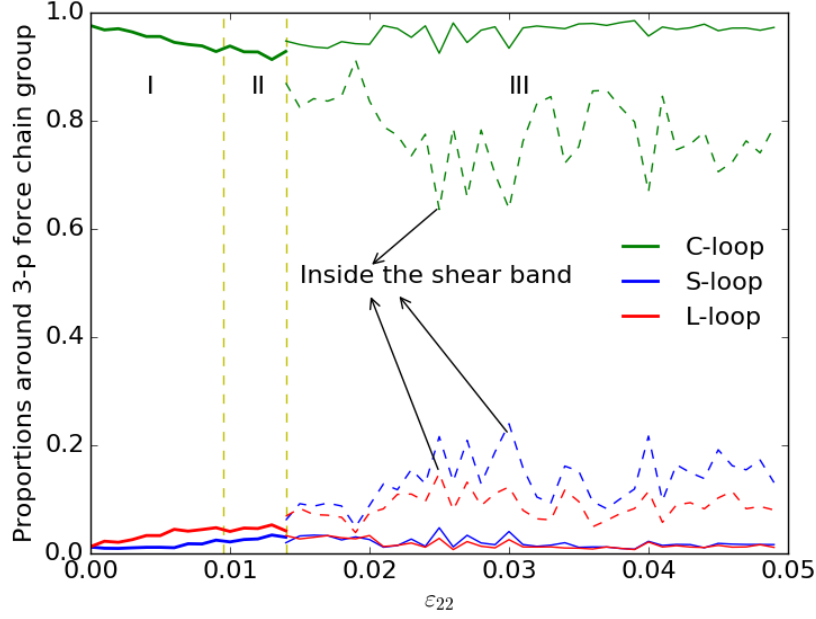


Figure 15: Proportions of topological loop exchanges around 3-p force chain groups. During Stage III, the dashed line shows the corresponding evolutions inside the shear band, while the solid line shows those outside the shear band.

326 (Stage I and II). These topological exchanges tends to indicate a dilatancy trend, however the volu-
327 metric strain does not behave like that during Stage I. To have a rational explanation of this incon-
328 sistency, it is necessary to look at the area changes for the topologically constant loops. As a result,
329 “C-loop” can be redivided into “C-loop-A0”, “C-loop-AS” and “C-loop-AL” to represent loops with
330 unchanged area, smaller area and larger area respectively, as shown in Figure 14(c). Figure 16 gives
331 the evolutions of average proportions of “C-loop-A0”, “C-loop-AS” and “C-loop-AL” around 3-p
332 groups (solid line) and for the whole system (dashed line). It can be seen that the crossing points
333 of proportion curves “C-loop-AS” and “C-loop-AL” are near to the characteristic point $\varepsilon_{22} = 0.01$,
334 before which the “C-loop-AS” owns a larger fraction (nearly Stage I). This is the mesoscopic origin
335 of the contractive behavior observed at first stage of hardening (Stage I). During this period, the loop
336 exchanges (or contact loss and gain) do not influence very much on the volumetric evolutions, but
337 the area evolutions of “C-loop” induce the contractancy hardening features. During Stage II, both
338 topological exchanges (Figure 15) and area evolutions (Figure 16) indicate a dilative trend, which
339 gives corresponding trends compared to the volumetric strain in Figure 2. Another interesting obser-
340 vation in Figure 16 is that the crossing point for 3-p groups comes earlier than for the whole system
341 which denotes once again the driving role played by the surrounding voids around force chains in
342 Figure 6(b). In Zhu et al. (2016b), loops surrounding force chains were also investigated, especially
343 the transformation from L3 (loops of 3 particles) to L6 (loops of 6 particles) was focused on. It

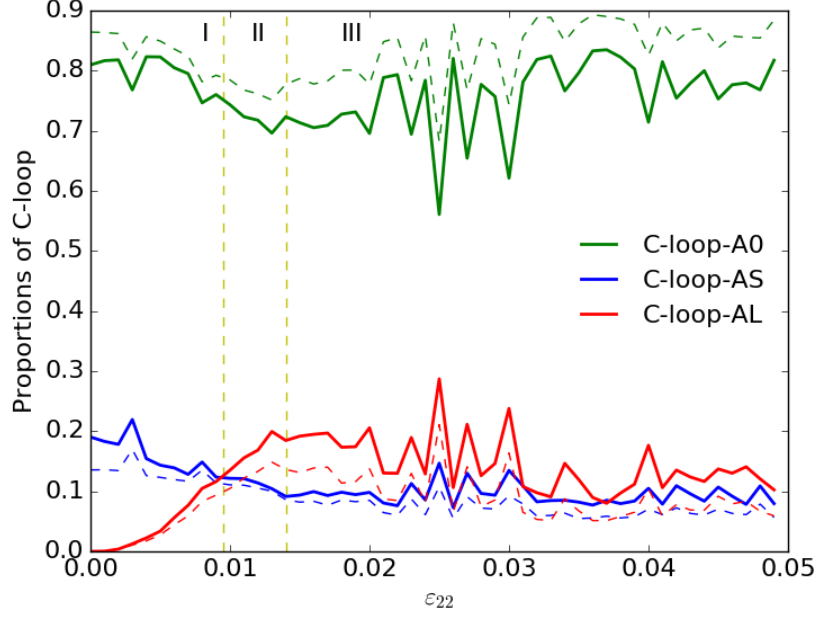


Figure 16: Proportions of “C-loop” with different area changes: around 3-p force chain group (solid line); for the whole system (dashed line).

344 was proved that geometrical and topological evolutions of loops surrounding force chains could be
 345 regarded as the key origin of the overall stress-strain responses in granular materials. This paper con-
 346 siders in a more general way by incorporating transformation types of all loops within the granular
 347 assembly, and combined to the results of defined mesoscopic stress and the force chain recti-linearity,
 348 the hardening phases with both the contractancy and dilatancy are further figured out.

349 In summary, we can conclude that the loop topology evolution and the area change of topologically
 350 constant loops play different roles in hardening phases. As the loop size and area both increase during
 351 Stage II, kinematic constraints around force chains are released and force chains are prompt to be
 352 destabilized, which could finally induce the softening process.

353 4. 3-p group bending and rotation in relation with macroscopic softening

354 The geometry of a 3-p group can be characterized by the two angles α_1 and α_2 , as shown in Figure
 355 17. Equivalently, the bending angle $\beta = |\alpha_1 - \alpha_2|$ and the mean orientation angle $\gamma = \frac{1}{2}(\alpha_1 + \alpha_2)$ can
 356 be considered. In addition to these angles, the principal stress orientation (as defined by diagonalizing
 357 $\sigma_{\Omega_{3-p}}$) is characterized by a third non coaxiality angle θ (Figure 17).

