Micromechanical aspects of soil plasticity:  
An investigation using a discrete model of polygonal particles.

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We investigate the quasistatic mechanical response of soils under monotonic loading using a discrete model of randomly generated convex polygons. The biaxial test is implemented using loading platens and confining stress applied through a membrane. These boundary conditions lead to strain localization as a typical mode of failure. Shear bands result from the buckling of chain forces, the length of those chain forces giving the characteristic width of the shear bands. The incremental response before failure is calculated from the numerical simulations. This response leads to nonlinear elasticity, non-associated plasticity, and instabilities strictly inside of the plastic limit surface. We explore the connection between the anisotropy of the contact network and the stiffness, and the role of the sliding contacts in the flow rule of plasticity.

1 INTRODUCTION

In his paper “The misery of constitutive modeling” Kolymbas wrote: "The main shortcoming in the field of constitutive modeling is that each researcher (or group or researchers) is developing his own constitutive model. This model is in most cases very intricate and, thus non-relocative, i.e. another researcher is unable to work with it. I can report from my own experience that it took me several months of hard work until I realized that I was unable to obtain anything with a constitutive model proposed by a colleague. How can relocativity be improved?” (Kolymbas 2004).

Let’s make clear from this remark that it is not completely true that there are as many constitutive models of soils as research groups working in soil deformation. In fact, some groups use more than one model in order to interpret their experimental results, or to implement their finite element codes. This is why there are probably more models than research groups.

Apart from the problem of proliferation of constitutive models, the large number of parameters they involved, most of which lack physical meaning, should also be mentioned. This problem has been pointed out by Scott in the workshop Constitutive Equations for Granular Non-cohesive Soils in 1988 (Scott 1988). He mentions that before 1960 the investigation of soils was restricted to the linear isotropic elasticity, which uses only two material parameters. He refers also to the important advance in the constitutive modeling starting with the Cam-clay model in 1968 (Roscoe and Burland 1968). This model led to the first non-linear representation of the plastic deformation of soils, containing five material parameters. Scott reports on subsequent constitutive models presented in 1978 and 1988 with 14 and 40 material parameters. These observations are presented in Fig. 1, which shows the number of parameters against the time. Using an exponential fitting of this data, Scott reported that the number of constants was growing at a Rate of 12% per year. Extrapolating this observation, he estimated that models developed in the year 2000 would have 184 constants! In contradiction to Scott’s predictions, no model has been reported with so many material parameters until now. However, the strong controversy concerning the validity of a large number of models and the lack of experimental meaning of the material parameters have led the practitioners to lost confidence in constitutive modeling. This has resulted in a gap between research and practice in
geotechnical engineering (Bolton 2002).

In geotechnical applications, it is desirable that the parameters of a constitutive relation depend directly on the properties of the grains. In the simple case of dry soils, granulometric properties can involve grain shape and angularity, distribution of grain sizes, friction coefficient and stiffness of the grains (Herle and Gudehus 1999). Instead of considering the granulometric properties, the existing models employ unfamiliar abstract quantities. This is probably due to the necessity to present a unified and rigorous formalism, without taking care of a direct relation of these quantities to the microstructure of the soils.

Recently, a large amount of work has been oriented toward the micromechanical aspects of soil deformation. This approach is motivated by the necessity to understand the effect of the geometry of the grains and the interparticle forces on the overall macromechanical response. There are however some limitations in this investigation, due to the difficulty to experimentally determine the micromechanical variables, such as contact forces and deformations at the grains. An alternative for the investigation of soils at the grain scale is the discrete element modeling (DEM) (Cundall and Strack 1979). Discrete approaches such as contact mechanics method (CM) (Jean and Moreau 1992; Moreau 1994) and the molecular dynamics (MD) (Thornton and Barnes 1986) take into account details like particle shape, size distribution, friction and cohesion between the grains. The interaction between the particles is modeled by the introduction of suitable contact forces. These forces are given in terms of a reduced number of parameters. The MD method introduces the normal and tangential stiffnesses, and the friction coefficients as the material constants of the grains. In CD the particles are supposed to be infinitely rigid, and the interactions between the grains are described by a Coulomb friction law with a single friction coefficient.

To compare simulations to the constitutive theories a homogenization technique is required. This is a formalism that allows one to derive macromechanical quantities from micromechanical variables. Different homogenization techniques have been used to derive the stress (Rothenburg and Selvadurai 1981; Goldenberg and Goldhirsch 2002; Bagi 1999) and the strain tensor (Lätzel, Luding, and Herrmann 2000; Bathurst and Rothenburg 1988; Kruyt and Rothenburg 1996; Bagi 1996) in terms of contact forces and deformations at the grains. There are some reasons why these average quantities are still not well determined: First, different averaging procedures lead to symmetric or anti-symmetric stress tensor (Bardet and Vardoulakis 2001). Second, the micromechanical definition of the strain tensor is still under discussion. However, it is expected that if the Representative Element Volume used to perform the averages is large enough, the different homogenization procedures converge to the same expression (Diebels and Steeb 2002).

From the derivation of the stress-strain relation one can bridge the gap between the discrete and continuum approaches. The incremental theory provides a simple method to obtain the incremen-
tal stress-strain relation directly from DEM simulations without recourse to any particular constitutive model (Darve, Flavigny, and Meghachou 1995). This method has been used to calculate the incremental response of disks (Bardet 1994) and spheres (Calvetti, Tamagnini, and Viggiani 2002; Kishino 2003). Some recent results seem to contradict many well-established concepts of the elastoplastic theory (Calvetti, Viggiani, and Tamagnini 2003; Kishino 2003). However, it should be addressed that the behavior of spherical packings is qualitatively different from realistic soil samples. For example, the friction angle of a packing of spheres is much lower than the experimental values for sand (Calvetti, Viggiani, and Tamagnini 2003). This is given by the fact that a sphere can rotate much more easily inside a packing rather than an arbitrarily shaped grain. It is, therefore, of obvious interest to study the incremental response of non-spherical particles.

In this paper we perform a micromechanical investigation of the soil deformation using a discrete model consisting of randomly generated polygons. The details of the particle generation, contact forces, boundary conditions and the molecular dynamics simulations are presented in Sec. 2. The deformation under biaxial test is investigated in Sec. 3. Here we emphasize in the role of the buckling of chain forces and the arising of sliding contacts on the shear band formation. In Sec. 4 we calculate incremental response of the polygonal assemblies before failure, we evaluate the relation between the elastic stiffness and the anisotropy of the contact network, as well as the role of the sliding contacts on the plastic flow rule. The conclusions are perspectives of this work are presented in Sec. 5.

