https://doi.org/10.1016/j.msea.2017.07.012

TITLE

Micromechanical modeling for mechanical properties of gradient-nanotwinned metals with a composite microstructure

Kai Wu[a], Xiang Guo[b, c], Haihui Ruan[d] and Linli Zhu[a, *]

[a] Department of Engineering Mechanics, and Key Laboratory of Soft Machines and Smart Devices of Zhejiang Province, Zhejiang University, Hangzhou 310027, Zhejiang Province, China

[b] School of Mechanical Engineering, Tianjin University, Tianjin 300072, China

[c] Tianjin Key Laboratory of Nonlinear Dynamics and Control, Tianjin 300072, China

[d] Department of Mechanical Engineering, The Hong Kong Polytechnic University, Hong Kong, China

[*] Corresponding author. E-mail address: llzhu@zju.edu.cn (Linli Zhu).

Abstract

Nanotwinned metals with a gradient microstructure have attracted a great deal of attention due to their excellent mechanical performance of combining high strength and high ductility. In this work, a micromechanical model is developed to describe the stress-strain response of gradient-nanotwinned metals with a composite microstructure. The deformation mechanisms originated from bimodal grain size distribution in nanostructured materials and nanoscale twin lamellae in a grain are involved in derivation of flow stress. The contributions from the gradient distribution of microstructural size and the microcracks during plastic deformation are taken into account in simulating the mechanical properties such as the yield strength and ductility. Using the proposed model, we figure out the stress-strain relation of gradient nanostructured metals and analyze the quantitative relation between the mechanical properties and the geometrical/physical parameters related to the gradient-nanotwinned composite copper. Numerical results show that, the strength and ductility of the gradient-nanotwinned bimodal metals are both improved as twins spacing decreases. With the volume fraction of coarse-grained phase decreased, the strength is improved significantly accompanied by slight reduction of the ductility. In addition, the simulated results are in a good agreement with experimental results. The present work could be helpful to describe and predict the elastic-plastic deformation behavior of gradient nanostructured composite -metals.

Keywords: Nanotwins; Bimodal grain size distribution; Gradient nanostructures; Yield strength; Ductility; Micromechanical modeling; Flow stress.

1. Introduction

As suggested by the Hall-Petch relation, refining grains is a useful method to realize the strengthening of metals [1]. When the grain size falls into nanoscale regime, the volume ratio of grain boundary increases sharply and grain boundaries-mediated plasticity becomes the primary deformation mechanism. Experiments have shown that compared with coarse-grained metals, the nanostructured and ultrafine-grained metals possess superior mechanical strength [2-4]. However, nanostructured metals have no strain hardening with rapid stress concentration, resulting in a significant reduction in the ductility. Some other strengthening methods such as strain hardening, solid solution strengthening can also improve the strength but greatly weaken the plasticity properties of the metals [5-7]. Therefore, it is important to find an effective methodology to achieve both high strength and high ductility in metallic materials.

Ultrafine-grained metals with nanoscale twins embedded in individual grain have recently been synthesized, achieving a strength increase to conventional coarse-grained metals. Twin boundaries are a special kind of low energy state coherency, each side lattice of which presents symmetry. They are major obstacles to dislocations movement for strengthening the nanotwinned metals [8-10]. Studies have addressed that both strength and ductility of the nanotwinned metals are improved as the twin-boundary spacing shrinks to nanometer scale [11-13]. Although both the twin boundary and the grain boundary are the interface defects, there are some differences in the aspects of the dislocation nucleation, propagation, and slipping [14-16]. In the process of increasing stress, the dislocations at the grain boundary will continue to accumulate until the new dislocations are generated in adjacent grains, leading to microcracks appearing at the grain boundaries with maximum stress concentration. For the twin boundaries, the partial dislocations can slip along the twin boundaries, and the interactions between the dislocations and the twin boundaries can significantly increase the number of the dislocations piled-up along the twin boundaries and improve the plastic properties of the metals. Theoretical models have been developed to explain the effects of dislocation nucleation and motion on plastic deformations in nanotwinned metals [17-19]. The grain size, twin spacing, and twin density are the important factors affecting the strength and plasticity of metals [9, 20, 21]. MD simulations [22-25], mechanism-based modeling [18, 19, 26-28] and numerical investigations based on finite element methods [29-31] were carried out to explore the deformation mechanisms and mechanical properties in nanotwinned metals.

Embedding the coarse grains into nanograined matrix to form a bimodal nanostructured metal is also an effective method to achieve high strength and high ductility in metallic materials [32-34]. Zhang et al. changed the cryomilling time to obtain bimodal nanostructured metals consisting of coarse grains and nanograins [32]. This bimodal metal combines the strengthening from the nanograins along with the strain hardening capability provided by dislocation activity in the coarse grains. Due to the coarse grains in the matrix of nanograins can prevent the propagation of microcracks along the grain boundaries, more microcracks could be produced in the nanograined matrix phase, which is beneficial to the plasticity when maintaining the high strength in bimodal metals [33-35]. According to the plastic deformation mechanism of each phase in bimodal nanostructured metals, the micromechanical models and finite element methods were proposed to describe and predict the mechanical properties of bimodal nanostructured materials [36-41].

In recent years, experimental studies showed that through altering the uniform distribution of microstructures into the gradient distribution in nanostructured metallic materials, the yield strength is improved significantly while keeping a good capability of strain hardening [42]. These gradient nanostructured metals can be prepared through surface mechanical attrition treatment (SMAT) [43, 44] and surface mechanical grinding treatment [45, 46]. With these techniques, the sizes of microstructures are in the nanometer scale on the topmost surface layer and increase gradually with an increasing depth from the treated surface. The microstructures in gradient-nanostructured metals include nanograins, nanotwins, nanolamellae, as well as the composite nanostructures. The strengthening mechanisms from these nanoscaled microstructures and the hardening mechanism of gradient distribution of microstructures attribute to the good combination of high yield strength and high ductility in gradient-nanostructured metals [47-50]. For example, the plastic deformation process of the gradient nanograined metals is gradually transited from coarse grains to nanograins, leading to reducing the possibility of stress concentration between neighboring grains [51]. Gradient changes of microstructural size in nanostructured metals produce additional strain hardening, which comes from the more geometrically necessary dislocations (GNDs) during the plastic deformation process [52-54]. These GNDs interact with the other dislocations during deformation, resulting in increasing the dislocations storage capacity to enhance the hardening behaviors [55]. For the mechanical performance of gradient-nanostructured metallic metals, some theoretical studies have been addressed to analyze the relation between the mechanical properties such as the strength and ductility, and the gradient distribution of microstructural size [56-58].

Since the metallic materials play an important role in infrastructural and overall economic development [59, 60], and the good combination of formability, hardenability, and ultimate strength is often expected [61-63]. The gradient nanostructured metals possess the excellent mechanical properties such as high yield strength and good ductility, to meet the increasing demands for high-performance materials. Recently, the topologically controlled SMAT was applied to fabricate a gradient-nanotwinned copper with a bimodal microstructure, which performs the improved yield strength while keeping a good ductility [64]. Inspired by this experimental study, a micromechanical model combining the above three strengthening mechanisms is developed in this work to describe the mechanical properties of gradient-nanotwinned metallic materials with a bimodal distribution of microstructural size. The simulated stress-strain responses based on the proposed model agree well with the experimental data of gradient-nanotwinned composite copper. The proposed model is further applied to predict the strength and ductility of such gradient-nanotructured composite metals with various gradient function of microstructural size and with different parameters in microcrack distribution function. It is believed that the present results could be helpful to achieve the improved mechanical properties of the gradient-nanotwinned metals with the bimodal microstructures by optimizing the size and distribution of microstructures.

2. A setup of theoretical model

To simulate the gradient-nanotwinned metals with a bimodal grain size distribution, the starting point of the model is to figure out the constitutive framework. The gradient-nanotwinned bimodal metals can be regarded as a superposition of *N*-layers of nanotwinned metals with a bimodal grain size distribution as shown in Fig. 1. The microstructural size and volume fraction change gradually along the depth. When the number of layers *N* is large enough, the properties of the gradient-nanotwinned structure can be approximated to vary continuously between each layer. Since the gradient-nanotwinned composite metal plane prepared by SMAT process is a symmetrical structure, it is only needed to analyze half of the SMATed plane. To describe the overall mechanical properties of such gradient-nanotwinned composite materials, the stress-strain relation of each phase and each layer must be identified. Therefore, the mechanism-based plasticity model is adopted to describe the stress-strain response for each phase, and the micromechanical method is used to reveal and predict the mechanical properties of each layer of nanotwinned composite metals. Due to the distinct deformation mechanisms in the nanograined phase, coarse-grained phase, and the twin lamellae in the grains, it is necessary to present the elasto-plastic constitutive relation of each phase. In the gradient-nanotwinned metals with a bimodal microstructure, the total strain rate of each phase in the composite microstructure of each layer is composed of two parts: elastic strain rate and plastic strain rate:

$$\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}^{e} + \dot{\boldsymbol{\varepsilon}}^{p} . \tag{1}$$

The elastic strain rate is obtained from the stress rate in a linear elastic relation as:

$$\dot{\boldsymbol{\varepsilon}}^{e} = \mathbf{M} : \dot{\boldsymbol{\sigma}} , \tag{2}$$

where M is elastic modulus of elasticity. Plastic strain $\dot{\boldsymbol{\varepsilon}}^{p}$ can be expressed as

$$\dot{\boldsymbol{\varepsilon}}^{p} = (3\dot{\varepsilon}^{p} / 2\sigma_{e})\boldsymbol{\sigma}' , \tag{3}$$

in which

$$\dot{\varepsilon}^{p} = \dot{\varepsilon}(\sigma_{e} / \sigma_{filow})^{m_0} . \tag{4}$$

Here, m_0 is the rate related parameter. $\dot{\varepsilon} = (2\dot{\varepsilon}_{ij}^{'}\dot{\varepsilon}_{ij}^{'} / 3)^{1/2}$ is the equivalent strain, in which $\dot{\varepsilon}_{ij}^{'} = \dot{\varepsilon}_{ij} - \dot{\varepsilon}_{kk}\delta_{ij} / 3$. $\sigma_{e} = (\sigma_{ij}^{'}\sigma_{ij}^{'} / 2)^{1/2}$ is the von Mises stress, and $\sigma_{ij}^{'} = \sigma_{ij} - \sigma_{kk}\delta_{ij} / 3$. σ_{flow} represents the flow stress of each phase, which will be given in the next section as below.

2.1 Flow stress in constituent phases of nanotwinned composite

For the coarse-grained phase, the volume occupied by the grain boundary is small in the total volume of the materials. Therefore, the contribution of grain boundaries on the flow stress can be negligible compared with the crystal internal dislocations activity. Thereby, the flow stress of the coarse-grained phase can be expressed as

$$\sigma_{flow} = \sigma_0 + M\alpha\mu b\rho_I^{1/2} + \sigma_b \,, \tag{5}$$

where σ_0 is the lattice friction stress, M represents the Taylor constant, α the empirical constant, μ the shear modulus, and b the Burgers constant. ρ_{I} is the dislocation density in the crystal interior of grains, given by [65,66]

$$\frac{\partial \rho_I}{\partial \varepsilon^{\mathrm{p}}} = M\left(\frac{k}{d_G(z)} + k_1\rho_I^{1/2} - k_2\rho_I\right). \tag{6}$$

Here, $k = 1/b; k_1 = \psi / b; k_2 = k_{20}(\dot{\varepsilon}^{\mathrm{p}} / \dot{\varepsilon}_0)^{-1/\mathrm{n}_0}$, ψ is a proportionality factor, k_{20}, $\dot{\varepsilon}_0$ and n_0 are the constants. $\sigma_b = M\mu b N_b / d_G(z)$ is back stress, in which d_G is the grain size varying with the depth z, and N_b is the number of dislocations blocked at the grain boundaries, following the evolution of the law as:

$$\frac{dN_b}{d\varepsilon^p} = \frac{\zeta}{b}\left(1 - \frac{N_b}{N_0}\right), \tag{7}$$

where ε_p is a plastic strain, ζ and N_0 are the average distance of the slip zone and the maximum number of dislocations blocked at grain boundaries, respectively.

Since nanoscale twins exist in the nanograined phase, the effects of twin boundaries and grain boundaries should be taken into account in the mechanical performance. During the plastic deformation, the dislocations activities occur in the region of crystal interior, grain boundaries, and twin boundaries. Hence, the flow stress can be described by Taylor's expression as:

$$\sigma_{flow} = \sigma_0 + M\alpha\mu b(\rho_I + \rho_{GB} + \rho_{TB})^{1/2}, \tag{8}$$

where ρ_{GB} is the density of dislocations related to the grain boundaries, given as

$$\rho_{GB} = k^{GB}\eta^{GB}/b \,. \tag{9}$$

Here, $k^{GB} = 6d_{GBDPZ} / \phi^{GB} d_G(z)$. ρ_{TB} is the dislocation density related to the twin boundaries and expressed as [26, 28]

$$\rho_{TB}(z) = \frac{c_1^T}{d_G^2(z)} + \frac{c_2^T}{d_G(z) d_{TB}(z)} - \frac{c_3^T}{d_{TB}^2(z)}, \tag{10}$$

where d_{TB} is the twin spacing, and $c_i^T (i = 1, 2, 3)$ are the size-independent constants.

The work hardening of the material consists of the isotropic strain hardening from ρ_{I} and the dynamic strain hardening from the back stress. The back stress is mainly due to the movement of the dislocations at the grain boundary. During the plastic deformation in the nanograined phase, there are few dislocations blocked at the grain boundaries so that the back stress can be neglected. However, in the case of the bimodal grain size distribution, the grain boundaries of the nanograined phase will produce a large number of nano/microcracks during the deformation, leading to a sudden increase in the number of dislocations blocked at the grain boundaries. Therefore, the back stress effect induced by the nano/microcracks in the nanograined phase should be considered in the flow stress of nanograined phase, which is modified as:

$$\sigma_{flow} = \sigma_0 + M\alpha\mu b(\rho_I + \rho_{GB} + \rho_{TB})^{1/2} + \sigma_b^*. \tag{11}$$

Here, σ_b^* is back stress originated from the nano/microcracks [38, 41]. In addition, the nano/microcracks can also change the stress-strain state near the cracks. Using the microcracks-based equivalent medium method [67], the equivalent modulus of the nanocrystalline phase can be given as

$$E = E_0[1+16(1-v_0^2)\rho/3]^{-1}; G = G_0[1+8(1+v_0)\rho / 3(1-v_0 / 2)]^{-1}, \tag{12}$$

where E_0 is the elastic modulus, G_0 shear modulus, and υ_0 Poisson's ratio of nanograined phase. ρ is the density of microcracks generated during deformation, which can be expressed as the function of plastic strain $\rho = \rho_0 p(f_w) = \rho_0[1 - f_w(\varepsilon_p)]$. Here, ρ_0 is a reference density of nano/microcracks, and $f_w(\varepsilon_p) = \exp(-(\varepsilon_p / \varepsilon_0)^m)$ is Weibull distribution function with *m* the Weibull modulus.

2.2 Composite model

The modified mean field method is applied here for developing a theoretical framework to describe the plastic deformation of bimodal nanotwinned layers in the gradient-nanostructured metals. The Young's modulus and Poisson's ratio of the *i*-phase are expressed as follows

$$E_i^s = E_i[1 + \frac{E_i \varepsilon^{(i)}}{\sigma_{flow}^{(i)}}(\frac{\sigma_{11}^{(i)}}{\sigma_{flow}^{(i)}})^{m_0 - 1}]^{-1}, \quad \upsilon_i^s = \frac{1}{2} - (\frac{1}{2} - \upsilon_i \frac{E_i^s}{E_i}) \tag{13}$$

which i=0 represents the nanograined phase, i=1 represents coarse-grained phase. σ_{flow} is the flow stress of each phase presented above. The corresponding bulk modulus and shear modulus for each phase can be given by

$$k_i^s = \frac{E_i^s}{3(1 - 2\upsilon_i^s)}, \quad \mu_i^s = \frac{E_i^s}{2(1 + \upsilon_i^s)}. \tag{14}$$

According to the modified mean field approach for two-phase metals, the relation between total hydrostatic strain and partial strain is

$$\sigma_{kk}^{(0)} = 3\kappa_0(a_0 + a_2)\bar{\varepsilon}_{kk}, \quad \sigma_{ij}^{(0)'} = 2\mu_0^s\left[(b_0 + b_2)\bar{\varepsilon}_{ij}' - c_1 b_2 \varepsilon_{ij}^{p(1)}\right]$$

$$\varepsilon_{kk}^{(1)} = a_0 \bar{\varepsilon}_{kk}, \quad \varepsilon_{ij}^{(1)'} = b_0 \bar{\varepsilon}_{ij}' + c_0 b_1 \varepsilon_{ij}^{p(1)}, \tag{15}$$

Here, $c_i\,(i\text{=}0,1)$ is the volume fraction of ith phase. The relation between the total hydrostatic stress and the partial stress is

$$\sigma_{kk}^{(0)} = 3\kappa_0 (a_0 + a_2)\bar{\varepsilon}_{kk}, \quad \sigma_{ij}^{(0)'} = 2\mu_0^s \left[(b_0 + b_2)\bar{\varepsilon}_{ij}' - c_1 b_2 \varepsilon_{ij}^{p(1)} \right]$$

$$\sigma_{kk}^{(1)} = 3\kappa_0 a_1 \bar{\varepsilon}_{kk}, \quad \sigma_{ij}^{(1)'} = \frac{2\mu_0^s}{\beta_0^s} b_2 \left[\bar{\varepsilon}_{ij}' - (1 - c_0 \beta_0^s)\varepsilon_{ij}^{p(1)} \right], \tag{16}$$

where

$$a_0 = \frac{\kappa_0}{c_0 \alpha_0^s (\kappa_1 - \kappa_0) + \kappa_0}, \quad a_1 = \frac{\kappa_1}{c_0 \alpha_0^s (\kappa_1 - \kappa_0) + \kappa_0}, \quad a_2 = \frac{\alpha_0^s (\kappa_1 - \kappa_0)}{c_0 \alpha_0^s (\kappa_1 - \kappa_0) + \kappa_0}$$

$$b_0 = \frac{\mu_0^s}{c_0 \beta_0^s (\mu_1 - \mu_0^s) + \mu_0^s}, \quad b_1 = \frac{\beta_0^s \mu_1}{c_0 \beta_0^s (\mu_1 - \mu_0^s) + \mu_0^s}, \quad b_2 = \frac{\beta_0^s (\mu_1 - \mu_0^s)}{c_0 \beta_0^s (\mu_1 - \mu_0^s) + \mu_0^s}$$

$$\alpha_0^s = (1 + \upsilon_0^s) / 3(1 - \upsilon_0^s), \quad \beta_0^s = 2(4 - 5\upsilon_0^s) / 15(1 - \upsilon_o^s).$$

Finally, the relation between stress and strain is obtained:

$$\bar{\sigma}_{kk} = 3\kappa_0 \left[1 + c_1 (a_1 - a_0) \right] \bar{\varepsilon}_{kk}, \quad \bar{\sigma}_{ij}' = 2\mu_0^s \left\{ (1 + \frac{c_1 b_2}{\beta_0^s}) \bar{\varepsilon}_{ij}' - \frac{c_1 b_1}{\beta_0^s} \varepsilon_{ij}^{p(1)} \right\}. \tag{17}$$

Suppose that the gradient-nanostructured metals are subjected to uniaixal uniform strain during tensile testing, the rule of mixtures (ROMs) of Voigt model is applied to calculate the effective stress in gradient-nanostructured metals [58, 68]. Owing to the equal strain in each layer of structures, the total stress $\tilde{\sigma}_{xx}$ of gradient-nanotwinned bimodal metal plate can be written as

$$\tilde{\sigma}_{xx} = (\sum_{j=1}^{\mathrm{N_G}} {}_j\bar{\sigma}_{xx} H_j) / H, \tag{18}$$

where j denotes the jth layer, N_{G} is the number of layers. ${}_j\bar{\sigma}_{xx}$ is the stresses applied on jth layer which is given by Eq. (17). $H_j (= H / \mathrm{N_G})$ and H are the thickness of jth layer and the entire gradient-nanostructured metals, respectively.

