



A strain–displacement–fabric relationship for granular materials

N.P. Kruyt^{a,*}, L. Rothenburg^b

^a Department of Mechanical Engineering, University of Twente, AE Enschede 7500, the Netherlands

^b Department of Civil Engineering, University of Waterloo, Waterloo, Canada

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ABSTRACT

In this micromechanical study of the behaviour of granular materials, relationships are investigated between deformation at the continuum macro-scale and at the micro-scale of interparticle contacts. Special attention is paid to the role of the microstructure, or fabric, as it is well known to have a strong influence on the behaviour of granular materials. Two-dimensional Discrete Element Method simulations of isobaric tests have been used to formulate truncated Fourier series representations for suitably-averaged relative displacement increment vectors at interparticle contacts and of parameters that describe the fabric. Based on a micromechanical expression for the average strain tensor that is valid in the two-dimensional case considered here and on these Fourier series representations, a Strain–Displacement–Fabric relationship has been derived that links the macro-scale dilatancy rate to the micro-scale relative displacements and fabric. Results of the Discrete Element Method simulations, using samples with different densities, have been employed to verify the accuracy of the proposed relationship for the dilatancy rate.

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1. Introduction

In many branches of science and engineering the behaviour of granular materials undergoing quasi-static deformation is important. This behaviour is described by a constitutive relation between (increments of) strain and stress. In the continuum-mechanical approach, such relations are often formulated heuristically. In the complementary micromechanical approach, relationships are studied between characteristics at the continuum macro-scale and the micro-scale of particles and interparticle contacts. Here, relationships are investigated between deformation (i.e. relative displacement) at the micro-scale of contacts and the strain at the continuum macro-scale. In particular, the dilatancy rate is studied, i.e. the change in volume induced by shear deformation (Reynolds, 1885), since it is an important characteristic of granular materials.

A large number of experimental studies (employing photoelastic materials; for example: Drescher and de Josselin de Jong, 1972; Oda, 1972a; Oda, 1972b; Oda, 1972c; Oda and Konishi, 1974; Oda et al., 1980) and computational studies (using the Discrete Element Method, DEM for short; for example: Cundall and Strack, 1979a; Thornton and Barnes, 1986; Rothenburg and Bathurst, 1989) have shown that granular materials may develop an anisotropic microstructure, even when the initial configuration is isotropic. This

microstructure, or *fabric*, can be characterised statistically by the contact distribution function (Biarez and Wiendieck, 1963; Horne, 1965) that describes the variation in the number of contacts oriented in various directions, or by a fabric tensor (Oda, 1972c; Satake and Satake, 1978; Kanatani, 1984). Relationships between the contact distribution function and fabric tensors are given by Kanatani (1984).

Based on the statics (in particular, the equilibrium equations for contact forces), a micromechanical expression for the average stress tensor in terms of the force vectors and the branch vectors at interparticle contacts has been formulated (for example, Weber, 1966; Rothenburg and Selvadurai, 1981; Christoffersen et al., 1981; Bagi, 1996; Kruyt and Rothenburg, 1996). The branch vector at an interparticle contact is the vector that connects the centres of the corresponding particles.

Using this micromechanical expression for the average stress tensor, Rothenburg and Bathurst (1989) derived an analytical relationship for the (relative) shear strength of two-dimensional granular materials (consisting of disk-shaped particles) in terms of the anisotropy in the contact distribution function, the anisotropy in the distribution of the normal forces and the (smaller) contribution due to tangential contact forces. This stress-force-fabric (SFF for short) relationship forms a cornerstone in micromechanics of granular materials.

Subsequent studies on SFF-relationships focussed on the influence of particle shape (two-dimensional ellipses by Rothenburg and Bathurst, 1993 and Nübel and Rothenburg, 1996;

* Corresponding author.

E-mail addresses: n.p.kruyt@utwente.nl (N.P. Kruyt), leo.rothenburg@uwaterloo.ca (L. Rothenburg).

polygon-shaped particles by Mirghasemi et al., 1995 three-dimensional ellipsoids by Oudafel and Rothenburg, 2001) and on general loading conditions (Li and Yu, 2013; 2014).

Based on the kinematics (in particular, the compatibility equations for relative displacements between particles in contact), Kruyt and Rothenburg (1996) formulated an expression for the average strain tensor in terms of the relative displacement vectors between particles in contact and geometrical vectors associated with contacts for the two-dimensional case. These geometrical vectors are described in detail in Section 3.

The objective of the current study is to develop a kinematic analogue of the stress-force-fabric relationship. This Strain–Displacement–Fabric (SDF for short) relationship connects deformation (i.e. relative displacement) at the micro-scale of interparticle contacts and fabric to continuum macro-scale strains. The kinematic analogue that is formulated here is more accurate than a previous analogue given by Kruyt and Rothenburg (2004), for reasons that are explained in detail in Section 4. For example, the expression by Kruyt and Rothenburg (2004) can not describe the critical state that is attained at large strains, where the volumetric strain increment becomes zero.

The outline of this study is as follows. In Section 2 DEM simulations are described, that have been employed to obtain detailed information at the micro-scale on particle displacements. The basics of micromechanics of granular materials are outlined in Section 3. The main result of the current study, a relationship between the continuum macro-scale dilatancy rate and the deformation characteristics at the micro-scale of interparticle contacts, is given in Section 4. In Section 5 this SDF-relationship is compared to results from DEM simulations. Finally, findings of this study are discussed in Section 6.

2. DEM simulations

Two-dimensional DEM simulations, as proposed by Cundall and Strack (1979b), have been performed, where the (unbreakable) particles are disk-shaped with variations in particle radius. The number of disks is 50,000. In these simulations the elastic part of the interparticle interactions is described by two linear springs, in directions normal and tangential to the contact, with spring stiffness k_n and k_t , respectively. This elastic part is complemented with the plastic (cohesionless) Coulomb friction criterion, according to which the (compressive) normal and tangential force components, f_n^c and f_t^c respectively, at the contact are constrained by $|f_t^c| \leq \mu f_n^c$ where μ is the interparticle friction coefficient.

Periodic boundary conditions have been imposed in order to increase the spatial homogeneity by eliminating wall effects and suppressing the formation of semi-permanent shear bands. Iso-baric tests have been performed where the deformation in one direction is imposed, with corresponding principal strain ϵ_1 (and principal stress σ_1), while in the perpendicular direction the principal strain ϵ_2 (with corresponding principal stress σ_2) is adjusted by a servo-mechanism such that the mean pressure $(\sigma_1 + \sigma_2)/2$ is kept constant.

In preparatory DEM simulations, a dense and a loose isotropic, initial sample have been created. The initial porosity n and coordination number (i.e. the average number of contacts per particle) Z are: $n = 0.15$, $Z = 4.18$ for the dense sample and $n = 0.21$, $Z = 3.40$ for the loose sample.

The deformation (or “overlap”) of the particles is fairly small as the value of the nondimensional ratio (in the two-dimensional case), $p/k_n = 5 \cdot 10^{-3}$. The value of the stiffness ratio $k_t/k_n = 0.5$ and the value of the interparticle friction coefficient $\mu = 0.5$.