2 DISCRETE MODEL

Here we present a two-dimensional discrete element model which will be used to investigate different aspects of the deformation of granular materials (Kun, D’Addetta, Ramm, and Herrmann 1999; Tillemans and Herrmann 1995). This model consists of randomly generated convex polygons, which interact via contact forces. There are some limitations in the use of such a two-dimensional code to model physical phenomena that are three-dimensional in nature. These limitations have to be kept in mind in the interpretation of the results and its comparison with the experimental data. In order to give a three-dimensional picture of this model, one can consider the polygons as a collection of prismatic bodies with randomly-shaped polygonal basis. Alternatively, one could consider the polygons as three-dimensional grains whose centers of mass all move in the same plane. It is the author’s opinion that it is more sensible to consider this model as an idealized granular material that can be used to check the constitutive models.
2.1 Generation of polygons

The polygons representing the particles in this model are generated by using the method of Voronoi tessellation (Kun and Herrmann 1999). This method is schematically shown in the left part of Fig. 2: First, a regular square lattice of side \( \ell \) is created. Then, we choose a random point in each cell of the rectangular grid. Then, each polygon is constructed assigning to each point that part of the plane that is nearer to it than to any other point. The details of the construction of the Voronoi cells can be found in the literature (Moukarzel and Herrmann 1992; Okabe, Boots, and Sugihara 1992).

Using the Euler theorem, it has been shown analytically that the mean number of edges of this Voronoi construction must be 6 (Okabe, Boots, and Sugihara 1992). The number of edges of the polygons is distributed between 4 and 8 for 98.7% of the polygons. Numerically, it is shown that the orientational distribution of edges is isotropic; and the distribution of areas of polygons is symmetric around its mean value \( \ell^2 \), as shown the right part of Fig. 2. The probabilistic distribution of areas follows approximately a Gaussian distribution with variance of \( 0.36\ell^2 \).

2.2 Contact forces

When two elastic bodies come into contact, a slight deformation in the contact region appears, and there is an interaction which transmits not only force but also torque between the bodies. In principle, this interaction can be obtained using standard technics such as finite elements methods. In our model this method would be computationally very expensive, and it is necessary to introduce some basic assumptions to simplify the calculation of this interaction. As it was presented before (Tillemans and Herrmann 1995), realistic contact forces and torques can be obtained by allowing the polygon to overlap and calculating them from this virtual overlap.

The first step for the calculation of the contact force is the definition of the line representing the flattened contact line between the two polygons in contact. This is defined from the contact points resulting from the intersection of the edges of the overlapping polygons. In most cases, we have two contact points, as shown in the left of Fig. 3. In such a case, the contact line is defined by the vector \( \vec{C} = \overrightarrow{C_1 C_2} \) connecting these two intersection points. In some pathological cases, the intersection of the polygons leads to four or six contact points. In these cases, we define the contact line by the vector \( \vec{C} = \overrightarrow{C_1 C_2} + \overrightarrow{C_3 C_4} \) or \( \vec{C} = \overrightarrow{C_1 C_2} + \overrightarrow{C_3 C_4} + \overrightarrow{C_5 C_6} \), respectively. This choice guarantees a continuous change of the contact line, and therefore of the contact forces, during the evolution of the contact.

The contact force is separated as

\[
\vec{f}^c = \vec{f}^e + \vec{f}^v, \tag{1}
\]

where \( \vec{f}^e \) and \( \vec{f}^v \) are the elastic and viscous contribution. The elastic part of the contact force is
decomposed as
\[ \ddot{\mathbf{f}} = f_n^e \hat{n}^e + f_t^e \hat{t}^e. \]  
(2)
The unit tangential vector is defined as \( \hat{t}^e = \mathbf{C}'/|\mathbf{C}'| \), and the normal unit vector \( \hat{n}^e \) is taken perpendicular to \( \mathbf{C}' \). The normal elastic force is calculated as
\[ f_n^e = -k_n A/L_c, \]  
(3)
where \( k_n \) is the normal stiffness, \( A \) is the overlapping area and \( L_c \) is a characteristic length of the polygon pair. Our choice is \( L_c = |\mathbf{C}'| \). This normalization is necessary to be consistent in the units of force (Kun and Herrmann 1999).

The frictional force is calculated using an extension of the method proposed by Cundall-Strack (Cundall and Strack 1979). An elastic force proportional to the elastic displacement is included at each contact
\[ f_t^e = -k_t \Delta x_t^e, \]  
(4)
where \( k_t \) is the tangential stiffness. The elastic displacement \( \Delta x_t \) is calculated as the time integral of the tangential velocity of the contact during the time where the elastic condition \( |f_t^e| < \mu f_n^e \) is satisfied. The sliding condition is imposed, keeping this force constant when \( |f_t^e| = \mu f_n^e \). The straightforward calculation of this elastic displacement is given by the time integral starting at the beginning of the contact:
\[ \Delta x_t^e = \int_0^t v_t^e(t') \Theta(\mu f_n^e - |f_t^e|) dt', \]  
(5)
where \( \Theta \) is the Heaviside step function and \( v_t^e \) denotes the tangential component of the relative velocity \( \mathbf{v}^e \) at the contact:
\[ v_t^e = \vec{v}_i - \vec{v}_j - \vec{\omega}_i \times \vec{\ell}_i + \vec{\omega}_j \times \vec{\ell}_j. \]  
(6)
Here \( \vec{v}_i \) is the linear velocity and \( \vec{\omega}_i \) is the angular velocity of the particles in contact. The branch vector \( \vec{\ell}_i \) connects the center of mass of particle \( i \) to the point of application of the contact force. Replacing Eqs. (3) and (4) into (2) one obtains:
\[ \ddot{\mathbf{f}} = -k_n A/L_c \hat{n}^e - k_t \Delta x_t^e \hat{t}^e. \]  
(7)
Damping forces are included in order to allow rapid relaxation during the preparation of the sample, and to reduce the acoustic waves produced during the loading. These forces are calculated as
\[ \ddot{\mathbf{f}} = -m(\gamma_n v_n^e \hat{n}^e + \gamma_t v_t^e \hat{t}^e), \]  
(8)
being \( m = (1/m_i + 1/m_j)^{-1} \) the effective mass of the polygons in contact. \( \hat{n}^e \) and \( \hat{t}^e \) are the normal and tangential unit vectors defined before, and \( \gamma_n \) and \( \gamma_t \) are the coefficients of viscosity. These forces introduce time dependent effects during the loading. We will show that these effects can be arbitrarily reduced by increasing the loading time, as corresponds to the quasistatic approximation.

The transmitted torque between two polygons in contact is calculated as \( \vec{\tau} = \vec{\ell} \times \ddot{\mathbf{f}} \). The so-called branch vector is taken as the vector connecting the center of mass of the particle to the center of mass of the overlapping polygon. Since this point is not collinear with the centers of masses of the interacting polygons, there is a contribution of the torque from both components of the contact force. This makes an important difference with respect to the interaction between disks or spheres: Polygons can transmit torques even in absence of frictional forces.
In order to solve the equations of motion, it is necessary to specify the forces acting on the particles on the boundary. Two different boundary conditions are used in the simulations. The floppy boundary method allows one to perform a stress-controlled test on the sample without imposing any restriction on the deformation of the assembly. Elastic walls can also be used to control the deformation of the polygonal assembly. These two boundary conditions are presented in the following sections.

