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How meso shear chains bridge multiscale shear behaviors in granular materials: a preliminary study

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Abstract

The “incremental shear strain chain” concept (simply called “shear chain”) has been proposed recently to quantitatively account for local kinematic features of granular materials. At the microscopic scale, contacts can slide and particles can rotate; while at the macroscopic scale, shear bands appear as a typical localized failure mode. Despite visual spatial distribution features, the direct links from microscopic to macroscopic shear behaviors are still missing. This paper investigates shear characteristics appearing at the micro, meso and macro scales in granular materials, and tries to elucidate how they can be correlated by adopting the shear chain concept. Based on the spatial statistics tools, the shear chain and the shear band orientations are compared by demonstrating that the shear band is influenced by the sample aspect ratio while shear chain orientation only depends on the stress state. Shear chains experience a relative steady and high fabric anisotropy, irrespective to the stress state. Micro contact sliding and particle rotation mainly exist in the shear chain connection positions, which gives possible clues on shear chain forming. In conclusion, the shear band is eventually conjectured to be formed of a collection of crossing shear chains at meso scale, according to detailed analysis and discussion on the correlations of shear behaviors across scales.

Keywords: granular materials, DEM, contact sliding, shear chain, shear band, particle rotation

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1. Introduction

For frictional granular materials, such as sands or coarse-grained soils, shear behaviors have been attracting much scientific attention for a long time. Indeed, the failure in geomaterials is closely related to the shear behavior, giving rise to mass-driven natural hazards [1, 2]. Under shearing loads, complex mechanical features are found in granular materials due to the disordered discrete structures and various components. The critical state [3, 4, 5], dilatancy [6, 7, 8], failure patterns [9, 10, 11] and many other phenomena are triggered by shearing but not well described in constitutive models, while multiscale investigations provide new clues for describing this constitutive complexity [12]. Shear banding, which relates to the macroscopic strain localization of a narrow band, is one of the typical failure patterns under shearing for granular materials. Although shear band orientation and width have been studied for a long time [13, 14], the intrinsic origin of this macroscopic strain localization still remains to be solved from the micro or meso scale explanations [15, 16, 17, 18, 19, 20]. Among the established results, the local meso slip structures have been observed within the granular assembly under shearing. They are suspected to play a major role in linking the local rearrangement and the macroscopic shear banding.

The granular micro-mechanics have been investigated from both numerical and experimental explorations during decades [21, 22, 23, 24], and then micromechanical models have been proposed [25, 26, 27, 28, 29]. Contacts between particles give rise to forces with or without the consideration of friction or cohesion, and the statistical characterization of forces and contact network finally result in the stress of the overall assembly. Microscopic features, such as particle size [30, 31, 32], particle shape [33, 34, 35] and particle breakage [36, 37, 38, 39], are also recognized to influence the macroscopic mechanical responses. For frictional granular materials, each contact is commonly assumed as elastoplastic, and the sliding is limited by the micro Coulomb friction at the contact scale. When one contact is sliding, i.e., two particles have relative tangential displacement, then it could be regarded as micro failure under shearing and related to local rearrangement [40]. Besides, at the microscopic scale, the rotation of particles will be triggered by the shear banding and concentrate within the localized area [41, 20, 42, 16]. So far, micromechanical ingredients like contact sliding and particle rotation have been involved in many researches on shear band forming, however, no direct links have been built to demonstrate that microscopic contact sliding or particle rotation trigger the macroscopic shear banding. Be-

32 fore shear band develops, the incremental deviatoric strain field already experiences a strain
33 localization pattern but at a local scale, where sliding and rotation also reflect some spatial
34 correlations to the incremental strain field [43]. It is therefore tempting to examine whether a
35 bridge exists between microscopic shear behaviors and macroscopic shear banding.

36 Between the grain scale and the sample scale, there is an intermediate scale referred to
37 as mesoscopic scale, where a few particles and relative voids form so-called mesostructures.
38 For example, force chains and contact-based loops (or cycles, in 2D) are examples of such
39 mesostructures. They have been defined to explore the force transmission and deformation
40 mechanisms of granular materials under various loading conditions [44, 45, 46, 11]. Small
41 localized patterns of the strain field before shear banding can be detected at the mesoscopic
42 scale, which are called “microbands” in some publications [41, 47]. They have been analysed
43 as meso-slip lines according to the solution of hyperbolic equations of plasticity theory [48]. In
44 recent work of authors [49, 48], this mesoscopic shear structure has been defined as “incremental
45 shear strain chain” (briefly “shear chain”) by connecting cells with large deviatoric strain in
46 the loop tessellation, which is inspired by force chain definition [44, 50]. The shear chain can
47 well describe the orientated meso slip features, as well as the plasticity generation of granular
48 materials during shearing. From a comprehensive comparisons of shear behaviors at micro,
49 meso and macro scale, it should be meaningful to correlate the shear chain distribution and
50 evolution to the contact sliding, grain rotation and shear banding. Once the link among the
51 shear behaviors of the three scales is specified, a door will be opened to meticulously investigate
52 the origin of shear banding.

53 Therefore in this paper, we try to identify the correlations from micro, meso to macroscopic
54 shear behaviors at the primary stage. The Discrete Element Method (DEM) is used to perform
55 the numerical tests, offering the advantage to obtain micro- and mesoscopic information inside
56 granular assemblies. Section 2 briefly introduces shear behaviors at micro, meso and macro
57 scales, particularly the shear chain structure which is defined in Liu et al. [49]. In Section 3,
58 the spatial distribution patterns of incremental strains, particle rotations and contact sliding
59 are compared for a typical biaxial test undergoing shear band formation. Then the orientation
60 features of shear chain and shear band are compared in Section 4, demonstrating that they are
61 different shear structures operating of different scales. The microscopic sliding and rotation
62 have a preferred location in the shear chain connection positions, as investigated in Section
63 5. Combined with the results gained in this paper and conclusions in other publications (e.g.,

[43, 47]), the connecting role of meso shear chains between micro and macro shear behaviors is tried to be established in Section 6. The intermediate mesoscale shear strain chain is proved to be the key bridge from the micro to macro scales for granular materials under shearing.

2. Shear behaviors at micro, meso and macro scales

At the micro scale of granular materials, the basic elements, i.e., particles and contacts, are considered. By adopting the Coulomb friction criterion at micro scale, the contact sliding should be regarded as the shear behaviors at micro scale. As for a single particle, its rotation will be triggered by the tangential forces, then the particle rotation could be another sign of shearing at the micro scale.

When shearing loads are applied for granular materials, a number of mesoscopic slip structures will appear within the sample, which have been observed from numerical analysis and experimental tests [41, 47]. In Liu et al. [49], these meso slip structures have been defined as “incremental shear strain chains” (briefly “shear chains”), providing a way to describe the mesoscopic shear behaviors concretely. The shear chain, as shown in Figure 1, is captured by searching connecting meso loops¹ with large meso deviatoric strains by some assumptions. Here are the simplified steps for shear chain definition and obtaining²:

1. Compute the incremental strain tensor for each meso loop cell, then collect meso loops with incremental deviatoric strains larger than the average value (the given threshold).
2. Within the group of loops of larger incremental deviatoric strains, search loop chains by judging whether the deviation (β in Figure 1) between the maximum shearing directions of two connecting loops (dash-dotted line in Figure 1) and the geometric directions joining the 2 barycenters (black solid lines in Figure 1) are close. The connection between the two loops are built if β fulfills a given limitation, in this paper it is set as $\beta \leq \beta_{th} = 22.5^\circ$. β_{th} denotes the threshold angle between these two directions.
3. If a chain of loops is composed of at least three loops, then it is regarded as a shear chain.

In Figure 1, there are key contacts and particles in forming a shear chain. The contact connecting two loops (red line in Figure 1) is called shear chain connection contact (“SCC” in Section 5.2), may exhibit significant features of sliding; the particles connected by shear chain

¹polygons tessellated from the contact network, more details can be found in [51, 52]

²more details can be found in Liu et al. [49]

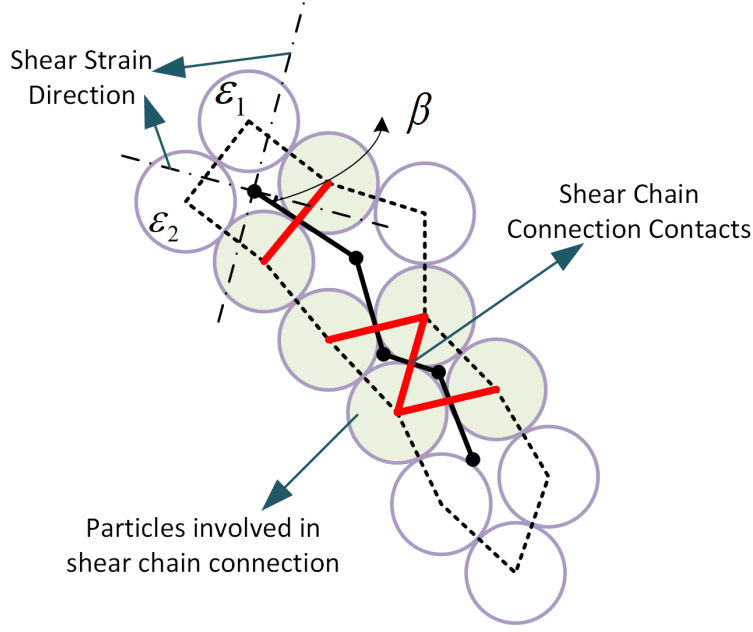


Figure 1: Schematic drawing of an incremental shear strain chain. β denotes the angle deviation between shear strain direction and the geometrical line connecting loop centers. Red lines are shear chain connection contacts, and their relative particles are marked in green.

92 contact (green sphere in Figure 1, “SC connex” in Section 5.3), could be imagined easier to
 93 rotate compared to other particles. In Section 5, these key micro matters will be carefully
 94 investigated.

95 The shear chain is a line-like structure, and we need to obtain its orientation angle θ . A
 96 representation of shear chains is achieved by joining the geometric barycenters of adjacent cells
 97 (dark thick line in Figure 1). For a shear chain of m adjacent mesoloops, the least square
 98 method defines the mean direction θ as:

$$\theta = \arctan \left(\frac{\sum_{i=1}^m (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^m (x_i - \bar{x})^2} \right) \quad (1)$$

99 where x_i and y_i corresponds to the x and y coordinates of the geometric barycenter of loop
 100 cell i , and \bar{x} and \bar{y} are the averages of the x_i and y_i , respectively. Within a sheared granular
 101 assembly, there should be a number of shear chains. Then we choose the average absolute value
 102 of θ , i.e., $\langle |\theta| \rangle$, to be an indicator for assessing the shear chain orientation of an assembly at
 103 a given state [49].

104 At the macro scale, shear bands are one of the typical failures for granular materials under
 105 shearing. The orientation and width of shear bands are usually focused on by researchers.
 106 Shear bands and shear chains are different but correlated somehow, which will be shown in
 107 Section 4 and 6.

108 3. Spatial distribution patterns during shear band forming

109 During deviatoric loading, dense granular materials usually experience a transition from a
110 homogeneous to a heterogeneous kinematic pattern with respect to the commonly considered
111 incremental deviatoric strain field. Besides, microscopic characterizations, such as particle
112 rotation and contact sliding, demonstrate corresponding distribution features to the strain
113 field. In this section, an example of biaxial drained test conducted by DEM is chosen, to show
114 the visual features of shear band forming and the related microscopic features.

115 3.1. An example of DEM biaxial test

116 A series of biaxial tests are performed for dense assemblies by using the open-source DEM
117 platform YADE [53]. Details of each DEM test are displayed in Appendix A. Here we select one
118 of the samples, Sample DP³, as an example to investigate the visual patterns of kinematic field.
119 Initially, 33 333 spherical particles are generated within a rectangle of aspect ratio $L/W=2.5$,
120 where L denotes the length and W denotes the width(the sketch of the sample is shown in
121 Figure 2); then the rectangle sample is densely packed to reach an isotropic stress state of
122 100 kPa by the combining method of particle growing and boundary compaction[40]. After
123 reaching the isotropic stress state, deviatoric loads are applied by compressing the upper and
124 lower boundaries with the strain rate of $-0.01/s$ while keeping the lateral stress constant to
125 100 kPa. Rigid walls are used for sample boundaries. The uniform distribution is chosen with
126 the ratio of the maximum diameter to the minimum $D_{max}/D_{min} = 1.98$ and the average size
127 $D_{50} = 8.4$ mm. Other parameters in the DEM simulations: the material density is set to
128 $\rho = 3,000$ kg.m⁻³; k_n/D_s is set to 300 MPa, where $D_s = 2R_1R_2/(R_1 + R_2)$ and R_1, R_2 are
129 the radii of particles in a given contact; k_t/k_n is set to 0.5. The information of other samples
130 are shown in Appendix A, and the only difference between all 16 samples is the sample aspect
131 ratio.

