Research on the yield function of sand based on thermodynamics

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Abstract. It is well known that stress-strain relation of sand is influenced by anisotropic fabric. In this paper, the relationship between macroscopic strain and shear strain and its pore structure is established by combining micromechanical theory and pore structure tensor. It is further confirmed that the stress-induced anisotropy and dilatancy of sand are inevitable. Based on this, with the help of thermodynamic theory, the inclined elliptic yield surface function in dissipative space is built, and there are three important lines in dissipative space for the influence of anisotropic fabric, normal consolidation line, phase transition line and peak line respectively corresponding to the three characteristic lines of real stress space: normal consolidation line, phase transition line and peak line which really reflects the mechanical properties of sand, especially dense sand.

1. Introduction
Particle mechanics is widely applied in engineering, but this theory is still very immature, and still many challenging problems are ready to study. Generally, we adopt continuum mechanics and micromechanics to derive the stress-strain relations of granular materials. And now, continuum mechanics is more used for existing models to describe the constitutive relations for granular materials, for example, treating soil as isotropic continuous medium to simulate soil behavior, and the framework of critical state soil mechanics is based on this. The second is on microscopic mechanics that considering soil as an aggregate of discrete particles with regular and irregular arrangement. Generally contact distribution of particles in a model usually is described with probability distribution functions to reflect their anisotropy\textsuperscript{[1][2][3]}.

Because the continuous plastic theory can not directly explain the microscopic properties of irreversible deformation of granular materials, and the detailed study of the microscopic properties of granular materials is very complex in mathematics, so that it is very limited to apply this method. In this paper, the pore fabric of sand is discussed from the theory of particle mechanics, and the relationship between the anisotropy of pore structure, the dissipation function and the yield function of real stress space is analyzed in detail.

2. Expression of strain tensor on pore fabric
The most meaningful study for granular material is not the reaction of individual particles but the arrangement mode in space and the whole reaction under external force. Here, we uniformly attribute...
the micro and meso-scale magnitude of the particles to the microstructure. In triaxial compression test of sand\cite{4}, it is observed that the granular materials have different strength due to different compression directions. and the direction along long axis of the non-spherical particles tends to rotate vertical to the direction of the maximum contact pressure, so the mechanical behavior of granular materials is significantly affected by their microstructure. The porosity ratio $e$ or porosity $n$ is usually used to express the compactness of the internal structure, but these quantities do not represent the directionality. The randomly arranged inner structure of granular materials can be illustrated by the geometry statistical character of the particles and their spatial distribution. The higher-order microstructure variables $d$ of the "fabric tensor" can usually represent the distribution and direction of the particles and pores $^{[4][5]}$. Bagi\cite{6} gave the mathematical description of the internal structure of granular materials based on the famous Voronoi-Delaunay chessboard mesh, and stated that the spatial distribution of particle contact points is the most fundamental factor when considering the shear expansion of materials. Li and Li$^{[7]}$ suggested a quantitative method for the inner structure of granular materials based on the mesh system formed by contact points. In three-dimensional space, the smallest pore elements form the continuous pore space, and the cell boundaries are all determinate structures. The microstructural formula of the strain tensor is expressed below.

![Figure 1. The boundary surface $S^{[7]}$](image)

Here any representative unit is defined as REV, and the volume $V$ is set, the boundary surface is closed. And for a representative unit REV, the compatibility conditions must be met, namely:

$$\oint_{S} d\left(u, S_{i}\right)=0$$

Among them, the continuous boundary surface of the representative element is represented as $S$, as shown in Figure 1, and $u$ denotes the displacement of the representative element. The pressure direction is positive according to the soil mechanics convention. Then the average displacement gradient tensor of the Rev. can be expressed as

$$\tilde{e}_{ij}=\frac{1}{V} \oint_{V} e_{ij} dV=-\frac{1}{V} \oint_{V} u_{i,j} dV$$

Based on the scatter theorem, the formula (2) can be re-expressed as

$$\tilde{e}_{ij}=\frac{1}{V} \oint_{V} u_{i,j} n(x) dS=\frac{1}{V} \oint_{S} u \otimes n dS$$