2.3 Floppy boundary

The method of floppy boundary is introduced to simulate the typical biaxial test used to investigate the strain localization (Marcher and Vermeer 2001): First, a rectangular shaped granular sample, surrounded by a latex membrane, is placed between two fixed walls to create plane strain condition. Then, the sample is subjected to axial loading, superimposed by a confining pressure applied on the membrane.

Let’s discuss how the latex membrane can be modeled. One way would be to apply a perpendicular force on each edge of the polygons belonging to the external contour of the sample. Actually, this does not work well, because the force will act on all the fjords of the boundary. This produces an uncontrollable growth of cracks during the loading that end up destroying the sample. With a latex membrane this cannot happen because the bending stiffness of the membrane does not allow the pressure to penetrate in all the fjords of the sample. To model such a membrane, we will introduce a criterion which restricts the boundary points that are subjected to the external stress.

The algorithm to identify the boundary is rather simple. The lowest vertex \( p \) from all the polygons of the sample is chosen as the first point of the boundary list \( B_1 \). In Fig. 4 \( P \) is the polygon that contains \( p \), and \( q \in P \cap Q \) is the first intersection point between the polygons \( P \) and \( Q \) in counterclockwise orientation with respect to \( p \). Starting from \( p \), the vertices of \( P \) in counterclockwise orientation are included in the boundary list until \( q \) is reached. Next, \( q \) is included in the boundary list. Then, the vertices of \( Q \) between \( q \) and the next intersection point \( r \in Q \cap R \) in the counterclockwise orientation are included in the list. The same procedure is applied until one surrounds the sample and reaches the lowest vertex \( p \) again. This is a very fast algorithm, because it only makes use of the contact points between the polygons, which are previously calculated to obtain the contact force in each time step.

Let’s define \( \{ B_i \} \) the set of points of the boundary and \( \{ M_i \} \) the set of boundary points that are in contact with the membrane. They are selected using a recursive algorithm. It is initialized with the vertices of the smallest convex polygon that encloses the boundary (see Fig. 5). The lowest point of the boundary is selected as the first vertex of the polygon \( M_1 = B_1 \). The second one \( M_2 \) is the boundary point \( B_2 \) that minimizes the angle \( \angle(B_1B_2,B_1) \) with respect to the horizontal. The third one \( M_3 \) is the boundary point \( B_3 \) such that the angle \( \angle(M_2B_3,M_1M_2) \) is minimal. The algorithm is recursively applied until the lowest vertex \( M_1 \) is reached again.
Figure 5: Floppy boundary obtained with threshold bending angle $\theta_{th} = \pi, 3\pi/4, \pi/2$ and $\pi/4$, the first one corresponds to the minimum convex polygon that encloses the sample.

The points of the boundary are iteratively included in the list $\{M_i\}$ using the bending criterion proposed by Astrøm (Astrom, Herrmann, and Timonen 2000; Alonso-Marroquin 2004). For each pair of consecutive vertices of the membrane $M_i = B_i$ and $M_{i+1} = B_j$ we choose that point from the subset $\{B_k\}_{1 \leq k \leq j}$ which maximizes the bending angle $\theta_k = \angle(B_kB_i, B_kB_j)$. This point is included in the list whenever $\theta_k \geq \theta_{th}$. Here $\theta_{th}$ is a threshold angle for bending. This algorithm is repeatedly applied until there are no more points satisfying the bending condition. The final result gives a set of segments $\{M_iM_{i+1}\}$ lying on the boundary of the sample as shown in Fig. 5.

On each segment of the membrane $\vec{T} = \Delta x_1\hat{x}_1 + \Delta x_3\hat{x}_3$, we apply a force

$$\vec{f}^m = -\sigma_1\Delta x_3\hat{x}_1 + \sigma_3\Delta x_1\hat{x}_3 - \gamma_b m_i\vec{v}\quad (9)$$

Here $\hat{x}_1$ and $\hat{x}_3$ are the unit vectors of the Cartesian coordinate system, $\sigma_1$ and $\sigma_3$ are the components of the stress we want to apply on the sample. This force is transmitted to the polygons in contact with it. For this purpose, the segments of the membrane are divided into two groups: A-type segments are those that coincide with an edge of a boundary polygon; B-type segments connect the vertices of two different boundary polygons. If the segment is A-type, this force is applied at its midpoint; if the segment is B-type, half of the force is applied at each one of the vertices connected by this segment. The last term in Eq. (9) is an additional damping force, which is included to reduce the acoustic waves produced during loading. Here $\gamma_b$ is the coefficient of viscosity of the floppy boundary. $m_i$ and $\vec{v}$ are the mass and the velocity of the polygon in contact with the membrane.
2.4 Walls as boundaries

Usually, the granular assemblies are loaded within a set of conning walls. These walls act as boundary conditions, and can be moved by specifying their velocity or the force applied on them. In our simulations, the interaction of the polygons with the walls is modeled by using a simple visco-elastic force. First, we allow the polygons to penetrate the walls. Then, for each vertex of the polygon $\alpha$ inside of the walls we include a force

$$\vec{f}_\alpha^b = -k_\alpha \delta \vec{n} - \gamma_\alpha m_\alpha \vec{v}_\alpha^b,$$

(10)

where $\delta$ is the penetration length of the vertex, $\vec{n}$ is the unit normal vector to the wall, $m$ is the mass of the polygon, and $\vec{v}_\alpha^b$ is the relative velocity of the vertex with respect to the wall.

2.5 Molecular dynamics simulation

The evolution of the position $\vec{x}_i$ and the orientation $\vec{\phi}_i$ of the polygon $i$ is governed by the equations of motion:

$$m_i \vec{x}_i = \sum_c \vec{f}_i^c + \sum_b \vec{f}_i^b + \sum_m \vec{f}_i^m,$$

$$I_i \vec{\phi}_i = \sum_c \vec{\phi}_i^c \times \vec{f}_i^c + \sum_b \vec{\phi}_i^b \times \vec{f}_i^b + \sum_m \vec{\phi}_i^m \times \vec{f}_i^m.$$

(11)

Here $m_i$ and $I_i$ are the mass and moment of inertia of the polygon. The first sum goes over all those particles in contact with this polygon; the second one over all the vertices of the polygon in contact with the walls, and the third one over all the edges in contact with the floppy boundary. $\vec{f}_i^m$ and $\vec{f}_i^b$ are the forces applied on the polygons in contact with the floppy boundary and the walls. They are defined by Eqs. (9) and (10). The interparticle contact forces $\vec{f}_i^c$ are given by replacing Eqs. (7) and (8) in Eq. (1). It results

$$\vec{f}_i^c = -(k_n A/L_c + \gamma_n m v_n^c) \vec{n} - (\Delta x_i^c + \gamma_l m v_i^c) \vec{v}_i^c.$$

(12)

We use a fifth-order Gear predictor-corrector method for solving the equation of motion (Allen and Tildesley 1987). This algorithm consists of three steps. The first step predicts position and velocity of the particles by means of a Taylor expansion. The second step calculates the forces as a function of the predicted positions and velocities. The third step corrects the positions and velocities in order to optimize the stability of the algorithm. This method is much more efficient than the simple Euler approach or the Runge-Kutta method, especially for problems where very high accuracy is a requirement.

