

A micromechanical model for deformation behavior of nanocrystalline copper

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Abstract. Molecular dynamics simulations have show that nanocrystalline (NC) materials can be treated as composite materials consisting of two phases of grain and grain boundary. In this paper, the incremental stress-strain relation is derived based on deformation mechanism of NC materials and internal variable theory from micromechanics point of view. The developed model is exemplified by the pure copper subjected to uniaxial tension. Implicated iteration algorithm is then employed to obtain the stress-strain relation. Moreover, the effects of grain shape and statistical distribution of grain sizes are also discussed, and predicted results are compared with experimental values to verify the model.

Introduction

Nanostructured materials refer to those whose microstructure characteristic length or its geometrical size, at least one dimension, is in the nanometer range^[1]. They have been the subject of considerable research in recent years due to their unique microstructure and appealing property.

Extensive experimental investigations^[2-3] and molecular dynamics simulation^[4-9] have show that NC materials can be considered as composite materials consisting of two phases of equiaxed grain and grain boundary. Due to smaller grains, the volume of grain boundary phase is comparable to the grain phase, so the role of grain boundary phase is not neglected regarding the mechanical properties compared with coarse grain materials. As we all know that the dislocation motion will ceased as the grain size decreases. So in this case, the dominant deformation mechanism is governed by grain boundary phase.

In this current investigation, NC materials are modeled as composites two phases of with grain and grain boundary. In order to calculate conveniently, we assume that both phases are isotropic, and the variation of temperature is neglected. The incremental stress-strain relation has been developed based on deformation mechanism of NC and internal variable theory. Then, the developed model was applied to pure copper subjected to uniaxial tension. The stress-strain relation predicted by the model and experimental data were also compared.

Micromechanical Model

It is assumed that the grains in NC materials are all spherical or spheroidal. When the grains are all spheroidal, we define the ellipsoidal domain as follows:

$$\frac{x_1^2}{a_1^2} + \frac{x_2^2}{a_2^2} + \frac{x_3^2}{a_3^2} \leq 1. \quad (1)$$

where a_i ($i = 1, 2, 3$) is one of the three semi-axes of the ellipsoid. Further, the grain shape is considered to be spheroidal when the condition $a_2 = a_3 = a \neq a_1$ is satisfied. The volume fraction of grains can be

given by $v_f = \frac{(\beta a - w)(a - w)^2}{\beta a^3}$, where $\beta = a_1/a$, $a = d/2\sqrt[3]{\beta}$, d is grain size, and w is grain boundary thickness.

Consider a unit volume element subjected to plastic deformation, we can describe the state of material using strain tensor ε_{ij} , absolute temperature T and internal variable ε_{ij}^p . From the point of thermodynamics^[10,11], the constitutive equation of the material and the evolution equation of internal variable are written as follows, respectively:

$$\sigma_{ij} = \frac{\partial \Xi}{\partial \varepsilon_{ij}} + \frac{1}{2} \left(\frac{\partial \Phi}{\partial \dot{\varepsilon}_{ij}} \dot{\varepsilon}_{ij} \right)^{-1} \Phi \frac{\partial \Phi}{\partial \dot{\varepsilon}_{ij}}. \quad (2)$$

$$\frac{\partial \Xi}{\partial \varepsilon_{ij}^p} + \frac{1}{2} \left(\frac{\partial \Phi}{\partial \dot{\varepsilon}_{ij}^p} \dot{\varepsilon}_{ij}^p \right)^{-1} \Phi \frac{\partial \Phi}{\partial \dot{\varepsilon}_{ij}^p} = 0. \quad (3)$$

In which Ξ is total Gibbs free energy, and Φ is the dissipation function.

In comparison with coarse grain materials, the deformation mechanism of grain boundary phase can not be ignored. The yield function can be described as:

$$f = \sqrt{J_2} - \frac{\sqrt{2}}{3} (\sigma_y + k_y d^{-0.5}) = 0. \quad (4)$$

where σ_0, k are material constants, and J_2 is second invariant of the stress deviator.