132 Figure 3 presents the curves of deviatoric stress and volumetric strain evolutions along the
133 biaxial drained test. Correspondingly, the incremental deviatoric and volumetric strain fields
134 are shown in Figure 4 for five key states (A, B, C, D, E in Figure 3). The local strain is defined
135 based on the contact loop tessellation. At the scale of a loop, incremental grain displacements
136 are adopted to define an incremental strain tensor of the given loop. Detailed information of the

³We choose this sample because two bands form with different orientations at the final stage, which make convenience for analyzing the distribution features of micro characterizations

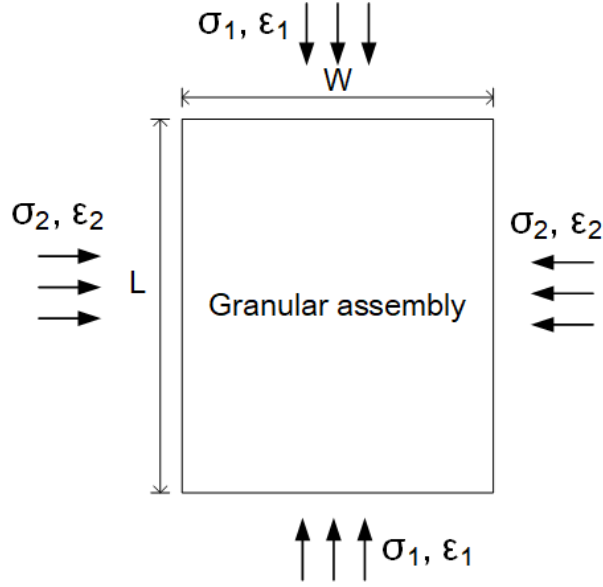


Figure 2: Schematic plot of DEM samples under the biaxial loading condition.

137 incremental strain definition used in this paper can be found in Liu et al. [52]. In Figure 3 and
 138 Figure 4, State D denotes the stress peak during biaxial loading, where several crossing shear
 139 bands firstly appear. Before State D, a strain structurization is already evident at small scale,
 140 and small crossing structures of relatively high incremental strain evenly distribute within the
 141 sample domain. These meso structures are observed in both experimental and numerical tests
 142 [41, 54, 47], and could be denoted as “incremental shear strain chain” from our previous work
 143 [49, 48]. After State D, two chronic shear bands finally form and the reflection is found at the
 144 left boundary, as shown in State E of Figure 4. Generally, the incremental deviatoric strain field
 145 is concerned to identify the strain localization of materials, and in Figure 4, the incremental
 146 volumetric strain field is also compared at the same stage. It can be seen that the incremental
 147 volumetric strain field demonstrates the same localized patterns as the incremental deviatoric
 148 strain field, and both the local dilation ⁴ (high negative value) and the local contraction (high
 149 positive value) concentrate within the local shear structures or shear bands. Therefore, not
 150 only shear deformation is triggered within the localization area, but also significant volumetric
 151 changes occur.

⁴in soil mechanics, the compression direction denotes the positive direction of strain, so the negative value of volumetric strain demonstrates dilation, and vice versa.

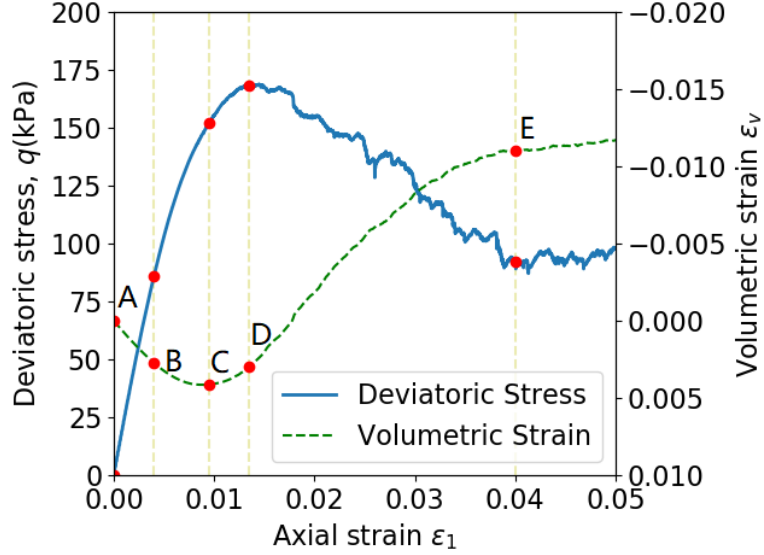


Figure 3: Deviatoric stress and volumetric strain evolutions of an example of the biaxial test (Sample DP in Appendix A). For the volumetric strain, the positive value denotes the compression and the negative value denotes the dilation of the sample.

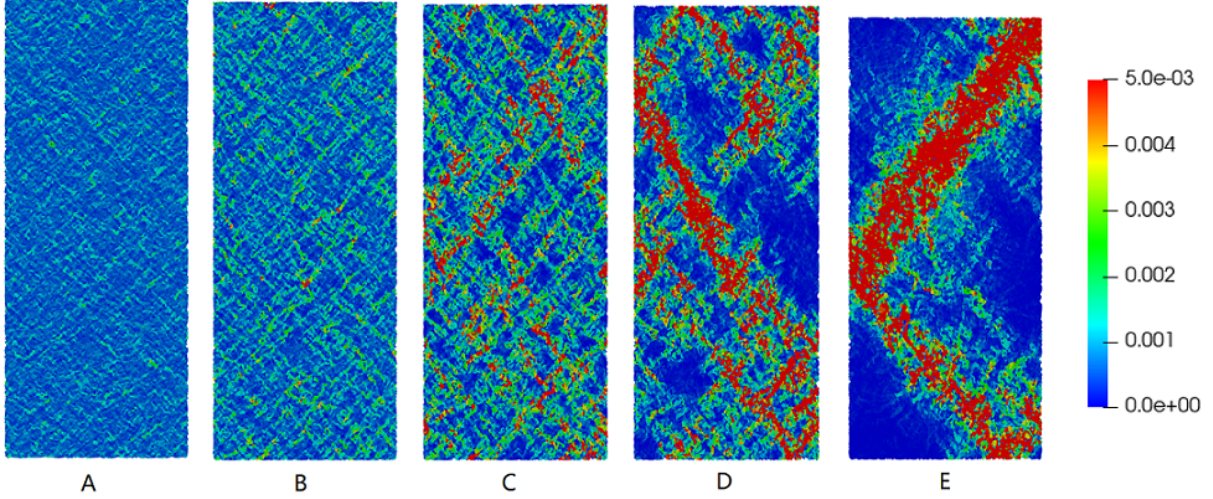
3.2. Spatial distributions of contact sliding and particle rotation

In Section 3.1, the evolution of the incremental strain field of granular sample from homogeneous to heterogeneous patterns has been highlighted under biaxial loading. This evolution could be compared with the microscopic failures such as contact sliding and particle rotation.

The sliding behavior between two connected particles could be simply identified by Coulomb friction criterion in contacts in DEM simulations. When the tangential contact force $|f_t|$ reaches the limit of μf_n ($\mu = \tan\phi_g$ denotes the friction coefficient and f_n is the normal contact force), the two connecting particles will experience relative sliding at the tangential direction. Figure 5 presents the sliding contact distribution for the 5 key states shown in Section 3.1. Initially sliding contacts are scarce at State A; then the sliding distribution becomes denser and prone to give rise to the meso shear features (micro bands or shear chains); finally the sliding contacts concentrate evidently within the shear band. Visually, the clustered sliding behaviors are strongly correlated to the macro shear band at State E, however they show less significant features relative to meso shear structures before the stress peak, especially for States A and B. At State C and D, the sliding behaviors already exhibit some clustering features, and their distribution features should be further explored by adopting the shear chain concept.

Besides contact sliding, the incremental rotation of particles is proved to be related to the incremental strain field, especially for the period before stress peak and when the meso shear structures are fluctuating [43]. In this study, the positive rotation represents counterclockwise

Deviatoric strain



Volumetric strain

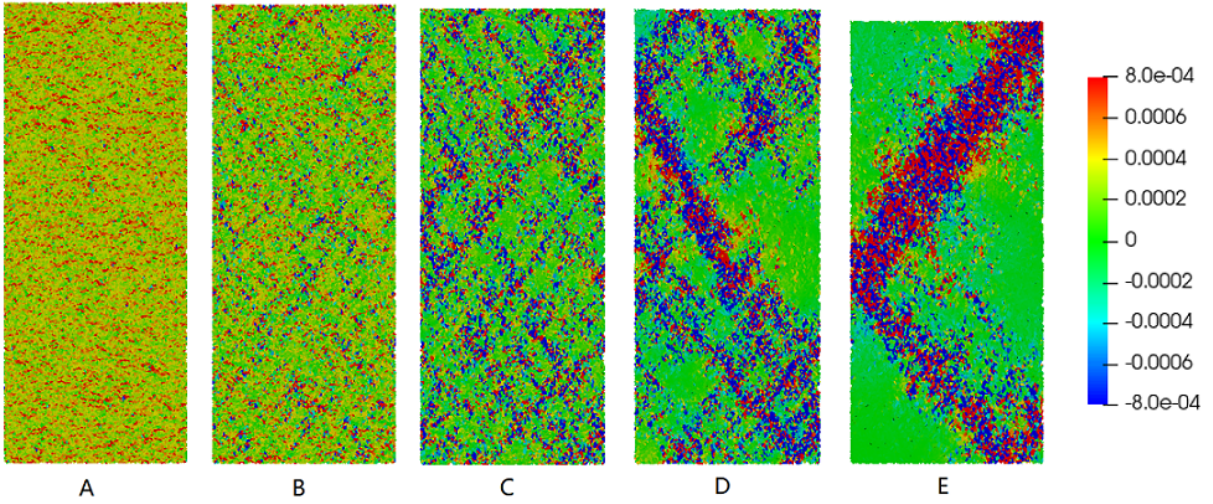


Figure 4: Spatial distributions of the incremental deviatoric and volumetric strain for different loading states in Figure 3. For the volumetric strain, the positive value denotes the compression and the negative value denotes the dilation.

171 direction and the negative rotation means the clockwise direction, and no background rotation is
 172 involved. Figure 6 shows the distributions of positive and negative particle rotation increments
 173 for the 5 states of Sample DP. Grey points shown in this figure denote particles with relative
 174 large absolute rotation increment (≥ 0.0005 rad, details of the threshold consideration are shown
 175 in Appendix B) between two steps (strain increment $d\varepsilon_1 = 0.0005$), which helps to distinguish
 176 the typical patterns of the distributions. Before the shear bands form (State A – D), it can be
 177 seen that large positive and negative incremental rotation points are clustered with opposite
 178 preferred inclinations, which is also observed by other publications [43, 55, 56, 57]; however at
 179 State E, the patterns of both positive and negative rotation increments show accordance with

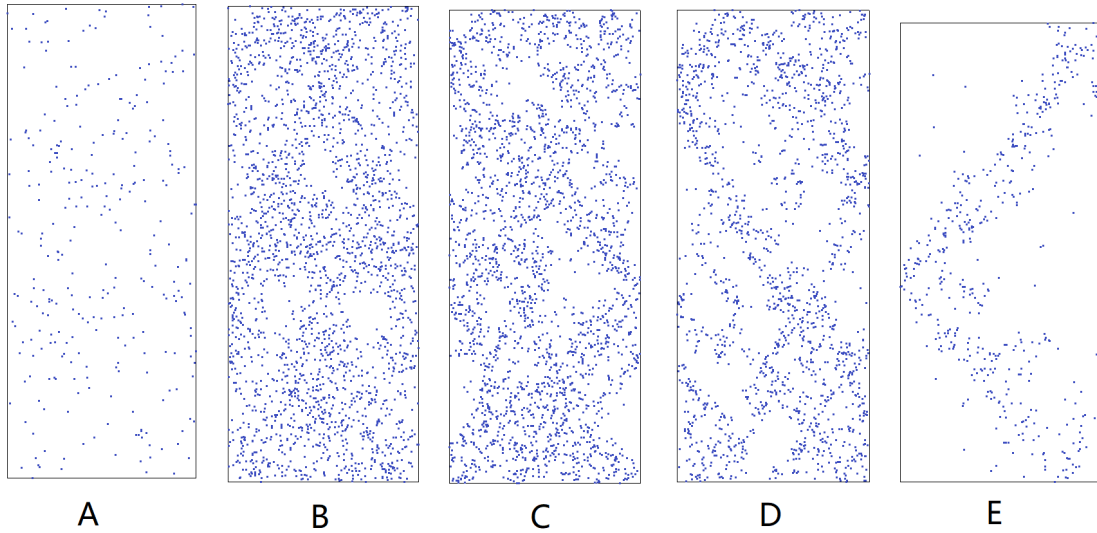


Figure 5: Spatial distributions of the contact sliding positions for different loading states.

the shear band area.