The evolution with imposed strain ϵ_1 of the (relative) shear strength $(\sigma_1 - \sigma_2)/(\sigma_1 + \sigma_2)$ and of the volumetric strain $\epsilon_1 + \epsilon_2$ in the isobaric tests is shown in Fig. 1 for the dense and the loose

sample (left and right, respectively). The dense sample shows a dilating volumetric response and a rapid increase in shear strength, followed by softening until a constant value is attained at large strains. The loose sample shows a compactive volumetric response and a gradual increase of the shear strength until a constant value is attained at large strains. At large strains the shear strength of the dense and the loose sample become (nearly) equal and the volumetric strains become nearly constant, consistent with critical state behaviour. In these simulations stress, strain and fabric tensors are coaxial.

3. Micromechanics

Since the particles in granular materials are generally very stiff, the kinematics of the system are determined by the displacement increments of the particle centres and their rotation increments, denoted for particle p by $d\mathbf{U}^p$ and $d\omega^p$ (in the two-dimensional case considered here the particle rotation is described by a scalar quantity) respectively. The relative displacement increment vector between particles p and q in contact, denoted by $d\Delta^{pq}$, describes the micro-scale deformation due to the increments of the displacements of the particle centres. It is defined by

$$d\Delta^{pq} = d\mathbf{U}^q - d\mathbf{U}^p. \quad (1)$$

Note that

$$d\Delta^{qp} = -d\Delta^{pq}. \quad (2)$$

Various micromechanical expressions have been proposed to express the (increment of) the average strain tensor in terms of interparticle relative displacement (increment) vectors. There are two categories: (i) approach based on the best-fit hypothesis (Liao et al., 1997) and (ii) equivalent continuum approach (Kruyt and Rothenburg, 1996; Bagi, 1996; Dedeker et al., 2000). Only the latter category is consistent with the average strain as determined by the boundary displacements (Kruyt and Rothenburg, 1996; Bagi, 2006) and gives expressions that are volume-additive. In the equivalent continuum approach in Bagi (1996) and Durán et al. (2010a) the system is divided into elementary cells (triangles and tetrahedra in the two and three-dimensional case, respectively) obtained from a Delaunay tessellation. This tessellation may introduce virtual contacts (i.e. non-physical contacts) whose deformation behaviour is very different from that at physical contacts (Durán et al., 2010b). Therefore, the approach in Kruyt and Rothenburg (1996) is employed here that is based on a tessellation involving only physical contacts.

In the two-dimensional case that is considered here, the total surface (occupied by particles and voids) can be tessellated into polygons (or loops), where the sides of the polygons correspond to interparticle contacts (as illustrated in Fig. 2 (left)). The polygons characterise the voids in the system of particles.

Such polygons are also considered in the formulation of micromechanically-based constitutive relations (for example, Nicot and Darve, 2011; Nguyen et al., 2016).

The branch vector $\mathbf{l}^{pq}$ of two particles p and q in contact is the vector that connects their centres: $\mathbf{l}^{pq} = \mathbf{X}^q - \mathbf{X}^p$, where $\mathbf{X}^p$ is the position vector of the centre of particle p , with an analogous definition for $\mathbf{X}^q$. Each (internal) contact c corresponds to two particles p and q as well as to two polygons R and S . The rotated polygon vector that connects the centres of adjacent polygons R and S is denoted by $\mathbf{g}^{RS} = \mathbf{Y}^S - \mathbf{Y}^R$, where $\mathbf{Y}^R$ is the position vector of the centre of polygon R , with an analogous definition for $\mathbf{Y}^S$. The polygon vector $\mathbf{h}^{RS}$ is obtained by rotating the vector $\mathbf{g}^{RS}$ counter-clockwise over 90° . Note that $\mathbf{g}^{SR} = -\mathbf{g}^{RS}$ and $\mathbf{h}^{SR} = -\mathbf{h}^{RS}$. The branch, rotated polygon and polygon vectors are illustrated in Fig. 2 (right).

Although the branch vector $\mathbf{l}^c$ and the polygon vector $\mathbf{h}^c$ may vary significantly between individual contacts, they are correlated

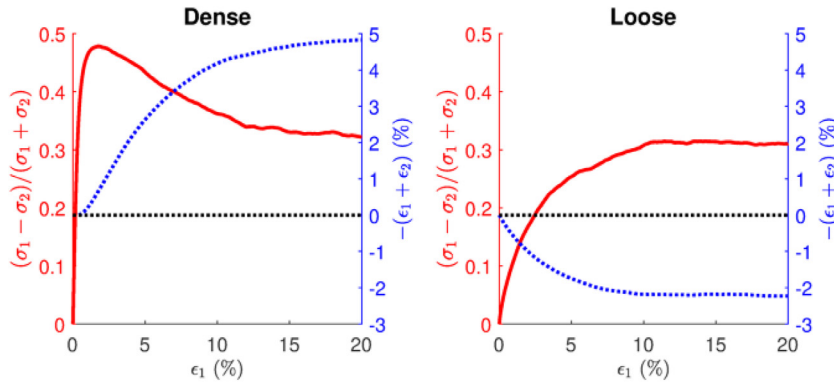


Fig. 1. Evolution with imposed strain ϵ_1 of (relative) shear strength $(\sigma_1 - \sigma_2)/(\sigma_1 + \sigma_2)$ (red, solid line) and volumetric strain $\epsilon_1 + \epsilon_2$ (blue, dotted line) in isobaric tests. Left: dense sample. Right: loose sample. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

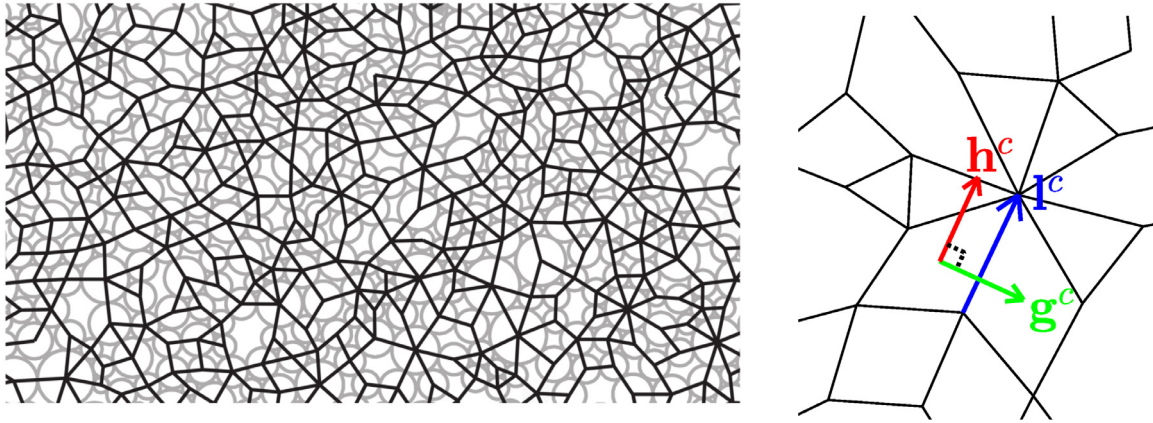


Fig. 2. Left: Tessellation of the total surface into polygons that are determined by the interparticle contacts. The contacts are indicated by black straight lines that connect the centres of particles in contact. The particles are shown as grey disks. Right: Branch vector $\mathbf{l}^c$, rotated polygon vector $\mathbf{g}^c$ and polygon vector $\mathbf{h}^c$ associated with a contact c . Particles are not shown here.

since they satisfy the average geometrical relationship (Krut and Rothenburg, 1996)

$$\delta_{ij} = \frac{1}{A} \sum_{c \in C} l_i^c h_j^c, \quad (3)$$

where δ_{ij} is the Kronecker symbol and the summation is over contacts c in the set of contacts C present in the region of interest with area A (consisting of particles and voids).