358 This section focuses on the relations between the geometric evolutions of 3-p groups (charac-
 359 terized by the orientation angle γ and the bending angle β) and the associated meso-stresses (charac-
 360 terized by the non coaxiality angle θ defined in Section 2 and the deviatoric meso-stress defined in

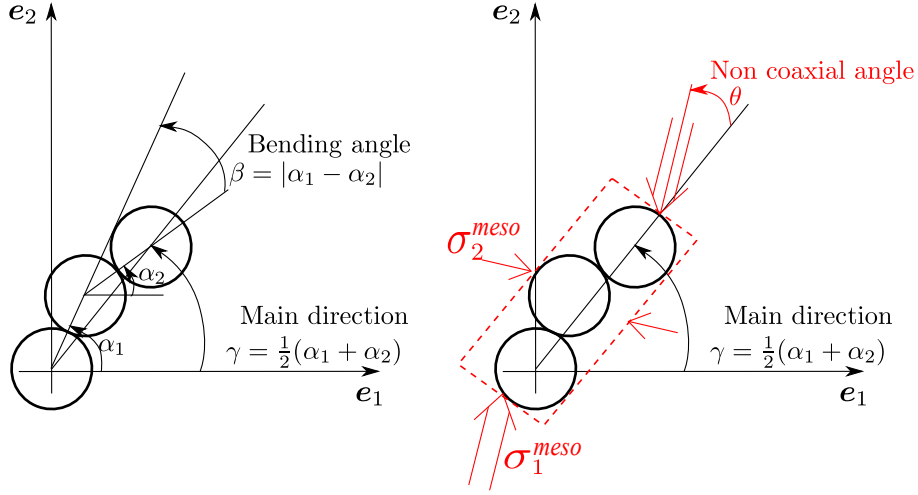


Figure 17: Geometrical and mechanical features of 3-p groups. The geometry is characterized by the bending angle β and orientation angle γ while the mesoscopic stress state is characterized by the major (σ_1) and minor (σ_2) stresses as well as the non coaxial angle θ .

361 Equation (4) for Ω_{3-p}^{\min}).

362 4.1. Force chain bending and buckling

363 In the wake of previous researches, e.g. [Tordesillas \(2007\)](#); [Zhu et al. \(2016b\)](#); [Zhang et al.](#)
 364 [\(2017\)](#), it is tempting to relate internal deformation of 3-p groups (in the form of bending) to force
 365 chain buckling (mesoscopic softening) and thus to macroscopic softening. In most of existing studies,
 366 buckling is defined as an increase in the bending angle β (see Figure 17). However, a rigorous
 367 definition of buckling needs to incorporate both a geometrical evolution and a force or stress saturation
 368 or decrease. As a result, a distinction is emphasized here between *bending* ($d\beta > 0$) and *buckling*
 369 which should incorporate an additional decreasing load information in usual definitions found in the
 370 literature.

371 To this respect, a possible mesoscale definition is to relate the bending of a 3-p group during
 372 the biaxial loading ($\frac{d\beta}{d\varepsilon_{22}} > 0$) to a simultaneous decrease in the deviatoric stress derived from $\sigma_{\Omega_{3-p}^{\max}}$
 373 ($\frac{dq_{\text{meso}}}{d\varepsilon_{22}} < 0$). Mathematically speaking a buckling definition is sought when both the conditions are
 374 reached:

$$\frac{d\beta}{d\varepsilon_{22}} > 0, \quad \text{and} \quad \frac{dq_{\text{meso}}}{d\varepsilon_{22}} < 0 \quad (8)$$

375 In Figure 18, the spatial distribution of $\frac{d\beta}{d\varepsilon_{22}}$ and $\frac{dq_{\text{meso}}}{d\varepsilon_{22}}$ is illustrated for two axial strain values
 376 (at the peak and in the softening regime). In this figure, the size of the symbols is proportional to

377 the absolute variation of the deviatoric stress $|\frac{dq_{\text{meso}}}{d\varepsilon_{22}}|$. Triangles pointing upward correspond to 3-p
378 groups with increasing deviatoric stress while triangles pointing downward correspond to 3-p groups
379 with decreasing deviatoric stress. 3-p groups undergoing bending are highlighted in dark. As a result,
380 3-p groups that fulfill the buckling definition of Equation 8 correspond to dark triangles pointing
381 downward in Figure 18.

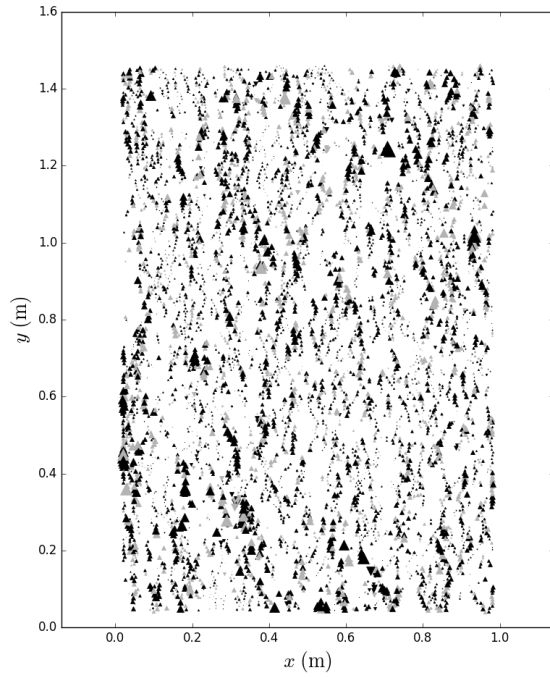
382 In Figure 18, the largest evolutions in $|\frac{dq_{\text{meso}}}{d\varepsilon_{22}}|$ (shown here) and in $|\frac{d\beta}{d\varepsilon_{22}}|$ (not shown here) con-
383 centrate in the shear band domain. Since 3-p groups are elementary parts constituting force chains,
384 a strong spatial correlation is observed between adjacent 3-p groups in terms of deviatoric stress rate
385 (adjacent triangles are of similar sizes). It is however not always the case for bending rate. In par-
386 ticular, 3-p groups subjected to a decrease in deviatoric stress and in bending angle (light triangles
387 pointing downward) are often located in between 3-p groups subjected to a decrease in deviatoric
388 stress together with an increase in bending angle (dark triangles).

