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Critical state and evolution of coordination number in simulated granular materials

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Abstract

A theory of critical state and of the evolution of coordination number during quasi-static deformations of granular materials is developed, based on the interpretation of several discrete element simulations of plane granular assemblies with a range of interparticle friction from nearly frictionless to infinitely rough. The theory is based on the concept that shear deformations tend to destroy interparticle contacts and create locally unstable configurations that regain stability by forming new or restoring old interparticle contacts. The process is operating in such a way that in a dense state the rate of contact disintegration exceeds the rate of contact creation, while in the critical state both rates are equalized. In a loose state more contacts are created than disintegrated until rates are equalized. Interparticle friction is viewed as an essential element that affects stability of local configurations. This explains the pronounced dependence of critical coordination number on interparticle friction as observed in two-dimensional discrete element simulations. The derived differential equation for the evolution of coordination number in biaxial tests is shown to describe the results of the discrete element simulations remarkably well. The paper also presents analyses of simulation data to investigate a relationship between packing fraction of granular assemblies and coordination number. The data suggest that the packing fraction is affected by the anisotropy of contact orientations as well as by the coordination number. The latter is the primary variable. Limited data also suggest that critical state is characterized by both critical coordination number and by critical anisotropy induced by shear deformations.

1. Introduction

The notion of critical state in granular materials was introduced by Casagrande (1936) in connection with observations that granular materials tend to reach the same void ratio in the course of shear deformations, irrespective of the initial void ratio. Dense granular materials reach the critical state as a result of dilation, while loose materials tend to reach the same state after volumetric contraction. When the steady state is reached, deformation continues without volume changes.

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Experimental studies indicate that the critical void ratio (or any other equivalent parameter, such as packing fraction) is not a unique characteristic of a material, but depends on many factors such as the consolidation stress in triaxial tests or possibly even on a loading path when more sophisticated testing devices are used (Been et al., 1991). Most continuum constitutive models for granular materials, starting from the critical state soil mechanics of Schofield and Wroth (1968), begin from the empirical concept of critical state. Many aspects related to critical state are presently not well understood, even empirically (Mooney et al., 1998). A micromechanical theory of critical state is not even in infancy yet.

Despite that many factors may affect the critical state, an intuitive reason for its existence is rather obvious: as no material can dilate or contract ad infinitum, the state of deformations without volume change must be reached at some point or another. If this argument is rationalized, it becomes clear that dilation is unavoidably associated with loss of particle stability. This leads to a spontaneous reduction in volume that compensates for the volume increase due to dilation. In this paper this mechanism is analysed deeper by examining a series of numerical simulations in which the particle stability is parametrically altered by varying interparticle friction. Based on this analysis, a simple analytical theory is developed for the evolution of coordination number, i.e. the average number of contacts per particle, in a plane granular assembly of disks. The theory leads to the characterization of critical state in terms of a critical coordination number that is shown to depend on interparticle friction. The analytical theory accurately describes the results of the numerical simulations.

In order to bring the theory of critical state formulated in terms of the coordination number into a conventional framework, a relationship between the coordination number and the packing fraction is examined, based on the numerical simulations. The simulation data point out that the link between packing fraction and coordination number may be affected by the degree of shear-induced anisotropy in contact orientations.

This study starts by describing several simulated biaxial tests with varying interparticle friction. These tests were augmented by unloading calculations at a number of points along the loading path in order to determine elastic parameters. These parameters are necessary in order to compute plastic strains in terms of which the theory of critical state is formulated. Theoretical relationships for the evolution of coordination number towards the critical state are compared with results from the simulations. A relationship between packing fraction and coordination number is examined and the main results presented in the paper are finally discussed.

2. Discrete element simulations

Two-dimensional discrete element simulations were performed using a code operating in a manner similar to that of Cundall and Strack (1979) with a slightly different dynamic relaxation procedure. Simulated biaxial tests employing periodical boundary conditions were performed on assemblies of 50,000 disks following a fairly wide log-normal particle-size distribution.

