The Mechanics Simulation of MSG Strain Gradient Plasticity Theory in Granular Material

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ABSTRACT

The size effect of granular material is related with its microstructure, of which discontinuity will cause the discontinuity of deformation, interfacial stress and energy space at the micro level. MSG strain gradient plasticity theory can correctly predict the size effect of granular material by considering the microstructure characteristics of granular material and introducing strain gradient which describes the discontinuity of physical quantities in the classic elastic-plastic constitutive relation. Based on the MSG strain gradient plasticity theory, we use the virtual work principle to derive the equilibrium equation and the boundary conditions, and then propose the incremental equations and the iterative process of finite element. It can be used as a method to simulate the deformation to failure process of granular material and predict its special mechanics behavior.

KEYWORDS: granular material; strain gradient; microstructure; size effect; finite element

INTRODUCTION

Granular material is a discontinuous material formed by accumulating of different sizes of particles in a certain way. Its mechanical property is closely related to the microstructure, and has an obvious particle size effect [1]. As a result of the discontinuity of microstructure, the deformation of micro level is extremely non-uniform although the stress field is uniform. The non-uniform and discontinuous deformation of the transition from inside the particles to the interface will lead to the totally difference of mechanic property between particle interface and its internal. Generally speaking, the solid energy band is superposed by numerous atomic energy levels. The energy level gap in the energy band is very small which is usually seen as continuous. But regarding the materials like nano-materials formed by accumulating of ultrafine particles, energy bands inside the materials split into discrete energy levels. The energy level gap increases with the decrease of particle size which leads to the deviation of physical and mechanical properties explained by energy band theory from the experimental result, even occurring the abnormal characteristics, like abnormal Hall-Petch relation in nano-materials. Therefore, so many special physical and mechanical properties of granular materials are caused by the space discontinuity of some physical quantities. Such as the discontinuity of deformation and energy bands, these discontinuities of physical quantities show the "gradient" phenomenon of physical quantities on particle interface, which is the phenomenon of changing sharply the physical quantities near interface. In the simulation of the material mechanical properties, based on the phenomenon of "gradient", strain gradient is introduced into the classic elastic-plastic constitutive relation to set up the strain gradient plasticity theory [2-3]. This theory takes into account the microstructure characteristics of particle material, and associates the change of physical quantities at a geometric point with neighborhood. It can explore the simulation of material performance and prediction of mechanical behavior to the micro range. For example, regarding the analysis of interface fracture of ceramic-metal material, the separation stress of interface directly calculated by the electron density functional theory ups to 10GPa [1, 4-5]. The test result also shows the interface separation stress can reach to a high value [6], while the interface separation stress can only reach 1GPa [1, 7] analyzed by the classic elastic-plastic constitutive theory. The crack front separation stress analyzed by the strain gradient plasticity theory is closed to the results calculated and tested by the electron density functional theory [8]. Another example, the result of studying the size effect of aluminum-silicon carbide particles reinforced materials shows [9-10], the stress-strain curve of particle reinforced materials corresponding to smaller diameter (7.5μm) carbide particles obviously higher than that of particle reinforced materials corresponding to larger diameter (16μm) carbide particles for the same particle volume percentage. But because the classical elastic-plastic theory does not contain the physical parameters describing particle size, it cannot predict above mentioned particle size effect, while strain gradient plasticity theory can correctly predict this kind of particle size effect relating with particles reinforced stress-strain relation and have the same result as test [10-11]. Starting from the phenomenon of gradient of granular material mechanics response, based on the constitutive relation of the MSG strain gradient plasticity theory, this paper uses the virtual work principle to derive the equilibrium equation and the boundary conditions and establish a mechanical simulation method suitable for granular material size effect.

