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MACROSCOPIC PARTICLE MODELING OF ELASTIC AND PLASTIC DEFORMATION IN METALS: A MULTISCALE APPROACH BASED ON INTERATOMIC POTENTIAL AND CRYSTAL STRUCTURE

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Abstract. *We formulate a macroscopic particle modeling analysis of metallic materials (aluminum and copper, etc.) based on theoretical energy and atomic geometries derivable from their interatomic potential. In fact, particles in this framework are presenting a large mass composed of huge collection of atoms and are interacting with each other. We can start from cohesive energy of metallic atoms and basic crystalline unit (e.g. face-centered cubic). Then we can reach to interparticle (macroscopic) potential function which is presented by the terms of exponent of inter-particle distance, like a Lennard-Jones potential used in molecular dynamics simulation. Equation of motion for these macroscopic particles has both dissipative term and fluctuation term, as well as the conservative term above, in order to express finite temperature condition. First, we determine the parameters needed in macroscopic potential function and check the reproduction of mechanical behavior in elastic regime. By using the present framework, we carry out uniaxial loading simulation of aluminum rod. The method can reproduce Young's modulus and Poisson's ratio as elastic behavior, though the result shows the dependency on division number of particles. Then, we proceed to include plasticity in this multiscale framework. As a result, a realistic curve of stress-strain relation can be obtained for tensile and compressive loading.*

Keywords: *Molecular dynamics, Particle method, Elasticity, Plasticity, Multiscale analysis*

1. INTRODUCTION

Recently, multiscale modeling of materials behavior with hierarchical approach has attracted much interests in research and development of materials science. Surveying existing computational methodologies, molecular dynamics (MD) has been established based on microscopic view, while traditional continuum-based approaches such as finite element (FE) analysis or particle methods (or sometimes called mesh-less methods) are provided from macroscopic viewpoint. In addition to these two separate approaches, in these days, a variety of combination between them has been proposed. For

example of solid state metallic material, it is basically hard task to model total mechanical behavior, including both macroscopic and microscopic viewpoints simultaneously. Limited to small strain or small deformation regime, it may be quite possible by configuring elastic constitutive law and parameters in materials modeling. Therefore, potential energy function between metallic atoms can be directly connected to macroscopic elastic constants, if theoretical harmonic approximation in small displacement is acceptable. However, for plastic deformation as subsequent stage of metallic material subject to larger deformation, it becomes hard to link directly between microscopic behavior (i.e. slip motion between atoms) and overall macroscopic constitutive law. Understanding plastic deformation of metal, as well as super-elastic deformation, which are usually observed in many materials, is one of difficult issues such that adequate computation model should help. Nowadays, not only macroscopic modeling but also microscopic modeling is important and is inevitable for the recent development of engineering materials [2]. We should note that total mechanical behavior of materials, in fact, might be sensitive to state-of-arts nanoscale structures. What is required here is to do analysis with nice coupling between microscopic and macroscopic methods.

In recent years, particle methods (or mesh-less methods), as a successor of on-mesh methods, has been developed extensively owing to increasing computation power. ”Particles” are treated in various sense, corresponding to size scale. In the smallest scale, particles are atoms or molecules (in MD method), whereas, in larger scale, they are only representative points embedded onto continuous body. However, there is common feature that all particle methods are solving an equation by chasing motion of particles. Therefore, computational combination between macroscopic and microscopic methods across spatial or time scale gap will be relatively easier by using particle modeling. Naturally, there may be two approaches as follows. One is that any macroscopic variable is used in evaluating atomistic simulation. For example, atomistic stress or strain is macroscopic variable which is defined from continuum relation, but is also adjusted to use in atomic simulations [1]. Another approach is that, to the contrary, any microscopic variable is applied in modeling and simulating macroscopic behavior. Actually, the latter idea has already been implemented as novel computational methodologies such as quasi-continuum (QC)[3][4] method or virtual atomic cluster (VAC)[5] method. In our opinion, the latter approach seems challenging and interesting. That is, interatomic potential function derived from microscopic relation is applied to macroscopic particle modeling (MPM), where the same type of equations of motion as atomic system (of course, their size is not equivalent to atomic size) is to be solved just like MD method.

In this paper, we propose an actual framework of MPM method, constructing from microscopic (atomic) potential energetics and dynamics. The framework is able to reproduce finite-temperature behavior by using Langevin-type equation of motion, where both dissipative force and fluctuating random force as well as conservative potential force are integrated. In our study, the conservative potential force is expressed by a simple power-law, just like an atomistic Lennard-Jones potential[6] for condensed matter. By using this new particle method, mechanical properties and thermal properties of materials will be evaluated, realizing multiscale approach. As a first stage of our study, in this paper, we would like to show the detailed derivation of equation and parameters settings. Then, computational results of simple uniaxial loading is verified.