389 As a result, and contrary to what is usually stated in the literature, 3-p groups are not the right
390 elementary structure to define buckling at the mesoscopic scale. As illustrated in Figure 19, we can
391 find indeed geometrical configurations in which a given 3-p group undergoes bending ($\frac{d\beta}{d\varepsilon_{22}} > 0$) while
392 the next 3-p group in the same force chain experience an opposite straightening evolution ($\frac{d\beta}{d\varepsilon_{22}} < 0$).
393 These two geometric evolutions are indeed a consequence of grain rolling (between chained grains,
394 sliding is unlikely to occur simply by definition of a force chain). Despite having two opposite geo-
395 metrical evolutions, the two 3-p groups have very similar meso-stress tensor because of spatial cor-
396 relation (Frenning and Alderborn, 2005). Therefore, for a given meso-stress evolution, both bending
397 and straightening can be observed simultaneously. For 3-p groups, the buckling condition consider-
398 ing β variations is thus not relevant and a proper definition should be sought while considering larger
399 mesostructures. 3-p groups can however still be used to analyze the impact of force chain rotations
400 onto the macroscopic behavior which is detailed in Section 4.2.

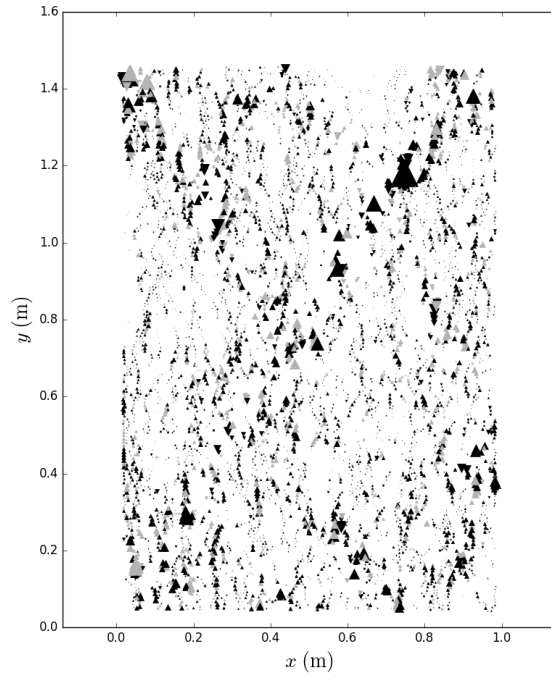
401 4.2. 3-p group rotations inside and outside shear band

402 Cumulative distributions of γ for three particular states are shown in Figure 20. In the coordinate
403 system recalled in Figure 17, 90° denotes a vertical direction aligned with the macroscopic loading
404 direction (e_2).

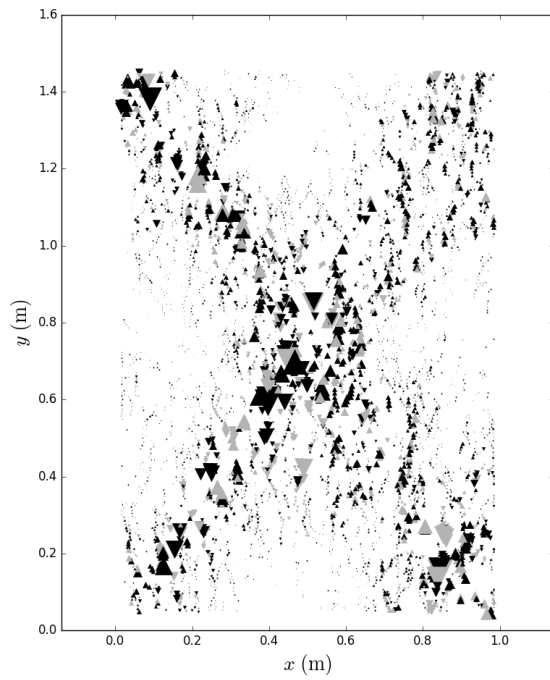
405 In the initial state (Figure 20(a)), the cumulative distribution of γ is typical of a uniform distribu-
406 tion between 0 and 180° which is consistent with the isotropic stress state imposed before any biaxial
407 loading and the spatial distribution of chained particles illustrated in Figure 9. As soon as the load



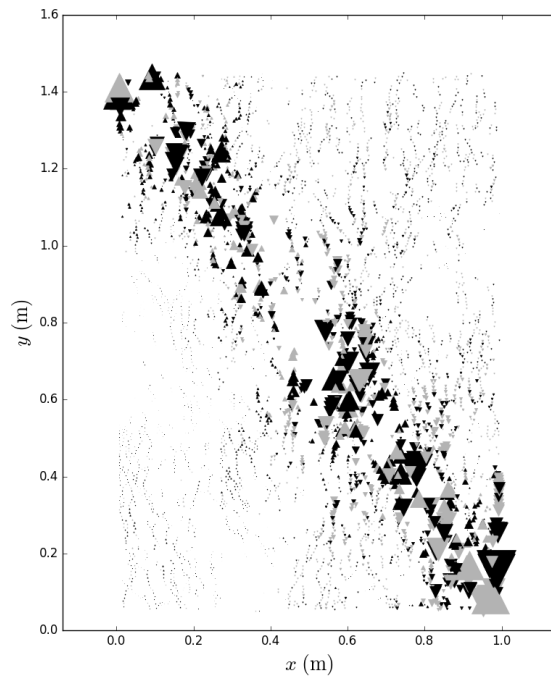
(a) Dense sample, $\varepsilon_{22} = 0.010$



(b) Dense sample, $\varepsilon_{22} = 0.013$



(c) Dense sample, $\varepsilon_{22} = 0.015$



(d) Dense sample, $\varepsilon_{22} = 0.025$

Figure 18: Spatial distribution of deviatoric stress rates in 3-p groups for different axial strain levels in the dense sample. The size of the symbols is proportional to the absolute variation of the deviatoric stress $|\frac{dq_{meso}}{d\varepsilon_{22}}|$. Triangles pointing upward correspond to 3-p groups with increasing deviatoric stress and vice versa. 3-p groups undergoing bending are shown in dark.