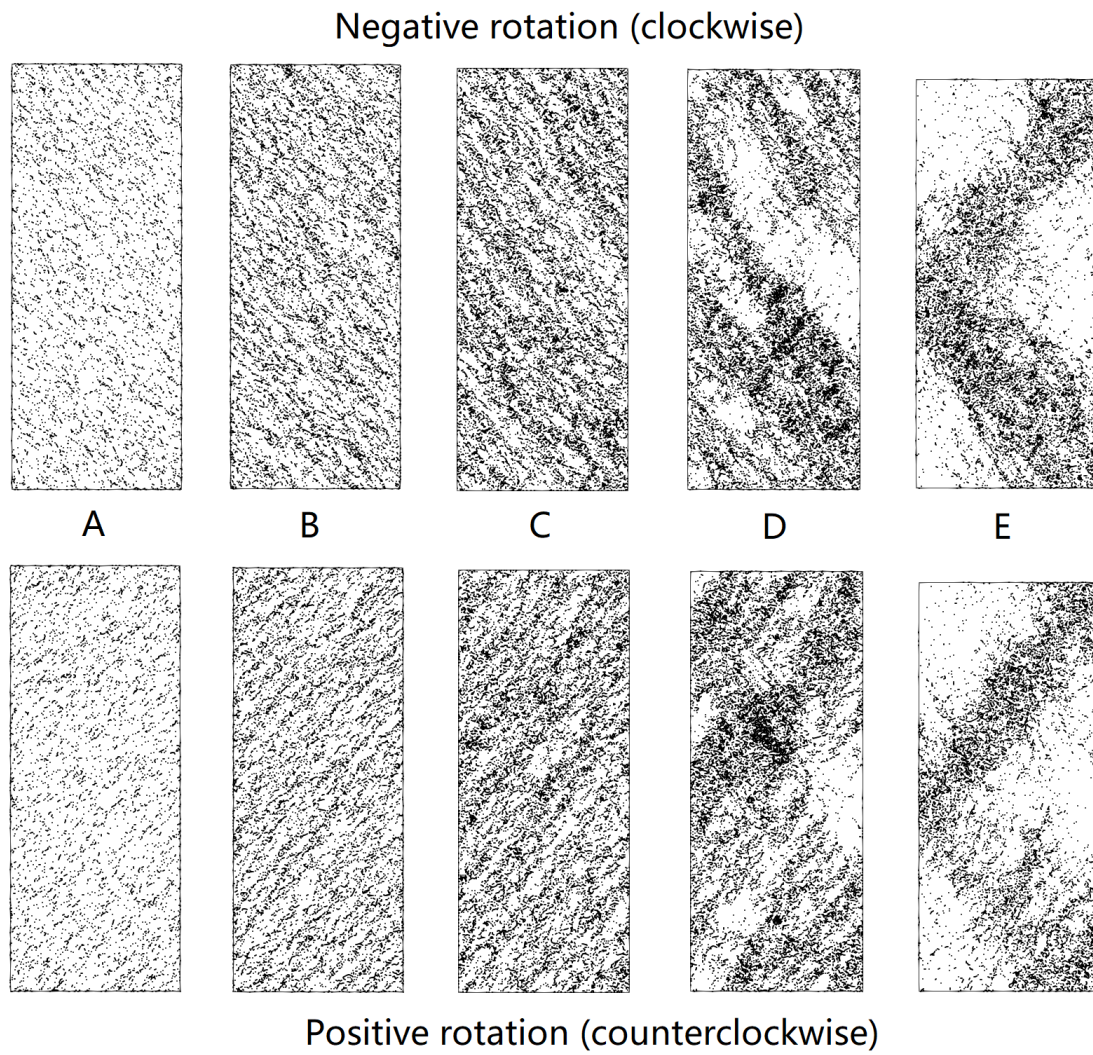


Figure 6: Spatial distributions of positive and negative particle rotation increments before stress peak for Sample DP in [Appendix A](#).

181 To better exhibit the rotation distribution features, we define the mean incremental rotation
 182 of the particles belonging to a particular meso loop k ⁵:

$$R_k = \frac{1}{A_k} \sum_{i=1}^{P_k} R_i A_i^{partial} \quad (2)$$

183 where A_k is the area of k , P_k means the particle number forming loop k , R_i is rotation increment
 184 of particle i , and $A_i^{partial}$ denotes the partial area of particle i included in loop k . R_k gives the
 185 information of the mean rotation increment at mesoscale and smooth the rotation increment
 186 fluctuating at the grain scale.

187 Figure 7 gives the distributions of the incremental rolling of loops for the 5 corresponding
 188 states. Similar but clearer than the pattern shown in Figure 6, the distribution of incremental
 189 rotation before State C not only corresponds to the strain field features shown in Section 3.1, but
 190 also exhibits the direction preference. In what follows, we name the shear structures “\” as left
 191 slip structures, and the shear structures “/” as right slip structures. It is clear that left shear
 192 structures contain most clockwise particle rotation while right shear structures contain most
 193 counterclockwise particle rotation. As the biaxial loading processes, the local slip structures are
 194 no more diffusely distributed but more and more clustered until the final shear band emerges,
 195 which is clearly illustrated in Figure 7 from State C to State E. When the shear band finally
 196 forms, it can be observed that the average incremental rotation direction is consistent with the
 197 shear band orientation: at State E, two bands of right and left orientations contains mostly
 198 clockwise (red points) and counterclockwise (blue points) rotations respectively. Moreover,
 199 Figure 7 indicates that right shear bands also contain a noticeable fraction of counterclockwise
 200 rotation increment and vice versa. This highlights the fact that mesoscale rotations are not
 201 limited in one direction of a single band, which may be a sign that shear bands are composed
 202 of a collection of smaller mesostructures with different orientations (discussion in Section 6.2).

203 Based on those observations, we can preliminarily conclude that contact sliding and particle
 204 rotations are related to the meso shear structures and probably control the shear band initiation
 205 from the meso scale. As we have defined the “incremental shear strain chain” (briefly “shear
 206 chain”) as the specific meso representative shear structures, in the following sections, we will

⁵Note that here the average rotation increment of one loop does not correspond to the rotation increment of the whole structure including void, R_k is considered for better showing the rotation features of meso slip structures with different directions.

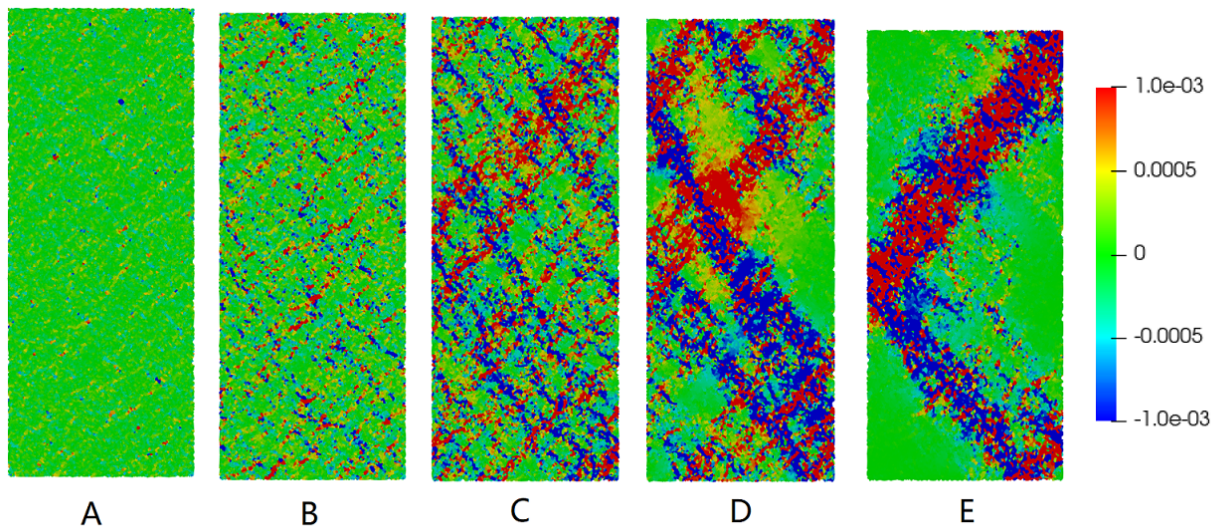


Figure 7: Spatial distributions of the large positive and negative incremental rotations of particles within Sample DP for different loading states (Positive: counterclockwise; Negative: clockwise).

207 use the shear chain concept to investigate the inmost mechanism.

208 4. Orientations of shear chains and shear bands

209 Inspired by force chain detection method [44, 45, 58, 50], the meso slips within granular
 210 materials have been defined as “incremental shear strain chains” in Liu et al. [49], which can
 211 basically describe the meso slip features within granular assemblies under shearing. Briefly,
 212 “incremental shear strain chain” is called “shear chain”, denoting that meso loops with large
 213 incremental deviatoric strain are connected to form a single shear chain structure with the
 214 consideration of the shear and geometrical directions. The precise definition of shear chain is
 215 shown in Section 2, and more details can be found in Liu et al. [49].

216 Under deviatoric loading, the spatial diversity of shear chains are initially homogeneous and
 217 random in space before the development of shear bands. In Figure 8, a large number of shear
 218 chains at State B and C of the sample are presented with different colors. At States B and
 219 C, the stress peak is not reached yet and the kinematic pattern is still diffuse and fluctuating
 220 (Figure 4). Shear chains detected in Figure 8 denote the areas of large incremental deviatoric
 221 strain triggered by local shearing, which reflects the main features of the meso slip structure.
 222 The preferred orientation $\langle |\theta| \rangle$ ⁶ of shear chains (proposed in Section 2) is near to $\pm 45^\circ$ to
 223 the horizontal plane from the beginning of the loading, and State C seems to show a little larger

⁶When we talk about the orientation for shear chains or shear bands, the acute angle to the plane of major compression is considered.

224 value of this angle than that in State B since the shear band is becoming initiated. In fact, the
 225 orientation of shear chains corresponds to the stress ratio at the macro scale and is independent
 226 from the loading path, boundary conditions and void ratios of the granular material, which has
 227 been carefully investigated in our previous study [49, 48]. This is a material property ruled by
 the continuum mechanics principles.



Figure 8: Shear chain distributions within the sample for States B and C.

228
 229 Unlike mesoscopic shear chains, shear bands denote a macroscopic band-like zone of fi-
 230 nite thickness where large shear deviatoric strains are intensely distributed. In a continuum
 231 framework, this zone is delimited by strain discontinuity surfaces with continuous strain dis-
 232 placements.

233 Based on the classical theory, the inclination of shear bands is related to the internal friction
 234 angle φ and the dilatancy angle ψ of the material considered. The angle of shear band to the
 235 direction of minor principal stress is usually expressed as $\theta_{sb} = 45^\circ + \frac{\varphi + \psi}{4}$. However, the
 236 boundary conditions may also have a strong influence on the shear band inclination, especially

237 when the boundary is rigid. Then in a discrete framework with a piecewise constant strain
 238 field, characterizing the shear band domain is a challenging task which is too often achieved
 239 only by naked eyes.

240 In order to determine the orientation of the shear band in an objective way, the Standard
 241 Deviatorial Ellipse method can be used. This method has been widely applied in geography
 242 sciences [59], and defines an ellipse with a preferred orientation based on the local gathering
 243 data in space. Lehoucq et al. [60] used the similar method to detect the cracks of rocks. In
 244 this study, we firstly select loop cells with incremental deviatoric strains larger than a given
 245 threshold (in this paper it is set as the average value of deviatoric strain) with the group size
 246 n , i.e., the number of loop cells which are selected; then examine the distribution pattern of
 247 these selected cells by observation roughly. If the observed pattern of selected cells show the
 248 existence of a single shear band in a particular zone, we can identify the orientation of this
 249 shear band by the following method:

- 250 1. Get positions of n selected loop cells with large incremental deviatoric strain, and compute
 251 the following matrix:

$$\mathcal{M} = \begin{bmatrix} var(x) & cov(x, y) \\ cov(x, y) & var(y) \end{bmatrix} = \frac{1}{n} \begin{bmatrix} \sum_{i=1}^n \tilde{x}_i^2 & \sum_{i=1}^n \tilde{x}_i \tilde{y}_i \\ \sum_{i=1}^n \tilde{y}_i \tilde{x}_i & \sum_{i=1}^n \tilde{y}_i^2 \end{bmatrix} \quad (3)$$

252 where x_i and y_i are the coordinates for each cell center, $\tilde{x}_i = x_i - \bar{x}$ and $\tilde{y}_i = y_i - \bar{y}$.