The micromechanical expression over the average strain increment tensor $d\epsilon$, in terms of the relative displacements $d\Delta^c$ and the polygon vectors $\mathbf{h}^c$ at the contacts, is given by Krut and Rothenburg (1996)

$$d\epsilon_{ij} = \frac{1}{A} \sum_{c \in C} d\Delta_i^c h_j^c, \quad (4)$$

where the summation is over the contacts c . The derivation of this expression consists of two steps. In the first step the average strain tensor is expressed in terms of the displacements at the boundary, using Gauss's theorem. In the second step, compatibility equations for relative displacements for the polygons are formulated that require that the sum of the relative displacements along the closed contours (i.e. the polygons) be equal to zero. Subsequently, moments are taken of these compatibility equations (by multiplication by the position vector of the centre of the polygon and summing over all polygons) and showing that the result is equal to the expression obtained from the first step. In this way an expression for the average strain tensor is obtained that is surface-additive (in the two-dimensional case considered here, rather than volume-additive in the three-dimensional case). Expression (4) is

actually an expression for the average displacement gradient tensor. For convenience, it is referred to by the shorter term strain tensor. The strain tensor is equal to the symmetric part of the displacement-gradient tensor. For the type of deformation analysed in detail here, the strain and displacement gradient tensors are equal.

The micromechanical expression for the stress tensor σ is given by (for example, Weber, 1966; Rothenburg and Selvadurai, 1981; Christoffersen et al., 1981; Bagi, 1996; Krut and Rothenburg, 1996)

$$\sigma_{ij} = \frac{1}{A} \sum_{c \in C} f_i^c l_j^c, \quad (5)$$

where the summation is over the contacts c and $\mathbf{f}^c$ is the interparticle force at contact c . Note the analogy between expressions (4) and (5): $\sigma \leftrightarrow d\epsilon$, $\mathbf{f}^c \leftrightarrow d\Delta^c$ and $\mathbf{l}^c \leftrightarrow \mathbf{h}^c$.

In the two-dimensional case, each contact c corresponds to two particles, p and q , as well as to two polygons R and S . Two geometrical vectors are associated with each contact: the branch vector $\mathbf{l}^c$ that is present in the expression (5) for the stress tensor and the rotated polygon vector $\mathbf{g}^{RS}$ that is involved in the expression (4) for the strain tensor (note that $\mathbf{h}^c$ and $\mathbf{g}^c$ are directly related, as they are perpendicular). Thus, an orientation of a contact c can be defined in two ways: based on the orientation (with respect to some reference direction) θ^c of the branch vector $\mathbf{l}^c$ or, alternatively based on the orientation φ^c of the rotated polygon vector $\mathbf{g}^c$. Direction φ^c gives the direction of the vector connecting the centres of the two adjacent polygons that correspond to contact c .

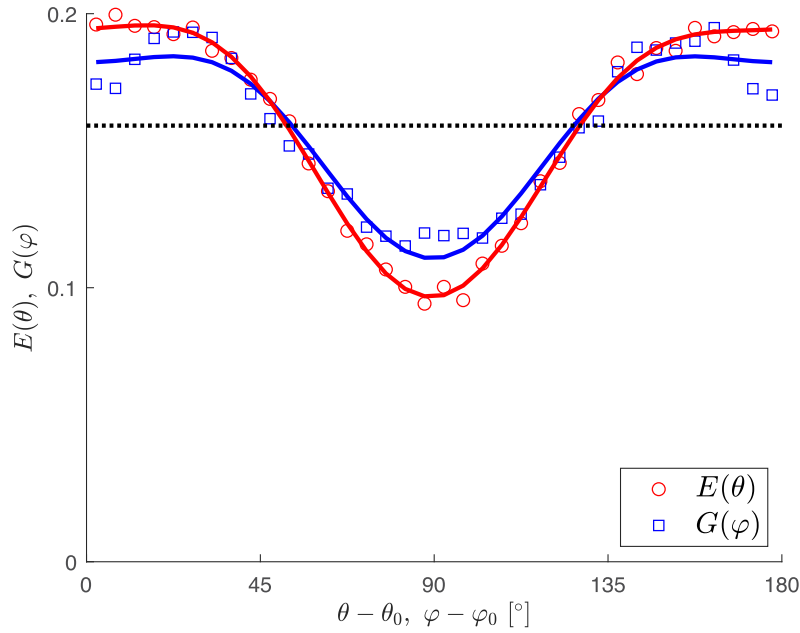


Fig. 3. Contact distribution functions $E(\theta)$ and $G(\varphi)$ (defined in Eq. (6)), obtained from results of the DEM simulation with the dense sample, at peak shear strength. The solid lines indicate fourth-order Fourier series least-squares approximations, Eq. (8). The black dotted line represents an isotropic distribution. Data are shown only for orientations in the interval $(0^\circ, 180^\circ)$, considering the symmetry implied by Eq. (7).

The distribution of contact orientations is usually based on orientations θ^c , giving the contact distribution function $E(\theta)$ (Horne, 1965). However, it is also possible to base the definition of a contact distribution function $G(\varphi)$ on orientations φ^c (Li and Li, 2009). The contact distribution function $E(\theta)$ is defined such that it gives the probability that the orientation θ^c of a contact c lies in an interval of width $\Delta\theta$ centred around θ . The contact distribution function $G(\varphi)$ based on the orientation φ^c is defined analogously

$$\begin{aligned} \text{Prob}\left[\theta - \frac{1}{2}\Delta\theta < \theta^c < \theta + \frac{1}{2}\Delta\theta\right] &= E(\theta)\Delta\theta \\ \text{Prob}\left[\varphi - \frac{1}{2}\Delta\varphi < \varphi^c < \varphi + \frac{1}{2}\Delta\varphi\right] &= G(\varphi)\Delta\varphi, \end{aligned} \quad (6)$$

for infinitesimally small $\Delta\theta$ and $\Delta\varphi$.

Since $E(\theta)$ and $G(\varphi)$ both are probability distributions, they satisfy the normalisation relations $\int_0^{2\pi} E(\theta)d\theta = 1$ and $\int_0^{2\pi} G(\varphi)d\varphi = 1$. As each contact c corresponds to two particles as well as to two polygons, it follows that contact orientations θ^c and φ^c are equivalent to contact orientations $\theta^c + \pi$ and $\varphi^c + \pi$, respectively. Hence

$$E(\theta + \pi) = E(\theta) \quad G(\varphi + \pi) = G(\varphi). \quad (7)$$

These contact distribution functions $E(\theta)$ and $G(\varphi)$ are shown in Fig. 3, as determined from the result of the DEM simulation at peak shear strength for the dense sample. They have the same qualitative features, but the anisotropy in $G(\varphi)$ is smaller than that in $E(\theta)$. For future reference, it is noted that $E(\theta)$ as well as $G(\varphi)$ can well be represented by a fourth-order Fourier series (for $E(\theta)$, see also Rothenburg and Bathurst, 1989)

$$\begin{aligned} E(\theta) &\cong \frac{1}{2\pi} [1 + a_c \cos 2(\theta - \theta_0) + b_c \cos 4(\theta - \theta_0)] \\ G(\varphi) &\cong \frac{1}{2\pi} [1 + A_c \cos 2(\varphi - \varphi_0) + B_c \cos 4(\varphi - \varphi_0)]. \end{aligned} \quad (8)$$

The reference angles θ_0 and φ_0 both correspond to the major principal stress direction. Note that due to the relations in Eq. (7), no odd-order Fourier terms are present. The parameters a_c and A_c describe the anisotropy in the contact distribution functions $E(\theta)$

and $G(\varphi)$, respectively. The higher-order terms involving parameters b_c and B_c are included here for completeness.