The grains with the plastic strain ε_{ij}^p are randomly distributed in the grain boundary phase. The strain filed caused by the applied force in the absence of plastic strain is denoted as ε_{ij}^0 . According to Colonnnet theory^[12], the total energy (Gibbs free energy) for the case of ε_{ij}^p and ε_{ij}^0 coexistence is the sum of energies for the conditions when the applied force and the plastic strain exist alone, respectively. So, the total Gibbs free energy can be written:

$$\Xi = \frac{1}{2} \int_D (\sigma_{ij}^0 + \sigma'_{ij}) (\varepsilon_{ij}^0 + \varepsilon'_{ij}) dv - \frac{1}{2} v_f \sigma_{ij} \varepsilon_{ij}^p = \Xi = \frac{1}{2} (\sigma_{ij}^0 \varepsilon_{ij}^0 - v_f \sigma_{ij}^0 \varepsilon_{ij}^*) - \frac{1}{2} v_f \sigma_{ij} \varepsilon_{ij}^p. \quad (5)$$

where ε_{ij}^0 is applied strain, σ_{ij}^0 is the corresponding stress field if the elastic modulus of two phase are equal, $\sigma'_{ij}, \varepsilon'_{ij}$ are perturbations of the stress and strain fields, σ_{ij} is the stress filed in the grain induced by plastic deformation, and ε_{ij}^* is the fictitious eigenstrain introduced by the equivalent inclusion theory^[12]. The expression of ε_{ij}^* is as follows:

$$\varepsilon_{ij}^* = \left[C_{ijmn} + (1 - v_f) (C_{ijab} - C_{ijab}^*) S_{abmn} \right]^{-1} (C_{mnl}^* - C_{mnl}) \varepsilon_{kl}^0. \quad (6)$$

where C_{ijkl} is elastic modulus tensor, and S_{ijkl} is Eshelby's tensor^[12].

For isotropic materials, Eq. (5) can be rewritten as:

$$\Xi = \frac{1}{2} (2\bar{\mu} I_{ijkl}^1 + \bar{\lambda} I_{ijkl}^2) \varepsilon_{ij}^0 \varepsilon_{kl}^0 - \frac{1}{2} v_f \sigma_{ij} \varepsilon_{ij}^p. \quad (7)$$

where

$$I_{ijkl}^1 = \frac{1}{2} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}). \quad (8)$$

$$I_{ijkl}^2 = \delta_{ij} \delta_{kl}. \quad (9)$$

$$\bar{\mu} = \mu - \frac{2\nu_f \mu (\mu - \mu^*)}{A_1}. \quad (10)$$

$$\bar{\lambda} = \lambda - \nu_f \left[\frac{2\lambda (\mu - \mu^*)}{A_1} + 2(\mu + \lambda) \left(\frac{\lambda - \lambda^*}{A_1} - \frac{2A_2 (\mu - \mu^*)}{A_1 (A_1 + 3A_2)} - \frac{3A_2 (\lambda - \lambda^*)}{A_1 (A_1 + 3A_2)} \right) \right]. \quad (11)$$

$$A_1 = 2(1 - \nu_f)(\mu^* - \mu)S_1 + 2\mu. \quad (12)$$

$$A_2 = 2(1 - \nu_f)(\mu^* - \mu)S_2 + (1 - \nu_f)(\lambda^* - \lambda)S_1 + 3(1 - \nu_f)(\lambda^* - \lambda)S_2 + \lambda. \quad (13)$$

with $\mu, \lambda, \mu^*, \lambda^*$ being Lamé coefficients of grain boundary and grain phases, respectively, and ν being Poisson's ratio of grain boundary.