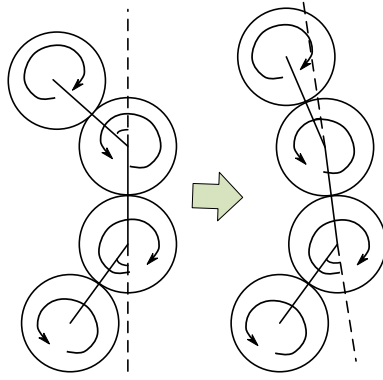


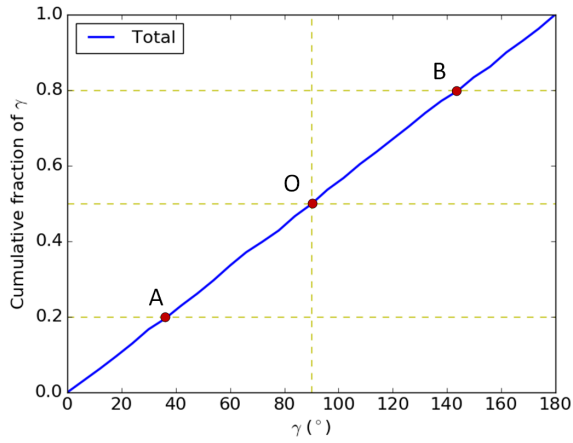
Figure 19: Example of simultaneous bending and straightening for two neighboring 3-p groups.

408 progresses, the force chain orientation changes ($\epsilon_{22} = 0.01$, Figure 9). The cumulative distribution
 409 shows a concentration of 3-p groups with mean orientation around 90° in Figure 20(b) (which is con-
 410 sistent with qualitative observations of Figure 9). After the shear band has formed, three cumulative
 411 distributions can be considered in Figure 20(c) for i) the domain inside the shear band, ii) the domain
 412 outside the shear band and iii) the whole sample. For the whole domain, γ is still aligned with the
 413 vertical direction on average, but slight deviations are observed while restricting the analysis inside
 414 and outside the shear band as illustrated in Figure 20(c) and 20(d):

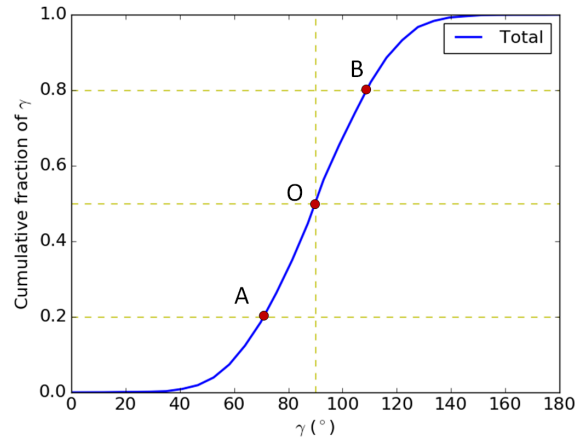
- 415 - inside the shear band γ tends to align to a direction less than 90° , denoting a clockwise rotation;
- 416 - outside the shear band γ shows the opposite trend, the counter clockwise rotation is identified.

417 To better show this trend, the strain evolution of the cumulative distribution is shown in Figure
 418 21 in the same form as used in Figure 10. Values corresponding to 20 % (γ at Point A in Figure
 419 20), 50 % (γ at Point O in Figure 20) and 80 % (γ at Point B in Figure 20) passing fraction of γ
 420 cumulative distributions are plotted together in Figure 21. Force chain geometrical directions of all
 421 passing percentages follow the same trend with clockwise rotation inside the shear band and counter-
 422 clockwise rotation outside the shear band (as illustrated in Figure 20(d)).

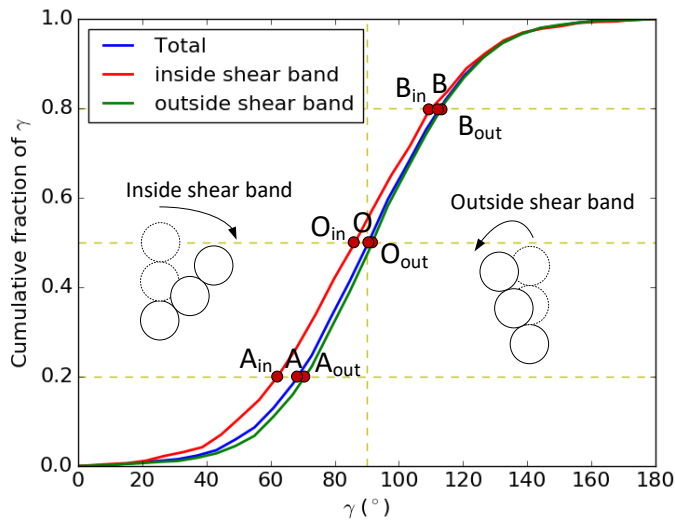
423 Note that the rotation of force chains here is not the same indicator as in previous studies. For
 424 example, Oda and Kazama (1998); Iwashita and Oda (2000) used individual particle rotations to
 425 identify fluctuation behaviors inside the shear band. Tordesillas et al. (2014, 2016) gave a vortex
 426 definition based on particle displacement field and explored the relations between vortices and force
 427 chain buckling. Kawamoto et al. (2018) found that major principal stress inside the shear band rotates
 428 differently compared to the major principal stress outside the shear band. The original signature of
 429 force chain geometrical rotation introduced in this paper corresponds to the rotation of mesostructures



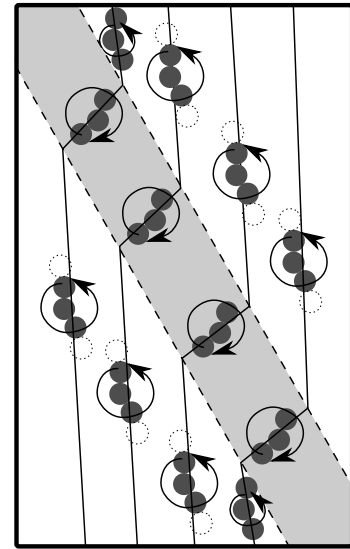
(a) Dense sample, $\epsilon_{22} = 0$



(b) Dense sample, $\epsilon_{22} = 0.01$



(c) Dense sample, $\epsilon_{22} = 0.04$



(d) 3-p groups rotations (Stage III)

Figure 20: γ cumulative distributions for three strain levels within the dense sample: (a) initial state; (b) characteristic state; (c) fully developed shear band state. (d) schematic diagram showing 3-p group rotations probably responsible for macroscopic softening.

430 of a few grains, while the internal changes (such as displacement of each sphere) within the 3-p group
 431 are ignored.