2. THEORY AND METHOD

2.1. Particle Modeling method: basic concept

Generally, in particle modeling, a material which occupys a certain space is replaced by assembly of discrete particles. This concept has been universal such as that in the former literature[7] and usual SPH (smoothed particle hydrodynamics) method [9][10][11][12][13][14] For example, when total volume is confined in a cube with dimension $L \times L \times L = V$ as shown in Fig.1, it is replaced by N particles. The particles have adequate mass,

$$M_i = \rho \frac{V}{N} \ , \tag{1}$$

so that the original density of the material ρ is retained. Motion of each particle is described by Newtonian equation of motion,

$$M_i \frac{\mathrm{d}^2 \boldsymbol{r}_i}{\mathrm{d}t^2} = \boldsymbol{F}_i \ , \tag{2}$$

where $\boldsymbol{F}_i$ includes interparticle force as well as additional forces induced by viscous friction and thermal fluctuation. Indeed, this equation is the same as that of molecular dynamics (MD) simulation. Thus, interparticle interaction can be configured from pairwise potential function $\phi_E(r)$, and then the conservative force is derived by

$$\boldsymbol{F}_i = \sum_{j=1}^{\text{Neighbor}} \boldsymbol{F}_{ij} = \sum_{j=1}^{\text{Neighbor}} \frac{\partial \phi_{E,ij}}{\partial r_{ij}} \frac{\boldsymbol{r}_{ij}}{r_{ij}} \ , \tag{3}$$

where $\phi_{E,ij} = \phi(E,r)|_{r_{ij}}$ means potential energy acting between two particles i and j. Separation r_{ij} is the absolute value of interparticle difference vector $\boldsymbol{r}_{ij} = \boldsymbol{r}_j - \boldsymbol{r}_i$.

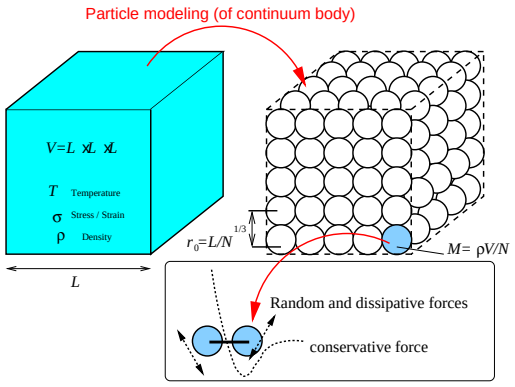


Figure 1. Concept of macroscopic particle modeling (MPM)

From the former study concerning "particle modeling" method [7][8], a power function expressed by

$$F_{ij} = \frac{G}{r_{ij}^p} - \frac{H}{r_{ij}^q} \tag{4}$$

has been used for interparticle force. In atomic simulation, the famous Lennard-Jones potential has the same function form as Eqn.(4) (corresponding to $p = 13, q = 7$). These macroscopic potential

parameters, G, H, p, q, in the function have to be determined. From energy-conservative mechanics, a potential function integrated from force function Eqn.(4) is given by

$$\phi_{E,ij} = -\frac{G}{p(r_{ij})^p} + \frac{H}{q(r_{ij})^q}. \tag{5}$$

2.2. Introducing of Langevin equation for particle modeling

In atomic system, Eqn.(2) is supposed to have only conservative force so that the total energy of the system should be conserved in principle. However, macroscopic particles' system should have additional treatment due to invisible effect from many disappeared degrees of freedom. Therefore, Langevin-type equation of motion can be applied to this particles' system, where energy dissipation and production of thermal energy by fluctuation are integrated. This type of equations have already used to dissipative particle dynamics (DPD) [17] and Brownian dynamics (BD)[18] simulations, which can analyze material behavior in slightly larger scale than atomic size. The Langevin equation is given by,

$$M_i \frac{\mathrm{d}^2 \boldsymbol{r}_i}{\mathrm{d}t^2} = \boldsymbol{F}_{i,C} + \boldsymbol{F}_{i,D} + \boldsymbol{F}_{i,R} = -\frac{\partial \Phi}{\partial \boldsymbol{r}_i} + \boldsymbol{F}_{i,D} + \boldsymbol{F}_{i,R} \tag{6}$$

where $\boldsymbol{F}_{i,D}$ and $\boldsymbol{F}_{i,R}$ are force vectors called dissipative and random forces, respectively. The conservative force on one particle is derived from

$$\Phi = \sum_{i=1}^{N} \sum_{j>i+1}^{N} \phi_{E,ij}, \tag{7}$$

which is total conservative energy of the system.