(3)

$n(x)$ denotes the normal direction of the point $x$ on the boundary surface $dS$ which points to the inside. Then, Thus, the displacement gradient along the direction $n$ is described by the statistical probability method$^{[7]}$:

$$\tilde{e}=\frac{1}{V} \sum_{c=1}^{c_{v}} \mu_{c} \otimes \Delta u=\frac{1}{V} \sum_{c=1}^{c_{v}} \mu_{c}(n) n \otimes \Delta \tilde{n}_{c} \Omega$$

$$=\frac{1}{V} E_{e} \Delta \tilde{n}_{c} \oint_{S} \mu_{c}(n) n \otimes n d\Omega$$

(4)

Here $\mu_{c}$ is a representative polygon vector of pore units$^{[7]}$ for granular materials which is closely related to the directional distribution of pore vector length. The integral range is the whole space $\Omega$.\[0x1088/1755-1315/580/1/012098]
and $E_0$ is defined as $E_0 = \frac{1}{\partial} \int \Omega d\omega$, as the standardization factor equals to $2\pi$ and $4\pi$ respectively in two and three dimensions. $\Delta u$ is set as a constant for the average relative displacement at the contact point of the microelement under the condition of uniform strain.

The fabric tensor $\mu$ can be expressed with the directional distribution of the pore vector. For the pore length $\mu(n)$ along $n$ is the average length of all pore vectors of the sample along the direction $n$. Therefore, based on the directional distribution of the average pore vector length, the structure tensor is set to illustrate the shape and direction of the mean pore unit: $\mu(n)$ the distance from the center of the space pore unit to the boundary of the pore unit $\partial\Omega$, $n$ the unit vector in the pore direction, pore vector $\mu(n)$ along the direction $n$ can be approximately as follows:

$$\mu(n) = \mu_0(1 + d) : (n \otimes n) = \mu_0(1 + n \cdot d \cdot n)$$ (5)

Here $\mu(n) = \mu_0(n)$, $d$ as the second order tensor of no trace symmetry, represents the anisotropy of pore structure. $\mu_0 = E_0 \int \Omega \mu(n) d\omega$, representing the average pore length, and substituting the formula (5) into the formula (4), we obtain:

$$\bar{\varepsilon} = \frac{1}{V} E_0 \int \Omega \mu(n) \otimes nd\omega = \frac{1}{V} E_0 \int \Omega \mu(n) (1 + n \cdot d \cdot n) \otimes nd\omega$$ (6)

Here removing the rotation tensor, then the strain tensor is expressed as:

$$\varepsilon_{ij} = (\bar{\varepsilon}_{ij} + \bar{\varepsilon}_{ij}) / 2$$ (7)

The volumetric strain along the directional $n$ with the action of compressive stress is as follows

$$\varepsilon_n(n) = \varepsilon_{ij} \delta_{ij} = \frac{1}{V} E_0 \int \Omega \mu(n) (1 + d \cdot n \cdot n) \cdot \delta_{ij} d\omega$$ (8)

Here $\varepsilon_0 = E_0 \int \Omega \mu_0 / V$, then formula (8) can be transformed into

$$\varepsilon_n(n) = \varepsilon_0 (1 + d \cdot n \cdot n)$$ (9)

Here $\varepsilon_0(n)$ represents the change rate of pore volume along the unit vector $n$.