432 In [Tordesillas et al. \(2016\)](#), the force chains are almost at the boundary of the vortices. Indeed,
 433 the geometrical rotation of force chains influences the surrounding particles and the confining loops.
 434 As a result, displacements and rotations of particles on both sides of a given force chain may differ
 435 and form structures like vortices. Because the rotation of 3-p group is more intense inside the shear
 436 band, more vortices are identified within the shear band zone which is consistent with the results of
 437 [Tordesillas et al. \(2016\)](#).

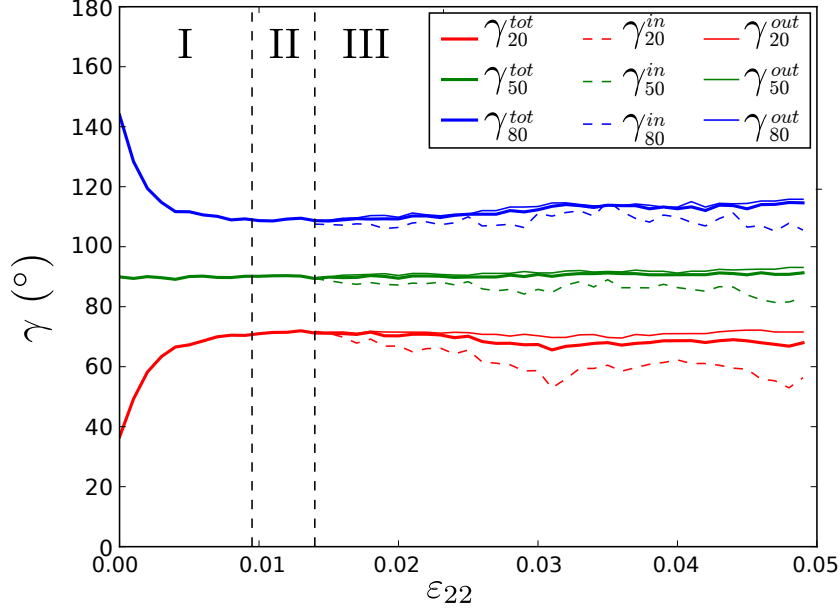


Figure 21: Strain evolution of the 20 %, 50 % and 80 % passing fractions of the cumulated distributions of the geometrical orientation γ of 3-p groups. After the stress peak, cumulative distributions are computed separately inside and outside the shear band.

4.3. Principal meso-stress rotations in force chains

Besides the geometrical rotation, a similar analysis can be carried out for the principal mesoscopic stress rotation as shown in Figure 22 for the angle $\gamma + \theta$. Stress also rotates in opposite directions inside (clockwise) and outside (counter clockwise) the shear band. A small difference is that principal stress orientations show less fluctuations around 90° as $(\gamma + \theta)_{80} - (\gamma + \theta)_{20} < \gamma_{80} - \gamma_{20}$. This means that the stresses of 3-p groups are on average more aligned with the axial loading direction than the geometrical orientation.

We do recall that, internal geometrical changes are induced by the evolution in the external forces applied to the 3-p groups. As a result the geometrical rotation of 3-p groups should be linked to an evolution of the non-coaxiality angle θ that is expected to take non-zero values. For the purpose of this analysis, the strain evolution of the mean absolute non coaxiality ($\langle |\theta| \rangle$) is shown in Figure 23.

During the hardening phases (Stage I and II), the geometrical orientation of 3-p groups tend to align to the axial loading direction. At the stress peak ($\epsilon_{22} = 0.014$), the mean absolute non-coaxiality reaches its minimum value $\langle |\theta| \rangle = 25^\circ$. As the major direction of stress is closer to the major loading direction than that of the geometry (Figure 21 and 22), the pilot role of the mesoscopic stress distribution in the loading direction is then identified before Stage III. After the stress peak, $\langle |\theta| \rangle$ increases both inside and outside the shear band. 3-p groups rotate under the plausible combined

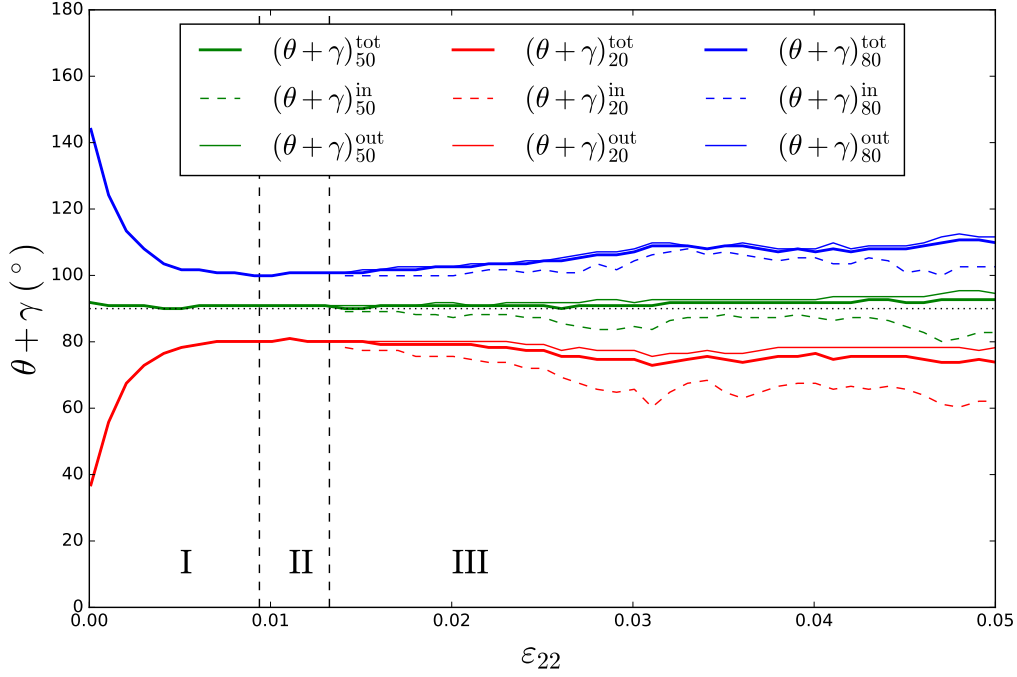


Figure 22: Strain evolution of the 20 %, 50 % and 80 % passing fractions of the cumulated distributions of the principal stress direction orientation $\gamma + \theta$ of 3-p groups. After the stress peak, cumulative distributions are computed separately inside and outside the shear band.