Continuum-mechanical considerations indicate that contact characteristics (such as the contact force $\mathbf{f}^c$ and the relative displacement increment vector $d\Delta^c$) will, on average, depend on the orientation, either θ^c or φ^c , of a contact c (Bathurst and Rothenburg, 1988; Rothenburg and Bathurst, 1989). Thus, it is meaningful to group contacts with similar orientations, either θ^c or φ^c , and determine averages for such groups of contacts. These group averages for the relative displacement increment vector are denoted by $\overline{d\Delta}(\theta)$ and $\overline{d\Delta}(\varphi)$, respectively.

For simplicity of notation, the type of group averaging, either based on orientation θ of the branch vector or that of the rotated polygon vector φ , is indicated by the argument: for an arbitrary contact quantity ψ^c , $\overline{\psi}(\theta)$ denotes the average when contacts are grouped by orientation θ^c and $\overline{\psi}(\varphi)$ denotes the average when contacts are grouped by orientation φ^c . Formally, the group averages are defined by

$$\overline{\psi}(\theta) = \frac{\sum_{c \in \mathcal{C}} \psi^c I_g(\theta^c)}{\sum_{c \in \mathcal{C}} I_g(\theta^c)} \quad \overline{\psi}(\varphi) = \frac{\sum_{c \in \mathcal{C}} \psi^c I_g(\varphi^c)}{\sum_{c \in \mathcal{C}} I_g(\varphi^c)}, \quad (9)$$

where the indicator function $I_g(\theta^c)$ equals 1 when orientation θ^c is in group g and 0 otherwise; $I_g(\varphi^c)$ is defined analogously.

In terms of these group averages the micromechanical expression Eq. (4) for the strain increment tensor $d\epsilon$ can be expressed as

$$\begin{aligned} d\epsilon_{ij} &= m_A \int_0^{2\pi} E(\theta) \overline{d\Delta_i h_j}(\theta) d\theta \\ &= m_A \int_0^{2\pi} G(\varphi) \overline{d\Delta_i h_j}(\varphi) d\varphi, \end{aligned} \quad (10)$$

where $m_A = N_{\text{cont}}/A$ is the contact density (with N_{cont} the number of contacts). In the first equality in Eq. (10) contacts have been grouped by orientation θ^c of the branch vector, while in the second for they have been grouped by orientation φ^c of the rotated polygon vector.

Two local, orthogonal coordinate systems associated with a contact c can be employed to define components of vectors, based

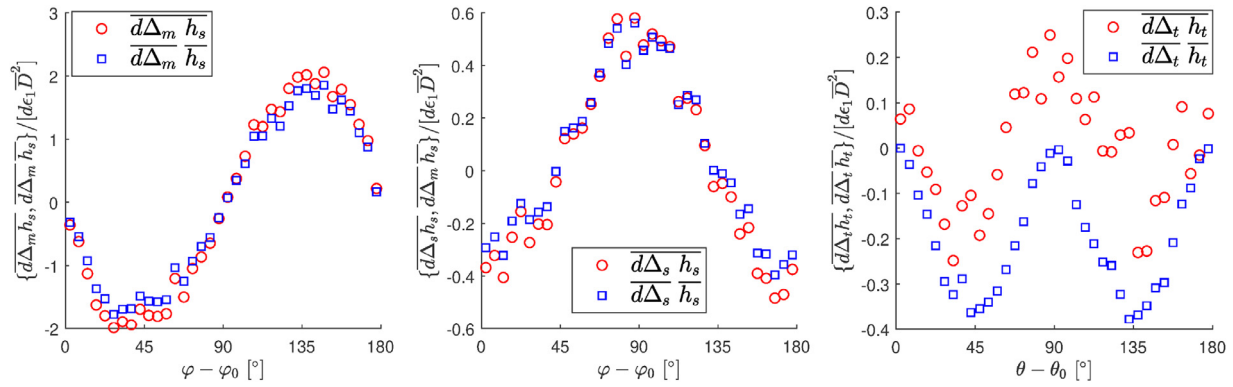


Fig. 4. Investigation of (lack of) correlation between components of the relative displacement increment and polygon vectors. Left: between m -component of relative displacement increment and s -component of polygon vectors. Middle: between s -component of relative displacement increment and s -component of polygon vectors. Right: between t -component of relative displacement increment and t -component of polygon vectors. Results have been scaled with the major principal strain increment $d\epsilon_1$ and the average particle diameter D_{avg}^2 . Data are shown only for orientations in the interval $(0^\circ, 180^\circ)$, considering the symmetry implied by Eqs. (7) and (12).

on the contact orientation θ^c or on φ^c . For the first system, the orthogonal unit vectors are denoted by $\mathbf{n}^c$ and $\mathbf{t}^c$, while those for the second system are $\mathbf{m}^c$ and $\mathbf{s}^c$. These vectors are defined by

$$\begin{aligned} \mathbf{n}^c &= (\cos \theta^c, \sin \theta^c)^T & \mathbf{t}^c &= (-\sin \theta^c, \cos \theta^c)^T \\ \mathbf{m}^c &= (\cos \varphi^c, \sin \varphi^c)^T & \mathbf{s}^c &= (-\sin \varphi^c, \cos \varphi^c)^T. \end{aligned} \quad (11)$$

With the $(\mathbf{n}^c, \mathbf{t}^c)$ local coordinate system, an arbitrary vector $\mathbf{b}^c$ associated with a contact c can be decomposed into normal and tangential components, b_n^c and b_t^c respectively, as $\mathbf{b}^c = b_n^c \mathbf{n}^c + b_t^c \mathbf{t}^c$. Note that the branch vector is given by $\mathbf{l}^c = l_n^c \mathbf{n}^c$. In this local coordinate system the normal and tangential components of the relative displacement increment vector $d\Delta^c$ are denoted by $d\Delta_n^c$ and $d\Delta_t^c$, respectively.

With the $(\mathbf{m}^c, \mathbf{s}^c)$ local coordinate system, an arbitrary vector $\mathbf{b}^c$ associated with a contact c can be decomposed into normal and tangential components, b_m^c and b_s^c respectively, as $\mathbf{b}^c = b_m^c \mathbf{m}^c + b_s^c \mathbf{s}^c$. Note that the rotated polygon vector is given by $\mathbf{g}^c = g_m^c \mathbf{m}^c$, and hence $\mathbf{h}^c = h_s^c \mathbf{s}^c$. In this local coordinate system the normal and tangential components of the relative displacement increment vector $d\Delta^c$ are denoted by $d\Delta_m^c$ and $d\Delta_s^c$, respectively.