MSG STRAIN GRADIENT PLASTICITY THEORY

Basic Assumption

MSG strain gradient plasticity theory adopts the multi-scale framework as shown in Fig. 1. In the micro cell, stress and strain are marked as $\tilde{\sigma}(\tilde{x})$ and $\tilde{\varepsilon}(\tilde{x})$ separately and $\tilde{x}$ is marked as the local coordinate of micro cell. In the meso cell, stress and strain are marked as $\sigma(x)$ and $\varepsilon(x)$ separately and x is marked as the global coordinates of meso cell. On the micro level, micro scale plasticity still follows the classical plasticity theory, and shear flow stress bases on the derivation of Taylor dislocation model. For establishing the relation between Taylor dislocation model of micro scale and strain gradient plasticity of meso scale, MSG strain gradient plasticity theory adopts the following basic assumptions:

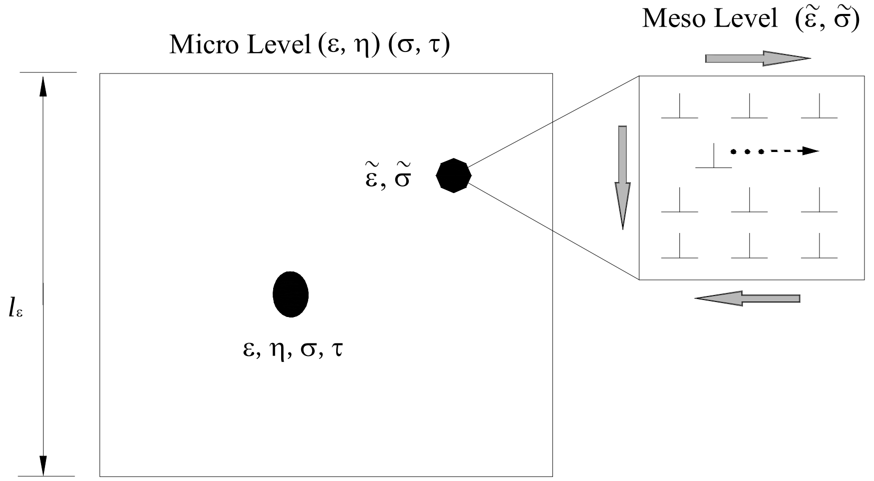

Figure 1: Microscopic and mesoscopic framework of MSG Strain gradient plasticity theory [12]

(1) The shear flow stress of micro scale is controlled by the dislocation motion and keeps the following Taylor harden relation.

$$\tilde{\sigma} = \sigma_v \sqrt{f^2(\tilde{\varepsilon}) + l\eta} \tag{1}$$

Where, σ_v is the reference stress, like the yield stress, etc.; f is the strain hardening function of uniaxial tension; η is the equivalent strain gradient; $l = M^2\alpha^2 b(\mu/\sigma_y)^2$ is the intrinsic material scale, α is the Taylor empirical constant (its value is about 0.3), b is the Burgers vector, μ is the shear modulus, M is the Taylor factor, relating with the yield criterion.

(2) The strain gradient plasticity is the meso scale description of dislocation motion, which can be derived from the micro scale plasticity based on the dislocation (like the Taylor model). So the meso cell scale l_ε must be smaller than the intrinsic material scale l, to make sure its strain approximately change linearly (could neglecting the higher-order strain gradient); at another side, l_ε should be large enough to guarantee containing large quantities of dislocation to make Taylor model be applied to the following virtual work principles based on consistent medium, to build up the relation between the strain gradient plasticity and the dislocation.