455 influence of the non coaxial stress and the release in kinematic constraints. Because the direction
 456 of the meso-stress is strongly influenced by the macroscopic boundary conditions, it does not rotate
 457 as much as the geometry and the non-coaxiality increases again. Besides, if we connect the present
 458 definition of force chain based on grain compression stresses with the other classical definition of
 459 force chains based on contact force networks (see Radjai et al. (1998) for instance), the geometrical
 460 rotation of 3-p groups is expected to change the internal stress distribution. Indeed, the meso-stress
 461 component initially aligned in vertical direction rotates and contribute to the lateral macro stress. As
 462 the macro lateral stress is imposed as constant (drained biaxial loading conditions), the meso-stress
 463 with the major direction oriented within a certain lateral sector will decrease accordingly. Therefore,
 464 large 3-p group rotations inside the shear band might be a contributor to the macro structural softening.

465 5. Conclusion and outlook

466 The structural strain softening observed in biaxial tests is revisited in this paper with mesoscopic
 467 analyses. Perspectives at the mesoscale are focused on, including geometrical and mechanical evo-
 468 lutions of basic force chain elements (3-p groups) and their surrounding loops. By investigating the
 469 stress, fabric, confining loops and rotations of force chains at this elementary mesoscale, new findings

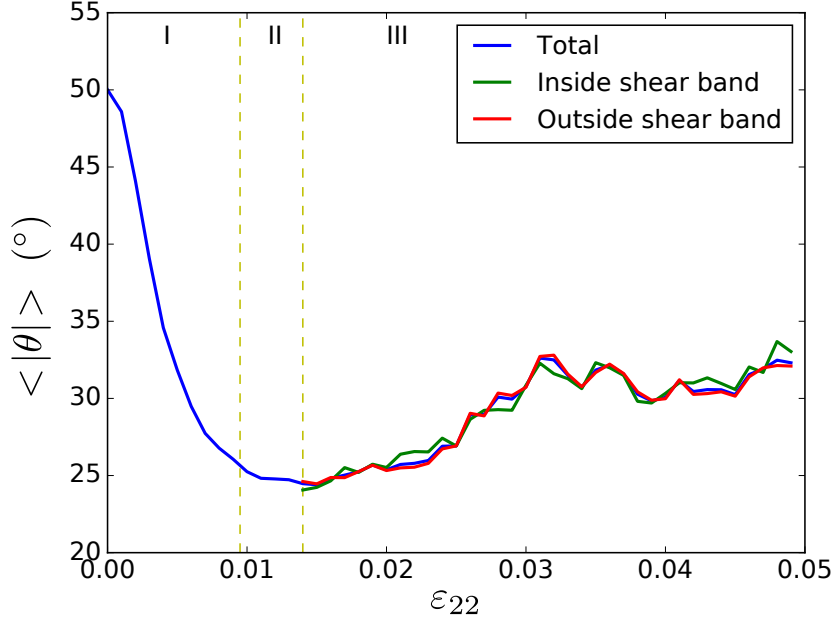


Figure 23: Evolution of the mean non coaxial angle $\langle |\theta| \rangle$ during the biaxial test for the dense sample. As the shear loading develops, $\langle |\theta| \rangle$ is computed separately inside and outside the shear band.

470 for both hardening and softening mechanisms are presented, which can be summarized as follows:

- 471 1. Dense and loose assemblies react differently as the deviatoric loads are applied. Structural
472 softening is identified for the dense specimen, with a final shear band forming. Using the meso-
473 stress definition based on 3-p groups, it has been shown that the meso softening also exists
474 locally in the solid phase of the granular sample. Also, the macroscopic softening is not simply
475 due to the geometric stress reduction coming from the increase in porosity.
- 476 2. The stress-strain relations for the dense assembly can be divided into three phases: hardening
477 with contractancy (Stage I), hardening with dilatancy (Stage II) and softening with dilatancy
478 (Stage III). At the mesoscale, the force chain population, relative stress, fabric and associated
479 topology exchanges are explored for all the three stages. For the first stage of hardening (Stage
480 I), the number of chained particles increases, force chains straighten and surrounding voids
481 shrink. This contributes to the robustness of the granular assembly and the persistence of the
482 force network, allowing for reversibility to a certain extent (quasi-elastic domain). For Stage II,
483 as dilatancy occurs, no new force chains are built and stress concentrates within existing force
484 chains. As contacts are continuously lost, force chains have more and more kinematic degrees
485 of freedom to evolve. At this stage, the persistence of the force network is more and more
486 compromised.

- 487 3. During Stage III, the meso-stress is highly concentrated on force chains, the recti-linearity of
488 which decreases (mesoscopic fabric anisotropy). As a shear band develops, the two homoge-
489 nous domains inside and outside the shear band are analyzed separately. Mesoscopic geometry
490 and stress rotations within the shear band are shown to differ from those outside the shear band
491 at the scale of 3-p groups. Finally, the non-coaxiality between geometry and stress contributes
492 to the mesoscopic softening.
- 493 4. At the level of 3-p groups, a meso-stress definition is proposed with and without taking into
494 account the surrounding voids. The corresponding statistics of meso-stresses give qualitative
495 correspondence to the macro stress, and with respect to the meso-stress of 3-p groups, the het-
496 erogeneity of force transmission is also identified. The force chain rotation of the 3-p group pro-
497 vides a sound micromechanical explanation for the observed macroscopic strain softening. 3-p
498 group rotation contributes to transfer the vertical load on the lateral boundaries. As the lateral
499 stress is imposed as constant, the vertical stress adapts accordingly, leading to the macroscopic
500 softening. This result connects material scale properties to the boundary conditions and relates
501 thus to structural softening. It has been derived here for a particular sample of aspect ratio 1.5
502 but a parametric study has shown that it can be generalized for other aspect ratios. The aspect
503 ratio influences however the shear band direction which will be discussed in a forthcoming
504 paper.

505 This study has shown once again the relevance of mesoscale structures to capture the physics of
506 granular materials. A number of statistical observations provide mesoscale clues to understand the
507 meso origin of hardening and softening in granular materials. 3-p group rotation has been shown to
508 contribute to this softening but this does not exclude other mesoscale mechanisms. By accounting
509 for spatial correlations between the introduced mesostructures, we envision to extend our mesoscale
510 description of granular materials in order to precise the mesoscale definition of buckling or softening
511 which has been shown to be irrelevant at the scale of 3-p groups.

512 The mesoscale analysis presented in this paper can also be used to bridge the gap between dis-
513 crete and continuum descriptions of granular materials at a scale where the concept of representative
514 elementary volume (REV) does not hold (the scale separation hypothesis required to define a REV is
515 not fulfilled at mesoscale). This will pave the way for a micromechanical analysis of slip lines and
516 shear bands as defined within continuum mechanics framework (discontinuities in the displacement
517 and strain fields respectively).