A linear elastic relationship between forces and interparticle displacements at contacts has been employed, i.e. $f_n^c = k_n \Delta_n^c$ and $f_t^c = k_t \Delta_t^c$, where f_n^c, f_t^c, are normal and tangential contact forces, Δ_n^c, Δ_t^c, are corresponding interparticle displacements and k_n, k_t are respective stiffnesses. Only compressive normal forces are allowed: if the normal force were to become tensile, the contact is considered to be broken for cohesionless materials. Furthermore, the tangential forces are limited by Coulomb friction, i.e. $\|f_t^c\| \leqslant \tan \phi_\mu f_n^c$ where ϕ_μ is the interparticle friction angle.

The values used for k_n and k_t ensure small compression at contacts, resulting in elastic strains typical of those observed in tests on silica sand under stresses of a few hundred kilopascals. The specific combination of consolidation stress, σ, normal stiffness, k_n, and the average particle diameter, $\overline{R}$, were selected in such a way that $\sigma/(k_n \overline{R}) = 5 \times 10^{-3}$ and $k_t/k_n = 0.5$. All data are presented in a non-dimensional form and interpretations are essentially independent of values of interparticle stiffnesses and consolidation stress.

Two isotropic initial assemblies were considered: a dense and a loose packing. The packing fractions ρ, i.e. the total area occupied by the particles divided by the area occupied by the assembly, are $\rho = 0.844$ for the dense packing and $\rho = 0.803$ for the loose packing. The corresponding coordination numbers Γ are $\Gamma = 3.97$ and $\Gamma = 3.31$, respectively.

This study refers to four biaxial compression tests, in which the minor principal stress σ_2 is kept constant. Two of them were carried out on dense and loose assemblies with the interparticle friction coefficient $\tan\phi_\mu = 0.5$. The other two simulations involved the same dense initial assembly but particles were assigned very small, $\tan\phi_\mu \to 0$, and very large, $\tan\phi_\mu \to \infty$, friction coefficients.

The test results are presented in Figs. 1 and 2 in terms of the ratio q/p, with p and q defined in terms of the principal stresses σ_1, σ_2 as $q = (\sigma_1 - \sigma_2)/2$ and $p = (\sigma_1 + \sigma_2)/2$. Both q/p and the packing fraction ρ are plotted against shear strain $\gamma = \varepsilon_1 - \varepsilon_2$, where ε_1 and ε_2 are the major and minor principal strains, respectively. The packing fraction plot replaces the more traditional volumetric strain, ε_v, versus shear strain relationship expressing dilation/contraction behavior. In terms of packing fraction ρ, the volumetric strain increment is given by $\dot{\varepsilon}_v = -\dot{\rho}/\rho$.

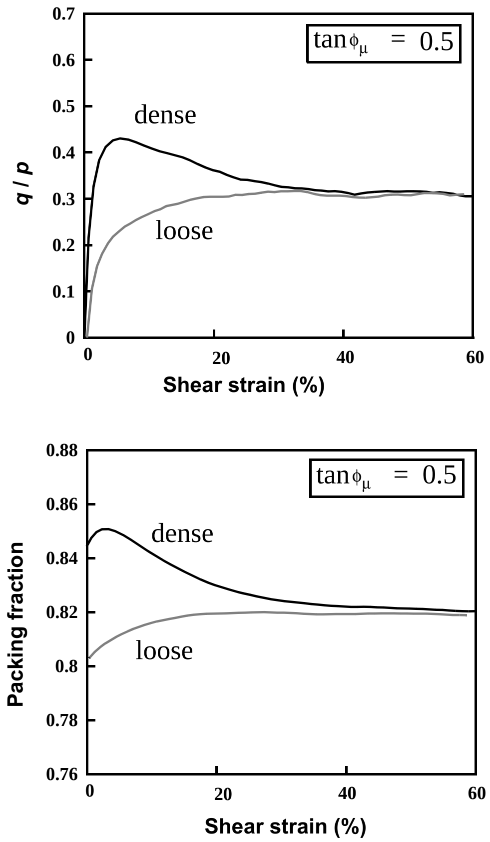

Fig. 1. Simulated tests on loose and dense assemblies with interparticle friction coefficient of 0.5.