3. Fabric changes caused by shear

The change of particle arrangement and pore fabric caused by shear is in fact the change of structure. Early researchers [8][9][10] have made a research on the relationship between fabric and strain. For granular material structure, the pore structure changes as the relative position between particles changes. The dual structural system [7] formed by pore and solid particles are dependent, and each of them can illustrate the inner structure of the granule. Numerical tests [7] have showed that the anisotropy for particle contact normal and pore structure is closely related, and the direction distribution of contact normal usually tends to that of pore structure. So, the relationship between pore fabric tensor and volume strain changes in compression is as follows

$$d\varepsilon_n(n) = d\varepsilon_i(1 + d \cdot n \cdot n)$$ (10)

Summation of the volume strain change rate of the pores along all directions:

$$d\varepsilon_n = d\varepsilon_i + d\varepsilon_i(1 \cdot d \cdot n \cdot n)$$

Horne [11] derived that directions of particle contact normal and its pore structure tended to the direction of the maximum principal stress that leads to anisotropy in the initial state of deformation. And the relative slippage among particles was no more limited to a certain direction as deformation occurred, and the degree of anisotropy decreased which not only caused the reduced dilatancy but also the stress ratio $\eta$ decreased too. Then, based on the above stated, the pore fabric tensor $d$ is a bias and varies with shear strain, we can express the theorem [11] using the isotropic tensor function $d(d) = d(d, d, d, d, d, d, d)$, relating the change of the fabric to shear strain $\varepsilon_j$, however, this function is...
very complicated, for easy, assuming the principal axis for $d_d$ and $d_{\varepsilon}$ are same \cite{12}, and the relationship between the two is as follows

$$\varepsilon_{i j} d(d_{n j} n) = \alpha d(\varepsilon_{i j} n n)$$ \hspace{1cm} (12)

Here $\alpha$ denotes the anisotropic parameter of the fabric reflecting its basic tendency of development. As partial strain $\varepsilon_{i j}$ is concerned, $d_{\varepsilon_{i j} n n}$ represents the shear strain increment under triaxial stress. Here, let's: $d(\varepsilon_{i j} n n) = d_{\varepsilon_{i j}}$, and integrating it into formula (11), we get

$$d_{\varepsilon_{i j}} = d_{\varepsilon_{i j}} + \alpha d_{\varepsilon_{i j}}$$ \hspace{1cm} (13)

It shows the increment of volumetric strain $d_{\varepsilon_{i j}}$ is coupled with the partial strain increment $d_{\varepsilon_{i j}}$ under compressive stress for granular materials.

4. decomposition of plastic strain

Generally, it is believed that the change in material volume is due to pore compression, while the plastic volume strain is only due to the action of compressive stress and is independent of the soil skeleton. As a matter of fact, the relationship between bulk strain and pore fabric analyzed above shows that volume change under shear stress consists of two processes for granular materials such as dense or medium dense sand. Firstly, when the axial strain is very small, dense or medium dense sand produces shear shrinkage under compressive stress $\varepsilon_{p i}$, and following with the development of anisotropic fabrics, additional volume changes $\alpha \varepsilon_{p i}$ will occur what is called "Reynolds dilatancy"\cite{13}. Therefore, for dense or medium dense sand, another source of plastic volume strain is shear-induced bulk deformation-dilatancy, the macroscopic plastic strain of granular material can be denoted as

$$d_{\varepsilon_{p i}} = d_{\varepsilon_{p i}} - \alpha d_{\varepsilon_{p i}}$$ \hspace{1cm} (14)

Seen from the formula above, the increment of macroscopic plastic volume strain consists of two components: one is the pore volume change-shear shrinkage $d_{\varepsilon_{p i}}$ caused by the direct change of compressive stress of granular material, the other is shear-induced volume change $(\alpha d_{\varepsilon_{p i}})$ -dilatancy. Because the pore structure of particles is anisotropic during loading, this part of the body is always in dilatant state and plays a major role in volume change. The volume strain in the modified Cambridge model generally means the first volume change-shear shrinkage which is completely obtained by the change of compressive stress, and does not consider the shear-induced dilatancy. Therefore, it has some limitations for the modified Cambridge to reflect the stress dilatancy relationship. The following we will further discuss the relationship between shear-induced volume change $(\alpha d_{\varepsilon_{p i}})$-dilatancy and dissipation function and yield function in real stress space based on thermodynamic framework.