518 **Acknowledgements**

519 This work was supported by National Key R&D Program of China (No. 2018YFC1508500),
520 China Scholarship Council (Joint PhD program, No. 201606270088) and China Postdoctoral Science
521 Foundation (No. 2018M642910)

522 We gratefully acknowledge the CNRS International Research Network GeoMech for having of-
523 fered the opportunity to kick start this project through the organization of many workshops with topics
524 connected to the concepts developed in this paper (<http://gdr-mege.univ-lr.fr/>).

525 We thank all the anonymous reviewers for their helpful suggestions on the quality improvement
526 of our paper.

527 **References**

- 528 Bagi, K., 1996. Stress and strain in granular assemblies. *Mechanics of materials* 22 (3), 165–177.
- 529 Been, K., Jefferies, M. G., 1985. A state parameter for sands. *Géotechnique* 35 (2), 99–112.
- 530 Bonelli, S., Millet, O., Nicot, F., Rahmoun, J., De Saxcé, G., 2012. On the definition of an average
531 strain tensor for two-dimensional granular material assemblies. *International Journal of Solids and*
532 *Structures* 49 (7-8), 947–958.
- 533 Cambou, B., Jean, M., Radjai, F., 2013. *Micromechanics of granular materials*. John Wiley & Sons.
- 534 Dafalias, Y. F., Jun 2016. Must critical state theory be revisited to include fabric effects? *Acta*
535 *Geotechnica* 11 (3), 479–491.
536 URL <https://doi.org/10.1007/s11440-016-0441-0>
- 537 Dedecker, F., Chaze, M., Dubujet, P., Cambou, B., 2000. Specific features of strain in granular mate-
538 rials. *Mechanics of Cohesive-frictional Materials* 5 (3), 173–193.
- 539 Frenning, G., Alderborn, G., 2005. Evolution of distributions and spatial correlations of single-
540 particle forces and stresses during compression of ductile granular materials. *Physical Review E*
541 71 (1), 011305.
- 542 Guo, N., Zhao, J., 2013. The signature of shear-induced anisotropy in granular media. *Computers and*
543 *Geotechnics* 47, 1–15.

- 544 Iwashita, K., Oda, M., 2000. Micro-deformation mechanism of shear banding process based on mod-
545 ified distinct element method. *Powder Technology* 109 (1-3), 192–205.
- 546 Kawamoto, R., Andò, E., Viggiani, G., Andrade, J. E., 2018. All you need is shape: Predicting shear
547 banding in sand with Is-dem. *Journal of the Mechanics and Physics of Solids* 111, 375–392.
- 548 Kruyt, N., Rothenburg, L., 1996. Micromechanical definition of the strain tensor for granular materi-
549 als. *Appi. Mech* 118, 706–711.
- 550 Kruyt, N. P., 2010. Micromechanical study of plasticity of granular materials. *Comptes rendus*
551 *mécanique* 338 (10-11), 596–603.
- 552 Kruyt, N. P., Millet, O., Nicot, F., 2014. Macroscopic strains in granular materials accounting for
553 grain rotations. *Granular matter* 16 (6), 933–944.
- 554 Kruyt, N. P., Rothenburg, L., 2016. A micromechanical study of dilatancy of granular materials.
555 *Journal of the Mechanics and Physics of Solids* 95, 411–427.
- 556 Kuhn, M. R., 1999. Structured deformation in granular materials. *Mechanics of materials* 31 (6),
557 407–429.
- 558 Lade, P. V., 1977. Elasto-plastic stress-strain theory for cohesionless soil with curved yield surfaces.
559 *International Journal of Solids and Structures* 13 (11), 1019–1035.
- 560 Li, X., Dafalias, Y. F., 2000. Dilatancy for cohesionless soils. *Géotechnique* 50 (4), 449–460.
- 561 Li, X., Yu, H.-S., 2009. Influence of loading direction on the behavior of anisotropic granular materi-
562 als. *International Journal of Engineering Science* 47 (11), 1284–1296.
- 563 Li, X., Yu, H.-S., 2013. On the stress–force–fabric relationship for granular materials. *International*
564 *Journal of Solids and Structures* 50 (9), 1285–1302.
- 565 Li, X. S., Dafalias, Y. F., 2012. Anisotropic critical state theory: Role of fabric. *Journal of Engineering*
566 *Mechanics* 138 (3), 263–275.
- 567 Liu, J., Nicot, F., Zhou, W., 2018. Sustainability of internal structures during shear band forming in
568 2d granular materials, accepted.
- 569 Love, A., 1927. *A treatise on the mathematical theory of elasticity*, cambridge university press. Cam-
570 bridge.

- 571 Ma, G., Regueiro, R. A., Zhou, W., Liu, J., 2018. Spatiotemporal analysis of strain localization in
572 dense granular materials. *Acta Geotechnica*, 1–18.
- 573 Ma, G., Zhou, W., Chang, X.-L., 2014. Modeling the particle breakage of rockfill materials with the
574 cohesive crack model. *Computers and Geotechnics* 61, 132–143.
- 575 Ma, G., Zhou, W., Regueiro, R. A., Wang, Q., Chang, X., 2017. Modeling the fragmentation of rock
576 grains using computed tomography and combined fdem. *Powder Technology* 308, 388–397.
- 577 Maeda, K., Kuwabara, N., Matsuoka, H., 2001. Micromechanical analysis on formation process of
578 microstructure in granular material during compression and shear. Kishino, éditeur: *Powders and*
579 *Grains*, 223–226.
- 580 Nguyen, N.-S., Magoaric, H., Cambou, B., 2012. Local stress analysis in granular materials at a
581 mesoscale. *International Journal for Numerical and Analytical Methods in Geomechanics* 36 (14),
582 1609–1635.
- 583 Nicot, F., Darve, F., 2011. The h-microdirectional model: accounting for a mesoscopic scale. *Me-*
584 *chanics of Materials* 43 (12), 918–929.
- 585 Nicot, F., Xiong, H., Wautier, A., Lerbet, J., Darve, F., 2017. Force chain collapse as grain column
586 buckling in granular materials. *Granular Matter* 19 (2), 18.
- 587 Oda, M., 1982. Fabric tensor for discontinuous geological materials. *Soils and Foundations* 22 (4),
588 96–108.
- 589 Oda, M., Kazama, H., 1998. Microstructure of shear bands and its relation to the mechanisms of
590 dilatancy and failure of dense granular soils. *Géotechnique* 48 (4), 465–481.
- 591 Peters, J. F., Muthuswamy, M., Wibowo, J., Tordesillas, A., 2005. Characterization of force chains in
592 granular material. *Physical review E* 72 (4), 041307.
- 593 Radjai, F., Jean, M., Moreau, J.-J., Roux, S., 1996. Force distributions in dense two-dimensional
594 granular systems. *Physical review letters* 77 (2), 274.
- 595 Radjai, F., Wolf, D. E., Jean, M., Moreau, J.-J., 1998. Bimodal character of stress transmission in
596 granular packings. *Physical review letters* 80 (1), 61.