Considering Eqs. (2) and (11), it follows that

$$\overline{d\Delta_m}(\varphi + \pi) = \overline{d\Delta_m}(\varphi) \quad \overline{d\Delta_s}(\varphi + \pi) = \overline{d\Delta_s}(\varphi). \quad (12)$$

4. Strain-displacement-fabric relationship

The micromechanical expressions (10) for the strain tensor $d\epsilon$ involve the group averages of a product, $\overline{d\Delta_i h_j}(\theta)$ and $\overline{d\Delta_i h_j}(\varphi)$. To proceed from these relationships (10) analytically, simplifying assumptions for the average of products must be made. Here it is assumed that the relative displacement increment vector $d\Delta$ and the polygon vector $\mathbf{h}$ are *uncorrelated*, and hence $\overline{d\Delta_i h_j}(\theta) \simeq \overline{d\Delta_i}(\theta) \overline{h_j}(\theta)$ and $\overline{d\Delta_i h_j}(\varphi) \simeq \overline{d\Delta_i}(\varphi) \overline{h_j}(\varphi)$.

The appropriateness of these assumptions has been investigated, using results of the DEM simulations at large strain for the dense sample. The terms $\overline{d\Delta_m h_s}(\varphi)$ and $\overline{d\Delta_s h_s}(\varphi)$ are shown in Fig. 4 (left and middle, respectively), together with the corresponding approximations, $\overline{d\Delta_m}(\varphi) \overline{h_s}(\varphi)$ and $\overline{d\Delta_s}(\varphi) \overline{h_s}(\varphi)$ respectively. These results show that $\overline{d\Delta_m}(\varphi)$ and $\overline{d\Delta_s}(\varphi)$ can be considered as being uncorrelated with $\overline{h_s}(\varphi)$, with sufficient accuracy. The term $\overline{d\Delta_t h_t}(\theta)$ and its approximation $\overline{d\Delta_t}(\theta) \overline{h_t}(\theta)$ are compared in Fig. 4 (right). The results show that the assumption of $\overline{d\Delta_t}(\theta)$ and $\overline{h_t}(\theta)$ being uncorrelated is generally *not* correct (as has already been noted by Kruyt and Rothenburg, 2004 for large strains in biaxial tests where the lateral stress is kept constant).

These results for the (lack of) correlations between relative displacement increment and polygon vectors show that it is prefer-

able to base analytical developments on the orientation φ of the rotated polygon vector, rather than θ of the branch vector. For future reference these observations about the lack of (or small) correlation when the orientations are based on that of the rotated polygon vector are expressed by

$$\overline{d\Delta_m h_s}(\varphi) \simeq \zeta_m \overline{d\Delta_m}(\varphi) \overline{h_s}(\varphi) \quad \overline{d\Delta_s h_s}(\varphi) \simeq \zeta_s \overline{d\Delta_s}(\varphi) \overline{h_s}(\varphi), \quad (13)$$

where ζ_m and ζ_s are correction factors (Bathurst and Rothenburg, 1988; Kruyt and Rothenburg, 2001). For perfect lack of correlation, $\zeta_m = \zeta_s = 1$. In general, $\zeta_m \simeq 1$ and $\zeta_s \simeq 1$; for the results shown in Fig. 4 (left and middle), $\zeta_m = 1.14$ and $\zeta_s = 1.11$. Note that the results shown in Fig. 4 (right) can not be described by such a multiplicative correction.

Using the assumption that the relative displacement increment and polygon vectors are uncorrelated, the micromechanical expression for the strain tensor Eq. (10) becomes

$$\begin{aligned} d\epsilon_{ij} &= m_A \int_0^{2\pi} G(\varphi) [\zeta_m \overline{d\Delta_m}(\varphi) m_i(\varphi) \\ &\quad + \zeta_s \overline{d\Delta_s}(\varphi) s_i(\varphi)] \overline{h_s}(\varphi) s_j(\varphi) d\varphi, \end{aligned} \quad (14)$$

where $\overline{\mathbf{h}}(\varphi) = \overline{h_s}(\varphi) \mathbf{s}(\varphi)$ and Eq. (13) have been used. Hence, expressions for $\overline{\Delta_m}(\varphi)$, $\overline{\Delta_s}(\varphi)$ and $\overline{h_s}(\varphi)$ are required that will now be formulated, based on results from the DEM simulations.

The quantity $\overline{h_s}(\varphi)$ represents the length of the polygon vector, which is equal to that of the rotated polygon vector. Hence $\overline{h_s}(\varphi)$ describes the distance between centres of adjacent polygons (voids). Results of the DEM simulations indicate (data not shown) that $\overline{h_s}(\varphi)$ is well represented by a second-order Fourier series

$$\overline{h_s}(\varphi) \simeq h_0 [1 + A_h \cos 2(\varphi - \varphi_0)], \quad (15)$$

where h_0 represents the isotropic part in the orientational distribution of the length of the polygon vector and A_h gives its anisotropy. For the isobaric tests considered here the reference orientation φ_0 corresponds to the direction of the major principle stress.

Similarly, the results from the DEM simulations for the components $\overline{d\Delta_m}(\varphi)$ and $\overline{d\Delta_s}(\varphi)$ of the group-averaged relative displacement increment vector $\overline{d\Delta}(\varphi)$ are shown in Fig. 5 for small and large strains for the dense sample. These results show that in both cases $\overline{d\Delta_m}(\varphi)$ and $\overline{d\Delta_s}(\varphi)$ can also be well described by second-order Fourier series

$$\begin{aligned} \overline{d\Delta_m}(\varphi) &\simeq d\Delta_0 \sin 2(\varphi - \varphi_0) \\ \overline{d\Delta_s}(\varphi) &\simeq d\Delta_0 [R_\Delta + A_\Delta \cos 2(\varphi - \varphi_0)]. \end{aligned} \quad (16)$$

Here $d\Delta_0$ represent an amplitude of the relative displacement increments, R_Δ and A_Δ give the isotropic and anisotropic parts of

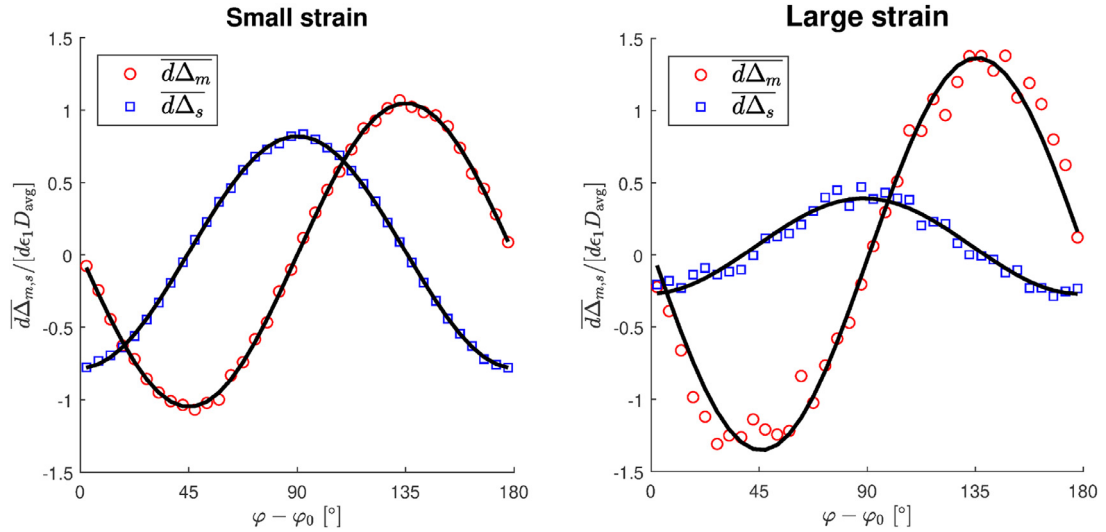


Fig. 5. Components $\overline{d\Delta_m}(\varphi)$ and $\overline{d\Delta_s}(\varphi)$ of the group-averaged relative displacement increment vector. Left: Small strain. Right: large strain. Results have been scaled with the major principal strain increment $d\epsilon_1$ and the average particle diameter D_{avg} . Data are shown only for orientations in the interval $(0^\circ, 180^\circ)$, considering the symmetry implied by Eq. (12). Results from DEM simulation with the dense sample.

the orientational distribution of the group-averaged relative displacement increment component $\overline{d\Delta_s}(\varphi)$. For the results shown in Fig. 5, $R_\Delta = -0.19$, $A_\Delta = 0.76$ (small strain) and $R_\Delta = -0.45$, $A_\Delta = 0.24$ (large strain).