5. Thermal analysis

Nowadays, there exist many constitutive models to illustrate the mechanical behavior of sand and other granular materials. For truly reflecting the mechanical phenomena tested in the lab, researchers generally solve these difficulties by adding model parameters. However, all these models can not be separated from fundamental mechanical concepts: critical state, stress-dilatancy theory and state parameters, and most of them are based on the classical theoretical framework of rate-independent, elastoplastic solids, so it is necessary to determine the yield surface, flow rule, etc. and the associated flow rule is adopted for many models, however, sand should conform to non-associated flow rule.

We adopt thermodynamic theory because it is a more rigorous method and does not require many human assumptions in traditional methods. Especially important is that the establishment of dissipation, yield functions and flow rules, as well as the close relationship between plastic-dilatancy and induced anisotropy. According to the dissipative part of the energy balance equation, we can infer the form of yield function, flow rule, non-associated flow rule, and naturally obtain the properties of friction materials in the real stress space.
6. Anisotropy model of sand

6.1 Shearing model of pure friction material

According to the thermodynamic principle, the two key points of establishing dissipation function $\delta \Phi$ are the selection of stress and strain variables. First of all, most isotropic hardening comes from compressive strain that makes the particles rearrange and crush as the pressure is large enough. The definition of sand or granular material as pure friction material is given in this paper [14]. This kind of material has a large shear deformation before shear failure occurs which means the normal consolidation stress $p_c$ applied should be large enough to make particles broken. Here particle breakage is not considered, the stress variables of the dissipation function $\delta \Phi$ in this paper are no longer dependent on consolidation pressure [14]. Secondly, through the mechanism analysis of plastic volume deformation of sandy soil in this paper, it can be seen that the macroscopic plastic volume increment $d e_q^p$ of dense sand or medium dense sand consists of two parts: one is volume compression $d e_q^p$ caused by the change of current compressive stress, the other is shear deformation $(d e_q^p)$ induced by shear deformation which is closely related to pore structure anisotropy. As a matter of fact, this part of the volume increment associated with the anisotropy of pore structure $d e_q^p$ is the result of the motion of granular rigid bodies, even if the particles are rigid and smooth, dilatancy will occur, then Collins [15], Collins and Muhunthan [14] concluded that reynolds dilatancy only represented the internal motion constraint of the material, and the storage energy generated by the pressure and shear component of the reaction force associated with it was balanced and offset, and the dissipation energy associated with this part of the shear expansion was zero. As a result, the dissipation function $\delta \Phi$ should be directly related to the stress-dependent volume change $d e_q^p$, independent of the shear-induced bulk strain-dilatancy [9][17]. For simplicity, $\alpha = \tan \theta$ is defined, based on the above two aspects of analysis, let the dissipation function $\delta \Phi$ be:

$$\delta \Phi = p \sqrt{(d e_r^p + \tan \theta d e_q^p)^2 + M^2 d e_q^p}$$  \hfill (15)

The complete expression of plastic work is:

$$\delta W^p = p d e_r^p + q d e_q^p$$

$$= (\rho d e_r^p + \bar{\xi} d e_q^p) + (\rho d e_r^p + \gamma d e_q^p)$$

$$= (\rho d e_r^p + \bar{\xi} d e_q^p) + \rho_n \sqrt{(d e_r^p + \tan \theta d e_q^p)^2 + M^2 d e_q^p}$$  \hfill (16)

If the two sides of the above equation are divided by $d e_r^p$, we can obtain the general dilatancy relationship of pure friction particle materials expressed by angle

$$\beta (\tan \bar{\theta} - \tan \psi) \sqrt{\tan \theta - \tan \phi_n} + \tan \phi_s^p \hfill (17)$$

Here $\tan \phi_n = q/p, \quad \beta = \rho/\bar{\rho}, \quad \bar{\theta} = \xi/\rho, \quad \phi_n, \quad \phi, \quad \psi$ respectively denote sliding friction angle, internal friction angle and dilatancy angle, and meet $d e_r^p / d e_q^p = -\tan \psi$.