$$\int_{V_{cell}} \tilde{\sigma}_{ij} \delta\tilde{\varepsilon}_{ij} dV = (\sigma_{ij}\delta\varepsilon_{ij} + \tau_{ijk}\delta\eta_{ijk})V_{cell} \tag{2}$$

where, V_{cell} is the meso cell volume; τ_{ijk} and η_{ijk} is for the higher-order strain and the strain gradient respectively; the relation between the micro scale virtual strain $\delta\tilde{\varepsilon}_{ij}$, meso scale virtual strain $\delta\varepsilon_{ij}$ and virtual strain gradient $\delta\eta_{ijk}$ is marked as:

$$\tilde{\varepsilon}_{ij}(x) = \varepsilon_{ij} + \varepsilon_{ij,k}\tilde{x}_k = \varepsilon_{ij} + \frac{1}{2}(\eta_{ijk} + \eta_{kji})\,\tilde{x}_k \tag{3}$$

where, the relation between meso strain ε_{ij}, strain gradient tensor η_{ijk} and displacement is marked as:

$$\varepsilon_{ij}(x)=\frac{1}{2}(u_{i,j}+u_{j,i}) \tag{4a}$$

$$\eta_{ijk}(x)=u_{k,ij}=\varepsilon_{ik,j}+\varepsilon_{jk,i}-\varepsilon_{ij,k} \tag{4b}$$

Constitutive Relation

Based on the above basic assumptions, we can derive the meso constitutive relation of MSG strain gradient plasticity theory [9]. Therefore, micro scale strain is broken down into 2 strains: volume and deflection.

$$\tilde{\varepsilon}_{ij}=\frac{1}{3}\tilde{\varepsilon}_{kk}\delta_{ij}+\tilde{\varepsilon}'_{ij} \tag{5}$$

where, the relation between volume strain and hydrostatic stress is:

$$\tilde{\varepsilon}_{kk}=\frac{1}{3K}\tilde{\sigma}_{kk} \tag{6}$$

In the formula, K is bulk modulus of elasticity. The deviator strain can be decomposed into elastic deviator strain and plastic deviator strain: $\tilde{\varepsilon}'_{ij}=\tilde{\varepsilon}'^{e}_{ij}+\tilde{\varepsilon}'^{p}_{ij}$. The elastic deviator strain $\tilde{\varepsilon}'^{e}_{ij}$ is proportionate to the deviator stress $\tilde{\sigma}'_{ij}$, namely $\tilde{\varepsilon}'^{e}_{ij}=\tilde{\sigma}'_{ij}/2\mu$; plastic deviator strain $\tilde{\varepsilon}'^{p}_{ij}$ is determined by the normal plastic flow rule, namely $\tilde{\varepsilon}'^{p}_{ij}=\lambda\tilde{\sigma}'_{ij}$ (λ is plasticity coefficient). Let coefficient $\lambda'=\lambda+1/2\mu$, then there is:

$$\tilde{\varepsilon}'_{ij}=\lambda'\tilde{\sigma}'_{ij} \tag{7}$$

On the micro scale level, the coefficient λ' is shown as:

$$\lambda'=\left[\frac{\tilde{\varepsilon}'_{ij}\tilde{\varepsilon}'_{ij}}{\tilde{\sigma}'_{ij}\tilde{\sigma}'_{ij}}\right]^{1/2}=\frac{3\tilde{\varepsilon}_e}{2\tilde{\sigma}_e} \tag{8}$$

In the formula, $\tilde{\varepsilon}_e=\sqrt{2\tilde{\varepsilon}'_{ij}\tilde{\varepsilon}'_{ij}/3}$, $\tilde{\sigma}_e=\sqrt{3\tilde{\sigma}'_{ij}\tilde{\sigma}'_{ij}/2}$ represent the equivalent strain and equivalent stress respectively under the micro scale. The yield criterion of micro scale is:

$$\tilde{\sigma}_e=\tilde{\sigma}=\sigma_y\sqrt{f^2(\tilde{\varepsilon})+l\eta} \tag{9}$$

Substituting Eq.3 into Eq.2 can result the meso stress σ_{ij} and higher-order stress τ_{ijk} showed by micro scale stress.

$$\sigma_{ij}=\frac{1}{V_{cell}}\int_{V_{cell}}\tilde{\sigma}_{ij}dV \tag{10}$$

$$\tau_{ijk} = \frac{1}{V_{cell}} \int_{V_{cell}} \frac{1}{2} (\tilde{\sigma}_{jk} \tilde{x}_i + \tilde{\sigma}_{ik} \tilde{x}_j) dV \tag{11}$$