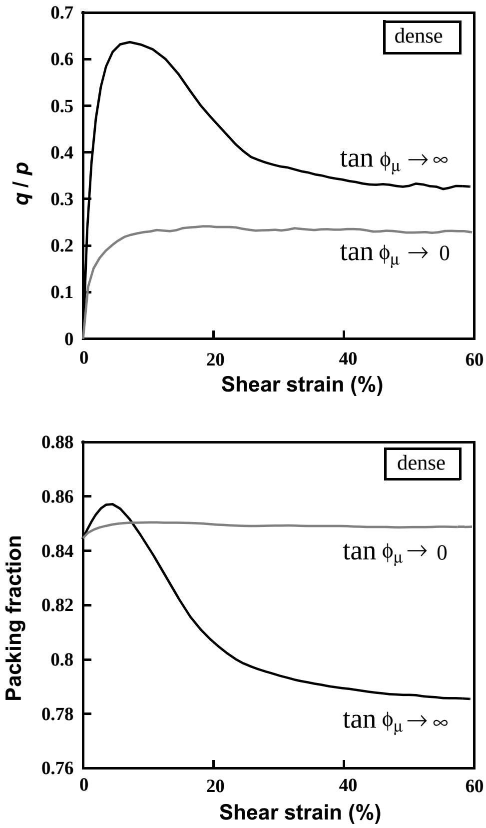

Fig. 2. Simulated tests on dense assembly with low and high interparticle friction coefficients.

3. Simulated unloading tests and elastic parameters

Due to stress changes in biaxial compression tests, strains are expected to contain a recoverable component. To determine recoverable strains, unloading tests were performed along the loading stress path of simulated tests, as illustrated in Figs. 3 and 4. These figures also illustrate variations of Young's moduli, E, and Poison's ratio, v, determined from initial slopes of unloading tests (using $d\sigma_1 = E\,d\varepsilon_1$ and $d\varepsilon_2 = -v\,d\varepsilon_1$). As loading and unloading slopes are essentially the same at initial test stages, the conclusion can be reached that the early behavior, typically characterized by a "dip" in the volumetric strain curve, is associated with recoverable strains. The term "elastic" is not strictly appropriate to characterize these strains, as both loading and unloading paths are associated with different microstructural changes, particularly at late test stages. Recognizing that an appropriate split of strains into "elastic" and "plastic" may be a far more complex issue than just calculating E and v as described above, this methodology is pursued in further analyses as a reasonable approximation that must be looked upon with a degree of caution. It should also be noted that due to anisotropy in contact orientations induced along loading and unloading paths, isotropic elastic relationship are, generally, inappropriate in all loading or unloading cases. However, since in biaxial tests one stress is kept constant, the second modulus (and the corresponding Poison's ratio) plays no role in describing the incremental response.

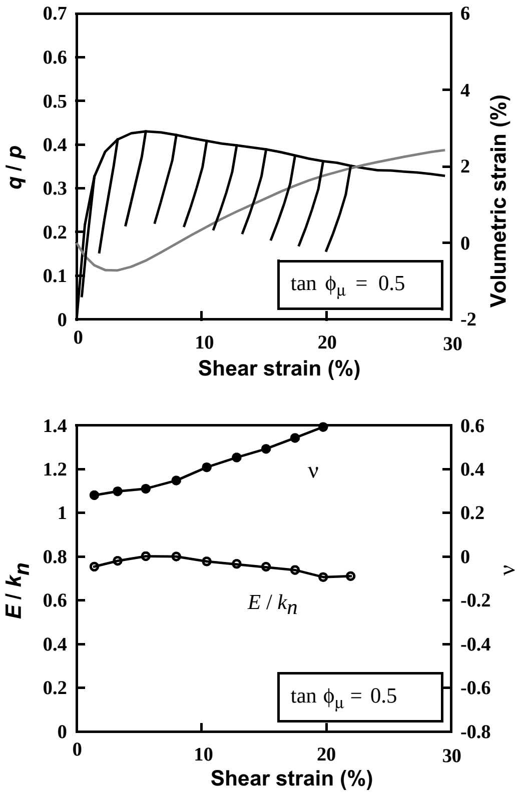

Fig. 3. Unloading tests and Young's moduli and Poisson's ratios at initial unloading stages for dense assembly with $\tan\phi_\mu = 0.5$.