The parameters of the molecular dynamics simulations were adjusted according to the following criteria: (1) guarantee the stability of the numerical solution, (2) optimize the time of the calculation, and (3) provide a reasonable agreement with the experimental data.

There are many parameters in the molecular dynamics algorithm. Before choosing them, it is convenient to make a dimensional analysis. In this way, we can keep the scale invariance of the model and reduce the parameters to a minimum of dimensionless constants.

As shown in Table 1, there are 2 dimensionless and 10 dimensional parameters. The latter ones can be reduced by introducing the following characteristic times of the simulations: the loading line $t_0$, the relaxation times $t_n = 1/\gamma_n$, $t_l = 1/\gamma_l$, $t_b = 1/\gamma_b$ and the characteristic period of oscillation $t_s = \sqrt{k_n/\rho \ell^2}$ of the normal contact.

Using the Buckingham Pi theorem (Buckingham 1914), one can show that the strain response, or any other dimensionless variable measuring the response of the assembly during loading, depends only on the following dimensionless parameters: $\alpha_1 = t_n/t_s$, $\alpha_2 = t_l/t_s$, $\alpha_3 = t_b/t_s$, $\alpha_4 = t_0/t_s$, the ratio $\zeta = k_l/k_n$ between the stiffnesses, the friction coefficient $\mu$ and the ratio $p_0/k_n$ between the confining pressure and the normal stiffness.
The variables $\alpha_i$ act as control parameters. They are chosen in order to satisfy the quasistatic approximation, i.e. the response of the system does not depend on the loading time. $\alpha_1 = 0.1$, $\alpha_2 = 0.5$ and $\alpha_3 = 0.5$ were taken large enough to have a high dissipation, but not too large to keep the numerical stability of the method. The ratio $\alpha_4 = t_0/t_s = 10000$ was chosen large enough to avoid rate-dependence in the mechanical response, corresponding to the quasistatic approximation. Technically, this is performed by looking for the value of $\alpha_4$ such that a reduction of it by half makes a change of the stress-strain relation less than 5%.

The parameters $\zeta$ and $\mu$ can be considered as material parameters. They determine the constitutive response of the system, so they must be adjusted to the experimental data. In this study, we have adjusted them by comparing the simulation of biaxial tests of perfect polygonal packings to the corresponding tests with dense Hostun sand (Marcher and Vermeer 2001). First, the initial Young modulus of the material is linearly related to the value of normal stiffness of the contact. Thus, $k_n = 1.6 \times 10^8 \text{N/m}$ is chosen by fitting the initial slope of the stress-strain relation in the biaxial test. Then, the Poisson ratio depends on the ratio $\zeta = k_t/k_n$. Our choice $k_t = 5.28 \times 10^7 \text{N/m}$ gives an initial Poisson ratio of 0.07. This is obtained from the initial slope of the curve of volumetric strains versus axial strain. The angles of friction and the dilatancy are increasing functions of the friction coefficient $\mu$. Taking $\mu = 0.25$ yields angles of friction of $30 - 40$ degrees and dilatancy angles of $20 - 30$ degrees. The experimental data yields angles of friction between $40 - 45$ degrees and dilatancy angles between $7 - 14$ degrees. A better adjustment would be made by including different void ratios in the simulations, but this is beyond the scope of this work.

### 3 BIAXIAL TEST

In this section we simulate the biaxial test in order to investigate the micromechanical rearrangements occurring during the deformation and failure of granular materials. The boundary conditions are chosen in order to mimic the experimental tests under plane strain conditions (Marcher and Vermeer 2001). A latex membrane surrounding the granular sample is modeled by using the method of floppy boundary explained in Subsec. 2.3. First, a confining pressure is applied to the sample through the floppy boundary. Then, two horizontal walls at the top and bottom of the packing are used to apply vertical loading with constant velocity.

The stress is calculated from the forces applied on the boundary as $\sigma_{ij} = \frac{1}{A} \sum_b f_i^b x_j^b$, where $\vec{x}^b$ is the point of application of the boundary force $\vec{f}^b$ and $A$ is the area enclosed by the floppy boundary (Cundall and Strack 1979). From the principal values of this tensor, one can define the pressure and the deviatoric stress as $p = (\sigma_1 + \sigma_3)/2$ and $q = (\sigma_1 - \sigma_3)/2$. The axial strain is calculated as $\epsilon_1 = \Delta H/H_0$, where $H$ is the height of the sample. The volumetric strain is given by $\epsilon_v = \Delta A/A_0$.

The evolution of the deviatoric stress and the volumetric strain are shown in Fig. 6 for different confining pressures. The stress response is characterized by a continuous decrease of the stiffness,
i.e. the slope of the stress-strain curve, from the very beginning of the load process. The failure is given by the peak stress value (i.e. the maximal stress reached during the loading). The volumetric strain has a compaction regime at the beginning of the load, and dilatancy before failure. The maximal dilatancy is observed around the failure. For large loadings, the sample reaches a stationary state where the stress and the volume remain approximately constant, except for some fluctuations which remain for large deformations.

The relation between the pressure and the deviatoric stress at failure is strictly non-linear, and it can be fitted by a power law (Alonso-Marroquin 2004)

\[
\frac{p}{p_r} = \alpha \left( \frac{q}{p_r} \right)^\beta,
\]

where \( p_r = 1 \times 10^6 \text{N/m} \), \( \alpha = 0.625 \) and \( \beta = 0.93 \). An interesting consequence of this non-linearity is that the envelope of all Mohr-Coulomb circles at failure cannot be represented by a single straight line, as shown in Fig. 7. However, one can use the Mohr-Coulomb failure criterion in a local sense, by approaching the envelope around each Mohr-Coulomb circle by a straight line. This line can be constructed by taking the common tangent of the two circles at pressure \( p - \Delta p \)

\[
\sigma = c(p) + \sigma_n \tan(\phi(p))
\]

Figure 6: Deviatoric stress and volumetric strain versus axial strain for different confining pressures. 1\( Pa \) corresponds to 1\( N/m \).

Figure 7: Mohr-Coulomb circles at the failure point for different pressures. The dotted line is tangent to the envelope curve of these circles.
and \( p + \Delta p \). As shown in Fig. 7, the resulting straight lines from these constructions lead to a dependence of the angle of friction and cohesive parameters with the pressure. For this reason they cannot be strictly considered as material parameters.