Using the basic equations of micro scale plasticity Eq.5 ~ Eq.9, the kinematics relation between micro scale and meso scale Eq.3 and the following relation Eq.12,

$$\frac{1}{V_{cell}} \int_{V_{cell}} \mathrm{d}V = 1, \quad \frac{1}{V_{cell}} \int_{V_{cell}} x_k \, \mathrm{d}V = 0, \quad \frac{1}{V_{cell}} \int_{V_{cell}} x_k x_m \, \mathrm{d}V = \frac{l_\varepsilon^2}{12} \delta_{km} \tag{12}$$

And calculating by Eq.9 ~ Eq.11 and keeping the minimum power l_ε, we get the micro constitutive relation of MSG strain gradient plasticity theory as:

$$\sigma_{ij} = K\varepsilon_{kk}\delta_{ij} + \frac{2\sigma}{3\varepsilon} \varepsilon'_{ij} \tag{13}$$

$$\tau_{ijk} = l_\varepsilon^2 \left[\frac{K}{6} \eta_{ijk}^H + \frac{\sigma}{\varepsilon} (\Lambda_{ijk} - \Pi_{ijk}) + \frac{\sigma_y^2 f'(\varepsilon) f(\varepsilon)}{\sigma} \Pi_{ijk} \right] \tag{14}$$

where,

$$\eta_{ijk}^H = \frac{1}{4} (\delta_{ik} \eta_{jpp} + \delta_{jk} \eta_{ipp}) \tag{15}$$

$$\Lambda_{ijk} = \frac{1}{72} \left[2\eta'_{ijk} + \eta'_{kji} + \eta'_{kij} + \frac{1}{2} \delta_{ij} \eta_{kpp} + \frac{1}{3} \eta_{ijk}^H \right] \tag{16}$$

$$\Pi_{ijk} = \frac{1}{54\varepsilon^2} \left[\varepsilon'_{mn} (\varepsilon'_{ik} \eta'_{jmn} + \varepsilon'_{jk} \eta'_{imn}) + \frac{1}{4} \eta_{qpp} (\varepsilon'_{ik} \varepsilon'_{jq} + \varepsilon'_{jk} \varepsilon'_{iq}) \right] \tag{17}$$

Meso strain deviator ε'_{ij} and strain gradient deviator η'_{ijk} represent as:

$$\varepsilon'_{ij} = \varepsilon_{ij} - \frac{1}{3} \varepsilon_{kk} \delta_{ij}, \ \eta'_{ijk} = \eta_{ijk} - \eta_{ijk}^H \tag{18}$$

Meso equivalent strain ε and meso flow stress σ represent as:

$$\varepsilon = \sqrt{\frac{2}{3} \varepsilon'_{ij} \varepsilon'_{ij}}, \ \sigma = \sigma_y \sqrt{f^2(\varepsilon) + l\eta} \tag{19}$$

where, η is the meso equivalent strain gradient, which is confirmed by Gao [3, 13].

$$\eta = \sqrt{\frac{1}{4} \eta'_{ijk} \eta'_{ijk}} \tag{20}$$

Equilibrium Equation and Boundary Conditions

Through the above analysis and deduction, the physical mechanical quantities of MSG strain gradient plasticity theory have been changed into that of meso scale. In order to get the solutions of MSG strain gradient plasticity theory questions, we still need the equilibrium equation and boundary conditions described by the meso physical mechanical quantities. Therefore, on the following parts, we use the virtual work equation of meso scale to derive these equations.