The group-averaged deformation component $\overline{\Delta_m}(\varphi)$ corresponds to the direction of the rotated polygon vector that is directed from polygon (void) centre to polygon (void) centre. As this vector is oriented in the “void direction”, it is expected that in deformations involving shear, this component $\overline{\Delta_m}(\varphi)$ is larger than the component $\overline{\Delta_s}(\varphi)$ in the perpendicular direction. Therefore in Eq. (16), the relative displacement increments have been scaled with the amplitude of the component $\overline{d\Delta_m}(\varphi)$. For small strain $\overline{\Delta_m}(\varphi)$ and $\overline{\Delta_s}(\varphi)$ are of equal magnitude (see Fig. 5 left), while for large strain $\overline{\Delta_s}(\varphi)$ is smaller than $\overline{\Delta_m}(\varphi)$ (see Fig. 5 right).

As dilatancy is an important characteristic of the behaviour of granular materials, the focus here is on the dilatancy rate $-d\epsilon_V/d\epsilon_S$, where the volumetric and shear strain increments, $d\epsilon_V$ and $d\epsilon_S$ respectively, are defined by $d\epsilon_V = d\epsilon_1 + d\epsilon_2$ and $d\epsilon_S = d\epsilon_1 - d\epsilon_2$.

Based on the micromechanical expression for the strain tensor (Eq. (14)) (where the assumption that the relative displacement increment and the polygon vectors are uncorrelated has already been incorporated) and the truncated Fourier-series representations for the contact distribution $G(\varphi)$ (Eq. (8)), the group-averaged length of the polygon vector (Eq. (15)) and the components of the relative displacement increment vector (Eq. (16)), it follows after some algebra and performing a second-order Taylor series expansion in parameters A_c , A_h , R_Δ and A_Δ that the dilatancy rate $-d\epsilon_V/d\epsilon_S$ is given by

$$-\frac{d\epsilon_V}{d\epsilon_S} \cong \frac{\zeta_s}{\zeta_m} \left[(2 + B_c)R_\Delta + \left(A_c + A_h - \frac{\zeta_s}{\zeta_m} 2R_\Delta \right) A_\Delta \right]. \quad (17)$$

Note that this result for the dilatancy rate only involves the ratio ζ_s/ζ_m of the correction factors ζ_m and ζ_s and that B_c (which quantifies the fourth-order component of $G(\varphi)$ in Eq. (8)) has no significant contribution to the dilatancy rate.

This strain-displacement-fabric expression (SDF for short) shows that the macro-scale dilatancy rate $-d\epsilon_V/d\epsilon_S$ is determined by: (i) the micro-scale fabric, in particular the geometrical anisotropy of the contact network as characterised by the parameters A_c and A_h and (ii) the micro-scale relative displacements, as characterised by the parameters R_Δ and A_Δ that describe the ori-

entational distribution of the component $\overline{d\Delta_s}(\varphi)$ of the relative displacement increment vector.

In the approach by Kruyt and Rothenburg (2004) the contact orientation was based on that of the branch vector, θ^c . A disadvantage of this approach is that the assumption of uncorrelated relative displacement increment and polygon vectors is not generally correct (see Fig. 4 (right)). For comparison with the current expression Eq. (17), their result for the dilatancy rate is given here as well

$$-\frac{d\epsilon_V}{d\epsilon_S} \cong \rho_h - 2\rho_\Delta, \quad (18)$$

where ρ_h and ρ_Δ are parameters in the truncated Fourier series representations for the normal and tangential components of the group-averaged polygon vector, $\overline{h_n}(\theta)$ and $\overline{h_t}(\theta)$, and of the relative displacement increment vector, $\overline{d\Delta_n}(\theta)$ and $\overline{d\Delta_t}(\theta)$

$$\begin{aligned} \overline{h_n}(\theta) &\cong h_{n0} \\ \overline{d\Delta_n}(\theta) &\cong d\Delta_{t0}[\rho_\Delta + a_\Delta \cos 2(\theta - \theta_0)] \\ \overline{h_t}(\theta) &\cong \rho_h h_{n0} \sin 2(\theta - \theta_0) \\ \overline{d\Delta_t}(\theta) &\cong -d\Delta_{t0} \sin 2(\theta - \theta_0). \end{aligned} \quad (19)$$

The accuracy of the theory Eq. (18) is limited, as will be shown in detail in Section 5.2. In particular, it does not describe the critical state where the dilatancy rate becomes zero.

5. Results

In this Section the accuracy of the developed SDF-relationship, Eq. (17), is evaluated. Since this relationship involves the parameters A_c and A_h that characterise the fabric as well as parameters R_Δ and A_Δ that characterise the micro-scale deformation, their evolution with imposed strain ϵ_1 is shown first in Section 5.1. The actual comparison of the developed SDF-relationship with results of the DEM simulations with the dense and the loose sample is presented in Section 5.2.

5.1. Evolution of micromechanical parameters

The results of the DEM simulations have been used to determine the parameters present in the SDF-relationship, Eq. (17). To this end, the group averages of relative displacement vector,

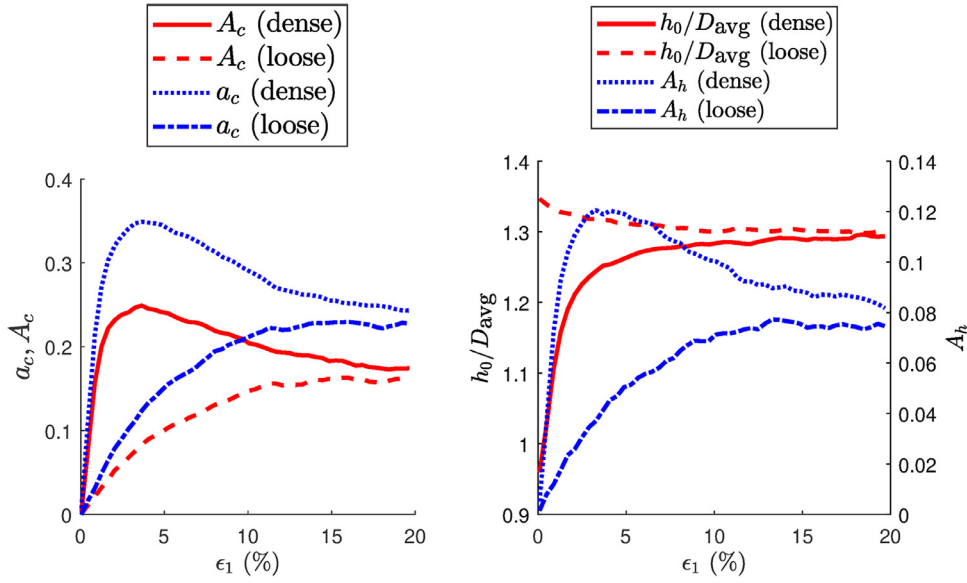


Fig. 6. Left: evolution with imposed strain ϵ_1 of parameters a_c and A_c in Eq. (8) that determine the anisotropy in the contact distributions $E(\theta)$ and $G(\varphi)$, respectively. Right: evolution with imposed strain ϵ_1 of parameters h_0 and A_h in Eq. (15) that determine the orientational distribution of the length of the group-averaged polygon vector $\bar{h}_s(\varphi)$. Data from DEM simulations with the dense and loose sample; h_0 is scaled with the average particle diameter D_{avg} .