This local Mohr-Coulomb analysis seems to be relatively consistent with the shear band orientation. Above the confining pressure of \( p_0 > 1.6 \times 10^5 \text{ N/m} \), we observed localization of strain as the typical mode of failure. This is given by a narrow zone in the sample where the dilatancy, the rotation of the particles, and the sliding between the grains are particularly intense. The shear band orientation for different confining pressures is shown in Fig. 8. The bars represent the uncertainty in the measure of the shear band, which is estimated as

\[
\Delta \theta = \arctan(\Delta w/\Delta l),
\]

where \( \Delta w \) and \( \Delta l \) are the width and the length of the shear band. The resulting orientations lie between the Mohr-Coulomb solution \( \theta_C = 45^\circ + \phi/2 \) and the Roscoe Solution \( \theta_R = 45^\circ + \Psi/2 \) (Vermeer 1990). The former one is defined in Fig. 7. The latter is defined by the angle of dilatancy \( \Psi = \arcsin(\delta V/\delta \gamma) \), being \( \delta V \) and \( \delta \gamma \) the increments of volumetric and deviatoric strains at the failure (Roscoe 1970). These limits are shown in Fig. 8. We observe that the inclination angles are between these two angles with a tendency towards the Mohr-Coulomb solution.

According to these results, the Mohr-Coulomb criterion can be used to describe with relative accuracy the onset of the failure and shear band orientation. However, it is important to remark that plastic deformations occur before failure. Sliding contacts are observed even under isotropic condition, and the strain localization seems to be an effect of a progressive concentration of slippage during the loading. This localization can be observed from the incremental plastic deformation between the grains. For each polygon, we calculate the plastic deformation between two loading stages separated by \( \Delta \xi_1 = 0.1\% \), as

\[
\xi = \sum_c |\Delta x^c - \Delta x^c_t|,
\]

where \( \Delta x^c \) is the tangential displacement at each contact and \( \Delta x^c_t \) is the elastic part of this displacement in this interval. The latter is calculated after Eq. (5).

Fig. 9 shows the distribution of plastic displacements in four different loading stages. Irreversible deformations are observed at the very beginning of the loading. The plastic deformation is approximately uniform for small loadings, and it presents a progressive localization during the loading process. At failure, the shear band is identified by a narrow zone where the sliding between the grains is more intense than on average. After failure, we observed two blocks moving one against another, separated by a shear band of some 6 – 8 grains diameters.

This continuous localization of plastic deformation makes difficult to determine where the shear band occurs. It has been almost always assumed that the shear band occurs at peak stress or beyond the failure (Vermeer 1990). In contradiction to this, we observe some signals of localization of plastic deformations before the failure, as shown in part (b) of Fig. 9. An explanation of this
Figure 9: Plastic deformation at the grain during a loading of $\Delta \epsilon_1 = 0.001$. The intensity of the color represents the plastic deformation. The snapshot is taken for loading stages with $\epsilon_1 = 0.01$, 0.02, 0.027 (failure) and 0.07.

apparent contradiction can be found by looking at the distribution of the stress around the shear band. We calculate the average of the stress tensor at each particle as $\sigma_{ij} = \frac{1}{A} \sum_c f^c_i \ell^c_j$ where $A$ is the area of the polygon, $f^c_i$ is the contact force and $\ell^c_j$ is the branch vector, connecting the center of mass of the polygon with the center of application of the contact force. The sum goes over all the contacts of the particle.

The principal stress direction at each grain is represented in Fig. 10 by a cross. The length of the lines represents how large the components are. During loading, we observe that the principal stress direction goes almost perpendicular to the load direction, forming columnlike structures which are called chain forces. At failure, these chain forces start buckling, and the buckled chains gradually concentrate as shear bands in the post-failure regime, which cause a growth of void ratio, and therefore a reduction of the strength in the shear band. For large deformations, one can see that the chain forces are perpendicular to the loading direction outside of the shear band, and they go almost perpendicular through the shear band, as is shown in the Fig. 10. Due to this fact, there is an abrupt change of the stress in the parallel direction to the shear band, in agreement with the bifurcation analysis (Vermeer 1990). Note from the Fig. 11 that the characteristic length of buckled chain forces proves to be of the same order of the width of shear band. This correlation has
Figure 10: Principal stress directions of the individual grains. The snapshot is taken for loading stages with $\varepsilon_1 = 0.01, 0.02, 0.027$ (failure) and 0.07.

been supported by experimental test on two-dimensional disks (Francois, Lacombe, and Herrmann 2001). It is also shown that a micromechanical analysis of the bucking of columns could provide a theoretical explanation of the finite width of shear bands (Satake 1998).

4 INCREMENTAL RELATION

Although the Mohr-Coulomb criterion is a simple and elegant approach to failure problems, this theory provides a too crude description of the behavior of granular materials before failure. In particular, the granular materials do not show a perfectly elastic behavior up to the failure condition, but they rather develop plastic deformations as a precursor behavior. Moreover, since the dilatancy occurs before failure, the volume expansion should be an integral part of the description of this failure. In the biaxial test simulations we have found a progressive localization of sliding contacts and a formation of chain forces before the sample fails. A micromechanical based constitutive model would require to determine what is the role of these micromechanical rearrangements on the overall elastoplastic deformation of the assembly.
4.1 Calculation of the incremental response

We will determine the incremental stress-strain relation of the polygonal samples used in the bi-axial test. The calculation of the average of the Cauchy stress tensor over a polygonal assembly leads to (Bagi 1999)

\[
\sigma_{ij} = \frac{1}{A} \sum_{e} x_{e}^{i} f_{j}^{e}
\]

(14)

The sum goes over all the forces acting over the boundary of the assembly. A is the area enclosed by the boundary and \( \bar{x}^{e} \) is the point of application of the boundary force \( \tilde{f}^{e} \). As it was shown in Subsec. 2.3, the forces are applied through a floppy boundary which encloses the sample. This boundary is given by an irregular polygon whose vertices are denoted by \( M_{i} = (x_{i}^{b}, y_{i}^{b}) \), where \( i = 1, 3, b = 1, \ldots N_{b} \), and \( N_{b} \) is the number of edges. In order to control the stress, we apply a force one each edge, as it was given by Eq. (9). Taking \( \tilde{f}^{e} = \tilde{f}^{b} \) and using the equilibrium condition \( \tilde{v}_{i} = 0 \), we obtain

\[
f_{i}^{e} = -\sigma_{1}(x_{3}^{b+1} - x_{3}^{b})\hat{x}_{1} + \sigma_{3}(x_{1}^{b+1} - x_{1}^{b})\hat{x}_{3}
\]

(15)

The point of application of this force is given by the center of the edge:

\[
x_{i}^{e} = \frac{1}{2}(x_{1}^{b+1} + x_{1}^{b})\hat{x}_{1} + \frac{1}{2}(x_{3}^{b+1} + x_{3}^{b})\hat{x}_{3}
\]

(16)