- 597 Rechenmacher, A. L., Abedi, S., Chupin, O., Orlando, A. D., 2011. Characterization of mesoscale
598 instabilities in localized granular shear using digital image correlation. *Acta Geotechnica* 6 (4),
599 205–217.
- 600 Rothenburg, L., Bathurst, R., 1989. Analytical study of induced anisotropy in idealized granular
601 materials. *Géotechnique* 39 (4), 601–614.
- 602 Roux, J.-N., 2000. Geometric origin of mechanical properties of granular materials. *Physical Review*
603 *E* 61 (6), 6802.
- 604 Satake, M., 1982. Fabric tensor in granular materials. In: *Proc., IUTAM Symp. on Deformation and*
605 *Failure of Granular materials*, Delft, The Netherlands.
- 606 Satake, M., 1992. A discrete-mechanical approach to granular materials. *International journal of en-*
607 *gineering science* 30 (10), 1525–1533.
- 608 Sibille, L., Hadda, N., Nicot, F., Tordesillas, A., Darve, F., 2015. Granular plasticity, a contribution
609 from discrete mechanics. *Journal of the Mechanics and Physics of Solids* 75, 119–139.
- 610 Sterpi, D., 1999. An analysis of geotechnical problems involving strain softening effects. *International*
611 *Journal for Numerical and Analytical Methods in Geomechanics* 23 (13), 1427–1454.
- 612 Suiker, A., De Borst, R., Chang, C., 2001. Micro-mechanical modelling of granular material. part 1:
613 Derivation of a second-gradient micro-polar constitutive theory. *Acta Mechanica* 149 (1-4), 161–
614 180.
- 615 Sun, Y., Gao, Y., Zhu, Q., 2017. Fractional order plasticity modelling of state-dependent behaviour of
616 granular soils without using plastic potential. *International Journal of Plasticity*.
- 617 Tordesillas, A., 2007. Force chain buckling, unjamming transitions and shear banding in dense gran-
618 ular assemblies. *Philosophical Magazine* 87 (32), 4987–5016.
- 619 Tordesillas, A., Muthuswamy, M., 2009. On the modeling of confined buckling of force chains. *Jour-*
620 *nal of the Mechanics and Physics of Solids* 57 (4), 706–727.
- 621 Tordesillas, A., Pucilowski, S., Lin, Q., Peters, J. F., Behringer, R. P., 2016. Granular vortices: iden-
622 tification, characterization and conditions for the localization of deformation. *Journal of the Me-*
623 *chanics and Physics of Solids* 90, 215–241.

- 624 Tordesillas, A., Pucilowski, S., Walker, D. M., Peters, J. F., Walizer, L. E., 2014. Micromechanics
625 of vortices in granular media: connection to shear bands and implications for continuum mod-
626 elling of failure in geomaterials. *International Journal for Numerical and Analytical Methods in*
627 *Geomechanics* 38 (12), 1247–1275.
- 628 Tordesillas, A., Walker, D. M., Lin, Q., 2010. Force cycles and force chains. *Physical Review E* 81 (1),
629 011302.
- 630 Šmilauer, V., et al., 2015. Yade Documentation 2nd ed. The Yade Project, <http://yade-dem.org/doc/>.
- 631 Walker, D. M., Tordesillas, A., 2010. Topological evolution in dense granular materials: a complex
632 networks perspective. *International Journal of Solids and Structures* 47 (5), 624–639.
- 633 Wan, R., Guo, P., 1998. A simple constitutive model for granular soils: modified stress-dilatancy
634 approach. *Computers and Geotechnics* 22 (2), 109–133.
- 635 Wang, J., Gutierrez, M. S., Dove, J. E., 2007. Numerical studies of shear banding in interface shear
636 tests using a new strain calculation method. *International Journal for Numerical and Analytical*
637 *Methods in Geomechanics* 31 (12), 1349–1366.
- 638 Wautier, A., Bonelli, S., Nicot, F., 2017. Scale separation between grain detachment and grain trans-
639 port in granular media subjected to an internal flow. *Granular Matter* 19 (2), 22.
- 640 Wautier, A., Bonelli, S., Nicot, F., 2018. Micro-inertia origin of instabilities in granular materials. *Int*
641 *J Numer Anal Methods Geomech*, 19.
- 642 Weber, J., 1966. Recherches concernant les contraintes intergranulaires dans les milieux pulvérulents.
643 *Bulletin de Liaison des Ponts-et-chaussées* 20, 1–20.
- 644 Xiong, H., Nicot, F., Yin, Z., 2017. A three-dimensional micromechanically based model. *Internat-*
645 *ional Journal for Numerical and Analytical Methods in Geomechanics*.
- 646 Yin, Z.-Y., Hicher, P.-Y., Dano, C., Jin, Y.-F., 2016. Modeling mechanical behavior of very coarse
647 granular materials. *Journal of Engineering Mechanics* 143 (1), C4016006.
- 648 Zhang, L., Nguyen, N. G. H., Lambert, S., Nicot, F., Prunier, F., Djeran-Maigre, I., 2017. The role of
649 force chains in granular materials: from statics to dynamics. *European Journal of Environmental*
650 *and Civil Engineering* 21 (7-8), 874–895.

- 651 Zhou, W., Yang, L., Ma, G., Chang, X., Cheng, Y., Li, D., 2015. Macro–micro responses of crushable
652 granular materials in simulated true triaxial tests. *Granular Matter* 17 (4), 497–509.
- 653 Zhu, H., Nguyen, H. N., Nicot, F., Darve, F., 2016a. On a common critical state in localized and
654 diffuse failure modes. *Journal of the Mechanics and Physics of Solids* 95, 112–131.
- 655 Zhu, H., Nicot, F., Darve, F., 2016b. Meso-structure organization in two-dimensional granular mate-
656 rials along biaxial loading path. *International Journal of Solids and Structures* 96, 25–37.