$\overline{d\Delta_m}(\varphi)$ and $\overline{d\Delta_s}(\varphi)$, and polygon vector $\bar{h}_s(\varphi)$ have been determined. Subsequently, the parameters in the Fourier representations Eqs. (15) and (16) have been evaluated by a least-squares method. Other parameters, such the contact distribution functions $E(\theta)$ and $G(\varphi)$, have been processed in an analogous manner. This process has been executed for each value of the imposed strain ϵ_1 .

The evolution of the anisotropies a_c and A_c in the contact distributions $E(\theta)$ and $G(\theta)$ respectively (see Eq. (8)), are shown in Fig. 6 (left). Although a_c is not present in the SDF-relationship (17), it is shown here for comparison with A_c . Initially, both anisotropies are nearly zero, as both the dense and the loose sample are isotropic. For the dense sample the contact anisotropy a_c in $E(\theta)$ rapidly increases up to the peak value, after which it decreases to a nearly constant value at large strains. For the loose sample the contact anisotropy a_c gradually increases. These findings are consistent with those presented by Rothenburg and Bathurst (1989) and Kruyt and Rothenburg (2014), for instance. At large strains, the contact anisotropy for the dense and the loose sample become nearly equal, consistent with the critical state for fabric (see for example, Zhao and Guo, 2013; Kruyt and Rothenburg, 2014; Li and Yu, 2014). The evolution of the anisotropy A_c in $G(\varphi)$ closely resembles that of a_c , for both the dense and the loose sample. For the dense and the loose sample the ratio A_c/a_c becomes almost constant ($\cong 0.7$) for $\epsilon_1 > 1.5\%$; no exact proportionality has been observed.

Parameter h_0 in Eq. (15) represents the isotropic part of the orientational distribution of the group-averaged length of the polygon vector $\bar{h}_s(\varphi)$. This parameter describes the distance between the centres of adjacent polygons (i.e. voids). A dense and a loose system are therefore expected to have a small and a large value of h_0 , respectively. This is confirmed by the results shown in Fig. 6 (right). For the loose sample, h_0 is nearly constant, while for the dense sample it rapidly increases with imposed strain ϵ_1 until its value becomes nearly constant at large strains. At large strains, the values are nearly equal for the dense and the loose sample, consistent with critical state behaviour.

Parameter A_h in Eq. (15) represents the anisotropy in the orientational distribution of the group-averaged length of the polygon vector $\bar{h}_s(\varphi)$. Initially, A_h is nearly zero, as both the dense and the loose sample are isotropic. The evolution with imposed strain ϵ_1

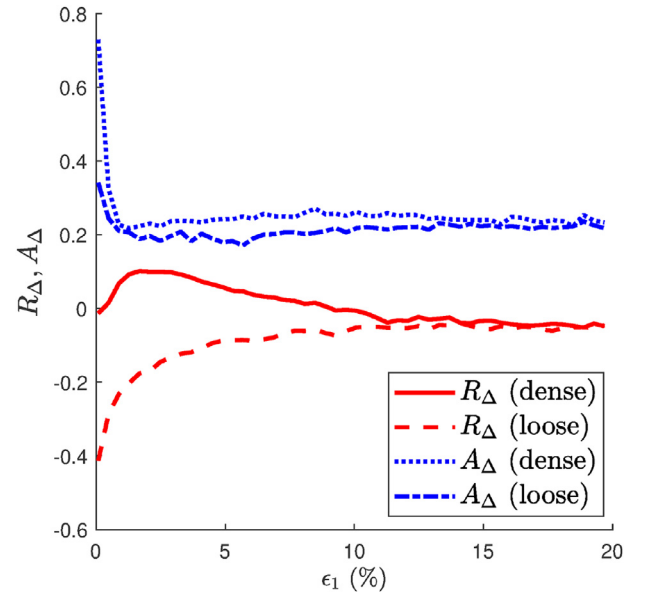


Fig. 7. Evolution with imposed strain ϵ_1 in isobaric tests of parameters R_Δ (red line, solid for the dense sample and dashed for the loose sample) and A_Δ (blue line, dotted for the dense sample and dot-dash for the loose sample) that characterise the orientational distribution of the component $\overline{\Delta_s}(\varphi)$ of the group-averaged relative displacement increment vector, see Eq. (16). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

shown in Fig. 6 (right) closely resembles that of the anisotropies a_c and A_c shown in Fig. 6 (left).

The parameters R_Δ and A_Δ in Eq. (16) determine the orientational distribution of the group-averaged component $\overline{\Delta_s}(\varphi)$ of the relative displacement increment vector. The parameters R_Δ and A_Δ determine the isotropic and the anisotropy of the orientational distribution, respectively. The evolution with imposed strain ϵ_1 of the parameters R_Δ and A_Δ is shown in Fig. 7.

For the dense sample the parameter R_Δ initially is positive. It reaches a peak and then decreases to a nearly constant (slightly negative) value at large strains. For the loose sample, R_Δ is neg-