Variations of E and v in Figs. 3 and 4 are quite complex but can be explained qualitatively. The early increase in the Young's modulus in the dense test with the "normal" $\tan\phi_\mu = 0.5$ (Fig. 3) is, most likely, related to an increase in contact anisotropy when there are relatively more contacts oriented in the direction of loading as compared to the perpendicular direction. The subsequent reduction in the modulus is due to the loss of contacts that accompanies dilation. The E-trend for the test with $\tan\phi_\mu \to \infty$ (Fig. 4) is qualitatively similar, but with a more drastic variation in the modulus due to much greater changes in microstructural characteristics (anisotropy and coordination number).

The increase in Poisson's ratio in the test with $\tan\phi_\mu = 0.5$ is likely controlled by a reduction in coordination number as is the case in strictly isotropic elastic assemblies (Kruyt and Rothenburg, 2002) with $k_t/k_n < 1$. A rather drastic initial reduction in Poisson's ratio into the negative range in the test with $\tan\phi_\mu \to \infty$ is somewhat surprising. For a dense and strictly elastic system Poisson's ratio is negative only when $k_t/k_n > 1$ (Bathurst and Rothenburg, 1988). This is not the case in this test. It appears, however, that high interparticle friction has the same effect as high tangential stiffness in the sense that both result in negative Poisson's ratio. At larger strain, when the assembly becomes loose due to dilation, the effect of apparent increase in tangential stiffness is no longer present. At shear strains of about 25% the Poisson's ratio is about the same for the assemblies with "normal" and high interparticle friction.

Due to the variation of the elastic parameters along the loading path, calculation of recoverable strains, e_1 and e_2, at any state has been performed by integration along the loading path, i.e. $e_1 = \int d\sigma_1/E$, and

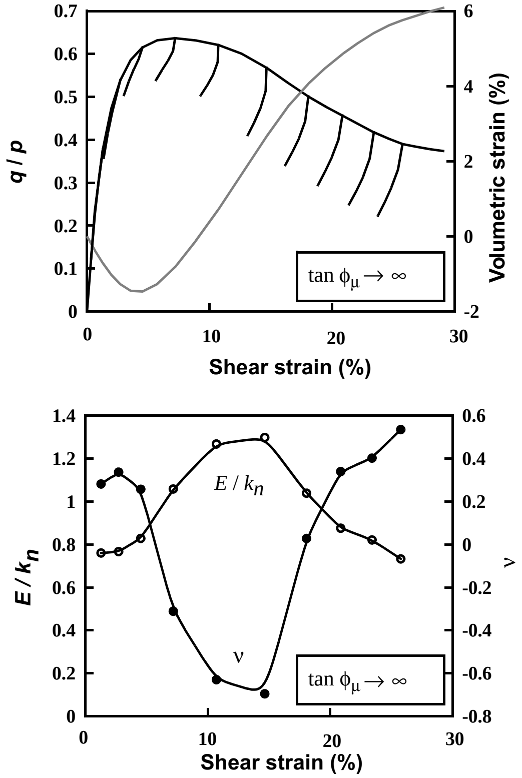

Fig. 4. Unloading tests and Young's moduli and Poisson's ratios at initial unloading stages for dense assembly with $\tan \phi_\mu \to \infty$.

$e_2 = -\int \nu \, d\sigma_1/E$. The computed recoverable strains were subtracted from total strains to obtain "plastic strains" in terms of which all subsequent interpretations are made.

4. Micromechanical theory of critical state

The packing fraction data illustrated in Fig. 1 represent a classical response in connection with which Casagrande introduced the concept of critical void ratio as corresponding to a unique packing at which the system evolves without volume change. The data in Fig. 2 for tests with drastically altered interparticle friction shed a somewhat different light on critical packing as a characteristic of non-geometric origin. The critical packing fraction in the test with small friction corresponds to what appears to be the densest packing for a given assembly of particles. On the other hand, the case of high friction apparently corresponds to the loosest packing. The rationale for such an interpretation will be clarified below.