The dissipative force term can be formulated by considering inherent resistance of a moving particle. In the meso- or micro-scale (relatively in smaller scale), that term is supposed to be caused by interparticle friction. When a particular viscosity μ is provided, the dissipative force should be estimated, from particles' velocity $\boldsymbol{v}_i, \boldsymbol{v}_j$, by

$$\boldsymbol{F}_{i,D} = \sum_{j=1}^{\text{neighbor}} \mu(\boldsymbol{v}_j - \boldsymbol{v}_i) \ . \tag{8}$$

On the other hand, in meso- and macro-scale (relatively in larger scale), the motion of particle should be through some other media, it is supposed that the dissipative force depends only on absolute velocity. In such a case, the friction force may be estimated by

$$\boldsymbol{F}_{i,D} = \gamma \boldsymbol{v}_i \ . \tag{9}$$

Random force induces fluctuation of particles and is formulated based on its randomness. Thus, in computation, numerically produced random numbers (pseudo-random numbers) with Gaussian distribution are utilized. The dissipative and random forces are working for a particle motion, so to speak, as brake and accelerator, respectively. All these three types of force in Langevin equation (Eqn.(6)) balance each other in equilibrium, or they evolve to make structural change (deformation and catastrophic fracture) in finite temperature condition.

2.3. Determination of potential parameters and mechanical properties

In the present MPM method, conservative force almost determines elastic properties. Therefore, based on existing elastic constants available from experiment or *ab initio* calculation, macroscopic potential parameters are determined. At first, total absolute amount of potential energy contained in one macroscopic particle is estimated. When atoms are condensed as solid material with density ρ, a lot of atoms are assigned to one macroscopic particle. For example, in solid state of fcc metal, each atom has cohesive energy e_0 which is calculated as the summation of twelve pairwise potential energies. If the number of atoms in one macroscopic particle is N_{atom}, collective energy in this macroscopic particle should be,

$$P_{atom} = N_{atom} e_0 \ . \tag{10}$$

When all the macroscopic particle have a spherical shape and they gather to make fcc structure of lattice constant a_0, N_{atom} is given by,

$$N_{atom} = \frac{\rho\pi}{6}\frac{r_0^3}{m}\frac{1}{0.74} \ , \tag{11}$$

where r_0 is equilibrium distance between macroscopic particles, m is atomic mass, the factor 0.74 means occupancy rate in fcc lattice. In most cases, e_0 and a_0 as well as structural type of crystal are easily available from experimental fact or *ab initio* evaluation. Thus, both e_0, a_0 and ρ are microscopic parameters, but N_{atom} and P_{atom} come to macroscopic variables to be configured next.

When macroscopic particles are separated by equilibrium distance $r = r_0$, their interparticle force should all vanish, and Eqn.(4) gives the condition,

$$F_{ij}|_{r=r_0} = \frac{G}{r_0^p} - \frac{H}{r_0^q} = 0 \ . \tag{12}$$

Equivalence between microscopic and macroscopic energies (Eqn.(10)) and equilibrium condition (Eqn.(12)) are both used to solve unknown potential parameters G, H by following equations.

$$\begin{aligned} G &= f(p,q) r_0^p \\ H &= f(p,q) r_0^p \\ f(p,q) &= \frac{P_{atom}}{6}\frac{pq}{p-q} \end{aligned} \tag{13}$$

Two undetermined exponents (powers) p, q which determine net shape of potential curve are needed and will be determined next.

Thus, energetic link between microscopic and macroscopic systems has been carried out. However, for mechanical response, the curve shape of potential function is crucial. Although there may be many choices for function type, we think that Eqn.(5) is reasonable because it furnishes three basic characteristics necessary for macroscopic particles. They are :(1)divergent feature of energy in closer separation than r_0, (2)equilibrium distance (energy minimum) at r_0, and (3)convergence to zero-energy in far larger separation.

The undertemined parameters p, q can be adjusted from elastic constant (i.e. Young's modulus) in the vicinity of equilibrium distance r_0 as follows.