According to above formula, corresponding dissipative stress components are

$$\tau = \frac{\partial (\delta \Phi)}{\partial (d e_r^p)} = p \sqrt{(d e_r^p + \tan \theta d e_q^p)} / \delta \Phi$$

$$\tau = \frac{\partial (\delta \Phi)}{\partial (d e_q^p)} = \rho_n \sqrt{(d e_r^p + \tan \theta d e_q^p) \tan \theta + M^2 d e_q^p} / \delta \Phi$$  \hfill (19)

Based on the above two formulas, it can be concluded that
\[
\tau - \tan \theta \pi = M^2 \frac{p}{\tau} \frac{d\varepsilon_p^v}{d\Phi}
\]

(20)

In this way, an inclined elliptic yield surface equation can be obtained in dissipative space \((\pi, \tau)\):

\[
\frac{\pi^2}{p^2} + \frac{(\tau - \tan \theta \pi)^2}{M^2 p^2} = 1
\]

(21)

As shown in figure 2, it is the yield function of dissipation space of pure friction material, an inclined ellipse with an inclined angle \(\theta\).

![Figure 2. The inclined ellipse in dissipative stress space](image)

Integrating formula (19), (20), (21), it can get

\[
d\varepsilon_p^v = \partial \Phi \left\{ \frac{\pi}{p} - \frac{(\tau - \tan \theta \pi) \tan \theta}{M^2 p^2} \right\} 
\]

Then dilatancy expression \(D\) can be derived as

\[
D = \frac{d\varepsilon_p^v}{d\varepsilon_q^v} = -\tan \psi = M^2 \frac{\pi}{\tau - \tan \theta \pi} - \tan \theta
\]

(23)

Shown in Figure 2, there exist three important lines rotating with shear. First is the "normal fixation line of motion" (KNCL), the plastic shear strain increment on this line is zero, but the stress state is not equidistant. And in the dissipative stress space : \(\tau/\pi = \tan \theta\). The second is the "Phase transformation line" (PTL), the total volumetric strain increment on this line is zero, that is to say \(d\varepsilon_v^v = 0\). At this point, dilatancy induced by shear is offset by stress induced shear contraction. Similarly, in the dissipative stress space: \(\tau/\pi = M^2 / \tan \theta + \tan \theta\). The third line is the "Reynolds-Taylor Line" (RTL) along which dissipative pressure equals to zero, that is \(\pi = 0, p = \rho\). According to formula (18), \(d\varepsilon_p^p + \partial \phi d\varepsilon_q^p = 0\), formula (23) can be transformed as:

\[
D = \frac{d\varepsilon_p^p}{d\varepsilon_q^p} \Rightarrow D_{\text{max}} = -\tan \psi = -\tan \theta
\]

(24)

6.2 bounded shear model for pure friction particle material

The analysis above is aimed at the general deformation of pure friction materials. For the research on the dilatancy Taylor \[18\] proposed, Collins and Muhunthan\[14\] defined the bounded shear deformation of a purely frictional particulate material which was considered from a thermodynamic point of view as plastic work storage without considering pre-consolidation pressure \(p_c\), and it was a pure shear flow with a volume part of zero dissipation increment and no plastic free energy stored, that was \(d\Psi^v = 0\), but the pressure and shear components of the reaction force were not equal to zero, and the energy stored in the force chain was rapidly dissipated due to frictional shear slip, so no plastic work was stored and all energy was dissipated. Collins\[14\] also showed that for pure friction particle materials, the
"quasi-steady state" shear deformation of dilatancy certainly occurred and no plastic properties were stored as long as anisotropy is considered in the model, but the reactive force component was not equal to zero.