The total strain of the element can be expressed:

$$\varepsilon_{ij} = \varepsilon_{ij}^0 + \varepsilon_{ij}^D. \quad (14)$$

where ε_{ij}^D is volume average strain created by plastic deformation, and can be determined by equivalent inclusion theory^[12]:

$$\varepsilon_{ij}^D = \varepsilon_{ij}^p - \nu_f B_{ijkl} \varepsilon_{kl}^p = (I_{ijkl}^1 - \nu_f B_{ijkl}) \varepsilon_{kl}^p. \quad (15)$$

where:

$$B_{ijkl} = B_1 I_{ijkl}^1 + B_2 I_{ijkl}^2. \quad (16)$$

$$B_1 = \frac{2\mu^*}{C_1}. \quad (17)$$

$$B_2 = \frac{\lambda^*}{C_1} - \frac{2\mu^* C_2}{C_1 (C_1 + 3C_2)} - \frac{3\lambda^* C_2}{C_1 (C_1 + 3C_2)}. \quad (18)$$

$$C_1 = 2 \left[\mu^* + (1 - \nu_f)(\mu^* - \mu)(S_1 - 1) \right]. \quad (19)$$

$$C_2 = \lambda^* + 2(1 - \nu_f) \left[2S_2 (\mu^* - \mu) + (S_1 - 1)(\lambda^* - \lambda) + 3S_2 (\lambda^* - \lambda) \right]. \quad (20)$$

By taking equivalent inclusion theory^[12], the stress field inside the grain induced by plastic deformation is derived as:

$$\sigma_{ij} = D_{ijkl} \varepsilon_{kl}^p. \quad (21)$$

where:

$$D_{ijkl} = D_1 I_{ijkl}^1 + D_2 I_{ijkl}^2. \quad (22)$$

$$D_1 = 2(1 - \nu_f) \mu (S_1 - 1) B_1. \quad (23)$$

$$D_2 = (1 - \nu_f) \left\{ 2B_2 \mu (S_1 - 1) + (B_1 + 3B_2) \left[2\mu S_2 + \lambda (S_1 - 1) + 3\lambda S_2 \right] \right\}. \quad (24)$$

Substitution of Eqs.(14), (15),(21) into Eq.(7), we have:

$$\Xi = \frac{1}{2} \left(2\bar{\mu} I_{ijkl}^1 + \bar{\lambda} I_{ijkl}^2 \right) \left[\varepsilon_{ij} - \left(I_{ijmn}^1 - \nu_f B_{ijmn} \right) \varepsilon_{mn}^p \right] \left[\varepsilon_{kl} - \left(I_{klmn}^1 - \nu_f B_{klmn} \right) \varepsilon_{mn}^p \right] - \frac{1}{2} \nu_f D_{ijkl} \varepsilon_{ij}^p \varepsilon_{kl}^p. \quad (25)$$

The energy dissipation in unit volume can be expressed as:

$$\Phi = (1 - \nu_f) \sigma_{ij}^c \dot{\epsilon}_{ij}^p \quad (26)$$

where σ_{ij}^c satisfies the yield condition of Eq.(4).

Substitution of Eqs.(25), (26) into Eqs.(2), (3) respectively gives:

$$\dot{\sigma}_{ij} = (2\bar{\mu}I_{ijkl}^1 + \bar{\lambda}I_{ijkl}^2) \left[\dot{\epsilon}_{kl} - (I_{klmn}^1 - \nu_f B_{klmn}) \dot{\epsilon}_{mn}^p \right] = \bar{C}_{ijkl} \left[\dot{\epsilon}_{kl} - (I_{klmn}^1 - \nu_f B_{klmn}) \dot{\epsilon}_{mn}^p \right] \quad (27)$$

$$\sigma_{ij}^c = \frac{\left[(I_{ijmn}^1 - \nu_f B_{ijmn}) \sigma_{mn} + \nu_f D_{ijmn} \epsilon_{mn}^p \right]}{1 - \nu_f} \quad (28)$$

The criterion for loading can be written in the form:

$$f(\sigma_{ij}^c) = 0 \quad \frac{\partial f}{\partial \sigma_{ij}^c} \cdot \dot{\sigma}_{ij}^c > 0 \quad (29)$$

Substitution of Eq.(28) into Eq.(27), and using Eq.(29), then we have:

$$\frac{\partial f}{\partial \sigma_{ij}^c} \left\{ (I_{ijkl}^1 - \nu_f B_{ijkl}) \bar{C}_{klmn} \dot{\epsilon}_{mn} + \left[\nu_f D_{ijmn} - (I_{ijkl}^1 - \nu_f B_{ijkl}) \bar{C}_{klab} (I_{abmn}^1 - \nu_f B_{abmn}) \right] \dot{\epsilon}_{mn}^p \right\} = 0 \quad (30)$$