2.3 Numerical framework of the model

Since the mechanical properties of gradient nanotwinned metals were measured by the uniaxial tensile testing, the axial loading conditions are applied to derive the stress-strain relation in each phase of the nanotwinned composite from Eqs. (1-4)[69]. The flow stresses in Eqs. (5) and (8) need to be substituted into Eq. (4). Here, the finite difference method is utilized to solve the differential equations in Eqs. (6) and (7) when we derive the flow stress in each phase. When the strain in each layer of the gradient structures applied, the stresses of each phase can be obtained as well as the effective stress of the composite microstructure from Eqs. (16-17), in which the corresponding elastic modulus can be calculated from Eqs. (13) and (14). Afterwards, substituting these effective stresses in each layer in Eq. (18), the overall stress of the gradient nanotwinned composite metals can be calculated.

Even though the nanotwinned metals have an essential anisotropy at the microscopic scale, the random orientation of crystals and nanotwins leads to the isotropic mechanical behavior in the macroscopic scale. Since the proposed model is applied to describe the mechanical properties of the bulk samples, it is reasonable to assume the isotropic mechanical performance of nanotwinned composite in each layer of gradient-nanotwinned metals.

3. Numerical results and discussion

We make use of the proposed model to simulate the mechanical properties of gradient-nanotwinned metals with bimodal microstructure. The material parameters used in all calculations are listed in Table 1. The existing experimental data of gradient-nanotwinned composite copper are provided to make a comparison with simulations [26, 64]. There are two sets of the gradient-nanotwinned coppers samples prepared by SMAT technique with the process time of 15 s and 30 s. The experimental results demonstrated that with the increase of the process time of SMAT, the percentage of nanotwinned region increases, and the twin spacing decreases [64]. With the decrease in the size of the twin lamellae, the strength and plasticity of the material are improved at the same time [64]. Fig. 2 shows the calculated results based on the proposed model and the experimental data. One can find that the model can describe the stress-strain relation of the gradient-nanotwinned metals with bimodal microstructures, and the theoretical results are in a good agreement with the experimental data of gradient-nanotwinned bimodal copper [64], including the yield strength, strain hardening, and the uniform elongation.

As described in the Section 2, the influence of microcracks is taken into account on the mechanical properties during the deformation, including the back stress effect caused by microcracks and the change of the stress/strain state of the microcracked-nanograined phase. Therefore, we examine the contribution of microcrack density in stress-strain relation of gradient-nanotwinned bimodal copper. Since the microcrack density is related to the parameters of reference density ρ_0 and the Weibull modulus *m*, Figs. 3a and 3b plot the stress-strain curves for different reference microcrack density and different Weibull modulus, respectively. It can be seen from the figures that, due to the microcracks only appearing during the plastic deformation, the reference microcrack density and Weibull modulus have no effect on the elastic property and yield strength of the material, but only on the failure strain and ultimate strength. With the increase of microcrack density and the decrease of Weibull modulus, the uniform elongation and ultimate strength are significantly reduced, as shown in Figs. 3c and 3d.

Since the microstructural sizes in gradient-nanotwinned bimodal metals are involved in the proposed constitutive model, we further analyze the effects of the size of the twin lamellae in the nanograined phase on the mechanical properties of this gradient-nanostructured copper. Suppose the twin spacing changes with the depth z as a function of $d_{TB} = 45 + \mathrm{B}exp(-z/2.0 \times 10^{-4})$nm, the corresponding stress-strain responses are shown in Fig. 4a. It can be noted that the yield strength of the material is improved and the ductility becomes better with the twin spacing reduced. Fig. 4b shows the yield strength and ultimate strength vary with the parameter *B* in the function of twin spacing. One can find that with the increase of *B*, the yield strength and ultimate strength are both reduced. Fig. 4c depicts the quantitative relation between the ductility and the parameter *B*. The ductility of the gradient-nanotwinned metals decreases with increasing the value of *B*. This is because with the increase in parameter *B*, the twin spacing in the gradient nanostructures becomes much larger, resulting in a decrease in material strength and toughness.

Due to the existence of two different grain size distributions in the gradient nanostructured metals with the bimodal microstructure, varying the volume fraction of each phase can change their mechanical properties. Therefore, we explore the influence of the gradient distribution of volume fraction of the constituent phases on the mechanical properties of the gradient-nanotwinned bimodal metals. Fig. 5a depicts the stress-strain curves with the volume fraction of coarse-grained phase following the gradient distribution function of $f_1 = Aexp(z/3.0 \times 10^{-3})$. It can be noticed that with the increase of the coarse-grained volume fraction, the strength of the gradient-nanotwinned bimodal metals turns weaker while the ductility is improved. Fig. 5b shows the quantitative relation between the yield strength and the parameter A in the function of the coarse grains volume fraction. It can be found that the volume fraction of the coarse-grained phase increases with the increase of A, leading to the strength of the material decreased. Fig. 5c further plots the ductility of the material varied with A. That is, with the increase of A, the uniform elongation of the material is enhanced slightly. Interestingly noted from Fig. 5 is that with a decrease in the volume fraction of coarse-grained phase a higher yield strength with good ductility can be achieved.

4. Conclusions

In summary, a micromechanical model is developed to analyze the size and volume fraction-dependent mechanical properties of gradient-nanotwinned metals with a bimodal microstructure. In the proposed model, the effects of the gradient distribution of microstructures, the bimodal grain size distribution, and the nano/microcrack on the mechanical performance are taken into account. The numerical results showed that the proposed model can describe the experimental results of the gradient-nanotwinned bimodal copper satisfactorily, and a good agreement between the simulations and experimental data is obtained. Moreover, we further analyze the influence of the parameters related to the microcracks density on the mechanical properties, and predict strength and ductility under different gradient distributions of volume fraction and various twin spacings in the gradient-nanotwinned bimodal metals. Our calculations demonstrate that the good combination of higher strength and good ductility can be achieved by reducing the twin spacing or decreasing the volume fraction of the coarse-grained phase in the gradient-nanotwinned metals with bimodal microstructures.

Acknowledgments

The authors gratefully acknowledge the support from the National Natural Science Foundation of China (Grant nos. 11472243, 11621062, 11372214), Doctoral Fund of Ministry of Education of China (20130101120175), the Early Career Scheme (ECS) of Hong Kong RGC (Grant no. 25200515) and the Departmental General Research Fund (G-UA2L) from the Hong Kong Polytechnic University.

References

[1] M.A. Meyers, A. Mishra, D.J. Benson, Mechanical properties of nanocrystalline materials, Prog. Mater. Sci. 51(4) (2006) 427-456.

[2] M. Dao, L. Lu, R.J. Asaro, J.T.M. De Hosson, E. Ma, Toward a quantitative understanding of mechanical behavior of nanocrystalline metals, Acta Mater. 55(12) (2007) 4041-4065.

[3] T. Zhu, J. Li, Ultra-strength materials , Prog. Mater. Sci. 55(7) (2010) 710-757.

[4] C. Suryanarayana, Mechanical behavior of emerging materials, Mater. Today 15 (11) (2012) 486-496.

[5] Y.T. Zhu, X.Z. Liao, Nanostructured metals: retaining ductility, Nat. Mater. 3(6) (2004) 351-352.

[6] R.O. Ritchie, The conflicts between strength and toughness, Nat. Mater. 10(11) (2011) 817-822.

[7] H.N. Kou, J. Lu, Y. Li, High-Strength and High-Ductility Nanostructured and Amorphous Metallic Materials, Adv. Mater. 26(31) (2014) 5518-5524.

[8] L. Lu, Y.F. Shen, X.H. Chen, L.H. Qian, K. Lu, Ultrahigh strength and high electrical conductivity in copper, Science 304(5669) (2004) 422-426.

[9] M. Dao, L. Lu, Y. Shen, S. Suresh, Strength, strain-rate sensitivity and ductility of copper with nanoscale twins, Acta Mater. 54(20) (2006) 5421-5432.

[10] L. Lu, K. Lu, Metallic materials with nano-scale twins, Acta Metall. Sin. 46(11) (2010) 1422-1427.

[11] L. Lu, X. Chen, X. Huang, K. Lu, Revealing the maximum strength in nano-twinned copper, Science 323(5914) (2009) 607-610.

[12] K. Lu, L. Lu, S. Suresh, Strengthening materials by engineering coherent internal boundaries at the nanoscale, Science 324 (2009) 349-352.

[13] X.Y. Li, Y.J. Wei, L. Lu, K. Lu, H.J. Gao, Dislocation nucleation governed softening and maximum strength in nano-twinned metals, Nature 464(7290) (2010) 877-880.

[14] R.J. Asaro, S. Suresh, Mechanistic models for the activation volume and rate sensitivity in metals with nanocrystalline grains and nano-scale twins, Acta Mater. 53(12) (2005) 3369-3382.

[15] P. Gu, M. Dao, R.J. Asaro, S. Suresh, A unified mechanistic model for size-dependent deformation in nanocrystalline and nanotwinned metals, Acta Mater. 59(18) (2011) 6861-6868.

[16] Y.M. Wang, F. Sansoz, T. LaGrange, R.T. Ott, J. Marian, T.W. Barbee, A.V. Hamza, Defective twin boundaries in nanotwinned metals, Nature Mater. 12(8) (2013) 697-702.

[17] Y.T. Zhu, X.L. Wu, X.Z. Liao, J. Narayan, L.J. Kecskes, S.N. Mathaudhu, Dislocation–twin interactions in nanocrystalline fcc metals, Acta Mater. 59(2) (2011) 812-821.

[18] Y.J. Wei, Scaling of maximum strength with grain size in nanotwinned fcc metals, Phys Rev B 83(13) (2011) 132104(1-4).

[19] P. Gu, M. Dao, S. Suresh, Analysis of size-dependent slip transfer and inter-twin flow stress in a nanotwinned fcc metal, Acta Mater. 67 (2014) 409-417.

[20] L.L. Zhu, X. Guo, H.H. Ruan, J. Lu, Prediction of mechanical properties in bimodal nanotwinned metals with a composite structure. Comp. Sci. Tech. 123 (2016) 222-231.

[21] X.Y. Li, M. Dao, C. Eherl, A.M. Hodge, H.J. Gao, Fracture, fatigue, and creep of nanotwinned metals, MRS Bulletin 41(4) (2016) 298-304.

[22] T. Zhu, J. Li, A. Samanta, H.G. Kim, S. Suresh, Interfacial plasticity governs

strain rate sensitivity and ductility in nanostructured metals, Proc. Natl. Acad. Sci. 104(9) (2007) 3031-3036.

[23] I. Shabib, R.E. Miller, Deformation characteristics and stress–strain response of nanotwinned copper via molecular dynamics simulation, Acta Mater. 57(15) (2009) 4364-4373.

[24] Z.S. You, X.Y. Li, L.G. Gui, Q.H. Lu, T. Zhu, H.J. Gao, L. Lu, Plastic anisotropy and associated deformation mechanisms in nanotwinned metals, Acta Mater. 61(1) (2013) 217-227.

[25] L.Q. Pei, C. Lu, X. Zhao, L. Zhang, K.Y. Cheng, G. Michal, K. Tieu, Brittle versus ductile behaviour of nanotwinned copper: A molecular dynamics study, Acta Mater. 89 (2015) 1-13.

[26] L.L. Zhu, H.H. Ruan, X.Y. Li, M. Dao, H.J. Gao, J. Lu, Modeling grain size dependent optimal twin spacing for achieving ultimate high strength and related high ductility in nanotwinned metals, Acta Mater. 59(14) (2011) 5544-5557.

[27] L.L. Zhu, X. Guo, J. Lu, Surface stress effects on the yield strength in nanotwinned fcc metallic nanowires, J. Appl. Mech. 81(10) (2014) 101002.

[28] L.L. Zhu, S.X. Qu, X. Guo, J. Lu, Analysis of the twin spacing and grain size effects on mechanical properties in hierarchically nanotwinned face-centered cubic metals based on a mechanism-based plasticity model, J. Mech. Phys. Solid. 76 (2015) 162-179.

[29] M. Dao, L. Lu, Y. Shen, S. Suresh, Strength, strain-rate sensitivity and ductility of copper with nanoscale twins, Acta Mater. 54(20) (2006) 5421-5432.

[30] A. Jerusalem, M. Dao, S. Suresh, R. Radovitzky, Three-dimensional model of strength and ductility of polycrystalline copper containing nanoscale twins, Acta Mater. 56(17) (2008) 4647-4657.

[31] H. Mirkhani, S.P. Joshi, Crystal plasticity of nanotwinned microstructures: A discrete twin approach for copper, Acta Mater. 59(14) (2011) 5603-5617.

[32] X. Zhang, H. Wang, R.O. Scattergood, J. Narayan, C.C. Koch, Modulated oscillatory hardening and dynamic recrystallization in cryomilled nanocrystalline Zn, Acta Mater. 50(16) (2002) 3995-4004.

[33] Y.M. Wang, M.W. Chen, F.H. Zhou, E. Ma, High tensile ductility in a nanostructured metal, Nature 419(6910) (2002) 912-915.

[34] Y.H. Zhao, T. Topping, J.F. Bingert, J.J. Thornton et al., High tensile ductility and strength in bulk nanostructured nickel, Adv. Mater. 20(16) (2008) 3028-3033.

[35] Z.H. Lee, V. Radmilovic, B. Ahn, E.J. Lavernia, S.R. Nutt, Tensile deformation and fracture mechanism of bulk bimodal ultrafine-grained Al-Mg alloy, Metall. Mater. Trans. A 41(4) (2010) 795-801.

[36] S. Berbenni, V. Favier, M. Berveiller, Impact of the grain size distribution on the yield stress of heterogeneous materials, Int. J. Plasticity 23(1) (2007) 114-142.

[37] S. Ramtani, G. Dirras, H.Q. Bui, A bimodal bulk ultra-fine-grained nickel: experimental and micromechanical investigations, Mech. Mater. 42(5) (2010) 522-536.

[38] L.L. Zhu, S.Q. Shi, K. Lu, J. Lu, A statistical model for predicting the mechanical properties of nanostructured metals with bimodal grain size distribution, Acta

Mater. 60(16) (2012) 5762-5772.

[39] X. Guo, R. Ji, G.J. Weng, L.L. Zhu, J. Lu, Micromechanical simulation of fracture behavior of bimodal nanostructured metals, Mater. Sci. Eng. A 618(2014) 479- 489.

[40] X. Guo, X.Y. Dai, G.J. Weng, L.L. Zhu, J. Lu, Numerical investigation of fracture behavior of nanostructured Cu with bimodal grain size distribution, Acta Mech. 225(4) (2014) 1093- 1106.

[41] L.L. Zhu, X. Guo, H.H. Ruan, Simulating Size and Volume Fraction-Dependent Strength and Ductility of Nanotwinned Composite Copper, J. Appl. Mech. 83(7) (2016) 071009.

[42] K. Lu, Making strong nanomaterials ductile with gradients, Science 345(6203) (2014) 1455-1456.

[43] N.R. Tao, K. Lu, Dynamic plastic deformation (DPD): A novel technique for synthesizing bulk nanostructured metals, J. Mater. Sci. Technol. 23 (6) (2007) 771-774.

[44] Y. S. Li, N. R.Tao, K. Lu, Microstructural evolution and nanostructure formation in copper during dynamic plastic deformation at cryogenic temperatures, Acta Mater. 56 (2) (2008) 230-241.

[45] A.Y.Chen, D.F.Li, J.B.Zhang, H.W.Song, J.Lu, Make nanostructured metal exceptionally tough by introducing non-localized fracture behaviors, Scripta Mater. 59(6) (2008) 579-582.

[46] H.L. Chan, H.H. Ruan, A.Y. Chen, J. Lu, Optimization of strain-rate to achieve

exceptional mechanical properties of 304 stainless steel using high speed ultrasonic SMAT, Acta Mater. 58 (15) (2010) 5086-5096.

[47] A.Y. Chen, H.H. Ruan, J. Wang, H.L. Chan, Q. Wang, Q. Li, J. Lu, The influence of strain rate on the microstructure transition of 304 stainless steel, Acta Mater. 59(9) (2011) 3697-3709.

[48] Y.J. Wei, Y.Q. Li, L.C. Zhu et al., Evading the strength–ductility trade-off dilemma in steel through gradient hierarchical nanotwins, Nature Comm. 5(4) (2014) 3580(1-8).

[49] H.T. Wang, N.R. Tao, K. Lu, Architectured surface layer with a gradient nanotwined structure in a Fe-Mn austenitic steel, Scripta Mater. 68(1) (2013) 22-27.

[50] X.L. Wu, M.X. Yang, F.P. Yuan, L. Chen, Y.T. Zhu, Combining gradient structure and TRIP effect to produce austenite stainless steel with high strength and ductility, Acta Mater. 112 (2016) 337-346.

[51] T.H. Fang, W.L. Li, N.R. Tao et al., Revealing extraordinary intrinsic tensile plasticity in gradient nano-grained copper, Science 331(6024) (2011) 1587-1590.

[52] G. Purcek, O. Saray, I. Karaman et al., High Strength and High Ductility of Ultrafine-Grained. Interstitial-Free Steel Produced by ECAE and Annealing, Metall. Mater. Trans. A 43(6) (2012) 1884-1894.

[53] H.W. Huang, Z.B. Wang, X.P. Yong et al., Enhancing torsion fatigue behaviour of a martensitic stainless steel by generating gradient nanograined layer via surface

mechanical grinding treatment, Mater. Sci. Tech. 29(10) (2013) 1200-1205.

[54] T.H. Fang, N.R. Tao, K. Lu, Tension-induced softening and hardening in gradient nanograined surface layer in copper, Scripta Mater. 77 (2014) 17-20.

[55] X.L. Wu, P. Jiang, L. Chen et al., Extraordinary strain hardening by gradient structure, Proc. Natl. Acad. Sci. 111(20) (2014) 7197-7201.