Internal virtual work of meso scale is presented as:

$$U = \int_V (\sigma_{ij}\delta\varepsilon_{ij} + \tau_{ijk}\delta\eta_{ijk})\,\mathrm{d}V \tag{21}$$

External forces include volume forces f_k, surface forces t_k and higher-order surface forces r_k, represented as:

$$E = \int_V f_k\delta u_k + \int_S (t_k\delta u_k + r_k n_i \delta u_{k,i})\,\mathrm{d}S \tag{22}$$

By the virtual work equation $U = E$ and step by step integration method, we derive the equilibrium equation

$$\sigma_{ik,i} - \tau_{ijk,ij} + f_k = 0 \tag{23}$$

and the boundary conditions

$$n_i(\sigma_{ik} - \tau_{ijk,j}) + n_i n_j (n_{l,l} - n_l n_k n_{l,k})\tau_{ijk} - (n_i\tau_{ijk})_{,j} + n_j n_l (n_i \tau_{ijk})_{,l} - t_k = 0 \tag{24}$$

$$n_i n_j \tau_{ijk} - r_k = 0 \tag{25}$$

where n_i is the normal unit vector of boundary surface.

MECHANICS SIMULATION OF GRANULAR MATERIAL

Basic Equations of Finite Element

Stress vector is presented as $\{\boldsymbol{\sigma}\}$, its component including stress σ_{ij} and higher-order stress τ_{ijk}; strain vector is presented as $\{\boldsymbol{\varepsilon}\}$, its component including strain ε_{ij} and strain gradient η_{ijk}. The incremental form of constitutive relation of MSG strain gradient plasticity theory is $\{\Delta\boldsymbol{\sigma}\} = [\boldsymbol{D}]\{\Delta\boldsymbol{\varepsilon}\}$, ($[\boldsymbol{D}]$ is material properties matrix). The geometric relation between strain vector $\{\boldsymbol{\varepsilon}\}$ and point displace vector $\{\mathbf{U}\}$ is $\{\boldsymbol{\varepsilon}\} = [\boldsymbol{B}]\{\mathbf{U}\}$, ($[\boldsymbol{B}]$ is strain matrix). When the material goes into a state of plastic flow, the constitutive relation is:

$$\{\Delta\boldsymbol{\sigma}\} = [\boldsymbol{D_e}]\{\Delta\boldsymbol{\varepsilon}^e\} = [\boldsymbol{D_e}](\{\Delta\boldsymbol{\varepsilon}\} - \{\Delta\boldsymbol{\varepsilon}^p\}) \tag{26}$$

where superscript and subscript "*e*" and "*p*" in the formula present separately the elastic part and the plastic party of related quantity. By the virtual work equation,

$$\int_V \{\delta(\Delta\boldsymbol{\varepsilon})\}^{\mathrm{T}}\{\Delta\boldsymbol{\sigma}\} = \int_V \{\delta(\Delta\mathbf{u})\}^{\mathrm{T}}\{\Delta\mathbf{f}\} + \int_S \{\delta(\Delta\mathbf{u})\}^{\mathrm{T}}\{\Delta\mathbf{t}\} \tag{27}$$

We derive the incremental equations of finite element:

$$[\mathbf{K}]\{\Delta\mathbf{U}\}=\int_V [\boldsymbol{B}]^{\mathrm{T}}[\boldsymbol{D}_e]\{\Delta\boldsymbol{\varepsilon}^p\}\mathrm{d}V+\int_V [\mathbf{N}]^{\mathrm{T}}\{\Delta\mathbf{f}\}\mathrm{d}V+\int_S [\mathbf{N}]^{\mathrm{T}}\{\Delta\mathbf{t}\}\mathrm{d}S \tag{28}$$

where, $\{\Delta\mathbf{f}\}$ and $\{\Delta\mathbf{t}\}$ present separately the vector increment of body force and surface forces; and elastic tangent modulus stiffness matrix is:

$$[\mathbf{K}]=\int_V [\boldsymbol{B}]^{\mathrm{T}}[\boldsymbol{D}_e][\boldsymbol{B}]\mathrm{d}V \tag{29}$$