Using Prandtl-Reuss flow rule^[13], the plastic strain rate can be written as:

$$\dot{\epsilon}_{mn}^p = \dot{\lambda} \frac{\partial f}{\partial \sigma_{mn}^c} \quad (31)$$

Substitution of Eq. (31) into Eq. (30) gives:

$$\dot{\lambda} = \Lambda_{mn}^m \dot{\epsilon}_{mn} \quad (32)$$

where:

$$\Lambda_{mn}^m = \frac{\frac{\partial f}{\partial \sigma_{ij}^c} (I_{ijkl}^1 - \nu_f B_{ijkl}) \bar{C}_{klmn}}{\frac{\partial f}{\partial \sigma_{ij}^c} \left[(I_{ijkl}^1 - \nu_f B_{ijkl}) \bar{C}_{klab} (I_{abmn}^1 - \nu_f B_{abmn}) - \nu_f D_{ijmn} \right] \frac{\partial f}{\partial \sigma_{mn}^c}} \quad (33)$$

Accordingly, Substitution of Eq. (32) into Eq.(27), and the incremental stress-strain relation can be described as:

$$\dot{\sigma}_{ij} = \bar{C}_{ijmn} \left(I_{mnkl}^1 - (I_{mnab}^1 - \nu_f B_{mnab}) \frac{\partial f}{\partial \sigma_{ab}^c} \Lambda_{kl}^m \right) \dot{\epsilon}_{kl} \quad (34)$$

Results

The developed model was applied to pure copper subjected to uniaxial tension. The stress-strain relation of pure Copper was investigated. The calculated parameters^[2] are: $\mu^* = 42.1\text{GPa}$, $\nu^* = 0.3$, $\mu = 25.26\text{GPa}$, $\nu = 0.33$. The applied macro strain rate is $\dot{\epsilon}^0 = 0.001\text{s}^{-1}$. The comparison between the predicted results and experimental data^[14, 15] is shown in Fig. 1. It is seen that they are in good agreement with each other.

The experiment results show that the stress-strain relation will take on a different phenomenon when the average grain size is the same. It may be provoked by the grain size distribution^[16]. So we will discuss the influence of grain distribution. The grain distributions^[17] are shown in Fig. 2. The effects of grain distribution on the stress strain relation are shown in Fig. 3. It is seen that the stress values are overestimated if grain distribution is not considered.

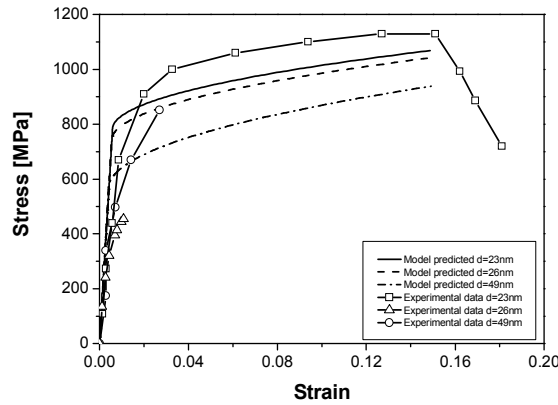


Fig. 1 Stress-strain relation predicted by present model in comparison with experimental data

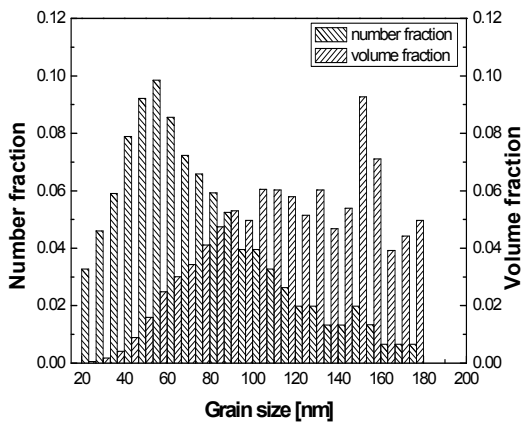


Fig. 2 Statistical distribution of grain size for Cu with average grain size of $\bar{d} = 75nm$ ^[17]