- 253 2. Compute the rotation angle of the ellipse γ

$$\tan \gamma = \frac{A + B}{C} \quad (4)$$

254 where

$$A = \left(\sum_{i=1}^n \tilde{x}_i^2 - \sum_{i=1}^n \tilde{y}_i^2 \right) \quad (5)$$

$$B = \sqrt{\left(\sum_{i=1}^n \tilde{x}_i^2 - \sum_{i=1}^n \tilde{y}_i^2 \right)^2 + 4 \left(\sum_{i=1}^n \tilde{x}_i \tilde{y}_i \right)^2} \quad (6)$$

$$C = 2 \sum_{i=1}^n \tilde{x}_i \tilde{y}_i \quad (7)$$

257 3. The equation of the standard deviational ellipse is then

$$\left(\frac{x}{r_x}\right)^2 + \left(\frac{y}{r_y}\right)^2 = s \quad (8)$$

258 where

$$\begin{aligned} r_x &= \sqrt{2} \sqrt{\frac{\sum_{i=1}^n (\tilde{x}_i \cos \gamma - \tilde{y}_i \sin \gamma)^2}{n}} \\ r_y &= \sqrt{2} \sqrt{\frac{\sum_{i=1}^n (\tilde{x}_i \sin \gamma + \tilde{y}_i \cos \gamma)^2}{n}} \end{aligned} \quad (9)$$

259 and $s > 0$ denotes the size of the ellipse ⁷.

260 In the above equations γ relates to the shear band direction when n selected cells belong to
 261 the shear band domain. The absolute value of shear band angle θ_{sb} is considered here: when
 262 $\gamma > 0$, $\theta_{sb} = 90^\circ - \gamma$; when $\gamma < 0$, $\theta_{sb} = 90^\circ + \gamma$. An example of the application of the Standard
 263 Deviational Ellipse can be found in the left side of Figure 9. For samples with multiple shear
 264 bands, this method can be used for different segments of selected zones, which is shown in
 265 Figure 10.

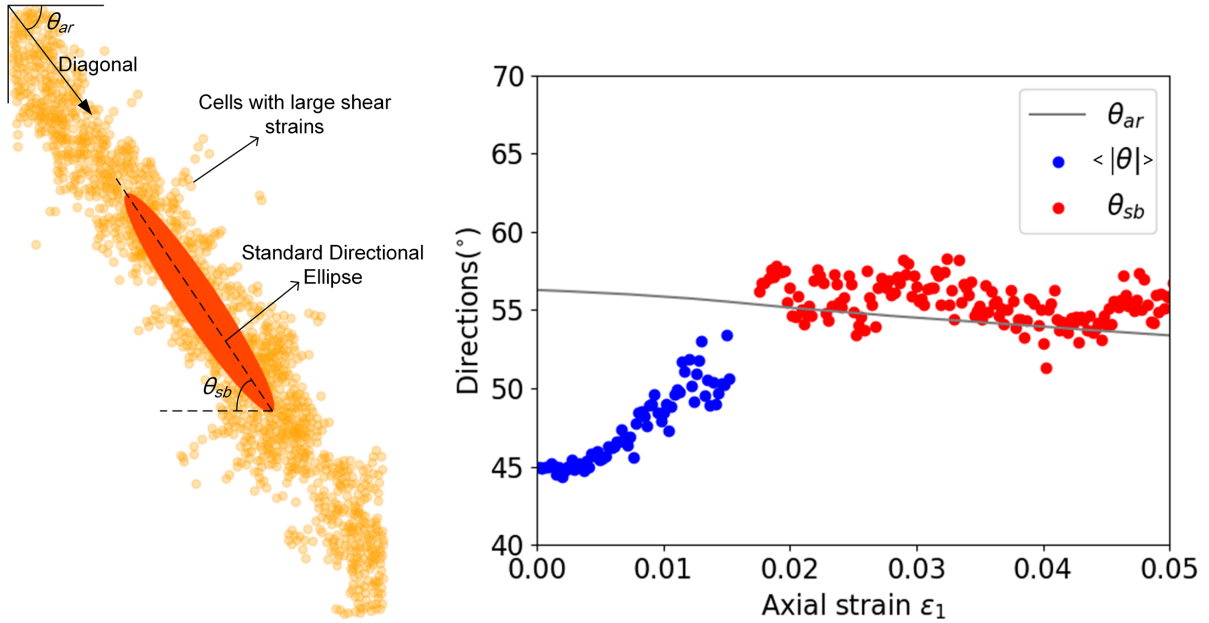


Figure 9: Example of single shear band (example of aspect ratio $L/W = 1.5$ in Appendix A) with the orientation determination based on the Standard Directional Ellipse method.

266 In Figure 9, the sample DF in Appendix A with a different aspect ratio $L/W = 1.5$ was
 267 selected to give an example of shear band orientation detection on the left side ⁸. The evolutions

⁷ s ($s > 0$) relates to the domain and density of data, and in this paper the value of s is not so important.

⁸It should be noted that the macro strain increment does not influence the evolution of shear chain and shear band orientations

268 of the average direction of shear chains $\langle |\theta| \rangle$ (blue points) and the shear band θ_{sb} (red points)
 269 are compared along the shearing process in the right side. Since the final shear band seems
 270 to connect the diagonal corners of the sample, the diagonal angle θ_{ar} evolution is also shown
 271 in Figure 9. It can be seen that θ_{sb} and θ_{ar} is close for this condition. Before the shear band
 272 forms, the shear chain direction $\langle |\theta| \rangle$ increases slightly from the beginning until the stress
 273 peak. After this stage, the shear chains are less easy to identify but the shear band orientation
 274 can be captured. The shear band orientation θ_{sb} is different from the initial mesoscopic shear
 275 chain direction $\langle |\theta| \rangle$ dictated by continuum mechanics principles.

276 If we consider biaxial tests of different aspect ratios (see details in Appendix A), the shear
 277 band orientations seem not unique although the particle size distribution, the density and
 278 the loading path are almost the same. For example, the granular assembly of aspect ratio
 279 $L/W = 2.5$ (Sample DP) gives rise to two shear bands of different orientations, as shown in
 280 Figure 10. The upper shear band and the lower shear band show reflecting features on the left
 281 boundary, while the orientations of them exhibit some differences during whole loading process
 282 (Figure 10): on the left of the figure, the crossing position of the two bands is not at the
 283 midpoint of the boundary; on the right of the figure, θ_{sb-up} and $\theta_{sb-down}$ evolve with different
 284 angles to the horizontal plane. Comparing to Figure 9, Figure 10 and the shear band patterns
 285 of all the samples in Appendix A, it should be concluded that the shear band orientation is
 286 not unique for a sample with given initial density and particle size distribution. The shear
 287 band orientation is then influenced by the sample aspect ratio, as also observed for Sample DI,
 288 DK and DL in Appendix A (shear band orientation evolution curves are not shown here). It
 289 turns out from the above findings that the shear band orientation is not a material property as
 290 such, although intrinsic properties still have some impacts [61]. Even for a single shear band
 291 of a given sample, the shear band orientation is not uniform and locally some kinks may occur
 292 [62]. We can see that in Figure 9 and Figure 10, the boundary of shear bands is not smooth
 293 but involves small crossing structures, and during softening stage these crossing structures are
 294 evolving. Then the macroscopic shear band might be a mixture of shearing behaviors at a
 295 lower scale, and the proposed shear chains could be regarded as a proper material body with
 296 an intrinsic orientation independent of the sample aspect ratios [49].

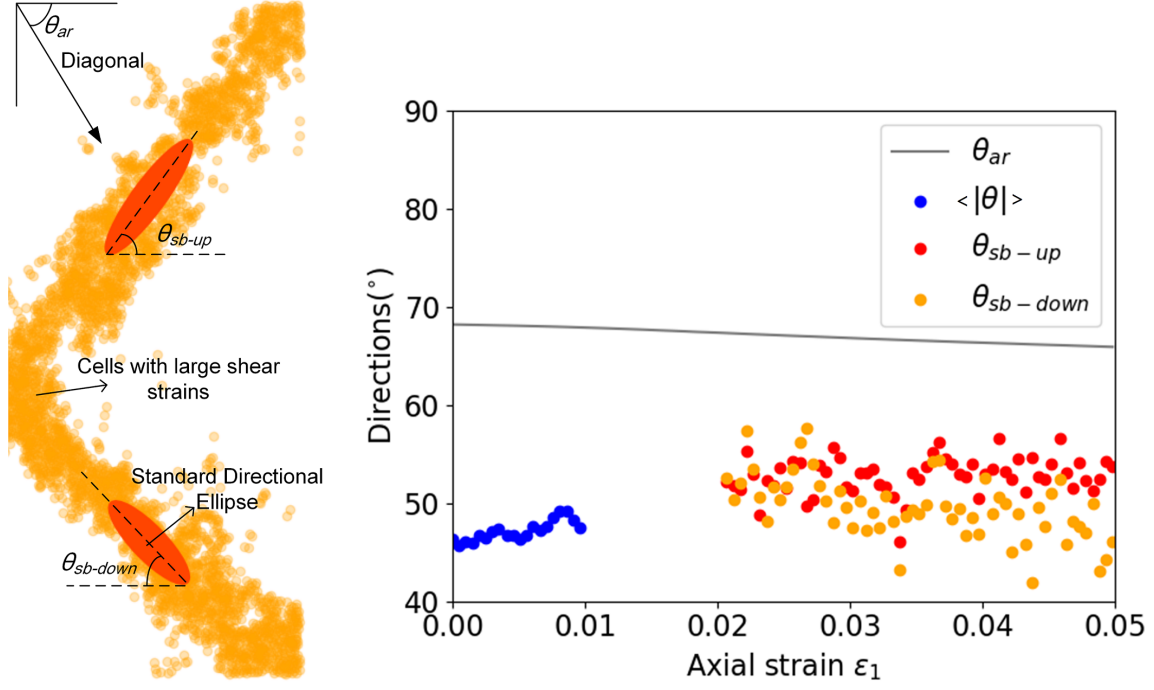


Figure 10: Granular sample with multiple shear bands of shear banding and evolutions of shear band and shear chain orientations ($L/W = 2.5$).

5. Microscopic fabric, sliding and rotation in shear chain

5.1. Fabric anisotropy within shear chains

Within the granular assembly, particles are connected by contact with forces, forming a fabric network on the whole. The fabric tensor Φ , defined from the normal directions to the contact planes between particles, has been widely used to describe the contact orientation density distribution in granular materials [27, 63, 64]:

$$\Phi_{ij} = \frac{1}{N_c} \sum_{c=1}^{N_c} n_i n_j \quad (10)$$

where N_c is the total number of contacts within the granular system, and $\Phi_{ii} = 1$.

As shown in Figure 1, shear chains are defined based on loop tessellation where a part of contact network is involved. Then each contact loop is eligible to be described by its own fabric tensor, similarly to Eq. 10:

$$\Phi_{ij}^l = \frac{1}{N_c^l} \sum_{c=1}^{N_c} n_i n_j \quad (11)$$

where N_c^l is the total number of contacts within a given loop. Under 2D conditions, the fabric anisotropy of each loop a^l is related to the deviations between the major and minor principal values of the fabric tensor Φ_{ij}^l , i.e., $a^l = \Phi_1^l - \Phi_2^l$, where $\Phi_1^l = 0.5(\Phi_{11}^l + \Phi_{22}^l) + ((0.5(\Phi_{11}^l -$

310 $\Phi_{22}^l))^2 + (\Phi_{12}^l)^2)^{0.5}$ and $\Phi_2^l = 0.5(\Phi_{11}^l + \Phi_{22}^l) - ((0.5(\Phi_{11}^l - \Phi_{22}^l))^2 + (\Phi_{12}^l)^2)^{0.5}$. In fact a^l describes
 311 the elongation of a given loop, the higher the value of a^l , the more elongated the shape of the
 312 loop [65].