Replacing Eqs. (15) and (16) into Eq. (14) leads to

\[
\sigma = \frac{1}{2A} \begin{bmatrix}
-\sigma_{1} \sum_{b} (x_{3}^{b+1} + x_{3}^{b})(x_{3}^{b+1} - x_{3}^{b}) & \sigma_{3} \sum_{b} (x_{1}^{b+1} + x_{1}^{b})(x_{1}^{b+1} - x_{1}^{b}) \\
-\sigma_{1} \sum_{b} (x_{3}^{b+1} + x_{3}^{b})(x_{3}^{b+1} - x_{3}^{b}) & \sigma_{3} \sum_{b} (x_{1}^{b+1} + x_{1}^{b})(x_{1}^{b+1} - x_{1}^{b})
\end{bmatrix}.
\]

(17)
By expanding this sums and using the formula for the area of irregular polygons

\[
A = \frac{1}{2} \sum_b \left( x_{1b}^b x_{3b}^{b+1} - x_{1b}^{b+1} x_{3b}^b \right),
\]

one obtains

\[
\sigma = \begin{bmatrix}
\sigma_1 & 0 \\
0 & \sigma_3
\end{bmatrix}.
\]

Thus, the stress controlled test is restricted to stress states without off-diagonal components. So we can simplify the notation introducing the pressure \( p \) and the deviatoric stress \( q \) in the components of the stress vector

\[
\tilde{\sigma} = \begin{bmatrix}
p \\
q
\end{bmatrix} = \frac{1}{2} \begin{bmatrix}
\sigma_1 + \sigma_3 \\
\sigma_1 - \sigma_3
\end{bmatrix}.
\]

The incremental strain tensor can be calculated from the average of the displacement gradient over the area enclosed by the boundary of the assembly. It has been shown (Bagi 1996) that it can be transformed in a sum over the boundary of the sample

\[
d_{ij} = \frac{1}{2A} \sum_b (\Delta u_b^b N_j^b + \Delta u_j^b N_b^b).
\]

Here \( \Delta \vec{u}^b \) is the displacement of the boundary segment, that is calculated from the linear displacement \( \Delta \vec{x} \) and the angular rotation \( \Delta \vec{\phi} \) of the polygons belonging to it, according to

\[
\Delta \vec{u}^b = \Delta \vec{x} + \Delta \vec{\phi} \times \ell.
\]

From the eigenvalues \( d_{e1} \) and \( d_{e3} \) of \( d_{ij} \), we define the volumetric and deviatoric components of the strain as the components of the incremental strain vector:

\[
d\varepsilon = \begin{bmatrix}
d e_1 \\
d e_3
\end{bmatrix} = \begin{bmatrix}
d e_1 + d e_3 \\
d e_1 - d e_3
\end{bmatrix}.
\]

By convention \( d e > 0 \) corresponds to a compression of the sample. We assume a rate-independent relation between the incremental stress and incremental strain tensor. In this case the incremental relation can generally be written as (Darve, Flavigny, and Meghachou 1995):

\[
d\varepsilon = M(\tilde{\theta}, \tilde{\sigma}) d\tilde{\sigma},
\]

where \( \tilde{\theta} \) is the unitary vector defining a specific direction in the stress space:

\[
\tilde{\theta} = \frac{d\tilde{\sigma}}{|d\tilde{\sigma}|} \equiv \begin{bmatrix}
\cos \theta \\
\sin \theta
\end{bmatrix}, \quad |d\tilde{\sigma}| = \sqrt{dp^2 + dq^2}.
\]

The constitutive relation results from the calculation of \( d\varepsilon(\theta) \), where each value of \( \theta \) is related to a particular mode of loading. Some special modes are listed in Table I.

In order to compare the resulting incremental response to the elastoplastic models, it is necessary to assume that the incremental strain can be separated into an elastic (recoverable) and a plastic (unrecoverable) component:

\[
d\varepsilon = d\varepsilon^e + d\varepsilon^p,
\]

\[
d\varepsilon^e = D^{-1}(\tilde{\sigma}) d\tilde{\sigma},
\]
Figure 12: Stress - strain relation resulting from the load - unload test. Gray lines represent the paths in the stress and strain spaces. The dash line shows the strain envelope response and the solid line is the plastic envelope response.

\[ d\tilde{\varepsilon}^p = J(\theta, \tilde{\sigma})d\tilde{\sigma}. \] 

(28)

Here, \( D^{-1} \) is the inverse of the stiffness tensor \( D \), and \( J = M - D^{-1} \) the flow rule of plasticity (Vermeer 1984). They can be obtained from the calculation of \( d\tilde{\varepsilon}^e(\theta) \) and \( d\tilde{\varepsilon}^p(\theta) \) as we will see below.

The method presented here to calculate the strain response has been used on sand experiments (Poo-rooshab, Holubec, and Sherbourne 1967). It was introduced by Bardet (Bardet 1994) in the calculation of the incremental response using discrete element methods. This method will be used to determine the elastic \( \tilde{\varepsilon}^e \) and plastic \( \tilde{\varepsilon}^p \) components of the strain as function of the stress state \( \tilde{\sigma} \) and the stress direction \( \theta \). First, it is isotropically compressed until it reaches the stress value \( \sigma_1 = \sigma_3 = p - q \). Next, it is subjected to axial loading in order to increase the axial stress \( \sigma_1 \) to \( p + q \). Loading the sample from \( \tilde{\sigma} \) to \( \tilde{\sigma} + d\tilde{\sigma} \) the strain increment \( d\tilde{\varepsilon} \) is obtained. Then the sample is unloaded to \( \tilde{\sigma} \) and one finds a remaining strain \( d\tilde{\varepsilon}^p \), that corresponds to the plastic component of the incremental strain. For small stress increments the unloaded stress-strain path is almost elastic. Thus, the difference \( d\tilde{\varepsilon}^e = d\tilde{\varepsilon} - d\tilde{\varepsilon}^p \) can be taken as the elastic component of the strain. This procedure is implemented on different "clones" of the same sample, choosing different stress directions and the same stress amplitude in each one of them.

This method is based on the assumption that the strain response after a reversal loading is completely elastic. However, numerical simulations have shown that this assumption is not strictly true, because sliding contacts are always observed during the unload path (Calvetti, Tamagnini, and Viggiani 2002; Alonso-Marroquin and Herrmann 2004). In our simulations, we observe that for stress amplitudes of \( |\tilde{\sigma}| = 0.001p \) the plastic deformation during the reversal stress path is less

<table>
<thead>
<tr>
<th>( \theta )</th>
<th>TEST</th>
<th>( dp &gt; 0 )</th>
<th>( dq &gt; 0 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0°</td>
<td>isotropic compression</td>
<td>( dp &gt; 0 )</td>
<td>( dq = 0 )</td>
</tr>
<tr>
<td>45°</td>
<td>axial loading</td>
<td>( d\sigma_1 &gt; 0 )</td>
<td>( d\sigma_3 = 0 )</td>
</tr>
<tr>
<td>90°</td>
<td>pure shear</td>
<td>( dp = 0 )</td>
<td>( dq &gt; 0 )</td>
</tr>
<tr>
<td>135°</td>
<td>lateral loading</td>
<td>( d\sigma_1 = 0 )</td>
<td>( d\sigma_3 &gt; 0 )</td>
</tr>
<tr>
<td>180°</td>
<td>isotropic expansion</td>
<td>( dp &lt; 0 )</td>
<td>( dq = 0 )</td>
</tr>
<tr>
<td>225°</td>
<td>axial stretching</td>
<td>( d\sigma_1 &lt; 0 )</td>
<td>( d\sigma_3 = 0 )</td>
</tr>
<tr>
<td>270°</td>
<td>pure shear</td>
<td>( dp = 0 )</td>
<td>( dq &lt; 0 )</td>
</tr>
<tr>
<td>315°</td>
<td>lateral stretching</td>
<td>( d\sigma_1 = 0 )</td>
<td>( d\sigma_3 &lt; 0 )</td>
</tr>
</tbody>
</table>

Table 2: Principal modes of loading according to the orientation of \( \theta \)
than 1% of the corresponding value of the elastic response. Within this margin of error, the method proposed by Bardet can be taken as a reasonable approximation to describe the elastoplastic response.