Young's modulus E can be estimated as the curvature of potential curve at equilibrium distance r_0, then,

$$E = \frac{1}{2r_0}\left.\frac{\partial^2 \phi_{E,ij}}{\partial r^2}\right|_{r=r_0} \ . \tag{14}$$

Substituting Eqn.(5) into this formula, it gives,

$$E = \pi\rho \frac{1}{0.74} \frac{pq}{72} \frac{e_0}{m} \quad . \tag{15}$$

This means that Young's modulus depends on the product between p and q. For the fcc metals (aluminum, copper, etc.), using each cohesive energy e_0, Young's modulus is estimated. They are tabulated on dependency on p, q as shown in Table 1. Actual Young's modulus obtained by uniaxial tensile test-

Table 1. Relation between potential parameters (p, q) and calculated Young's modulus

p	q	E_{Al} [GPa]	E_{Cu} [GPa]
3	9	51.6	76.2
4	8	61.1	90.4
4	**9**	**68.8**	**101.6**
4	10	76.4	112.9
5	9	95.5	117.2
experiment		70∼73	110∼130

ing are approximately 70∼73 GPa for aluminum and 110∼130 GPa. Referring these values, $p = 4$ and $q = 9$ may be the most suitable. Of course, we have another choices, but by this procedure we are able to set p, q to configure elastic response of macroscopic particles system.

2.4. Introducing plasticity in the present particle modeling framework

It is generally difficult to express both microscopic and macroscopic plasticity mechanisms at the same time. In macroscopic view, constitutive relation (sometimes complicated formula) can be responsible for plasticity. But, it contains lots of macroscopic parameters which are not immediately connected to microscopic dynamics or parameters. Energy dissipation or heat transport in plasticity, for example, has been one of difficult issues. We are challenging to introduce plasticity mechanism into macroscopic particles' system based on microscopic parameters, extending elastic method described above.

Fig.2 shows potential function including plastic regime. ϕ_U is the function representing "unloading behavior" after plastic deformation proceeds, which is expressed by

$$\phi_U(r_{ij}) = -\frac{G}{p(r_{ij} - \Delta r_0)^p} + \frac{H}{q(r_{ij} - \Delta r_0)^q} + C_\phi \quad , \tag{16}$$

where Δr_0 and C_ϕ are undetermined values until unloading starts. So, many different ϕ_U functions exist per unloading events. ϕ_Us connect each other as well as elastic potential ϕ_E by the function ϕ_P, which prescribes plastic route for between pair of particles. ϕ_P here is just a polynomial of interparticle separation r_{ij}. The ϕ_P should be determined microscopically (from MD simulation) or empirical values obtained by experimental elastic-plastic testing.

Actually, only the elemental framework of simulating in plastic regime has been shown here. It needs further verification and discussion, but let us omit the detailed description in the present paper, to avoid complication.

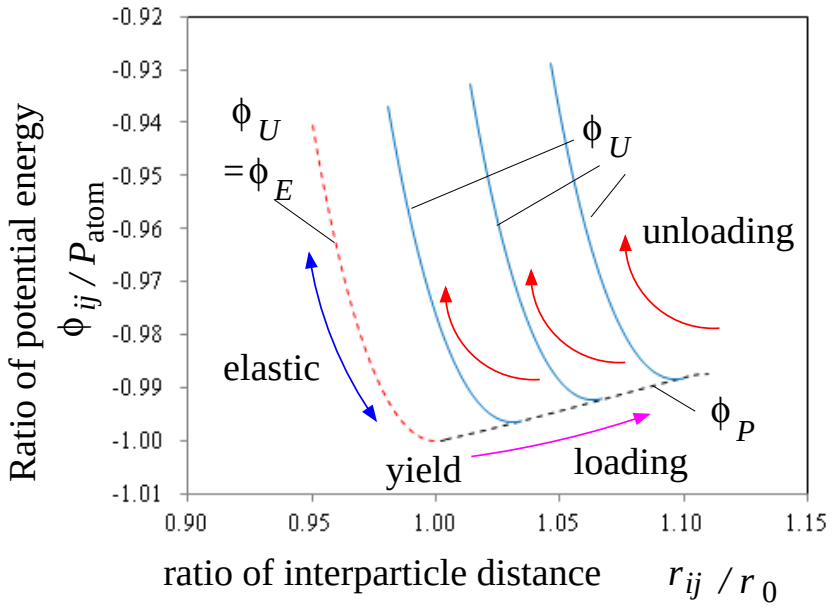


Figure 2. Interatomic potential functions representing elasticity and plasticity

2.5. Coarsening dissipative force and random force terms

In the field of MD study, a Langevin equation is sometimes used and is including Debye model for thermal conduction[19]. Dissipative term is formulated by,