313 In Figure 11, the evolutions of average fabric anisotropy for loops in shear chains A_{sc} and
 314 overall system A_{all} ⁹ are compared during biaxial loading (before shear banding). The 5 samples
 315 presented in Appendix A are selected for this analysis. It can be found that the average fabric
 316 anisotropy within shear chains shows mostly the unchanged trend along the deviatoric loading,
 317 while the average fabric anisotropy for the 5 samples overall stay increasing but lower than the
 318 shear chain anisotropy. The shear chain could be regarded as particular elongated zone with
 319 high average anisotropy in the granular assembly, irrespective to stress states and boundary
 320 conditions. In other words, the contacts in shear chain loops organized anisotropically in order
 321 to constitute meso shear structures.

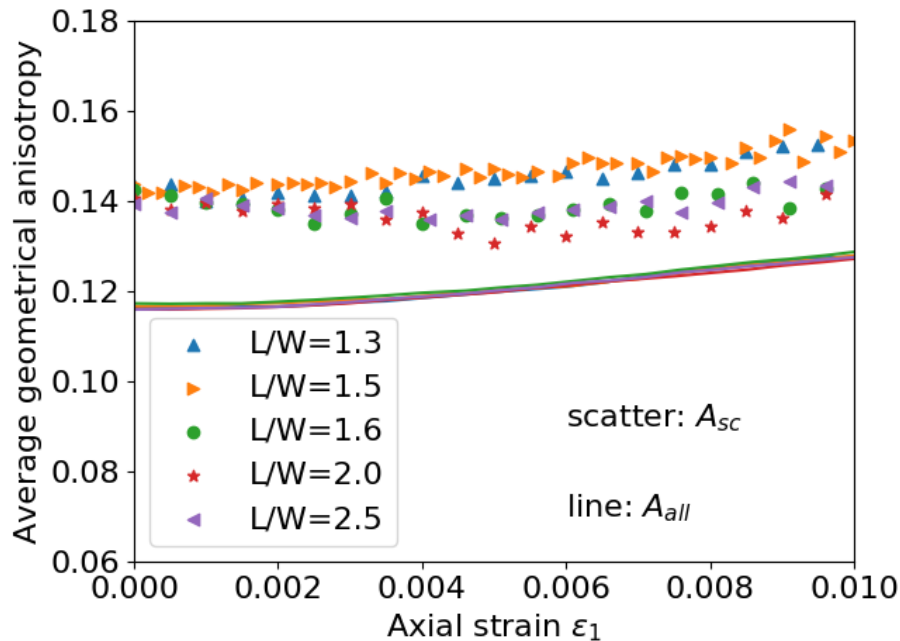


Figure 11: Average anisotropy comparisons for shear chain loops and overall system of 5 samples. Scatters are the anisotropy values for shear chains A_{sc} , and lines correspond to the anisotropy values of the overall system A_{all} . It should also be noted that nearly no difference can be found in A_{all} evolutions for the 5 samples.

322 5.2. Contact sliding statistics

323 At the macroscopic scale, failure occurs along a given loading path when a limit state is
 324 reached [46]. This means that for a particular choice of the loading parameters, a transition

⁹ $A_{sc} = \sum a^l / N_{SCL}$ and $A_{all} = \sum a^l / N_{ALL}$, where N_{SCL} is the number of loops in all shear chains and N_{ALL} is the number of loops within the whole granular assembly

325 from a quasi-static to a dynamic regime can occur [66]. At the microscale, contact sliding
 326 corresponds to the microscopic failures between two grains with relative tangent displacement.
 327 Being able to correlate microscopic and macroscopic failures is the corner stone to explain the
 328 origin of strain localization. Liu et al. [40] pointed out that contact sliding can be correlated
 329 with force chain bending, and when strain localization occurs, sliding contacts only exist within
 330 the shear band.

331 Since the shear chain can represent the slip lines, it is tempting to check whether the
 332 correlation exists between the contact sliding and shear chain structures. Based on the shear
 333 chain definition, contacts can be grouped as follows:

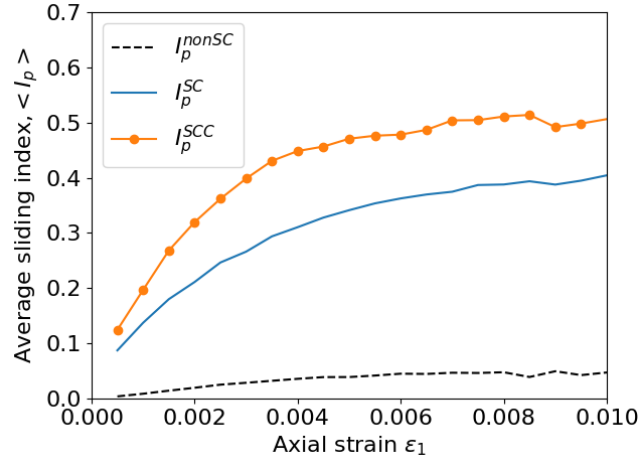
- 334 ► connection contacts (marked red in Figure 1) connecting two adjacent loops in shear
 335 chains, named “SCC”
- 336 ► contacts in shear chains but not belonging to connection contacts (dashed lines connecting
 337 particles in Figure 1), named “SC”
- 338 ► contacts not in shear chains, named “nonSC”

339 It should be noted that these 3 groups of contacts are mutually exclusive.

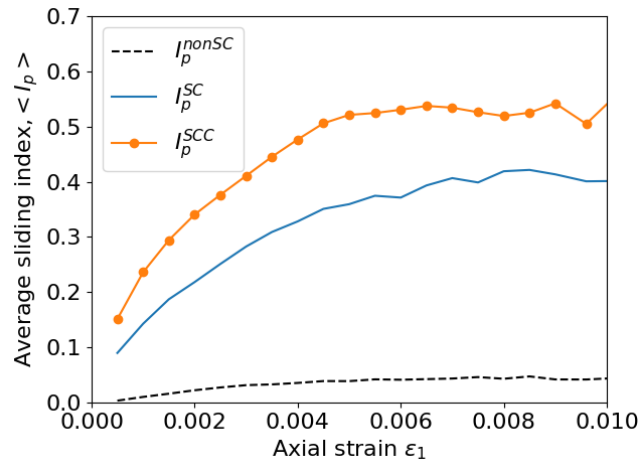
340 Evolutions of the average sliding index I_p ($I_p = \langle |f_t|/(\mu f_n) \rangle$) for these 3 groups are
 341 shown in Figure 12, and 3 samples of different aspect ratios in Appendix A are considered.
 342 Connection contacts “SCC” hold the highest magnitude of sliding index I_p , followed by the shear
 343 chain contact group “SC” and non-shear chain contact group “nonSC” respectively. Therefore
 344 connection contacts are like *bridges* in shear chains, their higher probability of sliding indicating
 345 the important role of sliding contacts in mesoscopic shear structure forming. Although sliding
 346 contacts have a preferred direction close to the lateral confining direction [49, 67], their influence
 347 on the incremental strain field involves geometric rearrangements captured at the mesoscale by
 348 shear chains. This observation strengthens the interpretation of shear chains as slip lines in
 349 continuum materials [48].

350 5.3. Particle rotation within shear chains

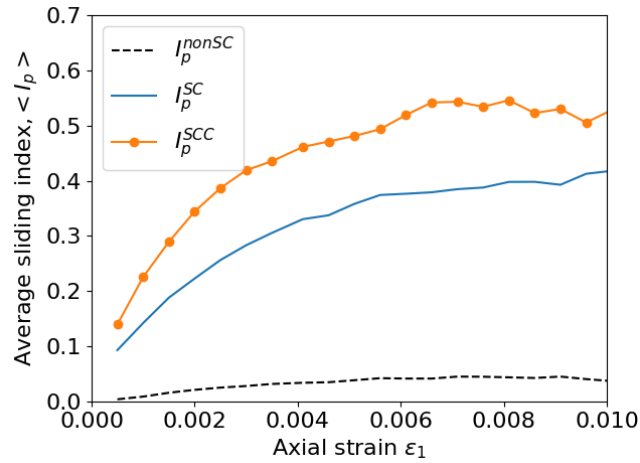
351 In Section 3.2, the incremental particle rotation distribution has been compared with the
 352 incremental deviatoric strain field. It has been proved that clockwise rotation and counterclock-
 353 wise rotation will concentrate along different (or opposite) orientations. Statistically, Figure 13



(a)



(b)



(c)

Figure 12: Average sliding index evolutions for connection contacts “SCC”, shear strain contacts “SC” and non shear chain contacts “nonSC”: (a) sample of aspect ratio $L/W = 1.3$; (b) sample of aspect ratio $L/W = 2.0$; (c) sample of aspect ratio $L/W = 2.5$.

354 ¹⁰ shows the average rotation evolutions of particles within left shear chain (oriented like “\\”),

¹⁰The green fluctuation points are due to some free particles of large rotations within the whole sample

355 right shear chain (oriented like “//”) and the overall system respectively for the sample of
 356 aspect ratio $L/W = 1.5$ (Sample DF in Appendix A). Particles in left shear chains almost own
 357 the negative value of rotation (clockwise) while particles in right shear chains have the mean
 358 rotation of positive value (counterclockwise), which corresponds to the observations in Section
 359 3.2 and also reported in Wang et al. [43]. For the overall system, the average rotation is nearly
 360 zero due to the offset of positive and negative rotations in general. The defined shear chain
 361 is proved to be able to capture the rotation features of meso shear behaviors. This observa-
 362 tion highlights the analogy between shear chains and slip lines where the slip motion generates
 363 rotation along the slip surface.

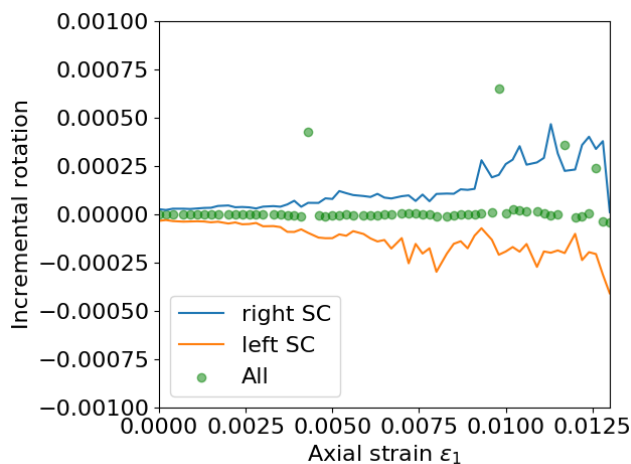
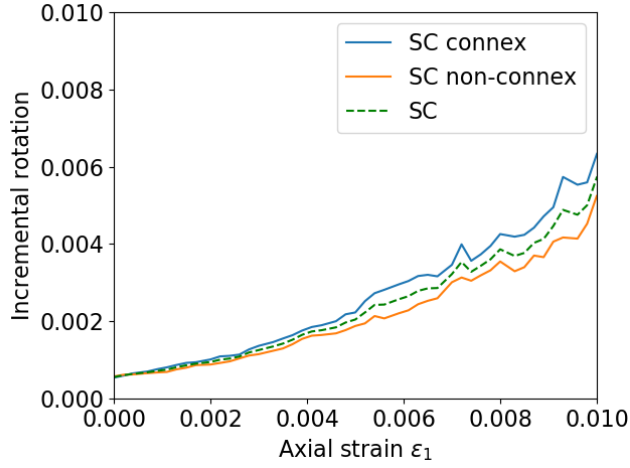
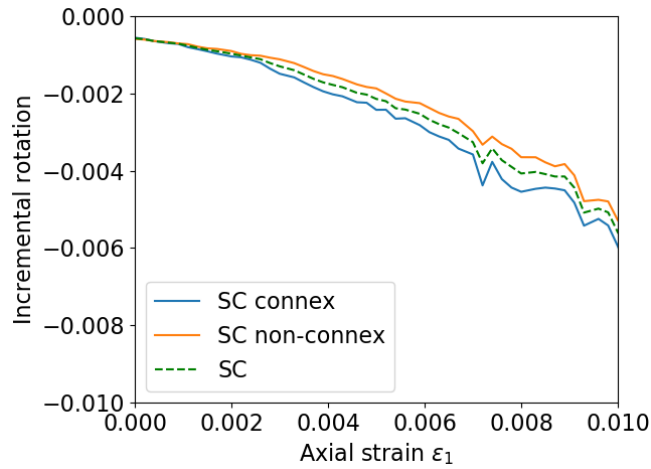


Figure 13: Average rotations for right shear chains “//”, left shear chains “\\” and all shear chains. “SC” means “shear strain chain” for simplification.