[56] J. Li, A.K. Soh, Modeling of the plastic deformation of nanostructured materials with grain size gradient, Int. J. Plasticity 39(4) (2012) 88-102.

[57] H.S. Liu, Jr. Mishnaevsky, Gradient ultrafine-grained titanium: Computational study of mechanical and damage behavior, Acta Mater. 71 (2014) 220-233.

[58] L.L. Zhu, H.H. Ruan, A.Y. Chen, X. Guo, J. Lu, Microstructures-based constitutive analysis of mechanical properties of gradient-nanostructured 304 stainless steels, Acta Mater. 128 (2017) 375-390.

[59] M. F. Ashby, Materials Section in Mechanical Design 2nd edn (Butterworth-Heinemann, 1999).

[60] Congressional Record, V. 148, Pt. 4, 11 April 2002 to 24 April 2002 (US Congress, Washington, D.C., 2006)

[61] G. Frommeyer, U. Brux, P. Neumann, Supra-ductile and high-strength manganese-TRIP/TWIP steels for high energy absorption purposes. ISIJ Int. 43(3) (2003) 438-446.

[62] B. C. De Cooman, K. G. Chin, J. K. Kim, High Mn TWIP steels for automotive applications. In: New Trends and Developments in Automotive System Engineering. (ed Chiaberge, M.) 101-128 (InTech, 2011).

[63] S. Allain, J. P. Chateau, O. Bouaziz, S. Migot, N. Guelton, Constitutive model of the TWIP effect in a polycrystalline high manganese content austenitic steel. Steel Res. 73 (6) (2002) 299-302.

[64] X.W. Liu, K. Wu, G. Wu, Y. Gao, L.L. Zhu, Y. Lu, J. Lu, High strength and high ductility copper obtained by topologically controlled planar heterogeneous structures, Scripta Mater. 124 (2016) 103-107.

[65] U.F. Kocks, H. Mecking, The physics and phenomenology of strain hardening, Prog. Mater. Sci. 48(3) (2003) 171-273.

[66] L. Capolungo, C. Jochum, M. Cherkaoui, J. Qu, Homogenization method for strength and inelastic behavior of nanocrystalline materials, Int. J. Plasticity 21(1) (2005) 67-82.

[67] M. Kachanov, Elastic solids with many cracks and related problems, Adv. Appl. Mech. 30 (1994) 259-445.

[68] L.L. Zhu, C.S. Wen, C.Y. Gao, X. Guo, J. Lu, A study of dynamic plasticity in austenite stainless steels with a gradient distribution of nanoscale twins, Scripta Mater. 133 (2017) 49-53.

[69] Huang, Y., Qu, S., Hwang, K.C., Li, M., Gao, H., 2004. A conventional theory of mechanism-based strain gradient plasticity. Int. J. Plasticity 20 (4-5) 753-782.

Table caption

Description, symbol, magnitude, and equation in which the different parameters of the models appear

Figure captions

Fig. 1. Schematic drawings of the gradient-nanotwinned metals with a bimodal microstructure separated into N layers. In each layer, a bimodal composite consists of the large-grained phase and the nanotwinned ultrafine/nanograined phase.

Fig. 2. Comparisons between the calculated stress and strain response and the experimental data [55] for the gradient-nanotwinned bimodal copper.

Fig. 3. Effects of reference microcrack density (a,c) and Weibull modulus (b,d) on stress-strain relation and mechanical properties of gradient-nanotwinned bimodal copper.

Fig. 4. Effects of gradient distribution of twin spacing on the strength and ductility of the gradient-nanotwinned bimodal copper. B is the parameter in the gradient function of twin spacing. The different value of B induces to the various gradient distribution of twin spacing.

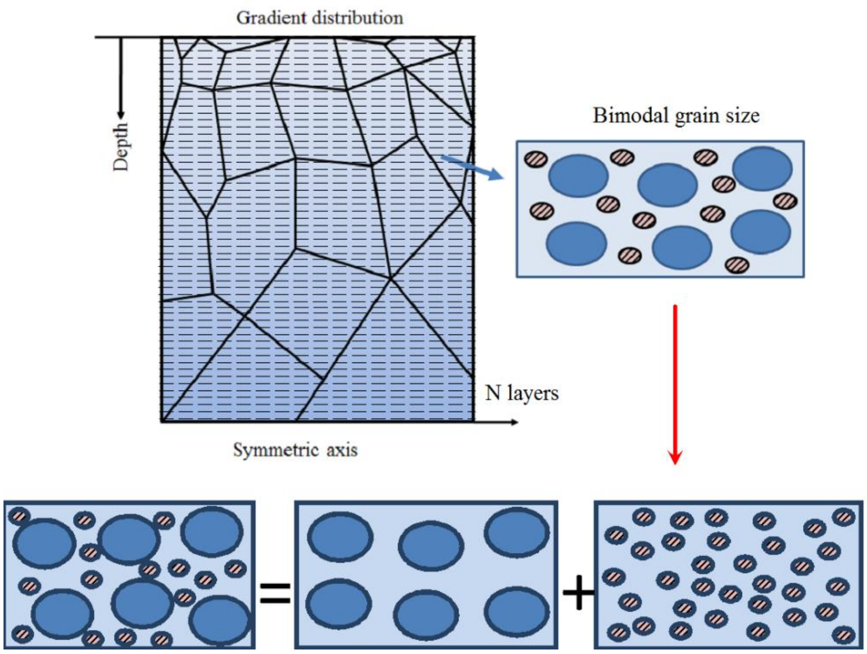
Fig. 5. Stress-strain relations under different gradient distributions of volume fraction

of coarse-grained phase (a), and the yield strength (b) and ductility (c) varying with the volume fraction relevant parameter *A*.

Table 1.

Description, symbol, magnitude, and equation in which the different parameters of the models appear

Parameter	Symbol	Ultrafine grain	Coarse grain
Elastic modulus	E	128 GPa	128 GPa
Shear modulus	μ	47.1 GPa	47.1 GPa
Poisson's ratio	υ	0.36	0.36
Burgers Vector	b	0.256 nm	0.256 nm
Taylor factor	M	1.732-3.06	1.732-3.06
Taylor constant	α	0.33	0.33
Dynamic recovery constant	n	21.25	21.25
Reference strain rate	$\dot{\varepsilon}_0$	1 s^{-1}	1 s^{-1}
Maximum number of dislocation	N_0	13	300
Reference density of nanomicrocracks	ρ_0	0.04	



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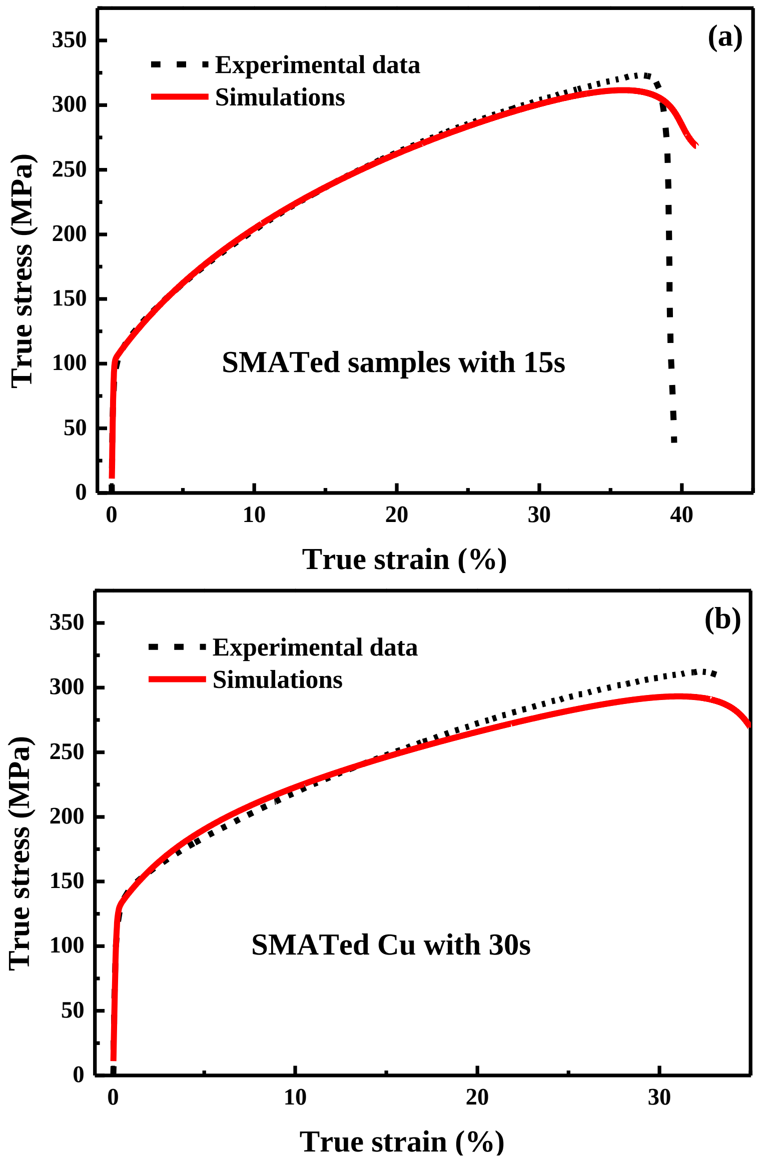
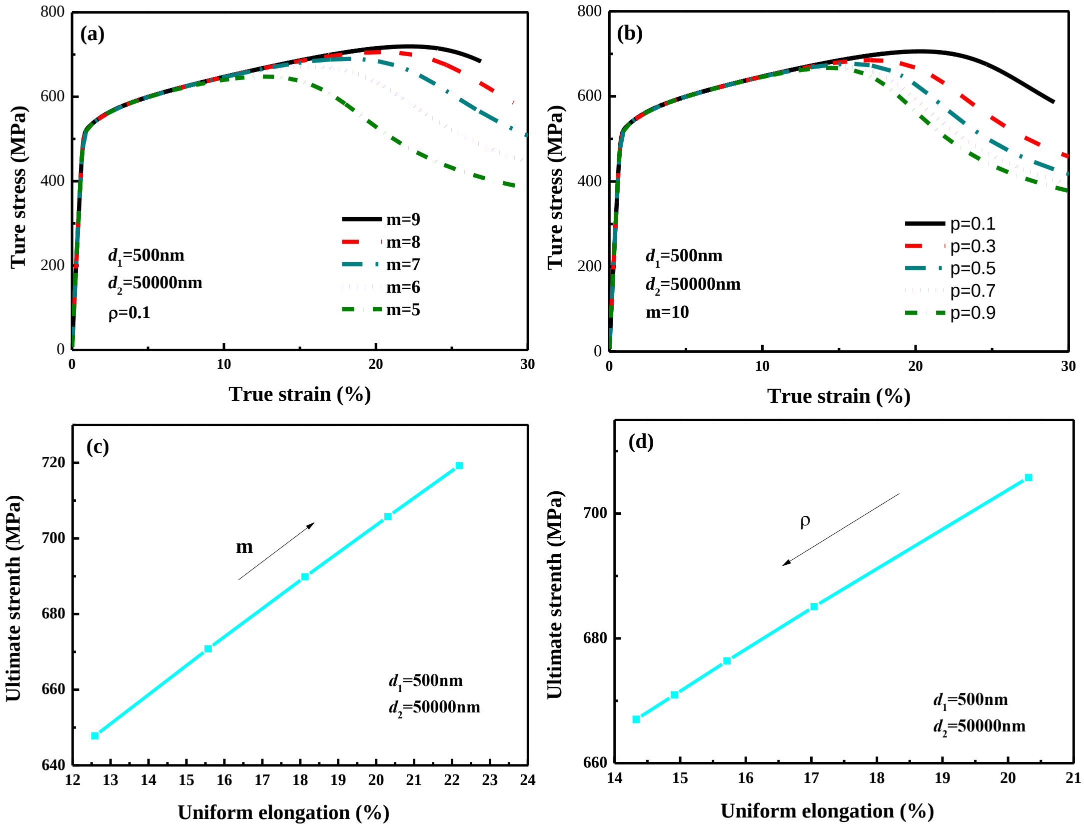


Fig. 2 Comparisons between the calculated stress and strain response and the experimental data [55] for the gradient-nanotwinned bimodal copper.



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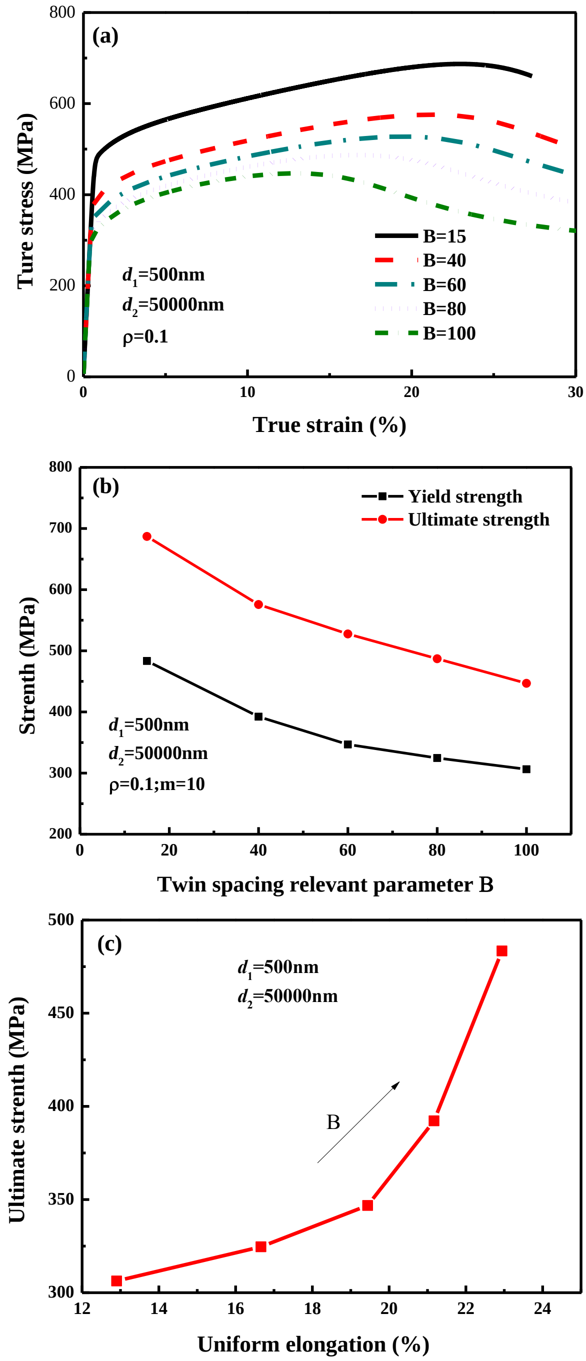


Fig. 4 Effects of gradient distribution of twin spacing on the strength and ductility of the gradient-nanotwinned bimodal copper. *B* is the parameter in the gradient function of twin spacing. The different value of *B* induces to the various gradient distribution of twin spacing.

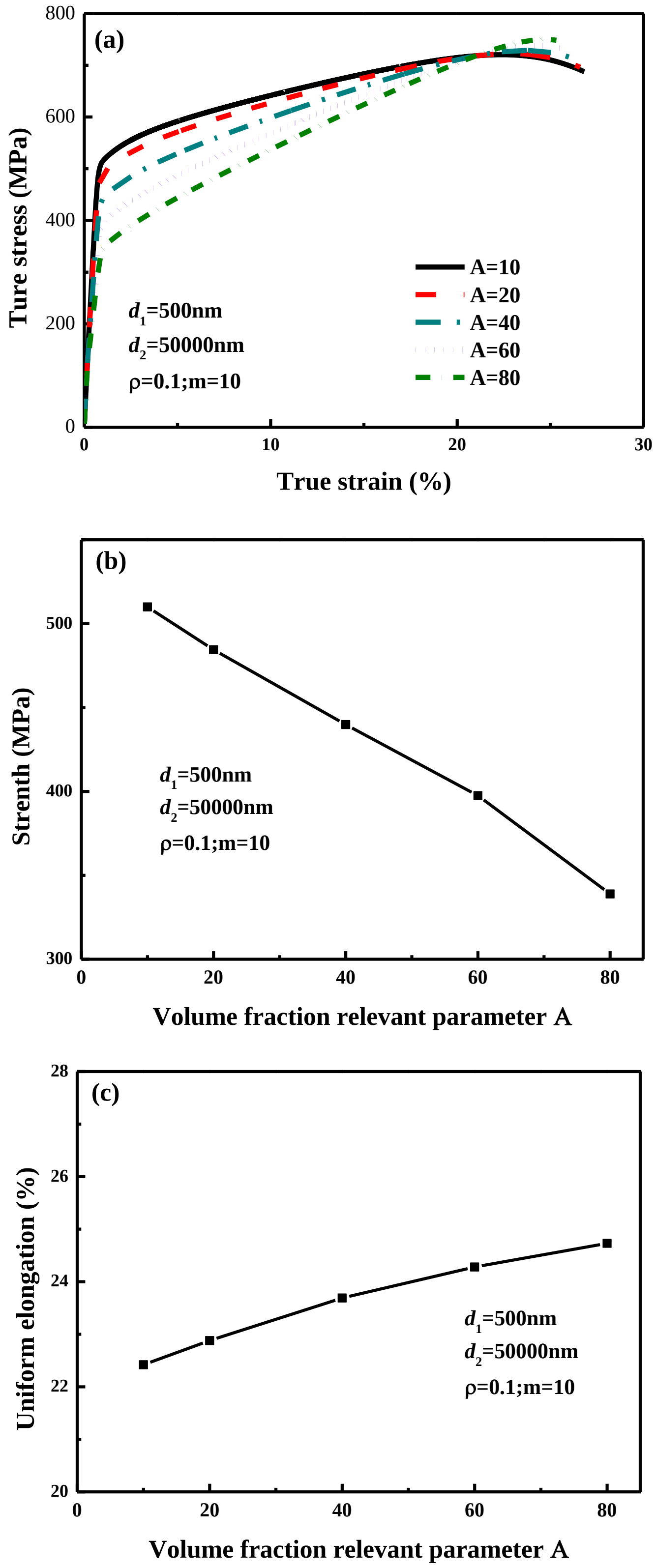


Fig. 5 Stress-strain relations under different gradient distributions of volume fraction of coarse-grained phase (a), and the yield strength (b) and ductility (c) varying with the volume fraction relevant parameter *A*.

TITLE

Micromechanical modeling for mechanical properties of gradient-nanotwinned metals with a composite microstructure

Kai Wu[a], Xiang Guo[b, c], Haihui Ruan[d] and Linli Zhu[a, *]

[a] Department of Engineering Mechanics, and Key Laboratory of Soft Machines and Smart Devices of Zhejiang Province, Zhejiang University, Hangzhou 310027, Zhejiang Province, China

[b] School of Mechanical Engineering, Tianjin University, Tianjin 300072, China

[c] Tianjin Key Laboratory of Nonlinear Dynamics and Control, Tianjin 300072, China

[d] Department of Mechanical Engineering, The Hong Kong Polytechnic University, Hong Kong, China

[*] Corresponding author. E-mail address: llzhu@zju.edu.cn (Linli Zhu).