In the test with low interparticle friction, see Fig. 6, the coordination number, Γ, remains at around 4 throughout the test as an assembly of *N frictionless disks* would generally require at least $2N$ contacts (i.e. $\Gamma = 4$) to be in static equilibrium when $2N$ equations of force equilibrium must be satisfied. This is because in assemblies of frictionless disks there is only one (normal) force component per contact and moment equilibrium equations are satisfied automatically. In principle, such a system could also be in a stable redundant state with $\Gamma > 4$, but such a state is apparently unattainable due to geometric restrictions on packing of practically rigid disks.

Shear deformations during biaxial tests are associated with extension strains and create a tendency for interparticle contacts to disintegrate. This tendency is clearly visible in the evolution of anisotropy in contact orientations. The latter is a consequence of the fact that contacts in the direction of maximum extension strain tend to disintegrate. Contact disintegration in an assembly of disks tends to reduce the coordination number below 4 and to send the assembly into a dynamic state, at least locally. Static equilibrium is eventually restored when a new contact or contacts are created. This mechanism is consistent with spurious local loss of equilibrium which is invariably observed in discrete element simulations, particularly close to critical state. This type of instabilities is manifested as fluctuations of coordination number evident in the figures above.

When there is friction between particles, an extra force component is available, making it easier for a system to remain in static equilibrium when contacts tend to disintegrate. In the same way, friction helps the system settle down after an instability. In the frictional case there are $3N$ equations of force and moment equilibrium that must be satisfied. In general, an assembly with M contacts and $2M$ force components can have an equilibrium state only when $2M \geqslant 3N$, which is equivalent to the condition $\Gamma \geqslant 3$. This means that a granular assembly cannot remain stable for coordination numbers below 3. In the biaxial test with high friction, when tangential forces are unrestricted, contacts indeed disintegrate down to the critical value close to 3, as Fig. 6 illustrates. When the range of tangential forces is limited, chances that contact disintegration would lead to instability increase. This limits the number of contacts that can disintegrate. As a result, assemblies with lower interparticle friction are expected to reach a critical state with a higher coordination number. The highest critical coordination number is 4 for frictionless particles.

According to the proposed mechanism, any macroscopic change in the number of contacts (expressed in terms of a change in coordination number, $\mathrm{d}\Gamma$) is the sum of the number of contacts disintegrated and of the number of contacts created during a strain increment, i.e. $\mathrm{d}\Gamma = \mathrm{d}\Gamma^- + \mathrm{d}\Gamma^+$. The number of contacts expected to disintegrate, $\mathrm{d}\Gamma^-$, during the shear strain increment $\mathrm{d}\gamma$ is likely proportional to the number of redundant contacts in the assembly and to the magnitude of the shear strain increment, i.e. $\mathrm{d}\Gamma^- = -f^-(\Gamma - 3)\,\mathrm{d}\gamma$, where f^- is a coefficient of proportionality, most likely a function of coordination number. The contact disintegrations are viewed as the primary cause of instabilities. During the same shear strain increment the number of contacts that would be created, $\mathrm{d}\Gamma^+$, during periods of instability is expected to be proportional to the number of vacant locations where contacts can be created. The latter number can be taken proportional to $4 - \Gamma$, resulting in $\mathrm{d}\Gamma^+ = f^+(4 - \Gamma)\mathrm{d}\gamma$, where f^+ is the corresponding coefficient of proportionality.

Coefficients f^- and f^+ reflect distances between neighbouring particles, as well as various probabilities of creating a stable contact or disintegrating one. In particular, both functions reflect how the macroscopic strain increment $\mathrm{d}\gamma$ translates into internal movements. As the free space within the assembly where contacts can be created was taken to be proportional to $4 - \Gamma$, the average internal movement per vacancy can be estimated as proportional to $\mathrm{d}\gamma/(4 - \Gamma)$. This suggests that the introduced coefficients of proportionality f^+ and f^- should be taken in the form $f^- = c^-/(4 - \Gamma)$ and $f^+ = c^+/(4 - \Gamma)$, where c^- and c^+ are constants that are independent of coordination number (but may depend on microscopic parameters such as interparticle friction and elastic parameters of particles k_n and k_t). Using these expressions, the coordination number increment $\mathrm{d}\Gamma$ can be written as $\mathrm{d}\Gamma = [c^+(4 - \Gamma) - c^-(\Gamma - 3)]\,\mathrm{d}\gamma/(4 - \Gamma)$, resulting in the following differential equation that describes the evolution of coordination number with shear strain:

$$\frac{\mathrm{d}\Gamma}{\mathrm{d}\gamma} = -c\frac{\Gamma - \Gamma_\infty}{\widetilde{\Gamma} - \Gamma}, \tag{1}$$

where, $c = c^+ + c^-$, $\widetilde{\Gamma} = 4$, $\underset{\sim}{\Gamma} = 3$ and $\Gamma_\infty = (c^+\widetilde{\Gamma} + c^-\underset{\sim}{\Gamma})/(c^+ + c^-)$ is the limiting value of the coordination number to which the solution of the above equation asymptotically approaches, i.e. the critical coordination number. Special notations $\widetilde{\Gamma}$ and $\underset{\sim}{\Gamma}$ for maximum and minimum coordination numbers are introduced for purposes of generalizing the above equation for particles shapes other than disks.

The solution of (1) can be obtained in an implicit form by separating variables and is as follows:

$$c\gamma = (\Gamma - \Gamma_0) - (\widetilde{\Gamma} - \Gamma_\infty)\ln\left(\frac{\Gamma - \Gamma_\infty}{\Gamma_0 - \Gamma_\infty}\right), \tag{2}$$

where Γ_0 is the initial coordination number.

Fig. 7 illustrates the comparison of the solution according to (2) with results from the discrete element simulations. In each individual case it is possible to obtain an almost perfect fit of the data shown previously (see Figs. 5 and 6) by taking the critical coordination number from data, using $\widetilde{\Gamma} = 4$ and selecting the constant c to achieve the best fit. With this approach there is about 10% variation in the optimum value of c. It was also noticed that the choice of $\widetilde{\Gamma} = 4.2$ minimizes differences between coefficients c from individual fits. This observation seems to imply that the maximum coordination number for the simulated system is higher than 4. This is not entirely implausible as simulated assemblies contain a reasonably wide range of particle sizes that may well result in a packing with the maximum coordination number greater than 4. The fit in Fig. 7 is with $\widetilde{\Gamma} = 4.2$ and $c = 9$ for the dense and loose assemblies with $\tan\phi_\mu = 0.5$ and for the dense assembly with $\tan\phi_\mu \to \infty$.

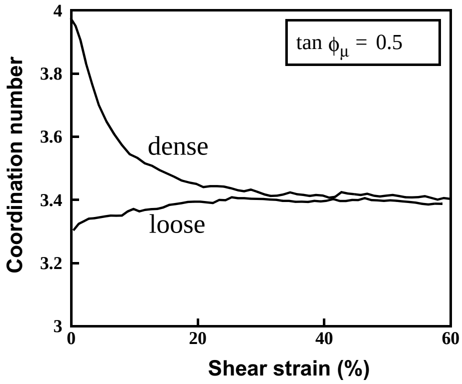

Fig. 5. Evolution of coordination number for dense and loose assemblies with interparticle friction coefficient of 0.5.

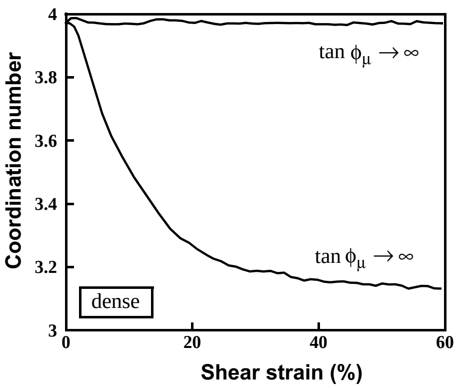

Fig. 6. Evolution of coordination number for dense assembly with low and high interparticle friction.