$$\boldsymbol{F}_D = -\alpha \boldsymbol{r}_i \ , \tag{17}$$

and random force is given by

$$\boldsymbol{F}_R = \boldsymbol{F}_R(\sigma) \ , \tag{18}$$

where α is a viscosity for atom and σ is the square root of variance. In MD scale, α and σ have the relation,

$$\sigma^{\text{micro}} = \left(\frac{2\alpha^{\text{micro}} k_B T}{\Delta t} \right)^{\frac{1}{2}} \tag{19}$$

and

$$\alpha^{\text{micro}} = m \frac{\pi}{6} \omega_D \ , \tag{20}$$

where $\omega_D = k_B \theta / \hbar$ is Debye frequency ($\theta, \hbar$ are Debye temperature and Planck's constant, respectively), k_B is Boltzmann's constant, Δt is time increment of MD and T is an equilibrium temperature. This MD system has to be coarsened and transformed to macroscopic particles' system, by virtue of scale factors. There is a trend of study to link microscopic parameters to macroscopic relation [15][16]. However, here, to start with, we assume very simple relations as follows. The scale factors are η_{CG} for α and ζ_{CG} for σ, and resulted expressions are

$$\sigma^{\text{macro}} = \eta_{CG} \left(\frac{2\alpha^{\text{macro}} k_B T}{\Delta t} \right)^{\frac{1}{2}} \tag{21}$$

and

$$\alpha^{\text{macro}} = \zeta_{CG} m \frac{\pi}{6} \omega_D \ . \tag{22}$$

Verifying these coasening parameters η_{CG} and ζ_{CG} should be required, but it will be done in further studies.

In this paper, as a first stage of this study, we think that the potential force (conservative force) is the most important factor for evaluation of material properties in solid. Therefore, we can omit those dissipative and random forces temporarily. It means that MPM simulation results discussed in the following section are carried in zero Kelvin condition. However, in principle, the MPM simulation in finite temperature T is also feasible by the framework shown in this section.

2.6. Calculation models and conditions

The calculation model is shown Fig.3, which has a rod-shape and is subject to uniaxial loading. The MPM parameters and structures are configured for pure aluminum crystal (Al). Velocity of particles in uppermost and lowermost layers is constrained so as to produce constant strain rate in the specimen. Calculation condition is shown in Table 2. Primarily, the effect of particles division number on elastic properties is shown and discussed. Division number in radial direction $n\phi$ and that in longitudinal direction nh vary, respectively. All the models have almost the identical diameter of 14 mm, but they have different logitudinal lengths, keeping spacing parameter r_0 constant. Accordingly, the number of particles are various based on combination between $n\phi = 2, 4, 8, 16$ and ratio $nh/n\phi = 1/8, 1/4, 1/2, 1, 2, 4, 8$.