Abstract

Nanotwinned metals with a gradient microstructure have attracted a great deal of attention due to their excellent mechanical performance of combining high strength and high ductility. In this work, a micromechanical model is developed to describe the stress-strain response of gradient-nanotwinned metals with a composite microstructure. The deformation mechanisms originated from bimodal grain size distribution in nanostructured materials and nanoscale twin lamellae in a grain are involved in derivation of flow stress. The contributions from the gradient distribution of microstructural size and the microcracks during plastic deformation are taken into account in simulating the mechanical properties such as the yield strength and ductility. Using the proposed model, we figure out the stress-strain relation of gradient nanostructured metals and analyze the quantitative relation between the mechanical properties and the geometrical/physical parameters related to the gradient-nanotwinned composite copper. Numerical results show that, the strength and ductility of the gradient-nanotwinned bimodal metals are both improved as twins spacing decreases. With the volume fraction of coarse-grained phase decreased, the strength is improved significantly accompanied by slight reduction of the ductility. In addition, the simulated results are in a good agreement with experimental results. The present work could be helpful to describe and predict the elastic-plastic deformation behavior of gradient nanostructured composite -metals.

Keywords: Nanotwins; Bimodal grain size distribution; Gradient nanostructures; Yield strength; Ductility; Micromechanical modeling; Flow stress.

1. Introduction

As suggested by the Hall-Petch relation, refining grains is a useful method to realize the strengthening of metals [1]. When the grain size falls into nanoscale regime, the volume ratio of grain boundary increases sharply and grain boundaries-mediated plasticity becomes the primary deformation mechanism. Experiments have shown that compared with coarse-grained metals, the nanostructured and ultrafine-grained metals possess superior mechanical strength [2-4]. However, nanostructured metals have no strain hardening with rapid stress concentration, resulting in a significant reduction in the ductility. Some other strengthening methods such as strain hardening, solid solution strengthening can also improve the strength but greatly weaken the plasticity properties of the metals [5-7]. Therefore, it is important to find an effective methodology to achieve both high strength and high ductility in metallic materials.

Ultrafine-grained metals with nanoscale twins embedded in individual grain have recently been synthesized, achieving a strength increase to conventional coarse-grained metals. Twin boundaries are a special kind of low energy state coherency, each side lattice of which presents symmetry. They are major obstacles to dislocations movement for strengthening the nanotwinned metals [8-10]. Studies have addressed that both strength and ductility of the nanotwinned metals are improved as the twin-boundary spacing shrinks to nanometer scale [11-13]. Although both the twin boundary and the grain boundary are the interface defects, there are some differences in the aspects of the dislocation nucleation, propagation, and slipping [14-16]. In the process of increasing stress, the dislocations at the grain boundary will continue to accumulate until the new dislocations are generated in adjacent grains, leading to microcracks appearing at the grain boundaries with maximum stress concentration. For the twin boundaries, the partial dislocations can slip along the twin boundaries, and the interactions between the dislocations and the twin boundaries can significantly increase the number of the dislocations piled-up along the twin boundaries and improve the plastic properties of the metals. Theoretical models have been developed to explain the effects of dislocation nucleation and motion on plastic deformations in nanotwinned metals [17-19]. The grain size, twin spacing, and twin density are the important factors affecting the strength and plasticity of metals [9, 20, 21]. MD simulations [22-25], mechanism-based modeling [18, 19, 26-28] and numerical investigations based on finite element methods [29-31] were carried out to explore the deformation mechanisms and mechanical properties in nanotwinned metals.

Embedding the coarse grains into nanograined matrix to form a bimodal nanostructured metal is also an effective method to achieve high strength and high ductility in metallic materials [32-34]. Zhang et al. changed the cryomilling time to obtain bimodal nanostructured metals consisting of coarse grains and nanograins [32]. This bimodal metal combines the strengthening from the nanograins along with the strain hardening capability provided by dislocation activity in the coarse grains. Due to the coarse grains in the matrix of nanograins can prevent the propagation of microcracks along the grain boundaries, more microcracks could be produced in the nanograined matrix phase, which is beneficial to the plasticity when maintaining the high strength in bimodal metals [33-35]. According to the plastic deformation mechanism of each phase in bimodal nanostructured metals, the micromechanical models and finite element methods were proposed to describe and predict the mechanical properties of bimodal nanostructured materials [36-41].

In recent years, experimental studies showed that through altering the uniform distribution of microstructures into the gradient distribution in nanostructured metallic materials, the yield strength is improved significantly while keeping a good capability of strain hardening [42]. **These gradient nanostructured metals can be prepared through surface mechanical attrition treatment (SMAT) [43, 44] and surface mechanical grinding treatment [45, 46]. With these techniques, the sizes of microstructures are in the nanometer scale on the topmost surface layer and increase gradually with an increasing depth from the treated surface.** The microstructures in gradient-nanostructured metals include nanograins, nanotwins, nanolamellae, as well as the composite nanostructures. The strengthening mechanisms from these nanoscaled microstructures and the hardening mechanism of gradient distribution of microstructures attribute to the good combination of high yield strength and high ductility in gradient-nanostructured metals [47-50]. For example, the plastic deformation process of the gradient nanograined metals is gradually transited from coarse grains to nanograins, leading to reducing the possibility of stress concentration between neighboring grains [51]. Gradient changes of microstructural size in nanostructured metals produce additional strain hardening, which comes from the more geometrically necessary dislocations (GNDs) during the plastic deformation process [52-54]. These GNDs interact with the other dislocations during deformation, resulting in increasing the dislocations storage capacity to enhance the hardening behaviors [55]. For the mechanical performance of gradient-nanostructured metallic metals, some theoretical studies have been addressed to analyze the relation between the mechanical properties such as the strength and ductility, and the gradient distribution of microstructural size [56-58].

Since the metallic materials play an important role in infrastructural and overall economic development [59, 60], and the good combination of formability, hardenability, and ultimate strength is often expected [61-63]. The gradient nanostructured metals possess the excellent mechanical properties such as high yield strength and good ductility, to meet the increasing demands for high-performance materials. Recently, the topologically controlled SMAT was applied to fabricate a gradient-nanotwinned copper with a bimodal microstructure, which performs the improved yield strength while keeping a good ductility [64]. Inspired by this experimental study, a micromechanical model combining the above three strengthening mechanisms is developed in this work to describe the mechanical properties of gradient-nanotwinned metallic materials with a bimodal distribution of microstructural size. The simulated stress-strain responses based on the proposed model agree well with the experimental data of gradient-nanotwinned composite copper. The proposed model is further applied to predict the strength and ductility of such gradient-nanotructured composite metals with various gradient function of microstructural size and with different parameters in microcrack distribution function. It is believed that the present results could be helpful to achieve the improved mechanical properties of the gradient-nanotwinned metals with the bimodal microstructures by optimizing the size and distribution of microstructures.

2. A setup of theoretical model

To simulate the gradient-nanotwinned metals with a bimodal grain size distribution, the starting point of the model is to figure out the constitutive framework. The gradient-nanotwinned bimodal metals can be regarded as a superposition of N-layers of nanotwinned metals with a bimodal grain size distribution as shown in Fig. 1. The microstructural size and volume fraction change gradually along the depth. When the number of layers N is large enough, the properties of the gradient-nanotwinned structure can be approximated to vary continuously between each layer. Since the gradient-nanotwinned composite metal plane prepared by SMAT process is a symmetrical structure, it is only needed to analyze half of the SMATed plane. To describe the overall mechanical properties of such gradient-nanotwinned composite materials, the stress-strain relation of each phase and each layer must be identified. Therefore, the mechanism-based plasticity model is adopted to describe the stress-strain response for each phase, and the micromechanical method is used to reveal and predict the mechanical properties of each layer of nanotwinned composite metals. Due to the distinct deformation mechanisms in the nanograined phase, coarse-grained phase, and the twin lamellae in the grains, it is necessary to present the elasto-plastic constitutive relation of each phase. In the gradient-nanotwinned metals with a bimodal microstructure, the total strain rate of each phase in the composite microstructure of each layer is composed of two parts: elastic strain rate and plastic strain rate:

$$\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}^e + \dot{\boldsymbol{\varepsilon}}^p . \tag{1}$$

The elastic strain rate is obtained from the stress rate in a linear elastic relation as:

$$\dot{\boldsymbol{\varepsilon}}^e = \mathbf{M} : \dot{\boldsymbol{\sigma}} , \tag{2}$$

where M is elastic modulus of elasticity. Plastic strain $\dot{\boldsymbol{\varepsilon}}^p$ can be expressed as

$$\dot{\boldsymbol{\varepsilon}}^p = (3\dot{\varepsilon}^p / 2\sigma_e)\boldsymbol{\sigma}' , \tag{3}$$

in which

$$\dot{\varepsilon}^p = \dot{\varepsilon}(\sigma_e / \sigma_{filow})^{m_0} . \tag{4}$$

Here, m_0 is the rate related parameter. $\dot{\varepsilon} = (2\dot{\varepsilon}_{ij}^{'}\dot{\varepsilon}_{ij}^{'} / 3)^{1/2}$ is the equivalent strain, in which $\dot{\varepsilon}_{ij}^{'} = \dot{\varepsilon}_{ij} - \dot{\varepsilon}_{kk}\delta_{ij} / 3$. $\sigma_e = (\sigma_{ij}^{'}\sigma_{ij}^{'} / 2)^{1/2}$ is the von Mises stress, and $\sigma_{ij}^{'} = \sigma_{ij} - \sigma_{kk}\delta_{ij} / 3$. σ_{flow} represents the flow stress of each phase, which will be given in the next section as below.

2.1 Flow stress in constituent phases of nanotwinned composite

For the coarse-grained phase, the volume occupied by the grain boundary is small in the total volume of the materials. Therefore, the contribution of grain boundaries on the flow stress can be negligible compared with the crystal internal dislocations activity. Thereby, the flow stress of the coarse-grained phase can be expressed as

$$\sigma_{flow} = \sigma_0 + M\alpha\mu b \rho_I^{1/2} + \sigma_b \, , \tag{5}$$

where σ_0 is the lattice friction stress, M represents the Taylor constant, α the empirical constant, μ the shear modulus, and b the Burgers constant. ρ_{I} is the dislocation density in the crystal interior of grains, given by [65,66]

$$\frac{\partial \rho_I}{\partial \varepsilon^{\mathrm{p}}} = M\left(\frac{k}{d_G(z)} + k_1 \rho_I^{1/2} - k_2 \rho_I\right). \tag{6}$$

Here, $k = 1/b; k_1 = \psi / b; k_2 = k_{20}(\dot{\varepsilon}^{\mathrm{p}} / \dot{\varepsilon}_0)^{-1/\mathrm{n}_0}$, ψ is a proportionality factor, k_{20}, $\dot{\varepsilon}_0$ and n_0 are the constants. $\sigma_b = M\mu b N_b / d_G(z)$ is back stress, in which d_G is the grain size varying with the depth z, and N_b is the number of dislocations blocked at the grain boundaries, following the evolution of the law as:

$$\frac{dN_b}{d\varepsilon^p} = \frac{\zeta}{b}\left(1 - \frac{N_b}{N_0}\right), \tag{7}$$

where ε_p is a plastic strain, ζ and N_0 are the average distance of the slip zone and the maximum number of dislocations blocked at grain boundaries, respectively.

Since nanoscale twins exist in the nanograined phase, the effects of twin boundaries and grain boundaries should be taken into account in the mechanical performance. During the plastic deformation, the dislocations activities occur in the region of crystal interior, grain boundaries, and twin boundaries. Hence, the flow stress can be described by Taylor's expression as:

$$\sigma_{flow} = \sigma_0 + M\alpha\mu b(\rho_I + \rho_{GB} + \rho_{TB})^{1/2}, \tag{8}$$

where ρ_{GB} is the density of dislocations related to the grain boundaries, given as

$$\rho_{GB} = k^{GB}\eta^{GB}/b \, . \tag{9}$$

Here, $k^{GB} = 6d_{GBDPZ} / \phi^{GB} d_G(z)$. ρ_{TB} is the dislocation density related to the twin boundaries and expressed as [26, 28]

$$\rho_{TB}(z) = \frac{c_1^T}{d_G^2(z)} + \frac{c_2^T}{d_G(z) d_{TB}(z)} - \frac{c_3^T}{d_{TB}^2(z)}, \tag{10}$$

where d_{TB} is the twin spacing, and $c_i^T (i = 1, 2, 3)$ are the size-independent constants.

The work hardening of the material consists of the isotropic strain hardening from ρ_I and the dynamic strain hardening from the back stress. The back stress is mainly due to the movement of the dislocations at the grain boundary. During the plastic deformation in the nanograined phase, there are few dislocations blocked at the grain boundaries so that the back stress can be neglected. However, in the case of the bimodal grain size distribution, the grain boundaries of the nanograined phase will produce a large number of nano/microcracks during the deformation, leading to a sudden increase in the number of dislocations blocked at the grain boundaries. Therefore, the back stress effect induced by the nano/microcracks in the nanograined phase should be considered in the flow stress of nanograined phase, which is modified as:

$$\sigma_{flow} = \sigma_0 + M\alpha\mu b(\rho_I + \rho_{GB} + \rho_{TB})^{1/2} + \sigma_b^*. \tag{11}$$

Here, σ_b^* is back stress originated from the nano/microcracks [38, 41]. In addition, the nano/microcracks can also change the stress-strain state near the cracks. Using the microcracks-based equivalent medium method [67], the equivalent modulus of the nanocrystalline phase can be given as

$$E = E_0[1 + 16(1 - v_0^2)\rho/3]^{-1}; G = G_0[1 + 8(1 + v_0)\rho / 3(1 - v_0 / 2)]^{-1}, \tag{12}$$

where E_0 is the elastic modulus, G_0 shear modulus, and υ_0 Poisson's ratio of nanograined phase. ρ is the density of microcracks generated during deformation, which can be expressed as the function of plastic strain $\rho = \rho_0 p(f_w) = \rho_0[1 - f_w(\varepsilon_p)]$. Here, ρ_0 is a reference density of nano/microcracks, and $f_w(\varepsilon_p) = \exp(-(\varepsilon_p / \varepsilon_0)^m)$ is Weibull distribution function with *m* the Weibull modulus.

2.2 Composite model

The modified mean field method is applied here for developing a theoretical framework to describe the plastic deformation of bimodal nanotwinned layers in the gradient-nanostructured metals. The Young's modulus and Poisson's ratio of the *i*-phase are expressed as follows

$$E_i^s = E_i[1 + \frac{E_i\varepsilon^{(i)}}{\sigma_{flow}^{(i)}}(\frac{\sigma_{11}^{(i)}}{\sigma_{flow}^{(i)}})^{m_0-1}]^{-1}, \quad \upsilon_i^s = \frac{1}{2} - (\frac{1}{2} - \upsilon_i\frac{E_i^s}{E_i}) \tag{13}$$

which i=0 represents the nanograined phase, i=1 represents coarse-grained phase. σ_{flow} is the flow stress of each phase presented above. The corresponding bulk modulus and shear modulus for each phase can be given by

$$k_i^s = \frac{E_i^s}{3(1-2\upsilon_i^s)}, \quad \mu_i^s = \frac{E_i^s}{2(1+\upsilon_i^s)}. \tag{14}$$

According to the modified mean field approach for two-phase metals, the relation between total hydrostatic strain and partial strain is

$$\sigma_{kk}^{(0)} = 3\kappa_0(a_0 + a_2)\bar{\varepsilon}_{kk}, \quad \sigma_{ij}^{(0)'} = 2\mu_0^s\left[(b_0 + b_2)\bar{\varepsilon}_{ij}' - c_1 b_2 \varepsilon_{ij}^{p(1)}\right]$$

$$\varepsilon_{kk}^{(1)} = a_0\bar{\varepsilon}_{kk}, \quad \varepsilon_{ij}^{(1)'} = b_0\bar{\varepsilon}_{ij}' + c_0 b_1 \varepsilon_{ij}^{p(1)}, \tag{15}$$

Here, $c_i\,(i\text{=}0,1)$ is the volume fraction of *i*th phase. The relation between the total hydrostatic stress and the partial stress is

$$\sigma_{kk}^{(0)} = 3\kappa_0(a_0 + a_2)\bar{\varepsilon}_{kk}, \quad \sigma_{ij}^{(0)'} = 2\mu_0^s\left[(b_0 + b_2)\bar{\varepsilon}_{ij}' - c_1 b_2 \varepsilon_{ij}^{p(1)}\right]$$

$$\sigma_{kk}^{(1)} = 3\kappa_0 a_1 \bar{\varepsilon}_{kk}, \quad \sigma_{ij}^{(1)'} = \frac{2\mu_0^s}{\beta_0^s} b_2\left[\bar{\varepsilon}_{ij}' - (1 - c_0\beta_0^s)\varepsilon_{ij}^{p(1)}\right], \tag{16}$$

where

$$a_0 = \frac{\kappa_0}{c_0\alpha_0^s(\kappa_1 - \kappa_0) + \kappa_0}, \quad a_1 = \frac{\kappa_1}{c_0\alpha_0^s(\kappa_1 - \kappa_0) + \kappa_0}, \quad a_2 = \frac{\alpha_0^s(\kappa_1 - \kappa_0)}{c_0\alpha_0^s(\kappa_1 - \kappa_0) + \kappa_0}$$

$$b_0 = \frac{\mu_0^s}{c_0\beta_0^s(\mu_1 - \mu_0^s) + \mu_0^s}, \quad b_1 = \frac{\beta_0^s\mu_1}{c_0\beta_0^s(\mu_1 - \mu_0^s) + \mu_0^s}, \quad b_2 = \frac{\beta_0^s(\mu_1 - \mu_0^s)}{c_0\beta_0^s(\mu_1 - \mu_0^s) + \mu_0^s}$$

$$\alpha_0^s = (1 + \upsilon_0^s)/3(1 - \upsilon_0^s), \quad \beta_0^s = 2(4 - 5\upsilon_0^s)/15(1 - \upsilon_o^s).$$

Finally, the relation between stress and strain is obtained:

$$\bar{\sigma}_{kk} = 3\kappa_0\left[1 + c_1(a_1 - a_0)\right]\bar{\varepsilon}_{kk}, \quad \bar{\sigma}_{ij}' = 2\mu_0^s\left\{(1 + \frac{c_1 b_2}{\beta_0^s})\bar{\varepsilon}_{ij}' - \frac{c_1 b_1}{\beta_0^s}\varepsilon_{ij}^{p(1)}\right\}. \tag{17}$$

Suppose that the gradient-nanostructured metals are subjected to uniaixal uniform strain during tensile testing, the rule of mixtures (ROMs) of Voigt model is applied to calculate the effective stress in gradient-nanostructured metals [58, 68]. Owing to the equal strain in each layer of structures, the total stress $\tilde{\sigma}_{xx}$ of gradient-nanotwinned bimodal metal plate can be written as

$$\tilde{\sigma}_{xx} = \left(\sum_{j=1}^{N_G} {}_j\bar{\sigma}_{xx} H_j\right)/H, \tag{18}$$

where j denotes the jth layer, N_G is the number of layers. ${}_j\bar{\sigma}_{xx}$ is the stresses applied on jth layer which is given by Eq. (17). $H_j(=H/N_G)$ and H are the thickness of jth layer and the entire gradient-nanostructured metals, respectively.