Fig. 12 shows the load-unload stress paths and the corresponding strain response when an initial stress state with \( \sigma_1 = 2.0 \times 10^5 \text{N/m} \) and \( \sigma_3 = 1.2 \times 10^5 \text{N/m} \) is chosen. The end of the load paths in the stress space maps into a strain envelope response \( \varepsilon^{e}(\theta) \) in the strain space. Likewise, the end of the unload paths maps into a plastic envelope response \( \varepsilon^{p}(\theta) \). This envelope consists of a very thin ellipse, nearly a straight line, which confirms the unidirectional aspect of the irreversible response predicted by the theory of elastoplasticity (Vermeer 1984). The yield direction can be found from this response, as the direction in the stress space where the plastic response is maximal. In this example, this is around \( \phi = 87.2^\circ \). The flow direction \( \psi \) is given by the direction of the maximal plastic response in the strain space, which is around \( 76.7^\circ \). The fact that these directions do not agree reflects a non-associated flow rule, as it is observed in experiments on realistic soils (Poorooshasb, Holubec, and Sherbourne 1967).

4.2 Elastic response

Another interesting aspect of the incremental stress-strain relation concerns the elastic response \( \varepsilon^e = \varepsilon - \varepsilon^p \). Fig. 13 shows the elastic envelope response for different stress ratios. For stress values such as \( q/p \leq 0.4 \) the stress envelope responses collapse on to the same ellipse. This response can be described by the isotropic linear elasticity by introducing two material Parameters i.e. the Young modulus \( E \) and the Poisson ratio \( \nu \) (Landau and Lifshitz 1986). For stress values satisfying \( q/p > 0.4 \) there is a reduction of the stiffness, and a rotation of the principal direction of the elastic tensor. In this case, the elastic response can not be described using linear isotropic elasticity.

It is not surprising that isotropic linear elasticity is not valid in the deformation of samples subjected to deviatoric loads. Indeed, numerical simulations (Thornton and Barnes 1986; Cundall, Drescher, and Strack 1982) and photo-elastic experiments (Drescher and de Josselin de Jong 1972) on granular materials show that loading induces a significant deviation from isotropy in the contact network. This anisotropy can be characterized by the distribution of the orientations of the branch

---

**Figure 13**: Elastic strain envelope responses \( \varepsilon^e(\theta) \). They are calculated for a pressure \( p = 160kPa \) and taking deviatoric stresses with \( q = 0.0p \) (inner), 0.1p, ..., 0.7p (outer).
vectors $\vec{\xi}$, as shown in Fig. 14. Each branch vector connects the center of mass of the polygon to the center of application of the contact force. Fig. 14 shows the branch vectors in the polygonal assembly for two different stages of loading. The structural changes of contact network are principally due to the opening of contacts whose branch vectors are oriented nearly perpendicular to the loading direction. Due to this open contacts, the strength under lateral compression is lower than the strength under further horizontal loads. That is why the elastic response becomes anisotropic.

Of course, the onset of anisotropy depends on the initial distribution of contact forces, and its evolution during loading. Fig. 15 shows the distribution of contact force in the polygonal assemblies for three different stages of loading. For low stress ratios, the contact forces is rather concentrated around their mean value. This distribution is qualitatively different to the heterogeneous distribution of force observed on highly polydisperse disks packings (Radjai, Jean, Moreau, and Roux 1996). This is due to the particular geometry of the polygonal packing, where the absence of voids and the low polydispersity of the grains reduces the disorder of the contact network.

From Fig. 15 we observe that loading induces an increase of the fluctuations of contact forces, which in turn implies the opening of contacts when the normal force $f_n$ vanishes. In particular, for stress values satisfying $q < 0.35p$ there is almost no open contacts. Above this limit a significant number of contacts are open, leading to an anisotropy in the contact networks, and hence, to an anisotropic linear response. It is observed that the parameters of the stiffness tensor are almost dependent on the averaged coordination number of the contact network (Alonso-Marroquin and Herrmann 2002). These correlation agrees with those theoretical models proposed to connects the elastic tensor to the so-called fabric tensor, measuring the anisotropy of the contact network (Cowin 1985).

### 4.3 Plastic response

An important aspect of our incremental calculation is that the plastic envelope response lies almost on a straight line, as predicted by the theory of elastoplasticity (Vermeer 1984). This property allows one to express the flow rule in Eq. (28) as (Alonso-Marroquin, Luding, and Herrmann 2004)

$$d\vec{\xi}^p(\theta) = J(\theta)d\vec{\sigma} = \frac{\langle \hat{\phi} \cdot d\vec{\sigma} \rangle}{h}\psi.$$  \hspace{1cm} (29)

Where $\langle x \rangle = x$ if $x > 0$; Otherwise $\langle x \rangle = 0$. This flow rule is given as a function of the three variables describing the plasticity: the yield direction $\hat{\phi}$, and the flow direction $\psi$, which were defined in Subsec. 4.1, and the plastic modulus $h = \max |d\vec{\xi}^p|$. The best fitting of the of these quantities leads to (Alonso-Marroquin, Luding, and Herrmann 2004)

$$\begin{align*}
\psi &= 46.0^\circ + 88.3^\circ \frac{q}{p},
\end{align*}$$  \hspace{1cm} (30)
Figure 15: Left: force distribution for the stress ratios $q/p = 0.1, 0.35, 0.65$. Here $f_t$ and $f_n$ are the tangential and normal components of the force. They are normalized by the mean value of $f_n$. Right: orientational distribution of the contacts $\Omega(\varphi)$ (outer) and of the sliding contacts $\Omega^s(\varphi)$ (inner). $\varphi$ represents the orientation of the branch vector.

$$\phi = 78.9^\circ + 59.1^\circ \frac{q}{p}$$

$$h = (1 - \frac{q}{0.85p})^{2.7}$$

These relations reproduce many features of realistic soils:

- **(1) The transition from contractancy to dilatancy before failure** (Nova and Wood 1979). According to Eq. (30), this transition occurs around $q = 0.5p$, where $\psi$ becomes $90^\circ$.