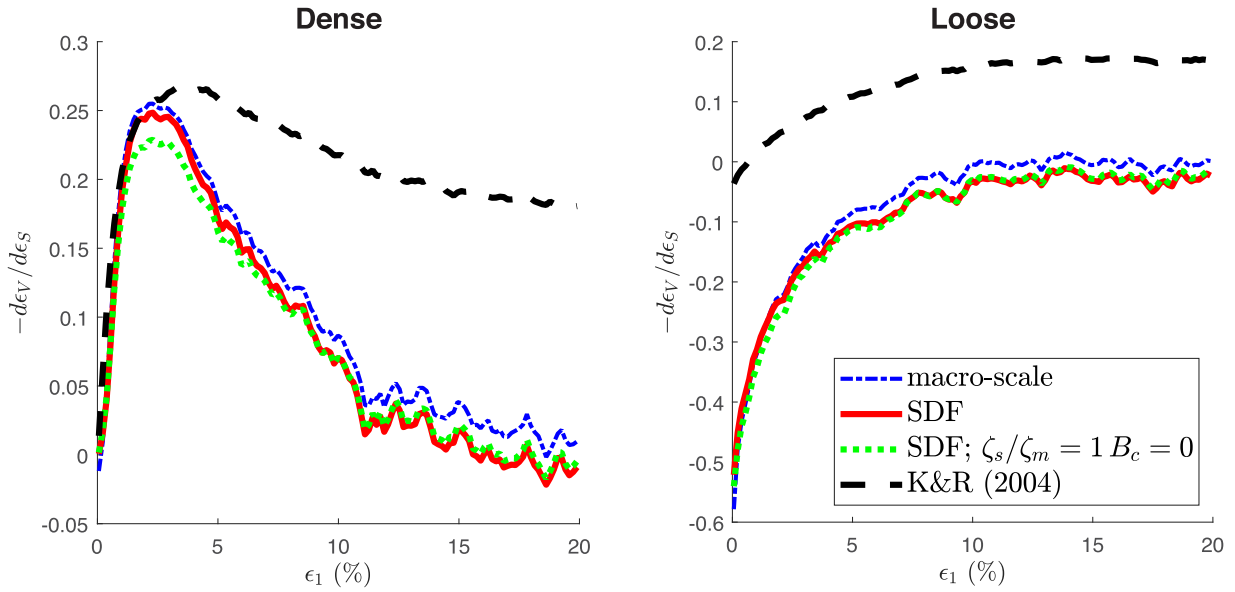


Fig. 8. Comparison of the dilatancy rate $-d\epsilon_v/d\epsilon_s$ from: continuum macro-scale deformation (blue dash-dot line), theory of Kruyt and Rothenburg (2004) (Eq. (18); black dashed line) and according to the SDF relationship (Eq. (17)). For the latter, results are shown when $\zeta_s/\zeta_m = 1$, $B_c = 0$ (green dotted line) and when ζ_s/ζ_m and B_c have been determined from the results of the DEM simulations (red solid line). Left: dense sample. Right: Loose sample. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

ative and decreases in magnitude with increasing strain. At large strains, R_Δ for the dense and for the loose sample become nearly equal.

For the dense and the loose sample A_Δ decreases (very rapidly for the dense sample) and becomes nearly constant for strain larger than about 1%. These values are nearly equal for the dense and the loose sample.

5.2. Accuracy of SDF-relationship

The results of the DEM simulations with the dense and the loose sample have been used to evaluate the accuracy of the developed SDF-relationship, Eq. (17), for the dilatancy rate $-d\epsilon_v/d\epsilon_s$, see Fig. 8. For comparison, results are also shown for the theory of Kruyt and Rothenburg (2004), Eq. (18). The macro-scale dilatancy rate has been determined from the deformation of the periodic box.

The dense sample shows a positive dilatancy rate (corresponding to dilation) which rapidly increases up to a peak value, after which the dilatancy decreases towards zero (corresponding to the critical state). For the loose sample, the dilatancy rate is negative (corresponding to compaction). With increasing imposed strain ϵ_1 the dilatancy rate decreases (in absolute value) towards zero (corresponding to the critical state).

The relationship by Kruyt and Rothenburg (2004) gives a qualitative agreement for the dense sample. For the loose sample their theory does not capture the compactive behaviour. In both cases this theory does not capture the critical state where the dilatancy rate approaches zero. Note that for the current isobaric tests, the parameter $\rho_\Delta \cong 0$ where ρ_Δ is defined through Eq. (19).

In contrast, the current SDF-relationship, Eq. (17), matches the dilatancy rate from the DEM simulations with good accuracy, for both the dense and the loose sample. Inclusion of the correction factors ζ_m and ζ_s and of the fourth-order Fourier series term (characterised by B_c) increases the accuracy of the SDF-relationship in reproducing the dilatancy rate from the DEM simulations somewhat, especially near the strain at which the peak dilatancy rate is attained. For large strains, the term ζ_s/ζ_m has only a very small influence. For both dense and loose sample the SDF-relationship

gives a dilatancy rate that approaches zero for large strains, consistent with critical state behaviour.

6. Concluding remarks

The micromechanical expression for the average strain tensor Eq. (4), in discrete form as a sum over contact quantities, has been used in order to establish a relationship between continuum macro-scale deformation on one hand and the fabric and suitable averages of the micro-scale deformation at interparticle contacts on the other hand.

Results of two-dimensional DEM simulations of isobaric tests have shown that it is advantageous to base the orientation of a contact on the orientation of the rotated polygon vector that connects the centres of adjacent polygons, as then the relative displacement increment and the polygon vectors are practically uncorrelated, Eq. (13). Truncated Fourier series representations for the relative displacement increment and the polygon vectors have been formulated, Eqs. (15) and (16), again employing the results of DEM simulations.

Combining these truncated Fourier representations and the micromechanical expression Eq. (14) for the strain tensor (in terms of the contact distribution function $G(\varphi)$ and of the group-averaged relative displacement increment and of polygon vectors), a strain-displacement-fabric (SDF) relationship, Eq. (17), has been derived that relates the continuum macro-scale dilatancy rate to the geometrical micro-scale parameters A_c and A_h in Eqs. (8) and (15) that describe the fabric and the micro-scale deformation parameters R_Δ and A_Δ in Eq. (16) that describe the orientational distribution of the group-averaged relative displacement increment Δ_s . This relationship for the dilatancy rate $-d\epsilon_v/d\epsilon_s$ forms a kinematic analogue to stress-force-fabric relationships.

The evolution with imposed strain ϵ_1 of the parameters associated with the developed SDF-relationship has been studied, using the results of the DEM simulations for the dense and the loose sample.

The dilatancy rate from the DEM simulations and according the SDF-relationship have been compared, showing good agreement for both the dense and the loose sample that show dila-

tive and compactive behaviour, respectively. For large strains, the dilatancy rate approaches zero, consistent with critical state behaviour.

The SDF-relationship connects the kinematics at the micro-scale to that at the macro-scale. Reflecting kinematics only, it does not directly involve a description of constitutive behaviour. However, the results support micromechanical constitutive modelling work by providing insights on the quantities at the micro-scale that are relevant and important to the macro-scale behaviour.

Expressions for the dilatancy rate can be considered as flow rules for the plastic strains. The SDF-relationship has been based on the micro-scale relative displacement at contacts, where no distinction has been made of elastic and plastic components. The basic ideas presented here, that are ultimately based on Eq. (10), can be employed to accomplish such micromechanical decompositions. Recent studies on the elastic-plastic decomposition of the strain tensor and on the extraction of such strains from the results of DEM simulations have been reported in Nicot and Darve (2006), Pouragha and Wan (2017), Pouragha and Wan (2018) and Kuhn and Daouadji (2018).

Kruij and Rothenburg (2016) developed an expression for the dilatancy rate in terms of coordination number and contact anisotropy, based on micromechanical considerations. Contrary to the current approach, this involved various modelling choices. It is recommended to further explore connections between these two approaches.

In the current study DEM simulations of isobaric tests with disk-shaped particles have been considered, with samples of different porosities. In these tests the principal directions of the fabric, stress and strain tensors are all coaxial. Hence, it is recommended to investigate SDF-relationships for other particle shapes and other loading conditions. The development of such SDF-relationships may benefit from previous work on SFF-relationships on these aspects (Rothenburg and Bathurst, 1993; Nübel and Rothenburg, 1996; Mirghasemi et al., 1995; Li and Yu, 2013; 2014).

The current SDF-relationship is restricted to the two-dimensional case. It is expected that many qualitative features of this two-dimensional SDF-relationship (in particular, the importance to the macro-scale dilatancy rate of the anisotropy in the microstructure and of the anisotropy in the orientational distribution of the micro-scale relative displacements) will also be present in three-dimensional SDF-relationships.

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