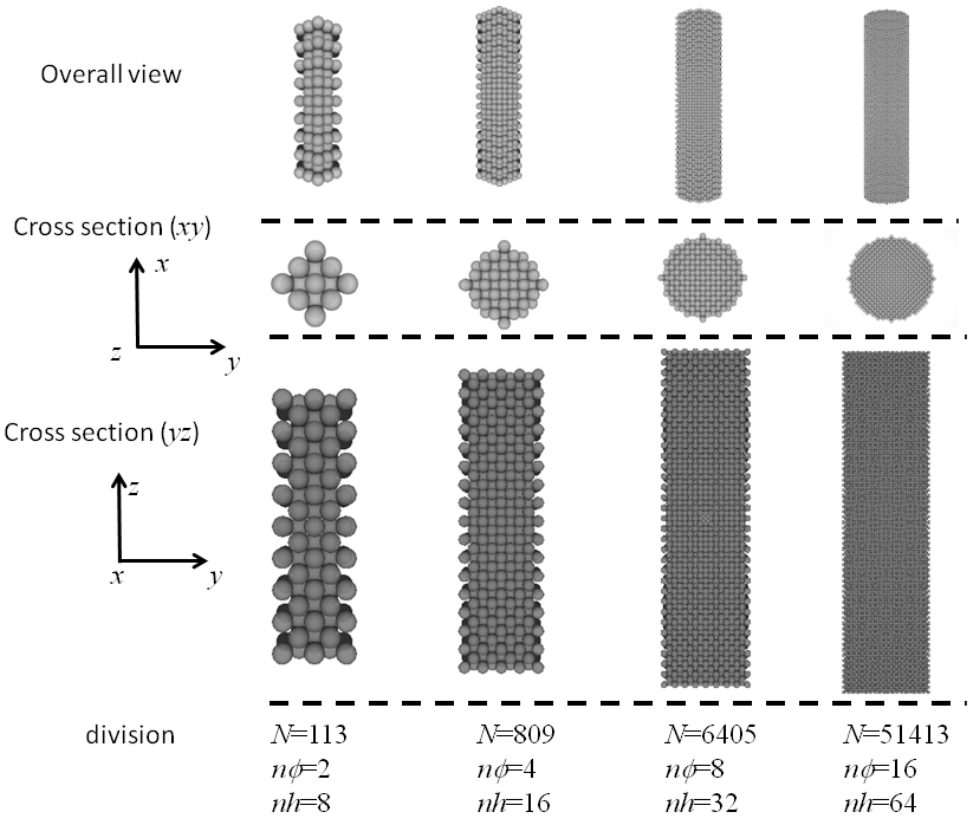


Figure 3. Calculation models for particle modeling ($n\phi$ and nh are the number of division along radial and longitudinal directions, respectively)

Table 2. Calculation condition for uniaxial tensile test by particle modeling

Property	unit	value
Diameter	mm	14.0
Longitudinal length	mm	2.26∼107
Particle equilibrium distance r_0	mm	0.592∼3.65
Number of steps	—	100000
Time increment Δt	sec	$4.58 \times 10^{-8} \sim 2.82 \times 10^{-7}$
Strain rate $\dot{\varepsilon}$	1/sec	$3.53 \times 10^{-2} \sim 2.18 \times 10^{-1}$

3. RESULTS AND DISCUSSIONS

3.1. Reproduction of elastic properties: Young's modulus and Poisson's ratio by macroscopic particle modeling (MPM) method

Figure 4 shows the relation between Young's modulus and the number of particle division. When the division parameters $n\phi$ and nh are small, the value fluctuates largely. However, enough division seems to result in a converged value, which is almost equivalent to the value fitted in constructing conservative potential. Poisson's ratio is shown in Fig.5. In spite of not fitting to any empirical value, Poisson's ratio ranges from 3.0 to 3.3, which is quite nice agreement with actual value of aluminum. There is a general tendency that, the larger the division number is, the larger is the Poisson's ratio. This is because dividing into finer particles numerically leads system to invest larger degrees of freedom, then constraint to particles becomes weaker.

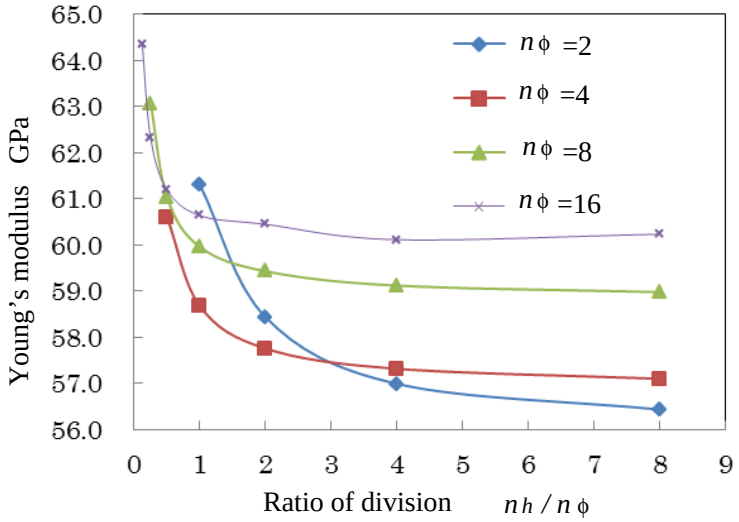


Figure 4. Relation between calculated Young's modulus and division number

3.2. Mechanical response from elastic deformation to plastic deformation

Fig.6 shows the stress-strain curve for uniaxial loading of aluminum specimen, including both elastic and plastic regime. 51413 ($n\phi = 16, nh/n\phi = 4$) is chosen as the division number of particles. Stress tensor is calculated by summing up dyadic product of force vector $\boldsymbol{F}_i$ and interparticle difference vector $\boldsymbol{r}_{ij}$. They are averaged over all particles in the specimen. In Fig.6, we are seeing the component