Iterative Solution Procedure

We use the incremental method to simulate the deformation to failure process of material. And classify the external load of body force $\mathbf{f}$ and external load of surface force $\mathbf{t}$ to grade m:

$$\mathbf{f}=\Delta\mathbf{f}_1+\Delta\mathbf{f}_2+\cdots+\Delta\mathbf{f}_m,\ \mathbf{t}=\Delta\mathbf{t}_1+\Delta\mathbf{t}_2+\cdots+\Delta\mathbf{t}_m \tag{30}$$

The load is applied step by step, and then we can gradually solve the displacement field, strain field and stress field of the whole process by Eq.28, to do the related analysis of mechanical behavior. Iterative solution procedure is as follows:

(1) Initial calculation: let $\Delta\boldsymbol{\varepsilon}^e=0$ and $\Delta\boldsymbol{\varepsilon}^p=0$, we get the initial displacement $\mathbf{U}^{(1)}=\Delta\mathbf{U}^{(1)}$ under the load of $\Delta\mathbf{f}=\Delta\mathbf{f}_1$, $\Delta\mathbf{t}=\Delta\mathbf{t}_1$. Then, we obtain the initial strain field $\varepsilon_{ij}^{(1)}$ and initial stress field $\sigma_{ij}^{(1)}$ by Eq.28.

(2) Judge whether there is any element gets into the yield: calculate the largest equivalent stress in all elements $\overline{\sigma}_{\max}=\max\limits_{e=1,2,\cdots}\{\sigma^{(1)}\}$, where $\sigma^{(1)}=\sqrt{3\sigma_{ij}'^{(1)}\sigma_{ij}'^{(1)}/2}$; if $\overline{\sigma}_{\max}>\sigma_T$ (σ_T is the meso flow stress), all elements get into the yield, adjusting initial displacement, strain and stress by multiplying coefficient $L_p=\sigma_T/\overline{\sigma}_{\max}$.

(3) The iterative calculation: adopting strain, plastic strain got from last iteration, Eq.28 is used to calculate the displacement, strain and stress increment under the current level of load, so to calculate the current displacement, strain and stress:

$$\left.\begin{aligned}\mathbf{U}^{(n)}&=\mathbf{U}^{(n-1)}+\Delta\mathbf{U}^{(n)}\\ \boldsymbol{\varepsilon}^{(n)}&=\boldsymbol{\varepsilon}^{(n-1)}+\Delta\boldsymbol{\varepsilon}^{(n)}\\ \boldsymbol{\sigma}^{(n)}&=\boldsymbol{\sigma}^{(n-1)}+\Delta\boldsymbol{\sigma}^{(n)}\end{aligned}\right\} \tag{31}$$

(4) Repeat the above calculating steps till to the finish of the whole loading procedure.

Finally, according to the displacement, strain and stress field of the whole process of loading, we can make an analysis and interpretation on the mechanical behavior of materials.

CONCLUSION

In this paper, we analyze the special physical and mechanical properties and its formed micro mechanism of granular materials, elucidate the basic reason why the classic mechanics theory of consistent medium cannot effectively predict the mechanical behavior of granular materials, discuss the constitutive relation of MSG Strain gradient plasticity theory based on Taylor dislocation model of micro scale, and derive related equilibrium equation and boundary conditions. Finally, we put forward the basic equations and the iteration steps of finite element simulating the deformation to failure process of granular material. The main results are summarized as follows:

(1) The size effect of granular material is caused by some discontinuous and non-uniform physical quantity such as strain and stress, etc. It performs as "gradient" phenomenon of physical quantity on particle interface, which leads to dramatically physical changes near the interface.

(2) MSG strain gradient plasticity theory established on the basis of Taylor dislocation model of micro scale contains the microstructure information of granular material and the strain gradient. It can be used in the mechanical simulation in micro range and the prediction of the special mechanical behavior produced by size effect.

(3) The incremental equations and the iterative process of finite element based on MSG strain gradient plasticity theory can be used as a method to simulate the deformation to failure process of granular material and predict its special mechanical behavior.

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