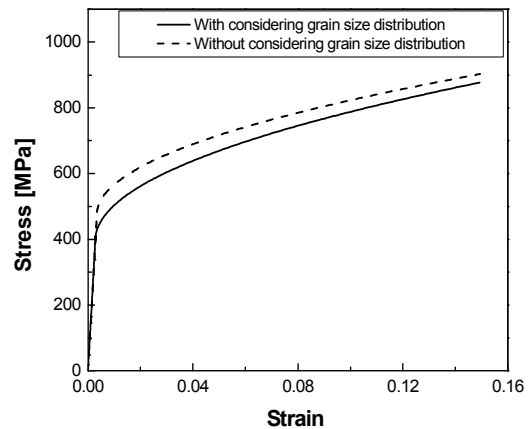


Fig.3 Stress-strain relation for average grain size of $\bar{d} = 75nm$.

The effects of parameter considering grain distribution are shown in Fig. 4 and 5. The same conclusions are taken on as without considering grain size distribution. The results show that the stress increases with the increasing parameter as $\beta \leq 1.0$, and it increases to the maximum at $\beta = 1.0$, when parameter β satisfies $\beta > 1.0$, the stress increases with the increasing parameter β .

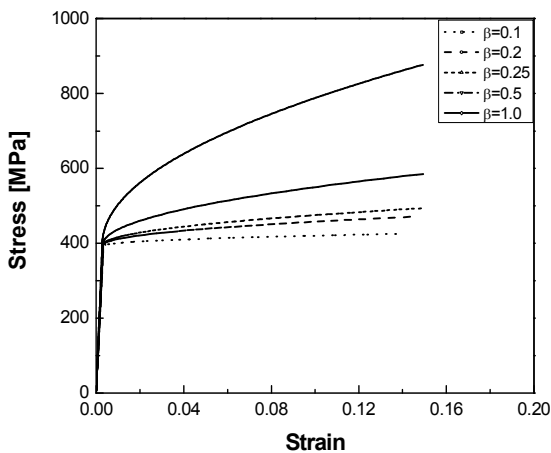


Fig. 4 Stress-strain relation for average grain size of $\bar{d} = 75nm$ $\beta \leq 1.0$

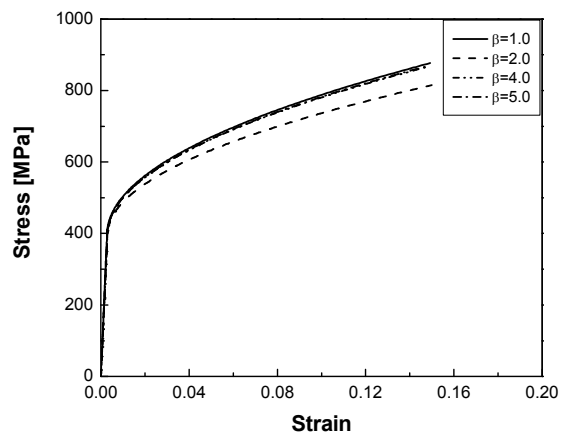


Fig. 5 Stress-strain relation for average grain size of $\bar{d} = 75nm$ $\beta \geq 1.0$

Conclusions

The constitutive relation of NC materials is developed from the micromechanics point of view. Then, the developed model is applied in pure copper subjected to uniaxial tension. Taking into account grain shape and statistical distribution of grain sizes, the stress-strain relation has been obtained. The results derived from the model are compared with the experimental data in literature, and show that they are in good agreement with each other. The stress is relative small considering grain distribution. The grain shape has influence on the stress-strain relation without considering gain size distribution. Stress increases with the increasing parameter as $\beta \leq 1.0$, but decreases as $\beta > 1.0$. When grain sizes distribution are considered, stress increases with parameter β , and arrives at the maximum as β is 1.0.

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