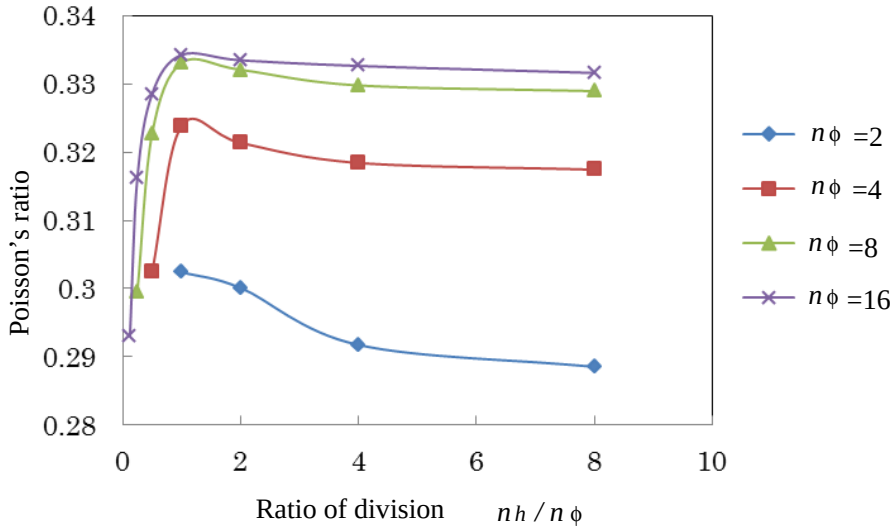


Figure 5. Relation between calculated Poisson's ratio and division number

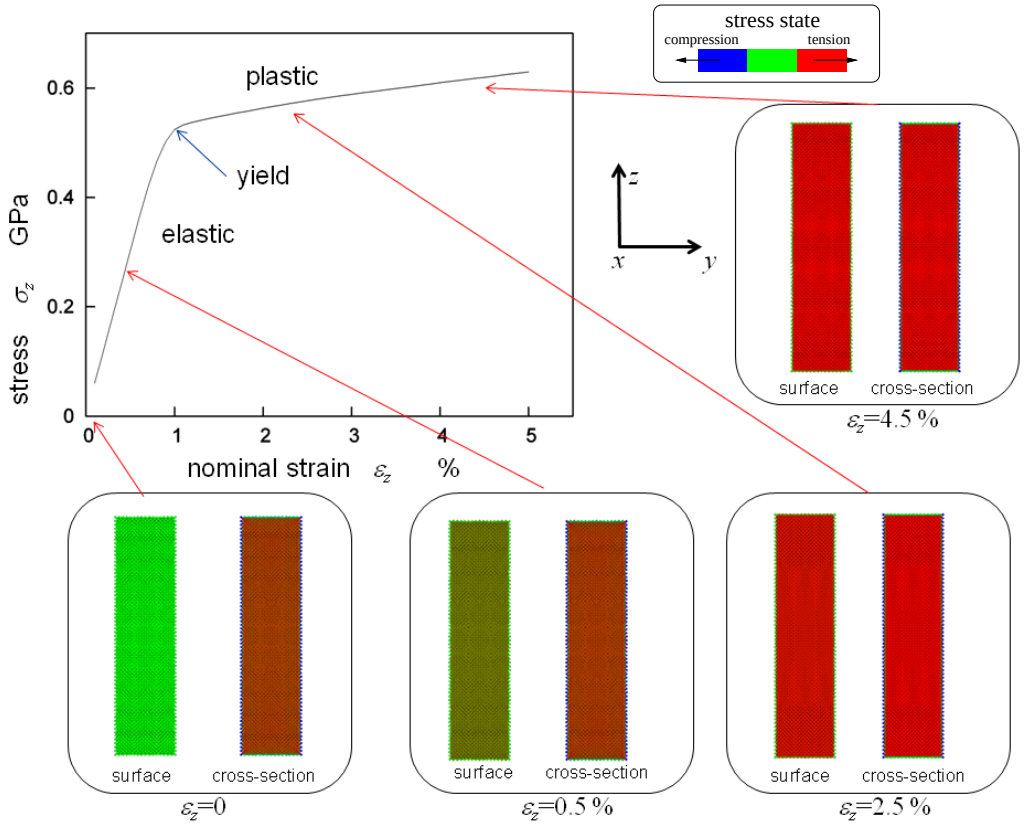
in loading (z) direction. In Fig.6, color of particle is corresponding to stress value (green=around zero, red:in tension, blue=in compressison).

In tensile loading as shown in Fig.6(a), the graph shows linear relation between stress and strain, then after yield occurs at about 1% of strain. Then, it changes to slower curve with strain-hardening behavior. The particles' configuration does not change so much, but stress increases especially inside the specimen. It is interesting that the stress on the surface of the rod is always vanishes. This is because force acting on a particle dwelling in surface region is spontaneously stabilized. In the strain regime shown here(up to 5%), plastic deformation seems not localized.