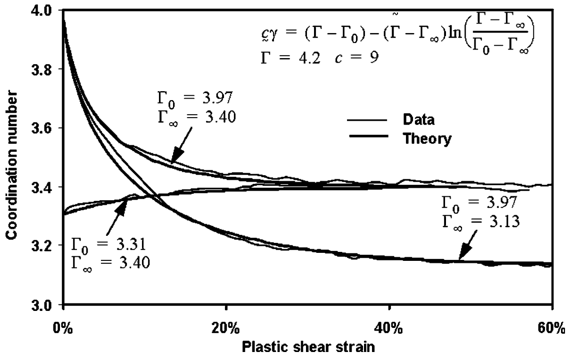

Fig. 7. Theoretical coordination number evolution relationships and simulations.

It should be noted that the elimination of elastic strains (see Section 3) is essential for achieving an accurate representation of the evolution of coordination number. Careful examination of the raw coordination number data in Figs. 5 and 6 indicates that at small values of total strain the slope of Γ versus the total shear strain is practically zero, while in terms of plastic strain the rate of reduction of Γ is maximum at zero plastic strain, precisely in accordance with (2). Elastic strains are, however, essential for creating preconditions for contact disintegration as well as for their creation. For a contact to disintegrate the normal force carried by this contact must be reduced to zero first. This reduction is associated with elastic strains that are also responsible for generating the contact forces when a new contact is formed. The presented theory associates plastic strains with particle movements that occur during periods of local instabilities.

5. Relation between packing fraction and coordination number

Formulation of the critical state theory in terms of coordination number rather than in terms of void ratio or packing fraction appears more natural as stability issues are addressed more readily in terms of coordination number. The latter, however, is not a convenient variable in applications and in this context the question arises if there is a unique relationship between packing fraction and coordination number. The question has a long history but no definitive answer.

First of all, a unique relationship between packing fraction and coordination number can only exist within an idealized context of rigid particles. In this case such a relationship has a statistico-geometric origin, as was demonstrated by Rothenburg (1980). When particles are compressible, the assembly volume can be altered by applied pressure without changing the coordination number. Secondly, even for rigid particles it was shown that the packing fraction depends not only on the coordination number of the assembly, but also on the degree of anisotropy in contact orientations. As the contact anisotropy varies along the loading path, it may not be possible to characterize the critical state in terms of packing fraction unless the critical state is characterized not only by the critical coordination number, but also by a unique *critical anisotropy* that remains the same whether the initial assembly is loose or dense. This seems to be the case, at least in the discrete element simulations described here.

Figs. 8 and 9 illustrate the evolution of anisotropy in contact orientations expressed in terms of parameter a. The frequencies $S(\theta)$ of contacts with angular orientation of normal vectors θ with respect to the direction of loading are given by the expression $S(\theta) = (1 + a \cdot \cos 2\theta)/2\pi$. In the case of the two tests with the same interparticle friction the same critical anisotropy is reached at large strains, along with

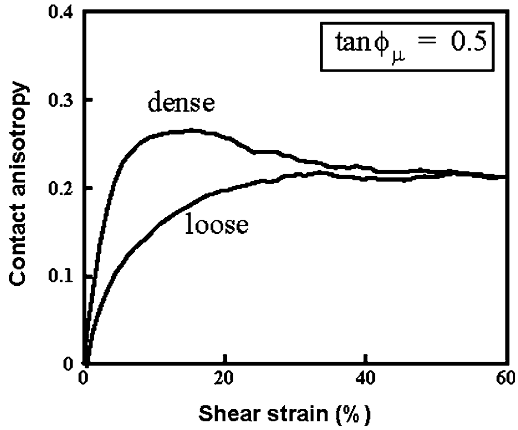

Fig. 8. Evolution of contact anisotropy for loose and dense assemblies with interparticle friction coefficient of 0.5.