364 Like different groups of contacts analysed in Section 5.2, particles can also be divided to
 365 different groups to investigate the particular rotation features. As shown Figure 1, all the
 366 particles involved in shear chains could be the “SC” particles; the particles colored in green
 367 which are in the connection positions in shear chains, they can be labeled as “SC connex”
 368 particles; while particles in shear chains but excluded by “SC connex” could be the “SC non-
 369 connex” particles which are not colored in the figure. For left shear chains and right shear
 370 chains, we plot the evolutions of average incremental rotation for “SC connex” contacts, “SC
 371 non-connex” contacts and “SC” contacts in Figure 14 for sample DF, respectively. Although
 372 the magnitudes of the 3 groups do not diverge significantly, the absolute values of incremental
 373 rotations are larger at shear chain connection positions. In other words, the grains undergoing
 374 different incremental rotation direction (clockwise and counterclockwise) could also play an
 375 important role in forming the meso shear structures, i.e., shear chains.



(a)



(b)

Figure 14: Average incremental rotation for particles in connection contacts (SC connex), not in connection contacts (SC non-connex) and in shear chains (SC): (a) right shear chains; (b) left shear chains.

376 In Figure 15, we select several shear chains near the initial state of biaxial loading, and par-
 377 ticles of large absolute incremental rotation are highlighted together. The threshold 0.0005 rad
 378 (threshold details in Appendix B) is used to highlight large incremental rotations, and different
 379 colors denote the sense of rotation. Shear chains (a) and (e) are right shear chains, where pos-
 380 itive incremental rotations (counterclockwise) frequently appear; on the contrary, shear chains
 381 (b)-(d) correspond to left shear chains where negative rotations (clockwise) mainly occupy the
 382 center in connection positions. Particles with large incremental rotations (both positive and
 383 negative) can be found for a particular shear chain, although the proportions and positions
 384 diverge. That explains why in Figure 14, the difference between the 3 groups is not very large.
 385 The shear chain (f) in Figure 15 is left chain with blue particles (clockwise rotation), moreover,
 386 several particles excluded by the shear chain (f) are also shown with counterclockwise rotation

387 (orange color). The particles of orange color are connected along the opposite direction of
 388 shear chain (f) with quasi-linear feature, then the meso loops related to these particles could
 389 also form a shear chain but not detected in our current algorithm [49] since chain branches are
 390 not considered ¹¹. Since the crossing slip structures are obvious in the incremental deviatoric
 391 strain field (Figure 4), a given left shear chain is prone to be crossed by one or more right shear
 392 chains. Then the rotation near the crossing place might be mixed with both large positive and
 393 negative values, which causes the co-existence of counterclockwise and clockwise rotations for
 394 one shear chain.

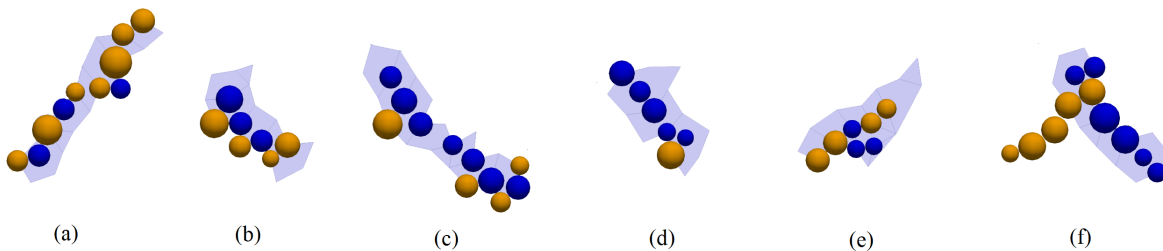


Figure 15: Examples of particles with large rotation (absolute value, orange denotes counterclockwise direction and blue denotes clockwise direction) and their spacial relations to the shear chains.

395 6. Discussion: links between multiscale shear behaviors

396 6.1. Shear chains and shear bands at different scales

397 Shear chains at meso scale can represent the meso slips during deviatoric loading. They
 398 relate to the concept of slip lines in plasticity (discontinuities in the displacement field), which
 399 is different from shear band (discontinuities in the strain field) [49, 48].

400 In Section 4, the orientation features are compared for shear chains and shear bands. Fur-
 401 thermore, the width and length are also important factors for comparison. In Figure 16, the
 402 zooming images of the shear strain field for shear chain area and shear band area are given
 403 for Sample DF. It can be observed that thin and quasi-linear shear chains are composed of
 404 loops with large incremental deviatoric strain, resulting in the width around a few times the
 405 particle diameter. While for the width of shear bands, it should be dozens of particle diameters

¹¹In Liu et al. [49], we developed the method for searching shear chains. Similar to the definition of force chains [44], the current algorithm for capturing shear chains is not perfect because only one branch can be extracted when the crossing point is met. Despite all this, significant features of shear chains are already well described by using the current method [49]. In our future work, the shear chain detection method will be improved from a topological perspective.

406 according to some publications [40, 68]. Besides, the direction of the incremental displacement
 407 of the particles is shown with unit arrows in Figure 16. It can be noted that the direction of the
 408 displacement field is slightly tilted when crossing the shear chain. As for the shear band, the
 409 incremental deviatoric strain field exhibits large fluctuations, and vortices exist as highlighted
 410 by the incremental displacement directions in Figure 16(b). These observations are consistent
 411 with results reported in [19, 69], indicating that shear chain and shear band are involved with
 412 different micro-structural features.

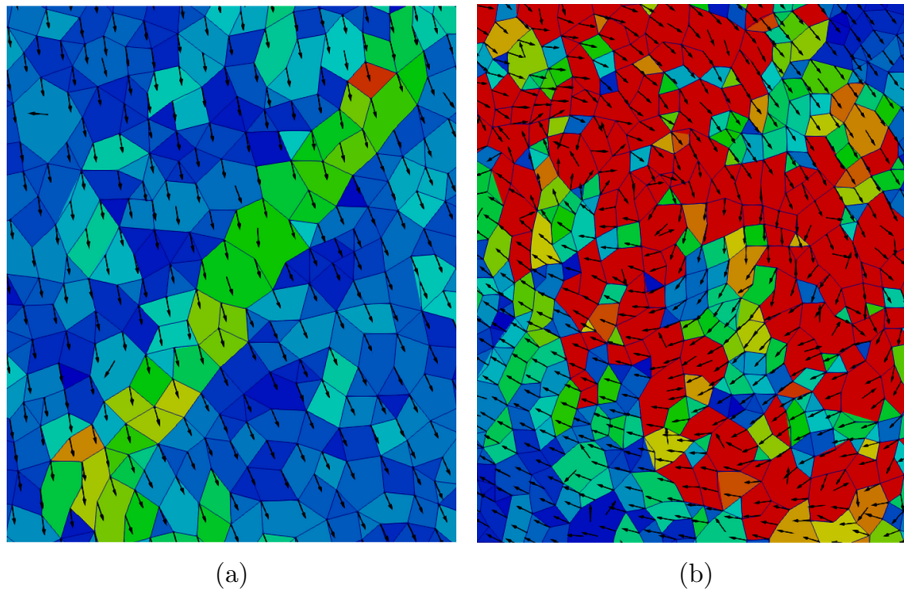


Figure 16: Zoomed images of incremental strain fields compared to the direction of the displacement field: (a) domain of a meso shear structure; (b) part domain of shear band.

413 According to the investigations till now, Table 1 reports the differences between these two
 414 structures. The length and width of shear chains and shear bands are described by the average
 415 diameter D_{50} of the granular samples. The shear chain length is evolving during the biaxial
 416 shearing, with a slight increasing trend.

Content	Shear band	Shear strain chain
Width	8-40 D_{50}	1-3 D_{50}
Length	Size of specimen	Several D_{50} , evolving
Direction	Affected by slip direction and boundary	Unique, maybe related to plastic theory
Displacement field	Evident vortex	Small rotation

Table 1: Comparisons of the shear band and the shear strain chain.

417 Although shear band and shear strain chain are different in terms of scales, they can be
 418 correlated under some reasonable assumptions. Shi and Horii [70] firstly proposed a simple
 419 microslip model to describe the origin of shear banding in sand deformations by assuming

420 internal defects within the specimen. In recent years, meso Mohr-Coulomb theory has been
421 adopted in describing the mesoscopic shear behaviors of amorphous materials [54, 71]. Houdoux
422 et al. [47] used two incremental scales (fast and slow temporal correlations) to explain the
423 evolutions of shear banding and micro-bands. Darve et al. [48] demonstrated that meso slip
424 lines and shear bands are distinct localized objects and discussed why and how the network of
425 meso-slip lines is bifurcating into a set of few macro-shear bands. The literature agrees that the
426 mesoscopic shear structure (micro-band or shear chain) and the ultimate chronic shear band
427 exhibit different geometrical and mechanical features, and it is often proposed that the meso
428 shear structures may aggregate in a dense distribution within the shear band to create this
429 larger structure. Therefore, we believe that shear band and shear chain should be strongly
430 correlated. Combining the micro failure distribution features analysed in Section 5, we can
431 assume the shear chain concept as the bridge connecting shear behaviors of multiscales.

432 *6.2. Bridging role of shear chains*

433 In Section 3, the microscopic failures are shown to concentrate within the shear band;
434 and in Section 5, the microscopic failures are proved to be correlated to the meso shear chain
435 formation. Therefore we can conjecture that meso shear chains triggered by sliding and rotation
436 are concentrated within shear bands. According to the present analysis and some literature
437 review (such as Houdoux et al. [47]), the possible relations between shear chains and shear
438 bands are drawn in Figure 17. Figure 17(a) corresponds to a regular arrangement of shear
439 chains and Figure 17(b) corresponds to a collection of shear chains of symmetric orientations
440 (with respect to the axial direction) in shear bands.

441 Figure 18 shows an example of the spatial distribution of large counterclockwise and clock-
442 wise incremental rotations for a shear band within a granular sample (Sample DF in Appendix
443 A). Within the shear band, particles with large rotation increments of different directions are not
444 arranged in order by two preferred orientations in Figure 18. At the stages before shear band-
445 ing, the incremental rotation fields are corresponding to shear chains of opposite orientations,
446 as shown in Figure 6 and Figure 7; examples in Figure 15 further demonstrate the correlation
447 between shear chains and particle rotations. Therefore, a stochastic-structured pattern of shear
448 chains in shear bands could be proposed from the perspective of kinematic rotation features,
449 which demonstrates that Figure 17(b) could approach the real situation. This hypothesis is
450 also supported by the fact that inside the shear band, the normal displacement field shows large

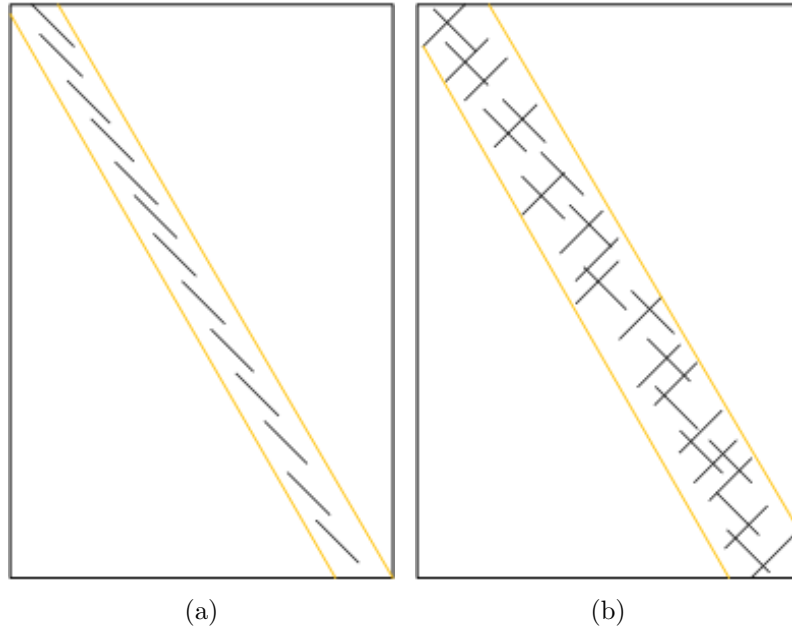


Figure 17: Schematic representation of the relationship between shear band and shear chains. Shear chains are denoted by dark straight short lines and the shear band zone is between the two yellow lines. Case (b) is conjectured to approach the actual situation compared to Case (a).

451 variations even vortices. As shown in Figure 16(b) and reported in literature [69], shear chains
 452 (or microbands) oriented in only one preferred direction could not induce large fluctuations like
 453 vortices. Houdoux et al. [47] also reported the same observation according to the spatial and
 454 temporal correlation analysis.