- **(2) The non-associativity of the plastic response.** This is given by the inequality $\psi < \phi$, which agrees with the flow rule of non-cohesive soils (Vermeer 1984).

- **(3) The existence of plastic deformations for extremely small deviatoric loads.** In particular, we obtain deviatoric plastic deformations for small deviatoric stresses as predicted by the Cam-clay theory (Roscoe and Burland 1968).

- **(4) The existence of instabilities strictly inside to the plastic limit surface.** This surface is given by the stress values where $h = 0$, which according to Eq. (32) corresponds to the line $q = 0.85p$. This does not agree with the failure surface given by Eq. (13). Experiments in soils report on the existence the instabilities before reaching the plastic limit condition. It proves to be a consequence of the non associativity of the plastic response (Darve and Laouafa 2000).

- **(5) The agreement with the stress-dilatancy relationships.** This is given by linear dependency of the angles of dilatancy and friction on the stress ratio. This linear relation fits with reasonable accuracy with experimental observations (Stroud 1971). In the context of the elastoplastic theories, this implies that the plastic potential functions and the yield surfaces have the same shape, independent on the stress level. This is a basic assumption for the isotropic hardening models (Roscoe and Burland 1968; Nova and Wood 1979).
Several constitutive models of elastoplasticity with work hardening start from the assumption that the material keeps its isotropy during loading (Nova and Wood 1979). In fact, one would expect that the material remains isotropic under small deviatoric loads. This assumption, however, contradicts the angle of dilatancy in Eq. (30). This establishes the existence of deviatoric plastic deformations under isotropic conditions, whenever the sample is initially subjected to the smallest deviatoric load! This departure from isotropy under extremely small loads deserves further micromechanical inspections of the contact network. Since the plastic deformations result from irreversible rearrangements at the contacts, it is interesting to examine the anisotropy induced by loading in the subnetwork of the sliding contacts.

The sliding condition at the contacts is given by \(|f_t| = \mu f_n\), where \(f_n\) and \(f_t\) are the normal and tangential components of the contact force, and \(\mu\) is the friction coefficient. When the sample is isotropically compressed, we observe a significant number of contacts reaching the sliding condition. If the sample has not been previously sheared, the distribution of the orientation of the branch vectors of all the sliding contacts is isotropic. This anisotropy is reflected in the fact that only volumetric plastic deformations are observed when the sample is subjected to isotropic loads. This anisotropy, however, is broken when the sample is subjected to the slightest deviatoric strain.

In effect, most of the sliding contacts whose branch vector is oriented nearly parallel to the loading direction leave the sliding condition at the very beginning of the loading.

The anisotropy of the sliding contacts is investigated by introducing the polar function \(\Omega^s(\phi)\), where \(\Omega^s(\phi)\Delta \phi\) is the number of sliding contacts per particle whose branch vector is oriented between \(\phi\) and \(\phi + \Delta \phi\). Fig. 15 shows this distribution for different stress ratios. For low stress ratios, the branch vectors \(\ell\) of the sliding contacts are oriented nearly perpendicular the loading direction. Sliding occurs perpendicular to \(\ell\), so in this case it must be nearly parallel to the loading direction. Then, the plastic deformation must be such as \(\Delta \varepsilon^P \ll \Delta \varepsilon^P\). It yields to a flow directions of \(\psi = \angle d\varepsilon^p \approx 45^\circ\), which agrees with Eq. (30).

Increasing the deviatoric strain results in an increase of the number of the sliding contacts. The average of the orientations of the branch vectors with respect to the load direction decreases with the stress ratio, which in turn results in a change of the orientation of the plastic flow in Eq. (30). Close to the failure, some of the sliding contacts whose branch vectors are nearly parallel to the loading direction open, giving rise to a butterfly shape distribution, as shown in Fig. 15. In this case, the mean value of the orientation of the branch vector with respect to the direction of the loading is around \(\varphi = 38^\circ\), which means that the sliding between the grains occurs principally around \(52^\circ\) with respect to the vertical. This provides a crude estimate of the ratio between the principal components of the plastic deformation as \(\Delta \varepsilon_3^P \approx -\Delta \varepsilon_1^P \tan(52^\circ)\). This gives an angle of dilatancy of \(\psi = \angle d\varepsilon^p \approx 97^\circ\). This crude approximation is reasonably close to the angle of dilatancy of 103.4° calculated from Eq. (30). The strong correlation between the orientational distribution of sliding contacts and the angle of dilatancy suggests that the plastic deformation of soils can be micro-mechanically described by the introduction of a new structure tensor, measuring the anisotropy of the subnetwork of sliding contacts. This would be an extension of the fabric tensor, which has been proposed to include the anisotropy in the to the constitutive relation of granular materials (Cowin 1985).

5 CONCLUDING REMARKS

The elastoplastic response of a Voronoi tessellated sample of polygons has been investigated in the case of monotonic and quasistatic loading. In spite of the simplicity of the model, it reproduces several aspects of realistic soils, such as strain localization, non-associated plasticity, anisotropic elasticity and the existence of instabilities strictly inside of the plastic limit surface. These aspects have been discussed in terms of the micromechanical rearrangements such as the onset of sliding contacts and the anisotropy of the contact network.

Numerical experiments on biaxial tests using floppy boundary condition and vertical loading at constant velocity yield strain localization as the typical mode of failure. The Mohr-Coulomb criterion is relatively consistent with the shear band orientations, but it is not sufficient to describe the progressive localization of plastic deformations during loading, and the buckling of the chain forces after failure. These buckled chains give the characteristic width of the shear band.

The role of the micromechanical rearrangements in the different aspects of the incremental re-
response has been examined. We report on a fairly good correlation between the incremental elastic response and the anisotropy induced during loading in the contact network. This correlation reflects the necessity to introduce the fabric tensor in the description of the anisotropic elastic response. The most salient aspects of the flow rule of plasticity can also be described from the anisotropy induced in the subnetwork of the sliding contacts.

Since the mechanical response of the granular sample is represented by a collective response of all the contacts, it is expected that the anisotropic elasticity and the non-associated flow rule of plasticity can be completely characterized by the inclusion of some internal variables, containing the information about the microstructural rearrangements between the grains. The traditional fabric tensor, measuring the distribution of the orientation of the contacts, can not fulfill a micromechanical description, because it does not make a distinction between elastic and sliding contacts. New structure tensors taking into account the statistics of the sliding contacts, must be introduced to give a micro-mechanical basis to the flow rule. The identification of these internal variables and the determination of their evolution equation and their connection to the macroscopic variables would be a key step in the development of a micromechanical inspired constitutive model for granular soils.

Acknowledgement We acknowledge the support of this work by the Deutsche Forschungsgemeinschaft (DFG) within the Research group Modellierung kohäsiver Reibungsmaterialien and the European Union project Degradation and Instabilities of Geomaterials with Application to Hazard Mitigation (DIGA) in the framework of the Human Potential Program, Research Training Networks (HPRN-CT-2002-00220).

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