2.3 Numerical framework of the model

Since the mechanical properties of gradient nanotwinned metals were measured by the uniaxial tensile testing, the axial loading conditions are applied to derive the stress-strain relation in each phase of the nanotwinned composite from Eqs. (1-4)[69]. The flow stresses in Eqs. (5) and (8) need to be substituted into Eq. (4). Here, the finite difference method is utilized to solve the differential equations in Eqs. (6) and (7) when we derive the flow stress in each phase. When the strain in each layer of the gradient structures applied, the stresses of each phase can be obtained as well as the effective stress of the composite microstructure from Eqs. (16-17), in which the corresponding elastic modulus can be calculated from Eqs. (13) and (14). Afterwards, substituting these effective stresses in each layer in Eq. (18), the overall stress of the gradient nanotwinned composite metals can be calculated.

Even though the nanotwinned metals have an essential anisotropy at the microscopic scale, the random orientation of crystals and nanotwins leads to the isotropic mechanical behavior in the macroscopic scale. Since the proposed model is applied to describe the mechanical properties of the bulk samples, it is reasonable to assume the isotropic mechanical performance of nanotwinned composite in each layer of gradient-nanotwinned metals.

3. Numerical results and discussion

We make use of the proposed model to simulate the mechanical properties of gradient-nanotwinned metals with bimodal microstructure. The material parameters used in all calculations are listed in Table 1. The existing experimental data of gradient-nanotwinned composite copper are provided to make a comparison with simulations [26, 64]. There are two sets of the gradient-nanotwinned coppers samples prepared by SMAT technique with the process time of 15 s and 30 s. The experimental results demonstrated that with the increase of the process time of SMAT, the percentage of nanotwinned region increases, and the twin spacing decreases [64]. With the decrease in the size of the twin lamellae, the strength and plasticity of the material are improved at the same time [64]. Fig. 2 shows the calculated results based on the proposed model and the experimental data. One can find that the model can describe the stress-strain relation of the gradient-nanotwinned metals with bimodal microstructures, and the theoretical results are in a good agreement with the experimental data of gradient-nanotwinned bimodal copper [64], including the yield strength, strain hardening, and the uniform elongation.

As described in the Section 2, the influence of microcracks is taken into account on the mechanical properties during the deformation, including the back stress effect caused by microcracks and the change of the stress/strain state of the microcracked-nanograined phase. Therefore, we examine the contribution of microcrack density in stress-strain relation of gradient-nanotwinned bimodal copper. Since the microcrack density is related to the parameters of reference density ρ_0 and the Weibull modulus *m*, Figs. 3a and 3b plot the stress-strain curves for different reference microcrack density and different Weibull modulus, respectively. It can be seen from the figures that, due to the microcracks only appearing during the plastic deformation, the reference microcrack density and Weibull modulus have no effect on the elastic property and yield strength of the material, but only on the failure strain and ultimate strength. With the increase of microcrack density and the decrease of Weibull modulus, the uniform elongation and ultimate strength are significantly reduced, as shown in Figs. 3c and 3d.

Since the microstructural sizes in gradient-nanotwinned bimodal metals are involved in the proposed constitutive model, we further analyze the effects of the size of the twin lamellae in the nanograined phase on the mechanical properties of this gradient-nanostructured copper. Suppose the twin spacing changes with the depth *z* as a function of $d_{TB} = 45 + \mathrm{B}exp(-z/2.0 \times 10^{-4})$nm, the corresponding stress-strain responses are shown in Fig. 4a. It can be noted that the yield strength of the material is improved and the ductility becomes better with the twin spacing reduced. Fig. 4b shows the yield strength and ultimate strength vary with the parameter *B* in the function of twin spacing. One can find that with the increase of *B*, the yield strength and ultimate strength are both reduced. Fig. 4c depicts the quantitative relation between the ductility and the parameter *B*. The ductility of the gradient-nanotwinned metals decreases with increasing the value of *B*. This is because with the increase in parameter *B*, the twin spacing in the gradient nanostructures becomes much larger, resulting in a decrease in material strength and toughness.

Due to the existence of two different grain size distributions in the gradient nanostructured metals with the bimodal microstructure, varying the volume fraction of each phase can change their mechanical properties. Therefore, we explore the influence of the gradient distribution of volume fraction of the constituent phases on the mechanical properties of the gradient-nanotwinned bimodal metals. Fig. 5a depicts the stress-strain curves with the volume fraction of coarse-grained phase following the gradient distribution function of $f_1 = Aexp(z/3.0 \times 10^{-3})$. It can be noticed that with the increase of the coarse-grained volume fraction, the strength of the gradient-nanotwinned bimodal metals turns weaker while the ductility is improved. Fig. 5b shows the quantitative relation between the yield strength and the parameter *A* in the function of the coarse grains volume fraction. It can be found that the volume fraction of the coarse-grained phase increases with the increase of *A*, leading to the strength of the material decreased. Fig. 5c further plots the ductility of the material varied with *A*. That is, with the increase of *A*, the uniform elongation of the material is enhanced slightly. Interestingly noted from Fig. 5 is that with a decrease in the volume fraction of coarse-grained phase a higher yield strength with good ductility can be achieved.

4. Conclusions

In summary, a micromechanical model is developed to analyze the size and volume fraction-dependent mechanical properties of gradient-nanotwinned metals with a bimodal microstructure. In the proposed model, the effects of the gradient distribution of microstructures, the bimodal grain size distribution, and the nano/microcrack on the mechanical performance are taken into account. The numerical results showed that the proposed model can describe the experimental results of the gradient-nanotwinned bimodal copper satisfactorily, and a good agreement between the simulations and experimental data is obtained. Moreover, we further analyze the influence of the parameters related to the microcracks density on the mechanical properties, and predict strength and ductility under different gradient distributions of volume fraction and various twin spacings in the gradient-nanotwinned bimodal metals. Our calculations demonstrate that the good combination of higher strength and good ductility can be achieved by reducing the twin spacing or decreasing the volume fraction of the coarse-grained phase in the gradient-nanotwinned metals with bimodal microstructures.

Acknowledgments

The authors gratefully acknowledge the support from the National Natural Science Foundation of China (Grant nos. 11472243, 11621062, 11372214), Doctoral Fund of Ministry of Education of China (20130101120175), the Early Career Scheme (ECS) of Hong Kong RGC (Grant no. 25200515) and the Departmental General Research Fund (G-UA2L) from the Hong Kong Polytechnic University.

References

[1] M.A. Meyers, A. Mishra, D.J. Benson, Mechanical properties of nanocrystalline materials, Prog. Mater. Sci. 51(4) (2006) 427-456.

[2] M. Dao, L. Lu, R.J. Asaro, J.T.M. De Hosson, E. Ma, Toward a quantitative understanding of mechanical behavior of nanocrystalline metals, Acta Mater.

55(12) (2007) 4041-4065.

[3] T. Zhu, J. Li, Ultra-strength materials , Prog. Mater. Sci. 55(7) (2010) 710-757.

[4] C. Suryanarayana, Mechanical behavior of emerging materials, Mater. Today 15 (11) (2012) 486-496.

[5] Y.T. Zhu, X.Z. Liao, Nanostructured metals: retaining ductility, Nat. Mater. 3(6) (2004) 351-352.

[6] R.O. Ritchie, The conflicts between strength and toughness, Nat. Mater. 10(11) (2011) 817-822.

[7] H.N. Kou, J. Lu, Y. Li, High-Strength and High-Ductility Nanostructured and Amorphous Metallic Materials, Adv. Mater. 26(31) (2014) 5518-5524.

[8] L. Lu, Y.F. Shen, X.H. Chen, L.H. Qian, K. Lu, Ultrahigh strength and high electrical conductivity in copper, Science 304(5669) (2004) 422-426.

[9] M. Dao, L. Lu, Y. Shen, S. Suresh, Strength, strain-rate sensitivity and ductility of copper with nanoscale twins, Acta Mater. 54(20) (2006) 5421-5432.

[10] L. Lu, K. Lu, Metallic materials with nano-scale twins, Acta Metall. Sin. 46(11) (2010) 1422-1427.

[11] L. Lu, X. Chen, X. Huang, K. Lu, Revealing the maximum strength in nano-twinned copper, Science 323(5914) (2009) 607-610.

[12] K. Lu, L. Lu, S. Suresh, Strengthening materials by engineering coherent internal boundaries at the nanoscale, Science 324 (2009) 349-352.

[13] X.Y. Li, Y.J. Wei, L. Lu, K. Lu, H.J. Gao, Dislocation nucleation governed softening and maximum strength in nano-twinned metals, Nature 464(7290)

(2010) 877-880.

[14] R.J. Asaro, S. Suresh, Mechanistic models for the activation volume and rate sensitivity in metals with nanocrystalline grains and nano-scale twins, Acta Mater. 53(12) (2005) 3369-3382.

[15] P. Gu, M. Dao, R.J. Asaro, S. Suresh, A unified mechanistic model for size-dependent deformation in nanocrystalline and nanotwinned metals, Acta Mater. 59(18) (2011) 6861-6868.

[16] Y.M. Wang, F. Sansoz, T. LaGrange, R.T. Ott, J. Marian, T.W. Barbee, A.V. Hamza, Defective twin boundaries in nanotwinned metals, Nature Mater. 12(8) (2013) 697-702.

[17] Y.T. Zhu, X.L. Wu, X.Z. Liao, J. Narayan, L.J. Kecskes, S.N. Mathaudhu, Dislocation–twin interactions in nanocrystalline fcc metals, Acta Mater. 59(2) (2011) 812-821.

[18] Y.J. Wei, Scaling of maximum strength with grain size in nanotwinned fcc metals, Phys Rev B 83(13) (2011) 132104(1-4).

[19] P. Gu, M. Dao, S. Suresh, Analysis of size-dependent slip transfer and inter-twin flow stress in a nanotwinned fcc metal, Acta Mater. 67 (2014) 409-417.

[20] L.L. Zhu, X. Guo, H.H. Ruan, J. Lu, Prediction of mechanical properties in bimodal nanotwinned metals with a composite structure. Comp. Sci. Tech. 123 (2016) 222-231.

[21] X.Y. Li, M. Dao, C. Eherl, A.M. Hodge, H.J. Gao, Fracture, fatigue, and creep of nanotwinned metals, MRS Bulletin 41(4) (2016) 298-304.

[22] T. Zhu, J. Li, A. Samanta, H.G. Kim, S. Suresh, Interfacial plasticity governs strain rate sensitivity and ductility in nanostructured metals, Proc. Natl. Acad. Sci. 104(9) (2007) 3031-3036.

[23] I. Shabib, R.E. Miller, Deformation characteristics and stress–strain response of nanotwinned copper via molecular dynamics simulation, Acta Mater. 57(15) (2009) 4364-4373.

[24] Z.S. You, X.Y. Li, L.G. Gui, Q.H. Lu, T. Zhu, H.J. Gao, L. Lu, Plastic anisotropy and associated deformation mechanisms in nanotwinned metals, Acta Mater. 61(1) (2013) 217-227.

[25] L.Q. Pei, C. Lu, X. Zhao, L. Zhang, K.Y. Cheng, G. Michal, K. Tieu, Brittle versus ductile behaviour of nanotwinned copper: A molecular dynamics study, Acta Mater. 89 (2015) 1-13.

[26] L.L. Zhu, H.H. Ruan, X.Y. Li, M. Dao, H.J. Gao, J. Lu, Modeling grain size dependent optimal twin spacing for achieving ultimate high strength and related high ductility in nanotwinned metals, Acta Mater. 59(14) (2011) 5544-5557.

[27] L.L. Zhu, X. Guo, J. Lu, Surface stress effects on the yield strength in nanotwinned fcc metallic nanowires, J. Appl. Mech. 81(10) (2014) 101002.

[28] L.L. Zhu, S.X. Qu, X. Guo, J. Lu, Analysis of the twin spacing and grain size effects on mechanical properties in hierarchically nanotwinned face-centered cubic metals based on a mechanism-based plasticity model, J. Mech. Phys. Solid. 76 (2015) 162-179.

[29] M. Dao, L. Lu, Y. Shen, S. Suresh, Strength, strain-rate sensitivity and ductility

of copper with nanoscale twins, Acta Mater. 54(20) (2006) 5421-5432.

[30] A. Jerusalem, M. Dao, S. Suresh, R. Radovitzky, Three-dimensional model of strength and ductility of polycrystalline copper containing nanoscale twins, Acta Mater. 56(17) (2008) 4647-4657.

[31] H. Mirkhani, S.P. Joshi, Crystal plasticity of nanotwinned microstructures: A discrete twin approach for copper, Acta Mater. 59(14) (2011) 5603-5617.

[32] X. Zhang, H. Wang, R.O. Scattergood, J. Narayan, C.C. Koch, Modulated oscillatory hardening and dynamic recrystallization in cryomilled nanocrystalline Zn, Acta Mater. 50(16) (2002) 3995-4004.

[33] Y.M. Wang, M.W. Chen, F.H. Zhou, E. Ma, High tensile ductility in a nanostructured metal, Nature 419(6910) (2002) 912-915.

[34] Y.H. Zhao, T. Topping, J.F. Bingert, J.J. Thornton et al., High tensile ductility and strength in bulk nanostructured nickel, Adv. Mater. 20(16) (2008) 3028-3033.

[35] Z.H. Lee, V. Radmilovic, B. Ahn, E.J. Lavernia, S.R. Nutt, Tensile deformation and fracture mechanism of bulk bimodal ultrafine-grained Al-Mg alloy, Metall. Mater. Trans. A 41(4) (2010) 795-801.

[36] S. Berbenni, V. Favier, M. Berveiller, Impact of the grain size distribution on the yield stress of heterogeneous materials, Int. J. Plasticity 23(1) (2007) 114-142.

[37] S. Ramtani, G. Dirras, H.Q. Bui, A bimodal bulk ultra-fine-grained nickel: experimental and micromechanical investigations, Mech. Mater. 42(5) (2010) 522-536.

[38] L.L. Zhu, S.Q. Shi, K. Lu, J. Lu, A statistical model for predicting the mechanical

properties of nanostructured metals with bimodal grain size distribution, Acta Mater. 60(16) (2012) 5762-5772.

[39] X. Guo, R. Ji, G.J. Weng, L.L. Zhu, J. Lu, Micromechanical simulation of fracture behavior of bimodal nanostructured metals, Mater. Sci. Eng. A 618(2014) 479- 489.

[40] X. Guo, X.Y. Dai, G.J. Weng, L.L. Zhu, J. Lu, Numerical investigation of fracture behavior of nanostructured Cu with bimodal grain size distribution, Acta Mech. 225(4) (2014) 1093- 1106.

[41] L.L. Zhu, X. Guo, H.H. Ruan, Simulating Size and Volume Fraction-Dependent Strength and Ductility of Nanotwinned Composite Copper, J. Appl. Mech. 83(7) (2016) 071009.

[42] K. Lu, Making strong nanomaterials ductile with gradients, Science 345(6203) (2014) 1455-1456.

[43] N.R. Tao, K. Lu, Dynamic plastic deformation (DPD): A novel technique for synthesizing bulk nanostructured metals, J. Mater. Sci. Technol. 23 (6) (2007) 771-774.

[44] Y. S. Li, N. R.Tao, K. Lu, Microstructural evolution and nanostructure formation in copper during dynamic plastic deformation at cryogenic temperatures, Acta Mater. 56 (2) (2008) 230-241.

[45] A.Y.Chen, D.F.Li, J.B.Zhang, H.W.Song, J.Lu, Make nanostructured metal exceptionally tough by introducing non-localized fracture behaviors, Scripta Mater. 59(6) (2008) 579-582.

[46] H.L. Chan, H.H. Ruan, A.Y. Chen, J. Lu, Optimization of strain-rate to achieve exceptional mechanical properties of 304 stainless steel using high speed ultrasonic SMAT, Acta Mater. 58 (15) (2010) 5086-5096.

[47] A.Y. Chen, H.H. Ruan, J. Wang, H.L. Chan, Q. Wang, Q. Li, J. Lu, The influence of strain rate on the microstructure transition of 304 stainless steel, Acta Mater. 59(9) (2011) 3697-3709.

[48] Y.J. Wei, Y.Q. Li, L.C. Zhu et al., Evading the strength–ductility trade-off dilemma in steel through gradient hierarchical nanotwins, Nature Comm. 5(4) (2014) 3580(1-8).

[49] H.T. Wang, N.R. Tao, K. Lu, Architectured surface layer with a gradient nanotwined structure in a Fe-Mn austenitic steel, Scripta Mater. 68(1) (2013) 22-27.

[50] X.L. Wu, M.X. Yang, F.P. Yuan, L. Chen, Y.T. Zhu, Combining gradient structure and TRIP effect to produce austenite stainless steel with high strength and ductility, Acta Mater. 112 (2016) 337-346.

[51] T.H. Fang, W.L. Li, N.R. Tao et al., Revealing extraordinary intrinsic tensile plasticity in gradient nano-grained copper, Science 331(6024) (2011) 1587-1590.

[52] G. Purcek, O. Saray, I. Karaman et al., High Strength and High Ductility of Ultrafine-Grained. Interstitial-Free Steel Produced by ECAE and Annealing, Metall. Mater. Trans. A 43(6) (2012) 1884-1894.

[53] H.W. Huang, Z.B. Wang, X.P. Yong et al., Enhancing torsion fatigue behaviour of

a martensitic stainless steel by generating gradient nanograined layer via surface mechanical grinding treatment, Mater. Sci. Tech. 29(10) (2013) 1200-1205.

[54] T.H. Fang, N.R. Tao, K. Lu, Tension-induced softening and hardening in gradient nanograined surface layer in copper, Scripta Mater. 77 (2014) 17-20.

[55] X.L. Wu, P. Jiang, L. Chen et al., Extraordinary strain hardening by gradient structure, Proc. Natl. Acad. Sci. 111(20) (2014) 7197-7201.

[56] J. Li, A.K. Soh, Modeling of the plastic deformation of nanostructured materials with grain size gradient, Int. J. Plasticity 39(4) (2012) 88-102.

[57] H.S. Liu, Jr. Mishnaevsky, Gradient ultrafine-grained titanium: Computational study of mechanical and damage behavior, Acta Mater. 71 (2014) 220-233.

[58] L.L. Zhu, H.H. Ruan, A.Y. Chen, X. Guo, J. Lu, Microstructures-based constitutive analysis of mechanical properties of gradient-nanostructured 304 stainless steels, Acta Mater. 128 (2017) 375-390.

[59] M. F. Ashby, Materials Section in Mechanical Design 2nd edn (Butterworth-Heinemann, 1999).

[60] Congressional Record, V. 148, Pt. 4, 11 April 2002 to 24 April 2002 (US Congress, Washington, D.C., 2006)

[61] G. Frommeyer, U. Brux, P. Neumann, Supra-ductile and high-strength manganese-TRIP/TWIP steels for high energy absorption purposes. ISIJ Int. 43(3) (2003) 438-446.