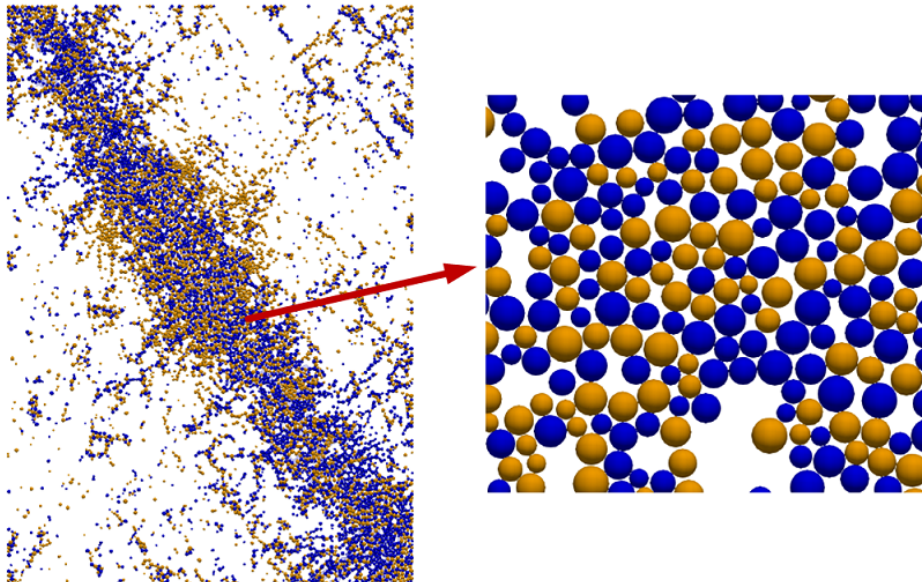


Figure 18: Particles of large incremental rotations (the orange denotes counterclockwise direction and the blue denotes clockwise direction) for a state when the shear band forms.

455 As shear banding has been a concerned issue in geomechanics for a long time, microscopic or
 456 mesoscopic representations inside the shear band have been studied from various perspectives.

457 For example, it has been shown that force chains rotate and bend inside shear band [52],
 458 sliding contacts and rotations accumulate inside the shear band [40, 62], and meso loops of
 459 large size appear inside shear band [11]. We define the shear chains as meso slips to represent
 460 the strain localization phenomena before shear band occurs [49], and manage to correlate
 461 this meso shear structure to shear behaviors at macro and micro levels. According to the
 462 analysis in this paper, the difference between shear band and shear chain has been clarified
 463 and the roles of microscopic shear behaviors on shear chains are preliminarily identified. Since
 464 microscopic failures commonly occur inside the shear band and they may trigger the shear chain
 465 formation, we assume that shear chains should be randomly distributed within the shear band,
 466 as illustrated in Figure 19. Microscopic failures such as sliding and particle rotation play key
 467 roles in forming shear chain structure (on the right of Figure 19), since the connection positions
 468 are commonly controlled by sliding contacts and particles of large rotation. The bridge from
 469 micro to macro shear behaviors could therefore be related to the meso shear chains. Shear
 470 chains could provide a missing link between micro to macro shear behaviors.

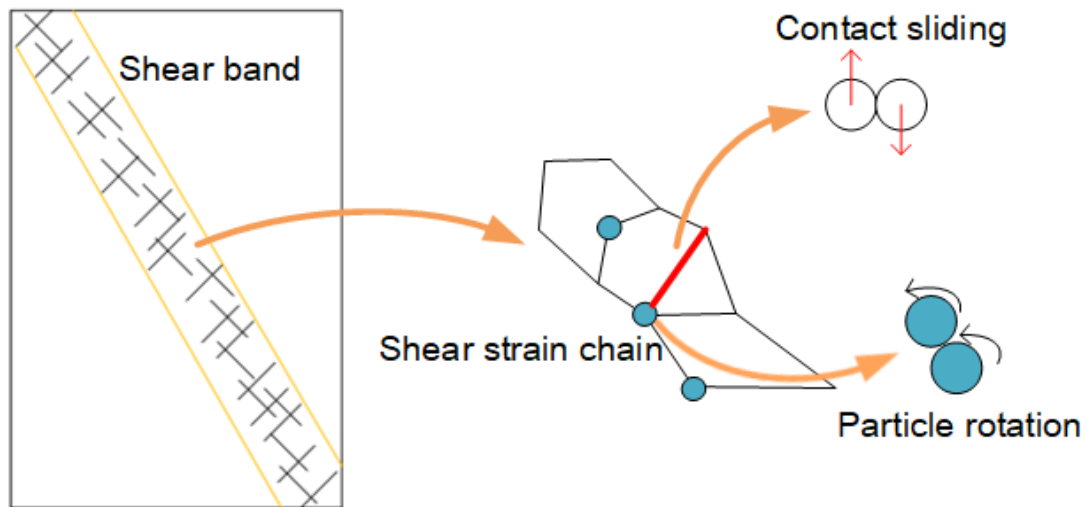


Figure 19: The bridge role of meso shear strain chains from microscopic to macroscopic shear failures.

471 This is our preliminary study and assumption of the bridge role of shear chains in linking
 472 macro and micro behaviors, and future work is necessary in terms of theory development and
 473 verification in 3D real cases, for example. Besides, we only considers the pure rotation of
 474 particles in this paper, the adaption of shear chains on the system with background rotation,
 475 as discussed in Singh et al. [72], should be further investigated.

476 7. Conclusion and outlook

477 This paper deals with the shear behaviors at micro, meso and macro scales in granular
478 materials and relates them thanks to the concept of shear strain chain defined in our previous
479 studies [49, 48]. A series of DEM biaxial tests are considered, providing rich detailed information
480 on the multiscale shear features. Shear chains are proved to be influenced by the concentration
481 of contact sliding and particle rotation, and they generally keep a steady anisotropy. Shear
482 bands are failure zones of a higher scale, and are shown to be very sensitive to sample aspect
483 ratios. Results presented in this paper support the idea that shear bands forms as a collection
484 of shear chains in a given domain driven by boundary effects. Meticulously, we conclude as
485 follows:

- 486 1. During the biaxial loading process of densely packed granular materials, both the incre-
487 mental deviatoric and volumetric strain fields experience the transition from meso-scale
488 diffuse localization to the final shear band. The spatial distributions of microscopic con-
489 tact sliding and particle rotation also confirm this trend.
- 490 2. The method based on the Standard Deviation Ellipse is used to measure the shear band
491 orientation. The orientations of shear chains and shear band are different, as shear chains
492 are mesoscopic features governed only by material properties while shear band orientation
493 are even more influenced by the aspect ratios of the rigid boundary.
- 494 3. In shear chains, average contact fabric anisotropy is kept almost steady and higher than
495 the anisotropy of the overall system. Contact sliding mostly occurs in the connection
496 contacts of shear chains. Particles of large rotation increment are frequent inside shear
497 chains, and these particles of opposite rotating directions are associated with shear chains
498 of opposite orientations, behaving as the main kinematic mechanism within shear chains.
- 499 4. Shear chains are different from the macro shear band in terms of thickness, orientation,
500 theoretical background and relations to displacement field. As contact sliding and particle
501 rotation are at the connection positions in shear chains and they also have a strong spatial
502 correlation to the shear bands, we conjecture that shear chains may be included inside the
503 developing shear band with the disordered distribution and shear chains appear therefore
504 as a bridge between micro and macro shear behaviors.

505 This paper presents the preliminary study on the bridging role of shear chains, which have
506 been defined as the shear structures at the meso scale [49]. Although qualitative findings are
507 obtained for 2D granular systems under biaxial loading, we still need to extend our conclusions
508 to more general conditions, for example, the 3D case and the complex loading path. The
509 existence of shear chains for critical conditions, e.g., the minimal sample size and the minimal
510 strain increment, should be clarified. The projection method [73] can be considered in the
511 future work, to better discern the shear band orientation differences. In addition, we need to
512 develop the theory for shear chains in granular materials, and reveal the mysterious origin of
513 shear banding by combining other characterizations such as the vortex and force chain analysis.
514 There are some cases where shear bands are prevented but shear chains emerges, e.g., periodic
515 boundary and loose sample, how the meso shear chains will transfer during this failure process
516 should also be the interesting future work.

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523 the quality improvement of our paper are really appreciated.

524 **Appendix A. Biaxial tests of different boundary conditions**

525 For this study, a set of quasi-2D ¹² biaxial drained tests of samples with different aspect
526 ratios (length vs. width) are conducted. Firstly, all specimens were randomly generated within
527 large rectangular domains of prescribed aspect ratios, before being compacted by moving the
528 bounding boundaries to a prescribed isotropic confinement. As shown in Figure 2, the aspect
529 ratio is represented as L/W , where L denotes the length and W denotes the width. Rigid walls
530 were set as boundaries. Although the specimen sizes are different, the particle size distribution
531 is kept almost the same. The unique uniform distribution is chosen for each specimen, and the
532 ratio of the maximum diameter to the minimum D_{max}/D_{min} is nearly 1.98 with the average

¹²by considering a single layer of 3D particles

533 size $D_{50} = 8.4$ mm. For other parameters in the DEM simulations, the material density is
534 set to $\rho = 3,000$ kg.m⁻³, k_n/D_s is set to 300 MPa, where $D_s = 2R_1R_2/(R_1 + R_2)$ and R_1 ,
535 R_2 are the radii of particles in a given contact, and k_t/k_n is set to 0.5. All the specimens are
536 compacted to a desired isotropic stress state with confining pressure of $\sigma_0 = 100$ kPa. During
537 compression process, the contact friction angle between particles for each sample is set as 2°
538 to reach a relative dense state. Gravity is not considered, and the boundary conditions are set
539 as rigid frictionless walls. After this isotropic compression, the friction angle ϕ is set to 35° for
540 the biaxial deviatoric loading. During the biaxial loading, the inertial number $I = D_{50}\dot{\gamma}\sqrt{\rho/p_0}$
541 ¹³ is lower than 2×10^{-6} which is small enough to meet quasi-static requirement.

542 The sample parameters for the drained biaxial tests are summarized in Table A.1. For
543 those 16 samples, only the aspect ratio L/W and the particle number are different at the initial
544 compacted states. The slight changes in void ratio V_r can be neglected. The sample chosen in
545 Section 2 is Sample DP. When conducting the drained biaxial loading, a compression is imposed
546 in the vertical direction with a constant strain rate of $\dot{\epsilon}_1 = 0.01$ s⁻¹ and the lateral pressure is
547 maintained constant to $\sigma_2 = 100$ kPa.

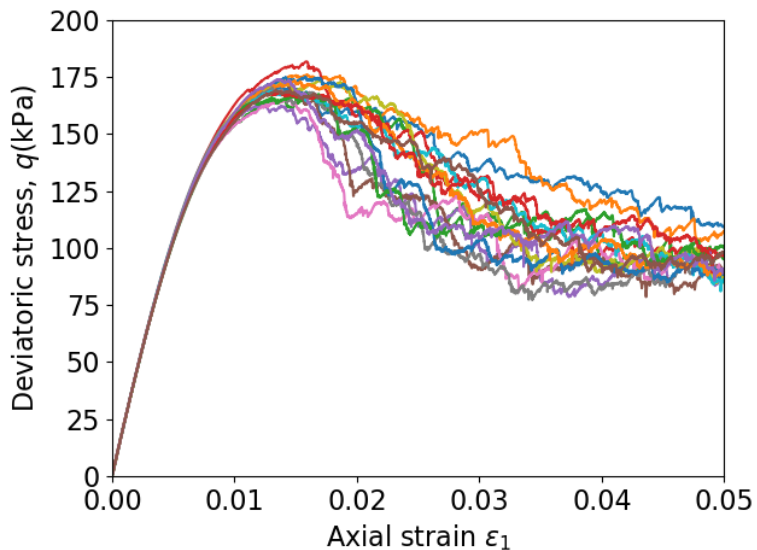
Sample	L/W	N_p	D_{max}/D_{min}	D_{50}	Initial void ratio V_r
DA	1.0	13333	1.98	8.4 mm	0.0162
DB	1.1	14667	1.98	8.4 mm	0.0161
DC	1.2	16000	1.98	8.4 mm	0.0161
DD	1.3	17333	1.98	8.4 mm	0.0161
DE	1.4	18667	1.98	8.4 mm	0.0161
DF	1.5	20000	1.98	8.4 mm	0.0161
DG	1.6	21333	1.98	8.4 mm	0.0161
DH	1.7	22667	1.98	8.4 mm	0.0160
DI	1.8	24000	1.98	8.4 mm	0.0161
DJ	1.9	25333	1.98	8.4 mm	0.0160
DK	2.0	26667	1.98	8.4 mm	0.0160
DL	2.1	28000	1.98	8.4 mm	0.0160
DM	2.2	29333	1.98	8.4 mm	0.0160
DN	2.3	30667	1.98	8.4 mm	0.0160
DO	2.4	32000	1.98	8.4 mm	0.0159
DP	2.5	33333	1.98	8.4 mm	0.0159

Table A.1: Sample parameters of drained DEM tests.