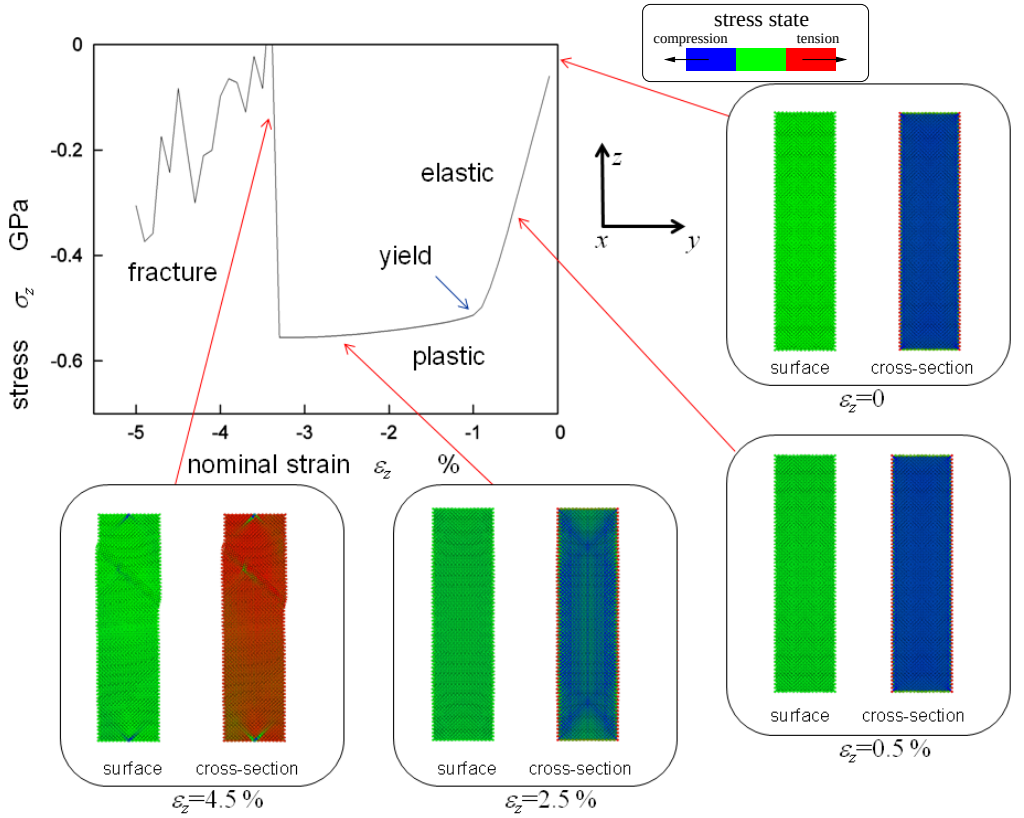
On the other hand, in Fig.6(b) shows the result obtained by compressive loading. As you can see, the tensile and compressive behavior is almost the symmetrical up to 3% of strain. However, in compression, sudden drop of stress value occurs approximately at 3.2% of strain. At this point, stress drops down to zero, which means the structure becomes unstable and, physically speaking, the structure fractures. By checking particles' configuration, it is recognized that slip motion between particles' layer certainly occurs. The slip deformation between these macroscopic particles is likely the same as that found between atoms in smaller size. Since, in this model, particles are arranged in the fcc lattice, the slip can occur along (111) planes. This result indicates that, in the present MPM method, anisotropy of plastic deformation is closely related to arrangement of particles.

4. CONCLUSION

In this study, we propose a computational framework by using macroscopic particles method (MPM). The MPM method is constructed from microscopic parameters such as cohesive energy and density of metallic materials. The interaction is composed of conservative, dissipative and random forces, along the theoretical probabilistic Langevin equation. In order to evaluate the possibility of the MPM method, the rod-shape model, in which interparticle force is configured only by conservative force, is checked as for the division number into particles. In elastic regime, Young's modulus and Poisson's ratio can be sufficiently reproduced. Plastic modeling in MPM is realized to be difficult issue. However, since plasticity mechanism is absolutely required for material modeling, we are first



(a) uniaxial tensile loading



(b) uniaxial compressive loading

Figure 6. Stress-strain curve obtained in uniaxial tensile simulation by macroscopic particle modeling (MPM)

challenging it by formulating a certain irreversible relation between particles in MPM framework. It is found that there is different stability in between tensile and compressive loadings for elastic-plastic deformation. Further sophistication of MPM method for elastic-plastic problem is quite possible and it is worth while studying.

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