[62] B. C. De Cooman, K. G. Chin, J. K. Kim, High Mn TWIP steels for automotive applications. In: New Trends and Developments in Automotive

System Engineering. (ed Chiaberge, M.) 101-128 (InTech, 2011).

[63] S. Allain, J. P. Chateau, O. Bouaziz, S. Migot, N. Guelton, Constitutive model of the TWIP effect in a polycrystalline high manganese content austenitic steel. Steel Res. 73 (6) (2002) 299-302.

[64] X.W. Liu, K. Wu, G. Wu, Y. Gao, L.L. Zhu, Y. Lu, J. Lu, High strength and high ductility copper obtained by topologically controlled planar heterogeneous structures, Scripta Mater. 124 (2016) 103-107.

[65] U.F. Kocks, H. Mecking, The physics and phenomenology of strain hardening, Prog. Mater. Sci. 48(3) (2003) 171-273.

[66] L. Capolungo, C. Jochum, M. Cherkaoui, J. Qu, Homogenization method for strength and inelastic behavior of nanocrystalline materials, Int. J. Plasticity 21(1) (2005) 67-82.

[67] M. Kachanov, Elastic solids with many cracks and related problems, Adv. Appl. Mech. 30 (1994) 259-445.

[68] L.L. Zhu, C.S. Wen, C.Y. Gao, X. Guo, J. Lu, A study of dynamic plasticity in austenite stainless steels with a gradient distribution of nanoscale twins, Scripta Mater. 133 (2017) 49-53.

[69] Huang, Y., Qu, S., Hwang, K.C., Li, M., Gao, H., 2004. A conventional theory of mechanism-based strain gradient plasticity. Int. J. Plasticity 20 (4-5) 753-782.

Table caption

Description, symbol, magnitude, and equation in which the different parameters of the models appear

Figure captions

Fig. 1. Schematic drawings of the gradient-nanotwinned metals with a bimodal microstructure separated into *N* layers. In each layer, a bimodal composite consists of the large-grained phase and the nanotwinned ultrafine/nanograined phase.

Fig. 2. Comparisons between the calculated stress and strain response and the experimental data [55] for the gradient-nanotwinned bimodal copper.

Fig. 3. Effects of reference microcrack density (a,c) and Weibull modulus (b,d) on stress-strain relation and mechanical properties of gradient-nanotwinned bimodal copper.

Fig. 4. Effects of gradient distribution of twin spacing on the strength and ductility of the gradient-nanotwinned bimodal copper. *B* is the parameter in the gradient function of twin spacing. The different value of *B* induces to the various gradient distribution of twin spacing.

Fig. 5. Stress-strain relations under different gradient distributions of volume fraction of coarse-grained phase (a), and the yield strength (b) and ductility (c) varying with the volume fraction relevant parameter *A*.

Table 1.

Description, symbol, magnitude, and equation in which the different parameters of the models appear

Parameter	Symbol	Ultrafine grain	Coarse grain
Elastic modulus	E	128 GPa	128 GPa
Shear modulus	μ	47.1 GPa	47.1 GPa
Poisson's ratio	υ	0.36	0.36
Burgers Vector	b	0.256 nm	0.256 nm
Taylor factor	M	1.732-3.06	1.732-3.06
Taylor constant	α	0.33	0.33
Dynamic recovery constant	n	21.25	21.25
Reference strain rate	$\dot{\varepsilon}_0$	1 s^{-1}	1 s^{-1}
Maximum number of dislocation	N_0	13	300
Reference density of nanomicrocracks	ρ_0	0.04	

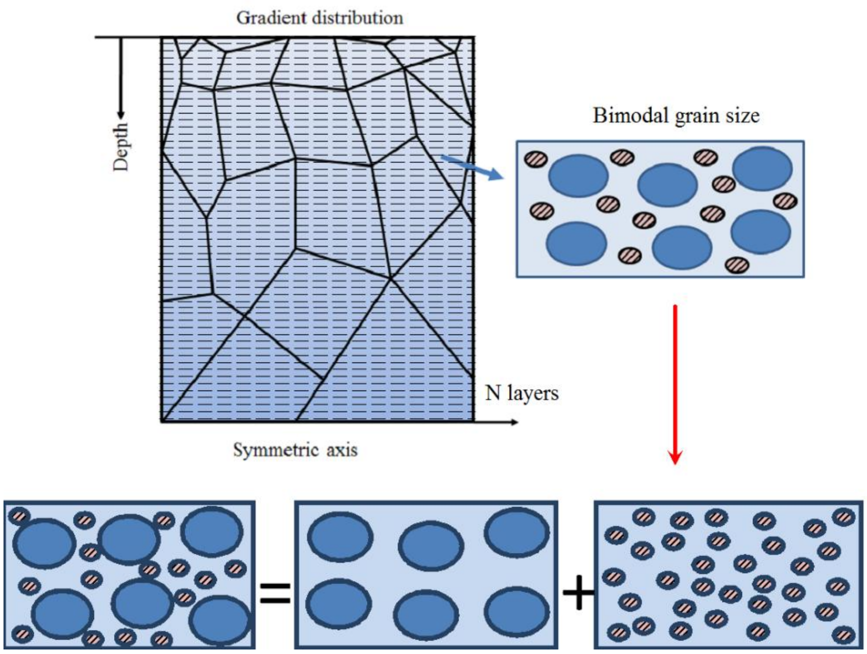


Fig. 1 Schematic drawings of the gradient-nanotwinned metals with a bimodal microstructure separated into *N* layers. In each layer, a bimodal composite consists of the large-grained phase and the nanotwinned ultrafine/nanograined phase.

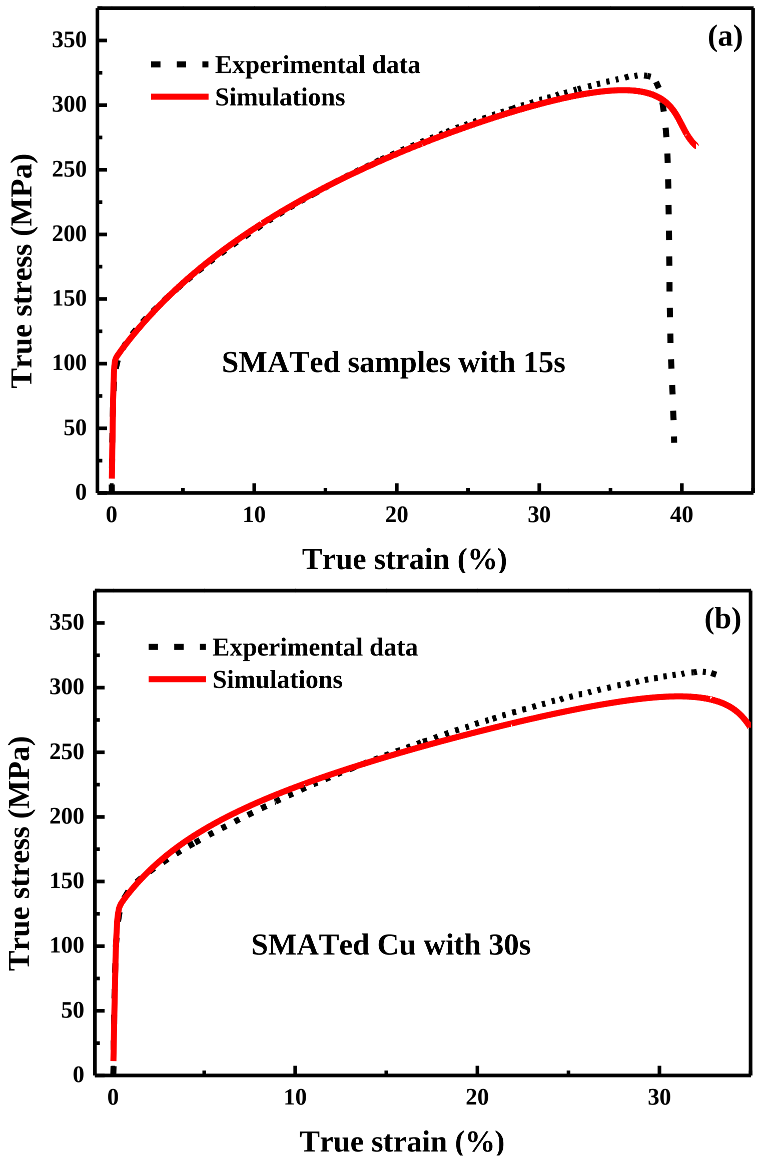


Fig. 2 Comparisons between the calculated stress and strain response and the experimental data [55] for the gradient-nanotwinned bimodal copper.

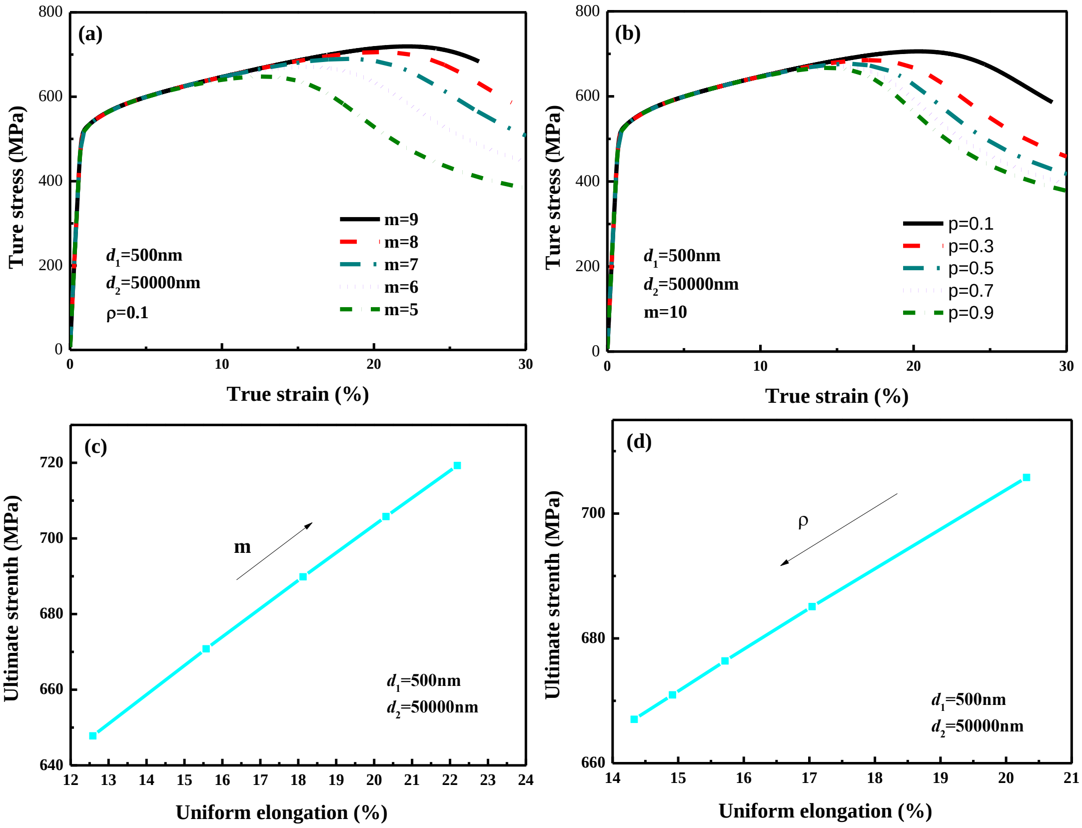


Fig. 3 Effects of reference microcrack density (a,c) and Weibull modulus (b,d) on stress-strain relation and mechanical properties of gradient-nanotwinned bimodal copper.

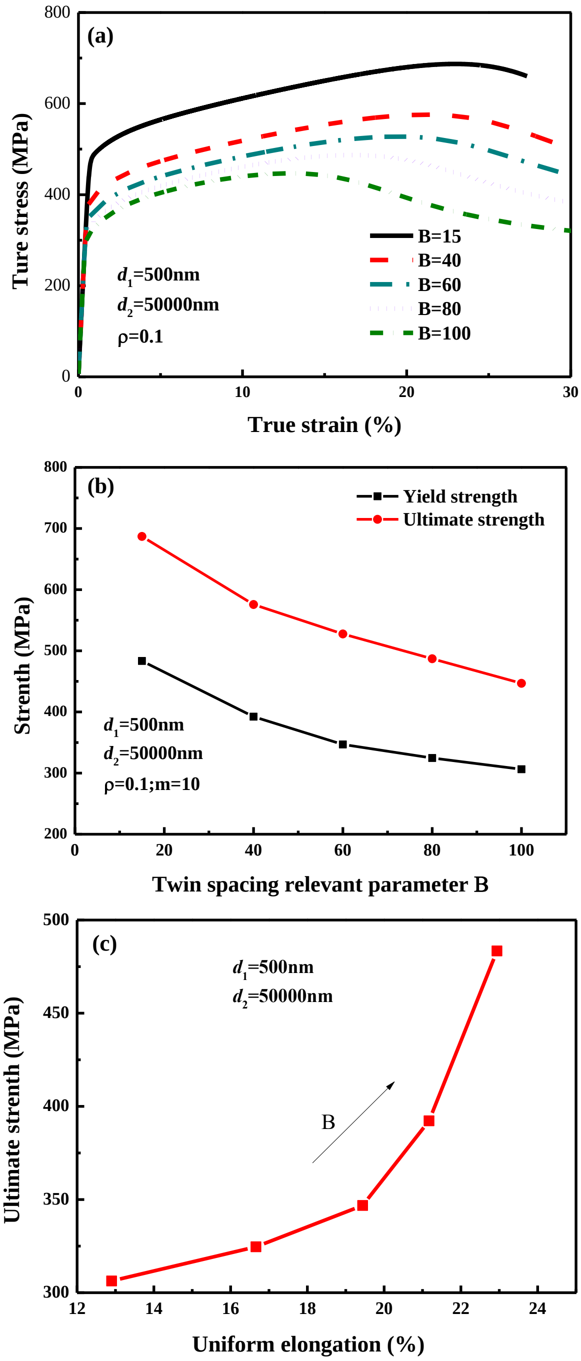


Fig. 4 Effects of gradient distribution of twin spacing on the strength and ductility of the gradient-nanotwinned bimodal copper. *B* is the parameter in the gradient function of twin spacing. The different value of *B* induces to the various gradient distribution of twin spacing.

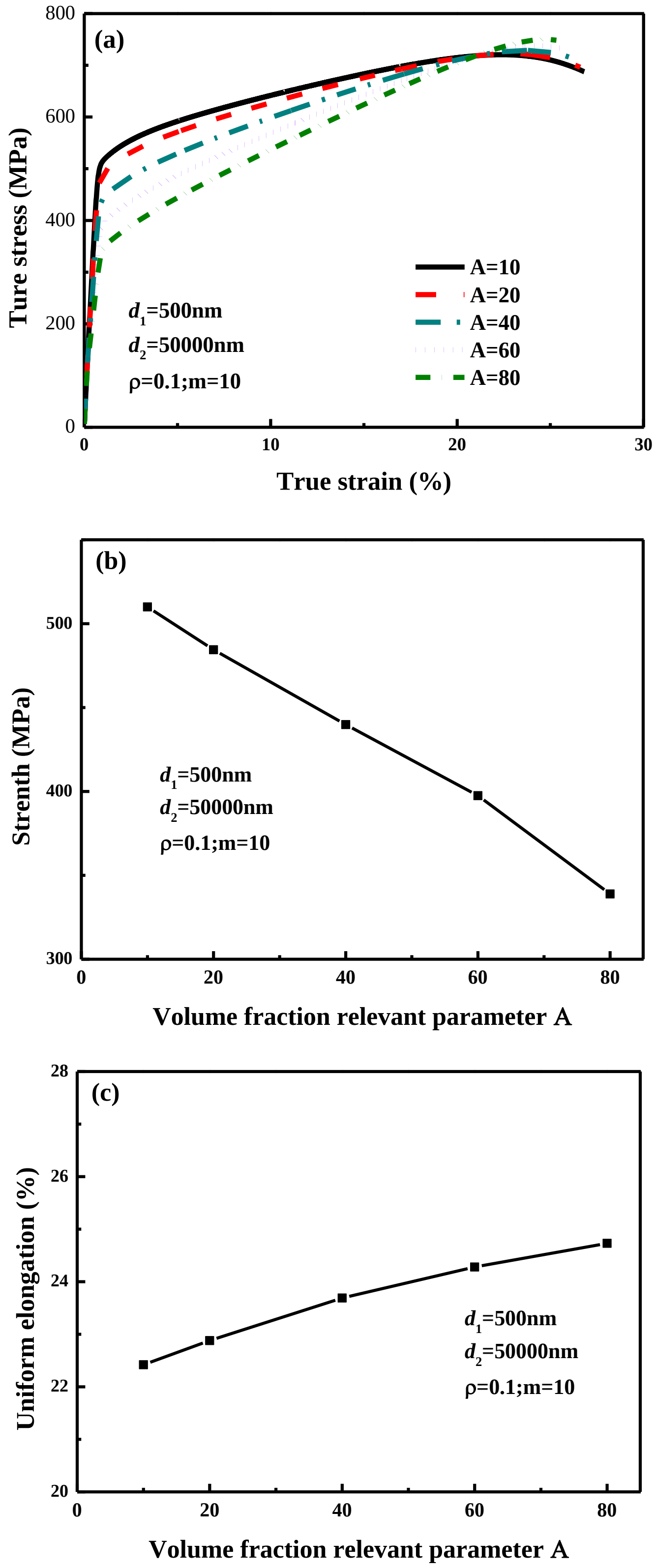


Fig. 5 Stress-strain relations under different gradient distributions of volume fraction of coarse-grained phase (a), and the yield strength (b) and ductility (c) varying with the volume fraction relevant parameter *A*.