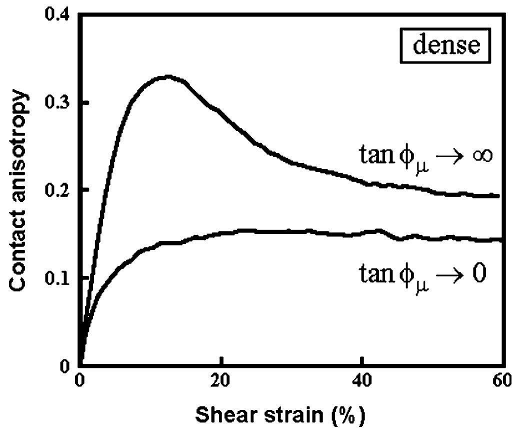

Fig. 9. Evolution of contact anisotropy for dense assembly with low and high interparticle friction.

the same coordination number. Critical packing fractions reached in both cases are also the same, see Fig. 1.

The uniqueness of the packing fraction versus coordination number relationship can be investigated based on simulation data, as both variables change simultaneously during tests. Fig. 10 summarizes the evolution of packing fraction during the four tests using a graph of packing fraction versus coordination number. Both variables evolve in each test tracing a path from the initial to critical states. The raw data show distinctly different paths reflecting considerably different histories of mean stress resulting in recoverable contraction. When the "recoverable" component of volume change is removed as described in Section 3, the results from the various simulations practically collapse onto the same graph. This type of volume correction does not result in a stress-independent relationship between density and coordination number, as the packing volume in the initial state is still stress-dependent. Only strain-related influences on packing volume are removed in such a way. Some differences between the curves still exist due to differences between anisotropy histories in the four tests. These differences are fundamental and demonstrate that the evolution of packing fraction cannot be described in terms of coordination number alone. As the main

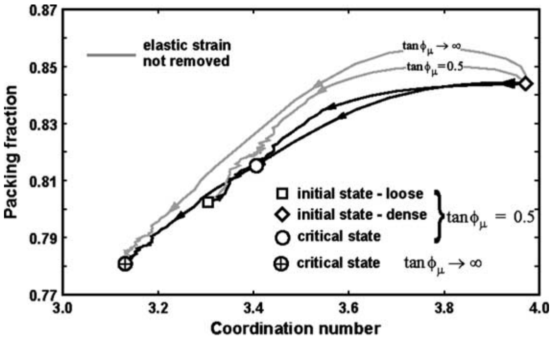

Fig. 10. Summary of packing fraction versus coordination number data.

result of this paper demonstrates in Fig. 7, the evolution of coordination number can be described uniquely, independently of other parameters.

6. Discussion

The micromechanical theory of critical state presented here is based on the notion that plastic deformations of granular materials are associated with instabilities created by disintegration of contacts during shear deformations. Intergranular contacts are also created as the system tends to restore stability. The critical state is reached when rates of contact disintegration and creation become equal. Restoration of equilibrium is facilitated by the presence of interparticle friction.

Based on this postulated mechanism, a differential equation for the evolution of coordination number is derived and solved, and its solution is compared to results of discrete element simulations. The critical coordination number appears in the derived equation as a quantity that depends on unspecified empirical constants that physically reflect probabilities of contact creation and disintegration and depend on interparticle friction. Other parameters involved in the equation include the coordination number at the densest state and a parameter that reflects the average strain necessary to disrupt or create a contact. The latter is likely dependent on consolidation stress and particle stiffnesses. Discrete element simulations confirm that the critical coordination number indeed depends on interparticle friction. The evolution of coordination number in all simulated tests is accurately described by the developed theoretical relationship using the same set of constants for all tests.

This study also addresses the possibility of formulating the theory of critical state in terms of packing fraction instead of coordination number. Analyses of simulation data tend to suggest that the relationship between packing fraction and coordination number is affected by anisotropy in contact orientations. From this point of view a theoretical description of changes in packing fraction cannot be achieved in terms of coordination number alone. A theory for describing the evolution of anisotropy is necessary for this purpose. Furthermore, a relationship between packing fraction and coordination number that also includes the degree of anisotropy in contact orientations is required. Despite of the influence of anisotropy on packing fraction, the critical packing fraction (or void ratio) is likely a unique characteristic of a granular material as the evolution of anisotropy is such that the same limiting anisotropy is reached at critical state, irrespective of the initial state. This also implies that a proper characterization of critical state should include the critical coordination number as well as the critical anisotropy. It is the combination of both characteristics that makes the critical state to be a unique state.

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