From the analysis above, we can obtain the relation of the bounded shear deformation of pure friction material:

\[ \pi \Delta e_p = 0, \quad \pi \Delta e_q = \Delta \theta = p \sqrt{(\Delta e_p + \tan \theta \Delta e_q)^2 + M^2 \Delta e_q^2} \] (25)

When the material is sheared, the volume strain increment is not zero, so it should meet \( \pi = 0 \) under this condition. According to the formula (21), when the dissipative stress is located at the two vertices of the yield trajectory \( A, B \), as shown in figure 2, and \( \rho = p \), that is, "Reynolds-Taylor line", according to formula (21) and (24), we get

\[ \tau = M \rho, \quad \tan \psi = \tan \theta \] (26)

And formula (17) can be transformed into

\[ \tan \phi_n = \tan \theta + \tan \phi \] (27)

Because the bounded shear deformation of the pure friction material is a pure shear flow, the plastic free energy stored in the pre-consolidation pressure \( p \) is not considered, so the increment of plastic free energy \( d\Psi^P \) is only related to the Reynolds effect. Based the description above, the plastic part of the free energy can be regarded as a function of \( \Delta e_p \)

\[ d\Psi^P (e_p) = d\Psi^P (e_q) \Delta e_p = (\Delta e_p + \alpha \Delta e_q) d\Psi^P (e_q) / \Delta e_p = (\Delta e_p + \alpha \Delta e_q) \Psi^P \] (28)

Therefore, the reaction force components are

\[ \rho = d\Psi^P / \Delta e_p = \Psi^P, \quad \xi = d\Psi^P / \Delta e_q = \alpha \Psi^P = \alpha \rho \] (29)

And the storage plasticity work related to the Reynolds effect is expressed as:

\[ \rho(-\alpha \Delta e_q) + \xi \Delta e_p = \rho(-\tan \theta \Delta e_q) + (\rho \tan \theta) \Delta e_q = 0 \] (30)

It shows that the storage plastic work related to the Reynolds effect is zero and satisfies \( \xi / \rho = \tan \theta = \tan \theta \). From the previous analysis, it can be seen that the normal consolidation line is also satisfied in the dissipation space: \( \tau / \pi = \tan \theta \), so the normal consolidation line (KNCL) of the dissipative stress space is a ray passing through the origin in \( p-q \) space. And formula (27) is further transformed into

\[ \tan \phi_n = \tan \theta + \tan \phi \] (31)

The formula above is the classic Reynolds-Taylor line \([13]\) commonly known as the failure line or peak strength line, passes through the origin in the real stress space \( p-q \) and describes the peak state of the sand in the case of drainage.

Figure 3. Yield function in true stress space for a bounded shear model of a purely frictional material

Shown in Figure 3, point \( C \) corresponds to the position of reactive force component \( (\rho, \xi) \) in the real
stress space. Comparing Fig.2 and Fig.3, it shows that for bounded shear deformation of pure friction materials, the three characteristic lines in the dissipative stress space correspond to the three characteristic lines starting from the origin in the real space, namely, the normal consolidation line (KNCL), the phase change line (PTL) and the peak line (RTL).

For simplicity, and meanwhile highlighting the force characteristics of the granular material, we set the yield function of real stress space as follows:

\[ f = q - \eta p = 0 \]  

Here \( \eta \) is the stress ratio, and although not present in this yield function, implies a close correlation between anisotropic parameters \( \alpha (\tan \theta) \) and changes with the change of stress ratio, in other words, dilatancy is inevitable under shear stress, and the corresponding stress-induced anisotropy-change \( \alpha \), also \( \alpha \) known as reaction force ratio .

On the basis of the above analysis, it can be found that the three characteristic lines of sand as pure friction material can be properly described by thermodynamic method: normal consolidation line (KNCL), phase change line PTL and peak line RTL, and the strain strengthening and softening characteristics of sand are well described, and is exactly matched with the mechanical characteristics reflected by the boundary plastic model of sand.

7. Summary

In this paper, from the point of view of micromechanics and using the averaging theory, the pore fabric of granular materials and the additional volume increase-dilatancy caused by structural changes are discussed. This part of the dilatancy should be reflected in the plastic model. Due to the influence of anisotropic fabric, there are three important lines in the dissipation space, namely: normal consolidation line, phase change line and peak line correspondingly extended to the three characteristic lines of the origin of the real stress space: normal consolidation line, phase change line and peak line which closely reflect the mechanical properties of sand, particularly for dense sand. Hence, the constitutive equation of sand based on thermodynamics accords with the boundary surface plastic model of sand.

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