Figure1
Click here to download high resolution image

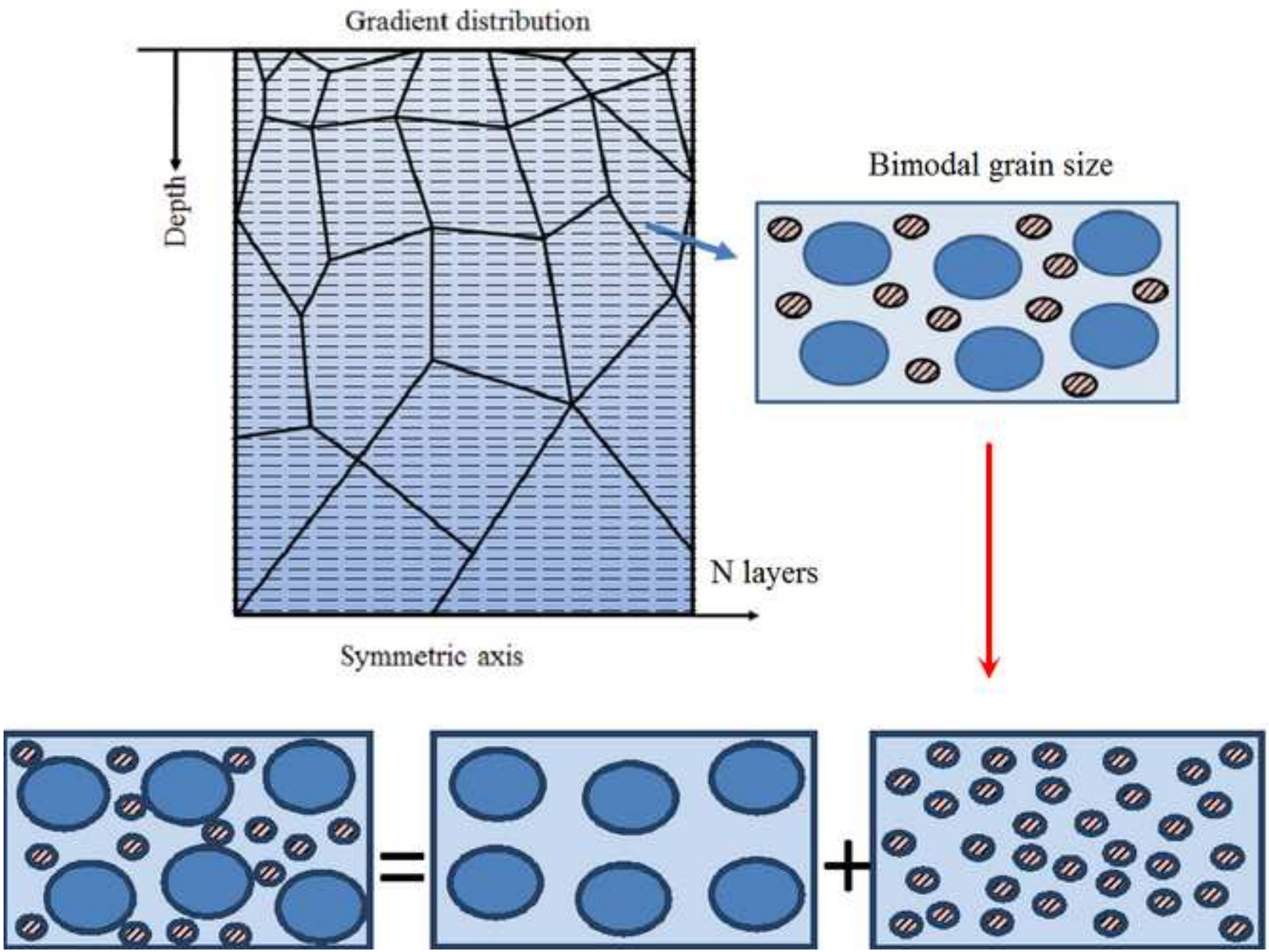


Figure2a

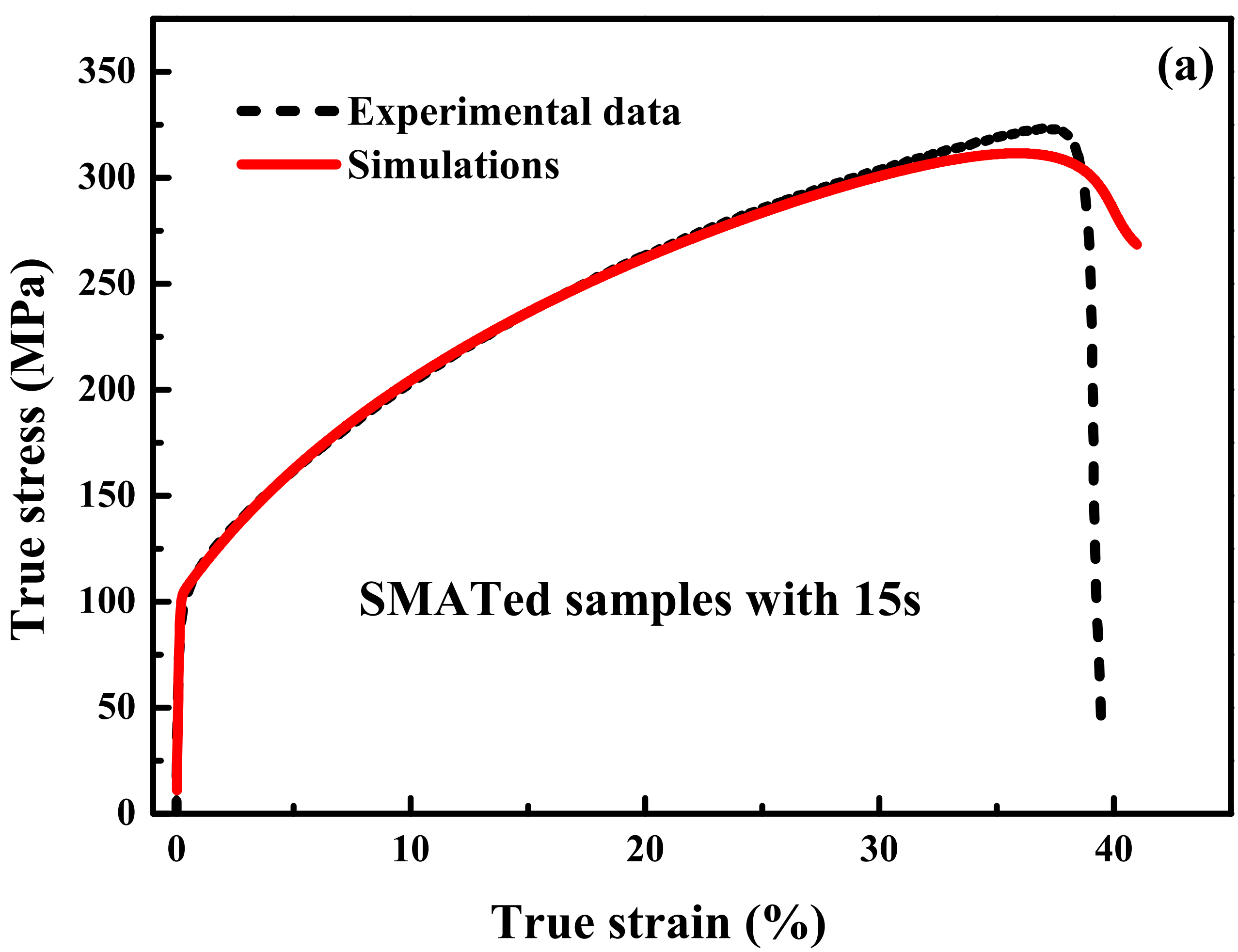

(a)
Experimental data
Simulations
SMATed samples with 15s
True stress (MPa)
True strain (%)
0
50
100
150
200
250
300
350
0
10
20
30
40

Figure2b

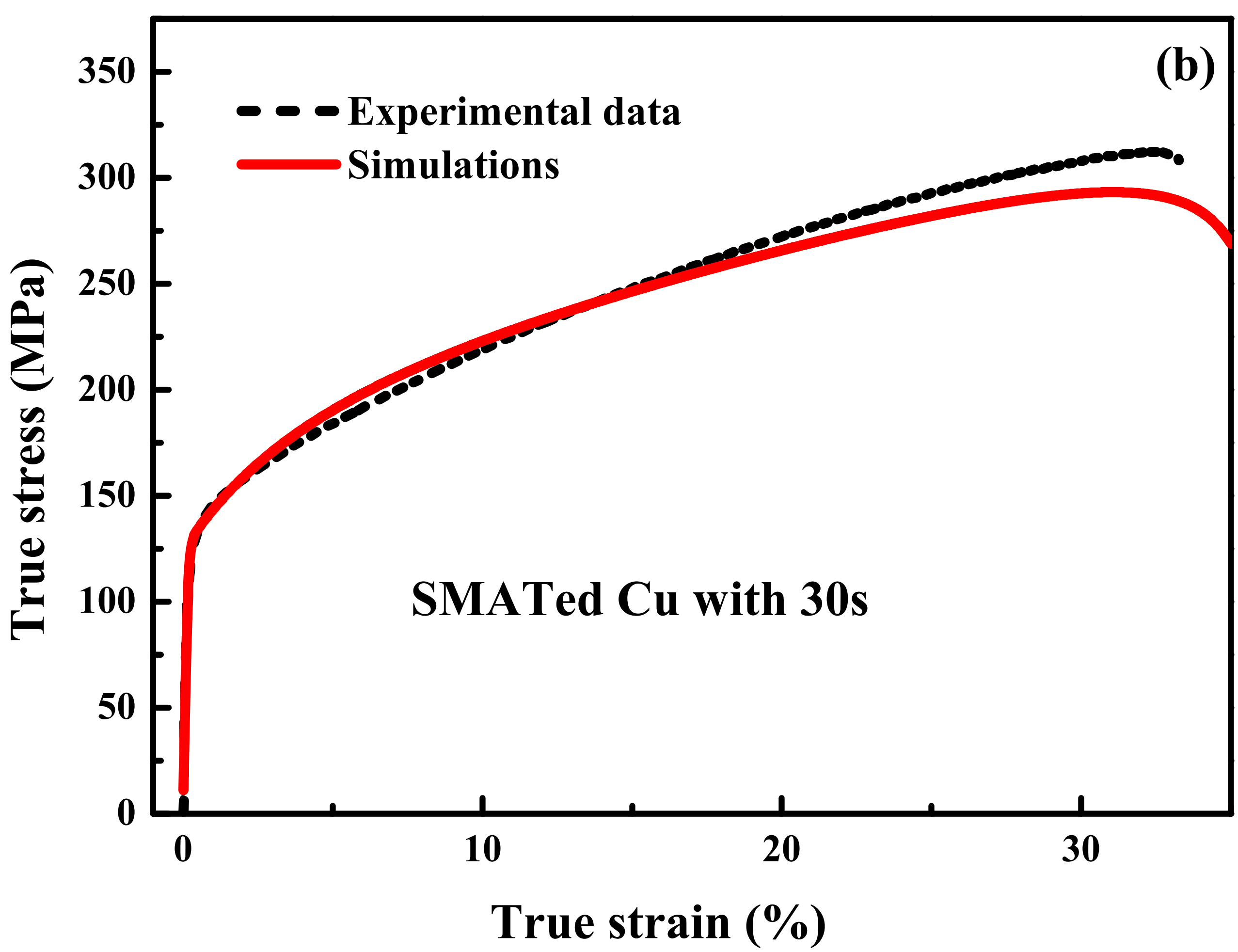
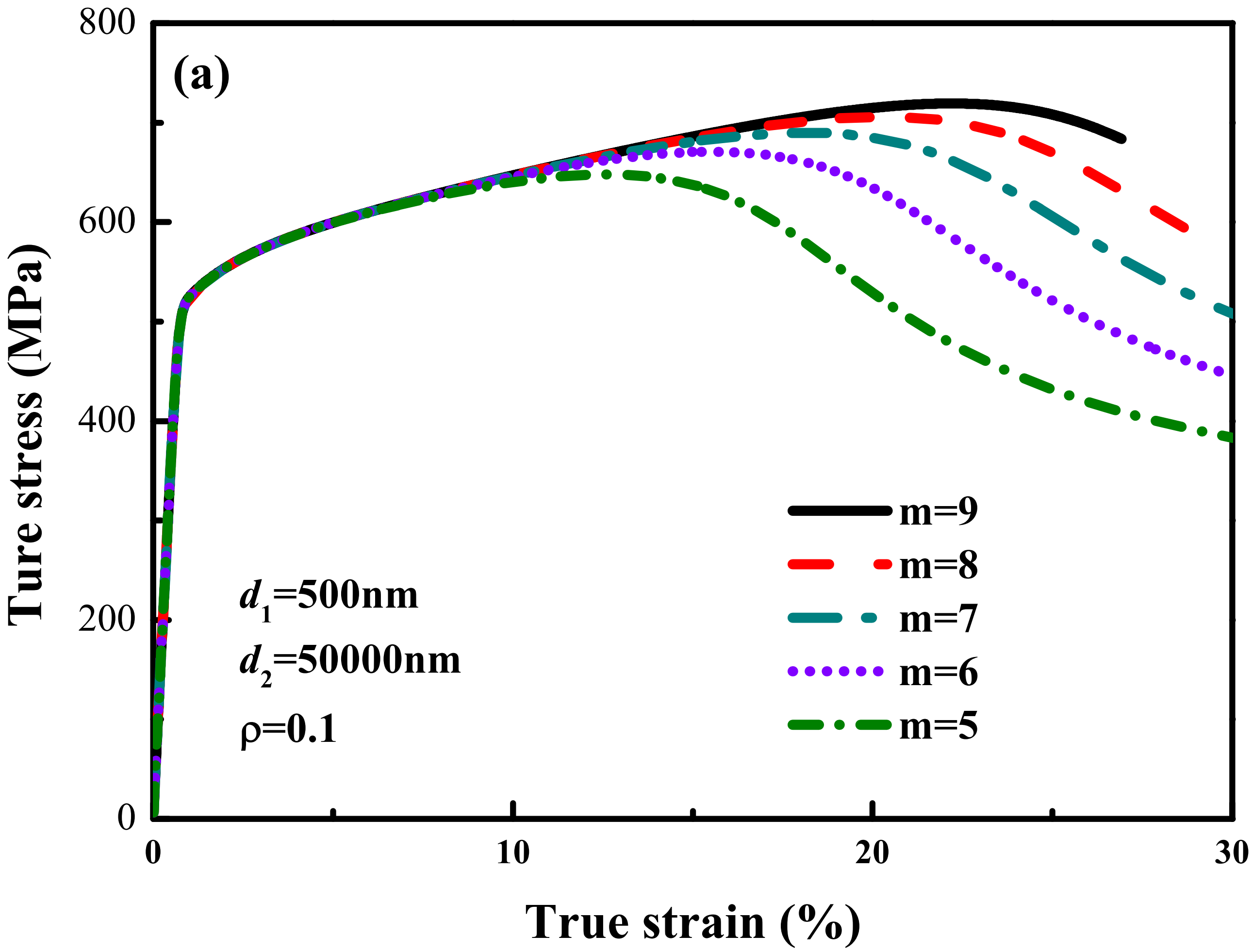

(b)
Experimental data
Simulations
SMATed Cu with 30s
True stress (MPa)
True strain (%)
0
50
100
150
200
250
300
350
0
10
20
30

Figure3a



(a)
Ture stress (MPa)
True strain (%)
800
600
400
200
0
0
10
20
30
d1=500nm
d2=50000nm
ρ=0.1
m=9
m=8
m=7
m=6
m=5

Figure3b

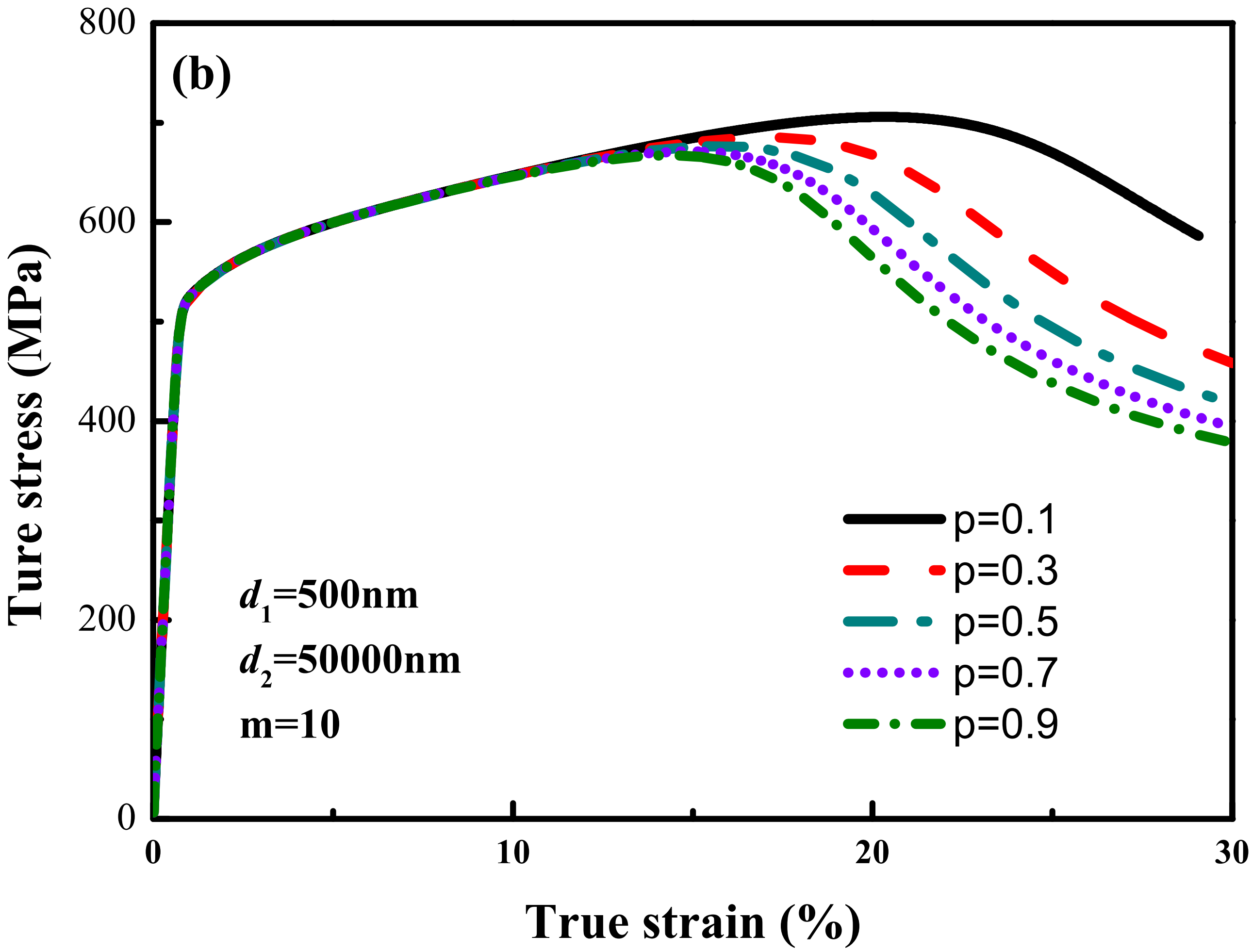

(b)
Ture stress (MPa)
800
600
400
200
0
0
10
20
30
True strain (%)
d_1=500nm
d_2=50000nm
m=10
p=0.1
p=0.3
p=0.5
p=0.7
p=0.9