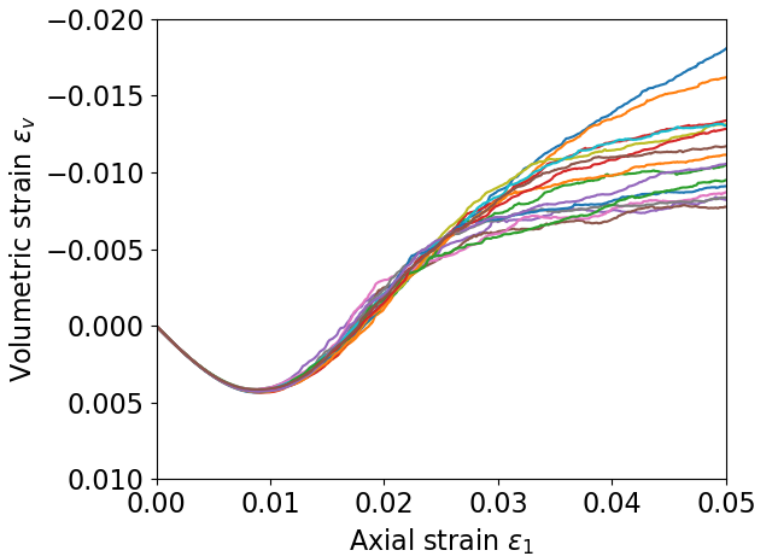
548 Under biaxial loading, the overall stress-strain responses of the drained biaxial tests of
549 different L/W are shown in Figure A.1. It can be observed that nearly no differenc can
550 be found for the deviatoric stress evolution curves before the stress peak state (the onset of

¹³ D_{50} denotes the average diameter; $\dot{\gamma}$ is the shearing rate; p_0 means the average stress.

551 softening) of 16 samples, and the large divergences after the stress peak could be attributed to
 552 the bifurcation development.



(a)



(b)

Figure A.1: Evolutions of deviatoric stress q (a) and volumetric strain ε_v (b) during drained biaxial tests with axial strain rate $\dot{\varepsilon}_1 = 0.01 \text{ s}^{-1}$ and lateral confinement $\sigma_2 = 100 \text{ kPa}$. Different curves correspond to different aspect ratios L/W . We ignore the labels of the samples since all the curves share the same period before the stress peak.

553 For all the drained biaxial tests of dense samples, chronic shear band appears from the point
 554 near stress peak to the final state. The patterns of shear bands are diverse, as shown in Figure
 555 [A.2](#). Under some conditions, a single shear band is identified (aspect ratio $L/W=1.4, 1.5, 1.6,$
 556 $1.7, 2.0$ and 2.1); while multiple shear bands with reflections can be found for other cases. It is
 557 clear that the shear band event does not hold unique features when the aspect ratio is changed.

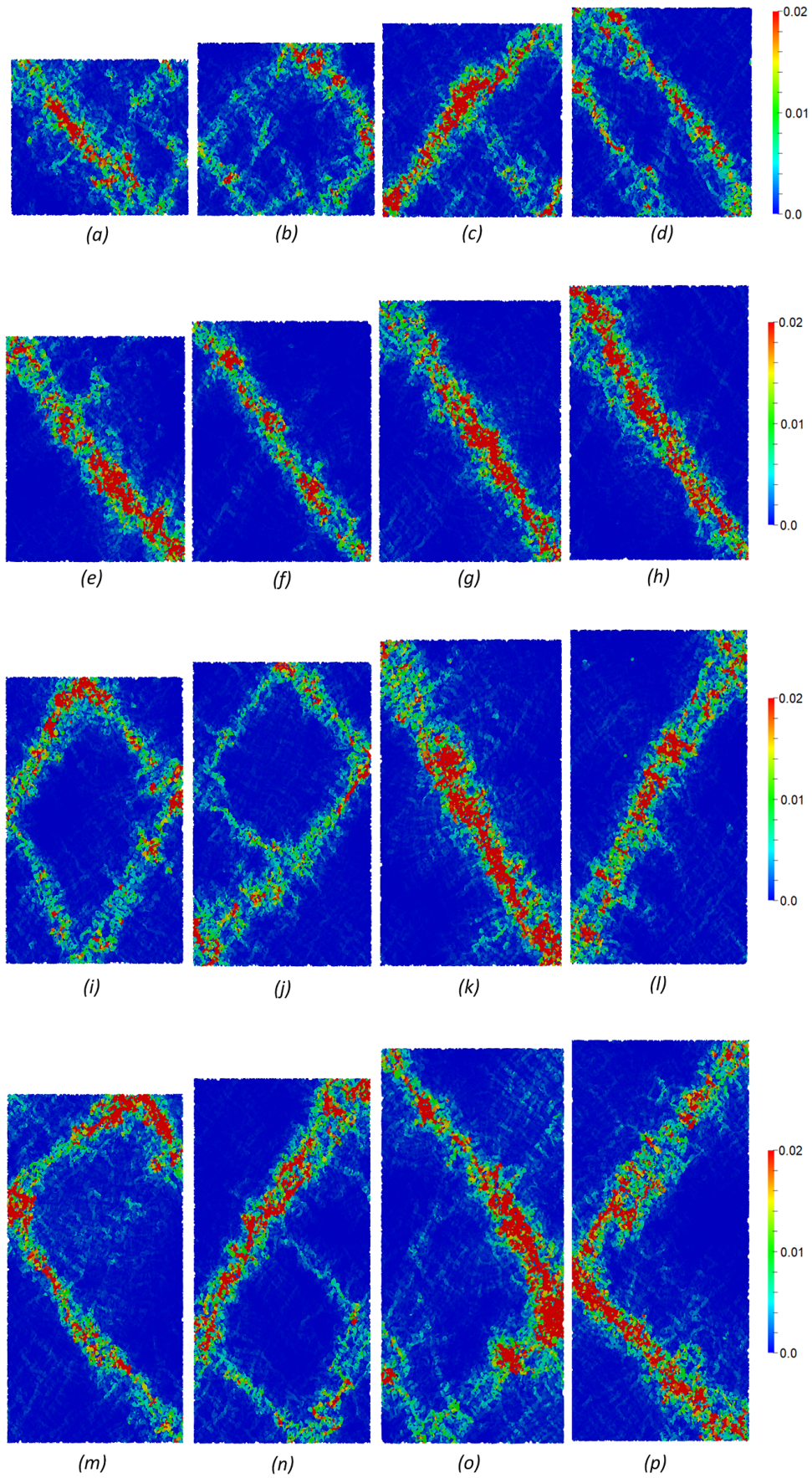


Figure A.2: Shear band patterns for specimens of different aspect ratios: (a) $L/W = 1.0$; (b) $L/W = 1.1$; (c) $L/W = 1.2$; (d) $L/W = 1.3$; (e) $L/W = 1.4$; (f) $L/W = 1.5$; (g) $L/W = 1.6$; (h) $L/W = 1.7$; (i) $L/W = 1.8$; (j) $L/W = 1.9$; (k) $L/W = 2.0$; (l) $L/W = 2.1$; (m) $L/W = 2.2$; (n) $L/W = 2.3$; (o) $L/W = 2.4$; (p) $L/W = 2.5$.

558 **Appendix B. Threshold of large rotation increments in sheared granular assembly**

559 In this paper, a number of quantities for meso or micro structures are calculated by the
560 incremental form. All the increments are compared by two successive states with the macro
561 strain increment of 0.0005, as well as the incremental rotation of particles. When defining
562 particles of large rotation increment (absolute value) in this paper, a threshold 0.0005 rad is
563 used. The chosen value results in clear images of featured patterns of rotation increment field.
564 Figure B.1 gives an example of rotation increment distributions by using different thresholds
565 for Sample DP in Appendix A at State B. When the threshold is too small (0.0001 rad) or too
566 large (0.01 rad), the featured pattern of rotation increment field can not be well captured. We
567 choose the value of 0.0005 rad to measure the large rotation increment in this paper, since the
568 field pattern is clear and a large number of particles are included. It should be noted that the
569 threshold 0.0005 rad is applicable for simulations of this study, when considering other cases a
570 new threshold should be given with the respect to the strain increment between two successive
571 states.

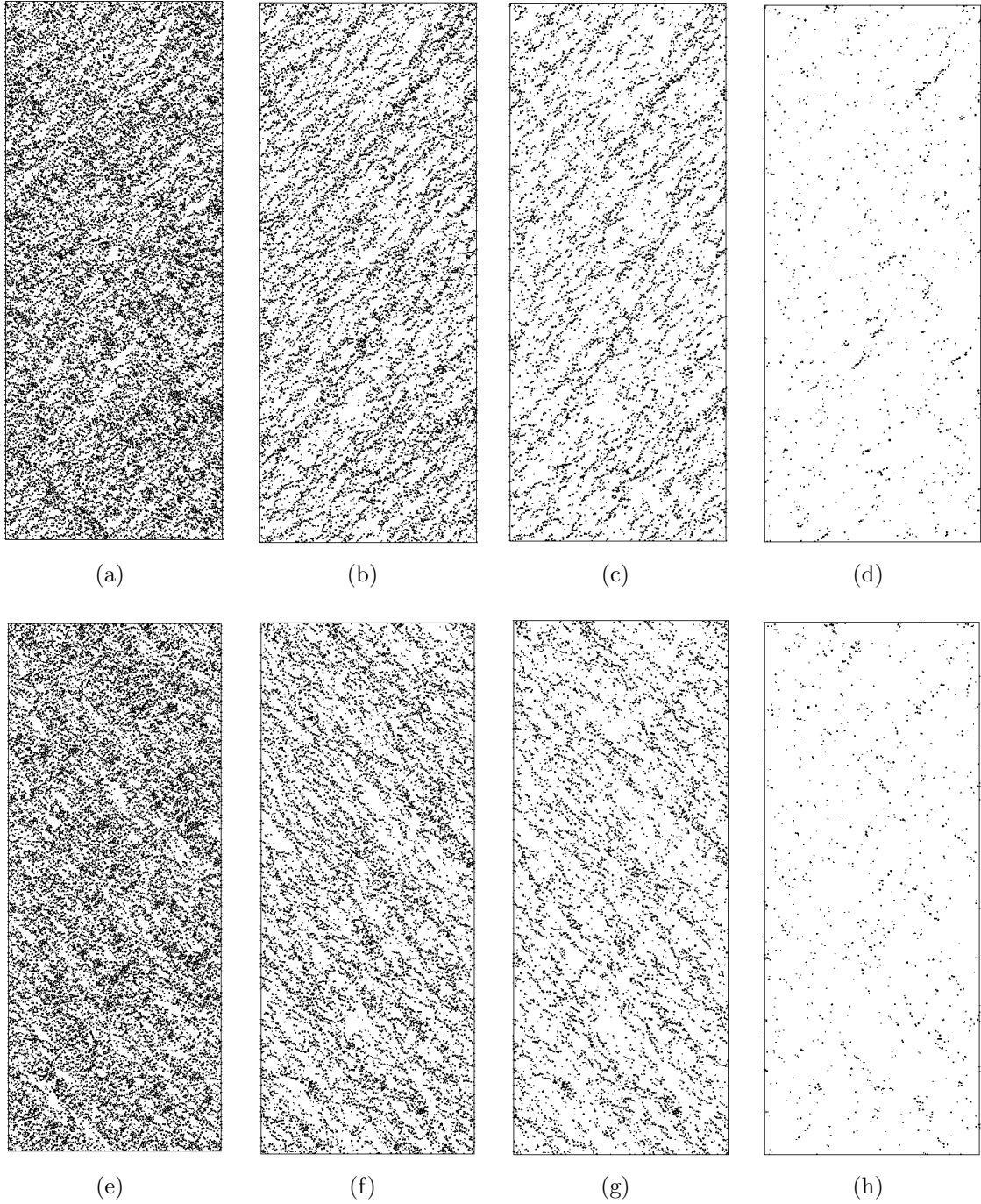


Figure B.1: Distribution maps of particles with large rotation increments. Different thresholds are set as: threshold 0.0001 rad for (a) positive and (e) negative rotation increment; threshold 0.0005 rad for (b) positive and (f) negative rotation increment; threshold 0.001 rad for (c) positive and (g) negative rotation increment; threshold 0.005 rad for (d) positive and (h) negative rotation increment.

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