Figure3c

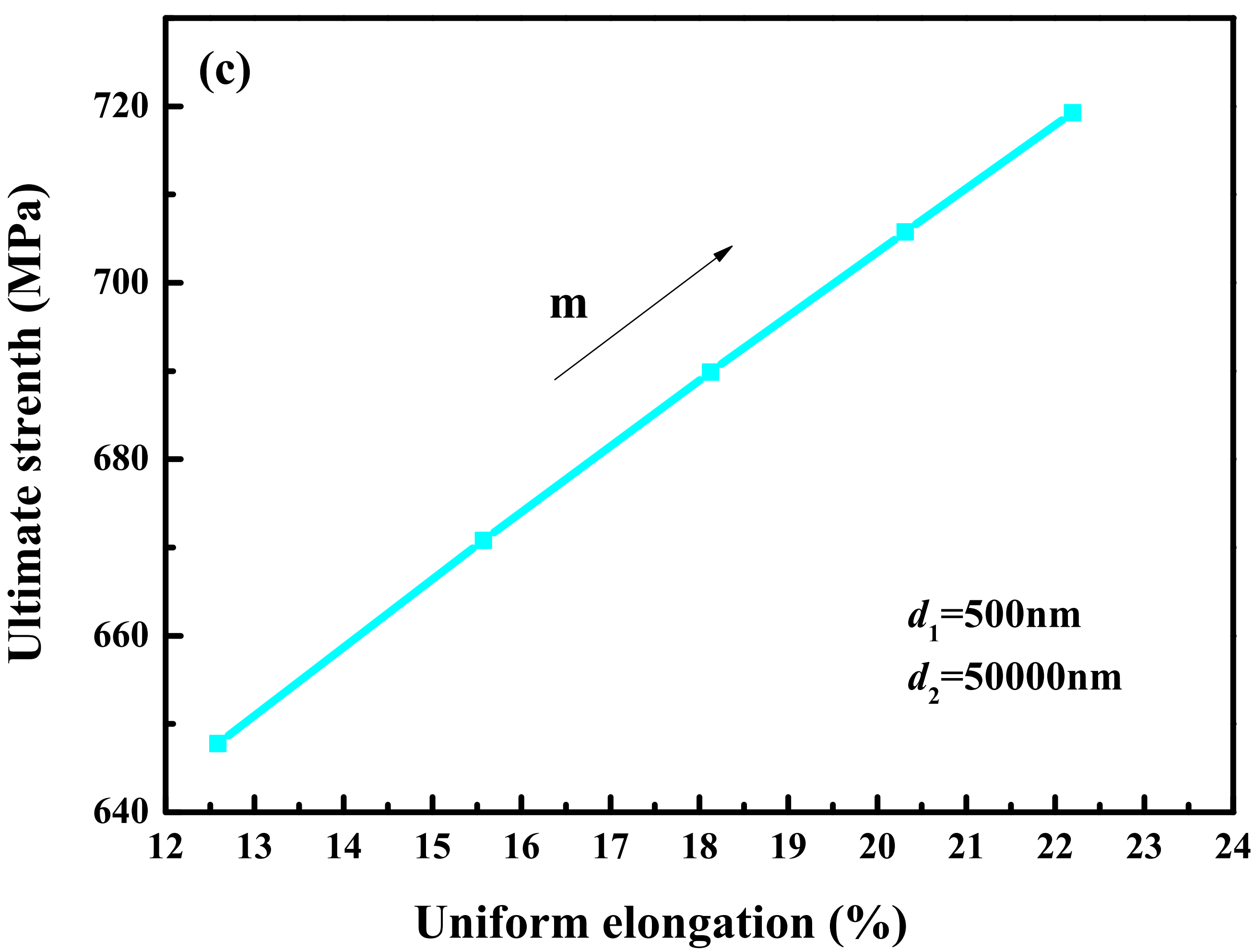

(c)
m
d_1=500nm
d_2=50000nm
Ultimate strenth (MPa)
720
700
680
660
640
12
13
14
15
16
17
18
19
20
21
22
23
24
Uniform elongation (%)

Figure3d

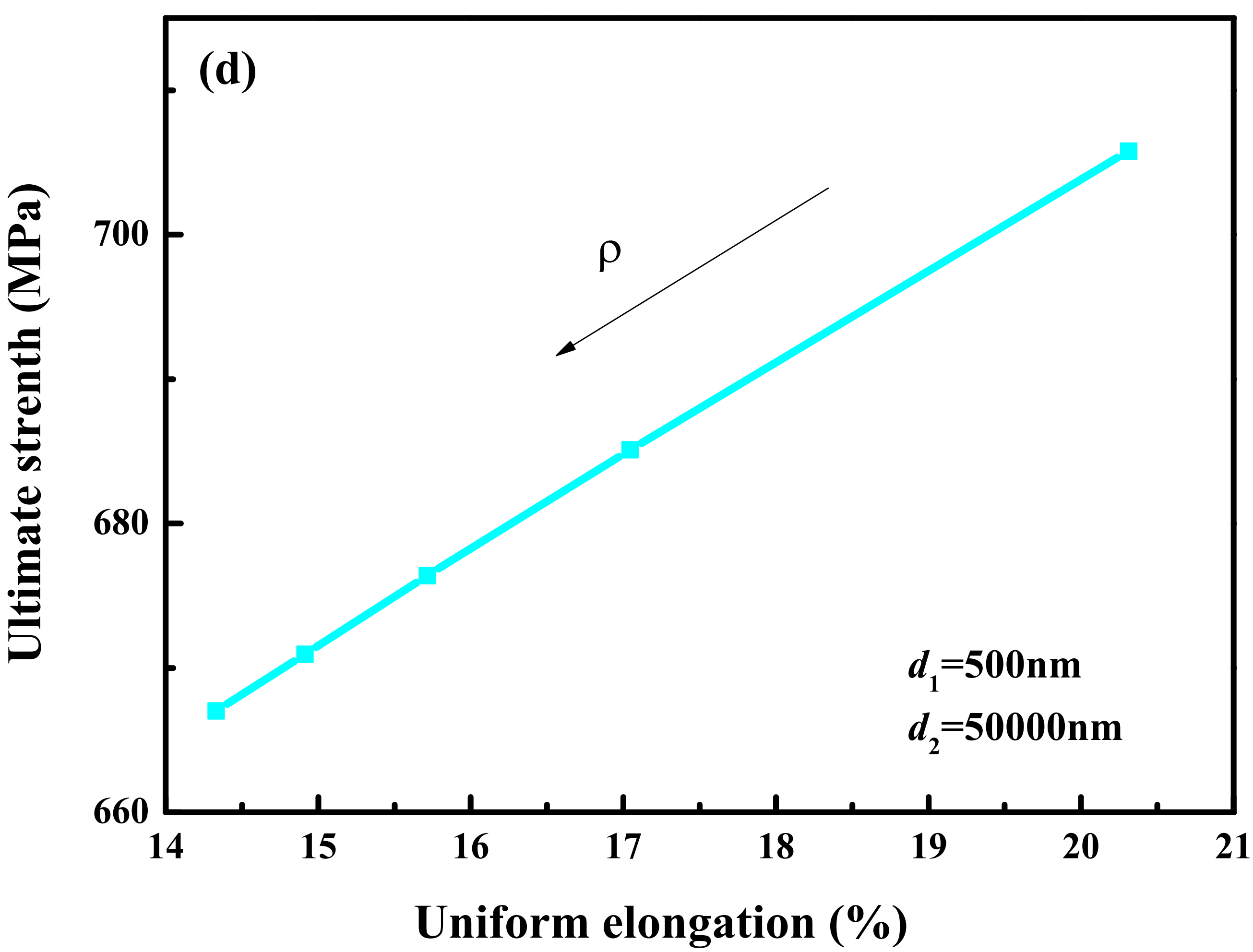
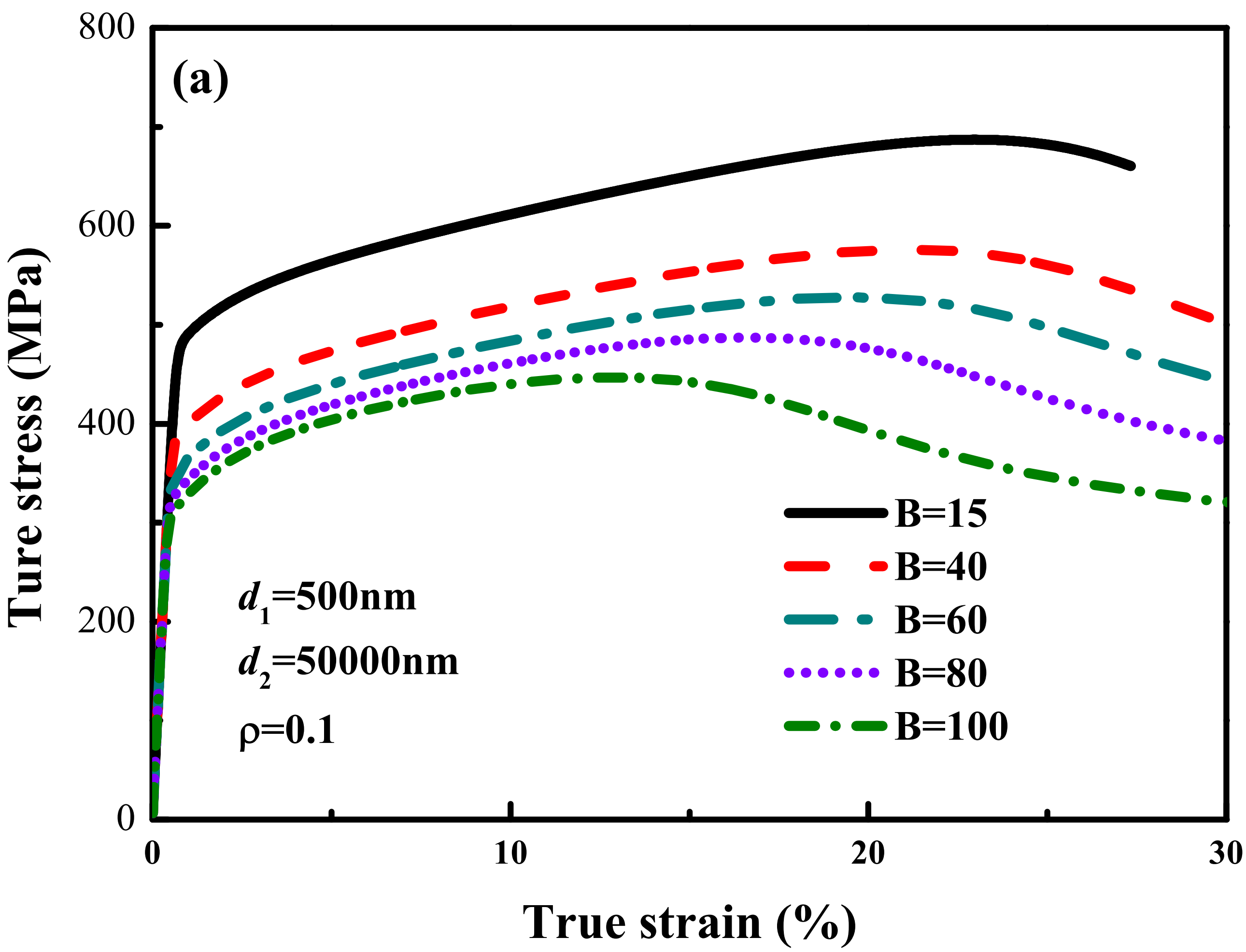

(d)
ρ
d_1=500nm
d_2=50000nm
700
680
660
14
15
16
17
18
19
20
21
Ultimate strenth (MPa)
Uniform elongation (%)

Figure4a



(a)
Ture stress (MPa)
True strain (%)
0
200
400
600
800
0
10
20
30
d_1=500nm
d_2=50000nm
ρ=0.1
B=15
B=40
B=60
B=80
B=100

Figure4b

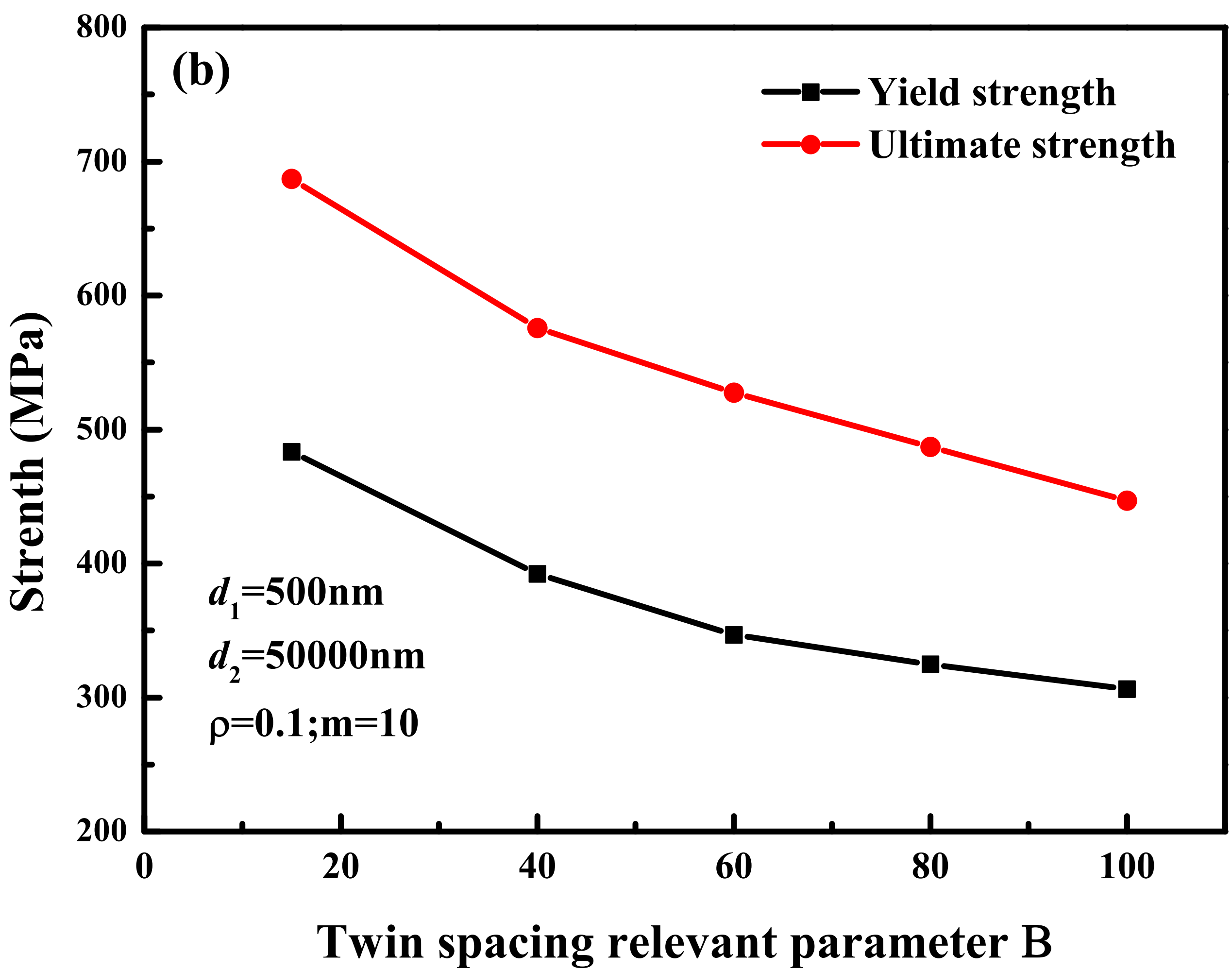
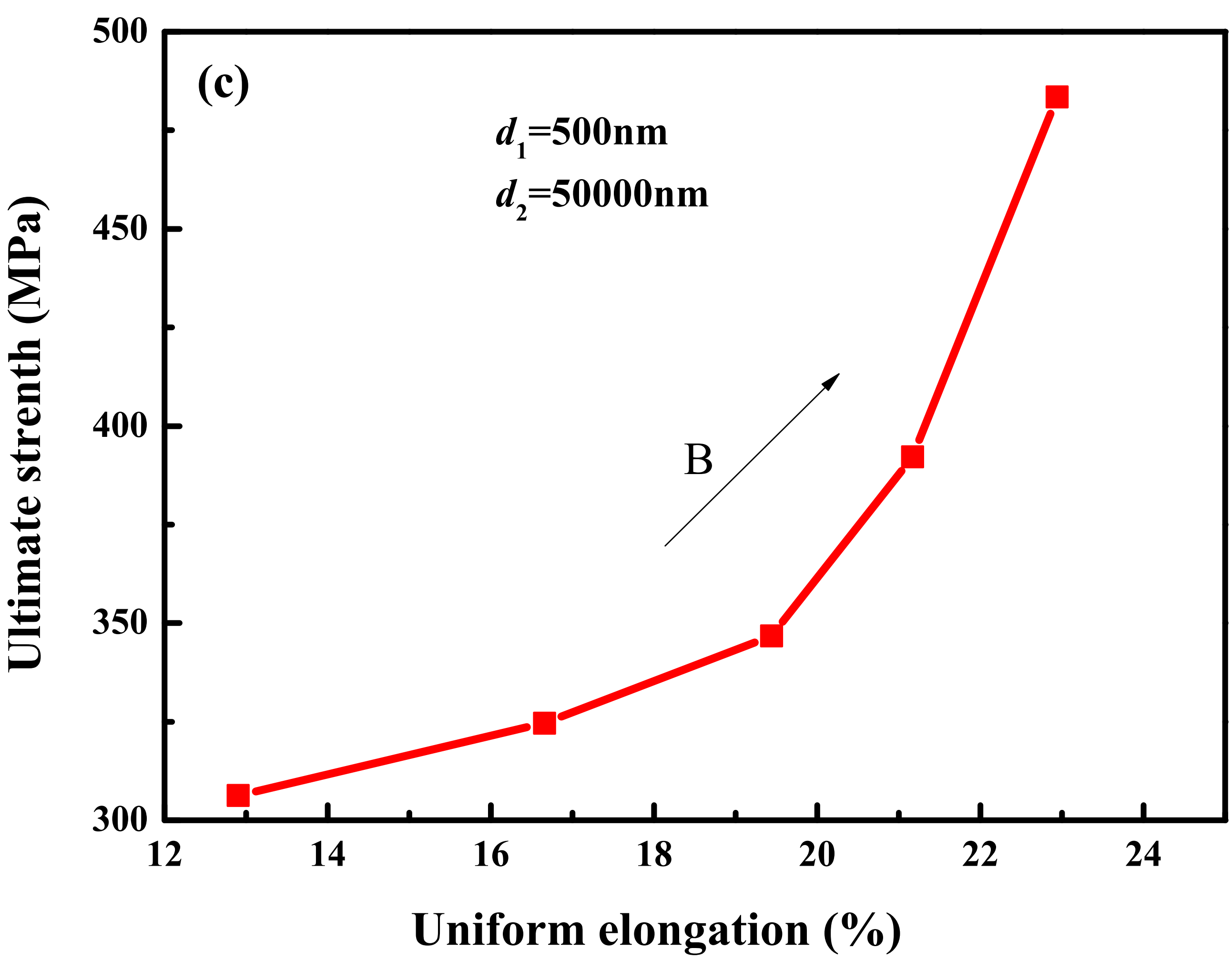

(b)
Yield strength
Ultimate strength
d_1=500nm
d_2=50000nm
ρ=0.1;m=10
Strenth (MPa)
Twin spacing relevant parameter B
800
700
600
500
400
300
200
0
20
40
60
80
100

Figure4c



(c)
d_1=500nm
d_2=50000nm
B
Ultimate strenth (MPa)
Uniform elongation (%)
500
450
400
350
300
12
14
16
18
20
22
24

Figure5a

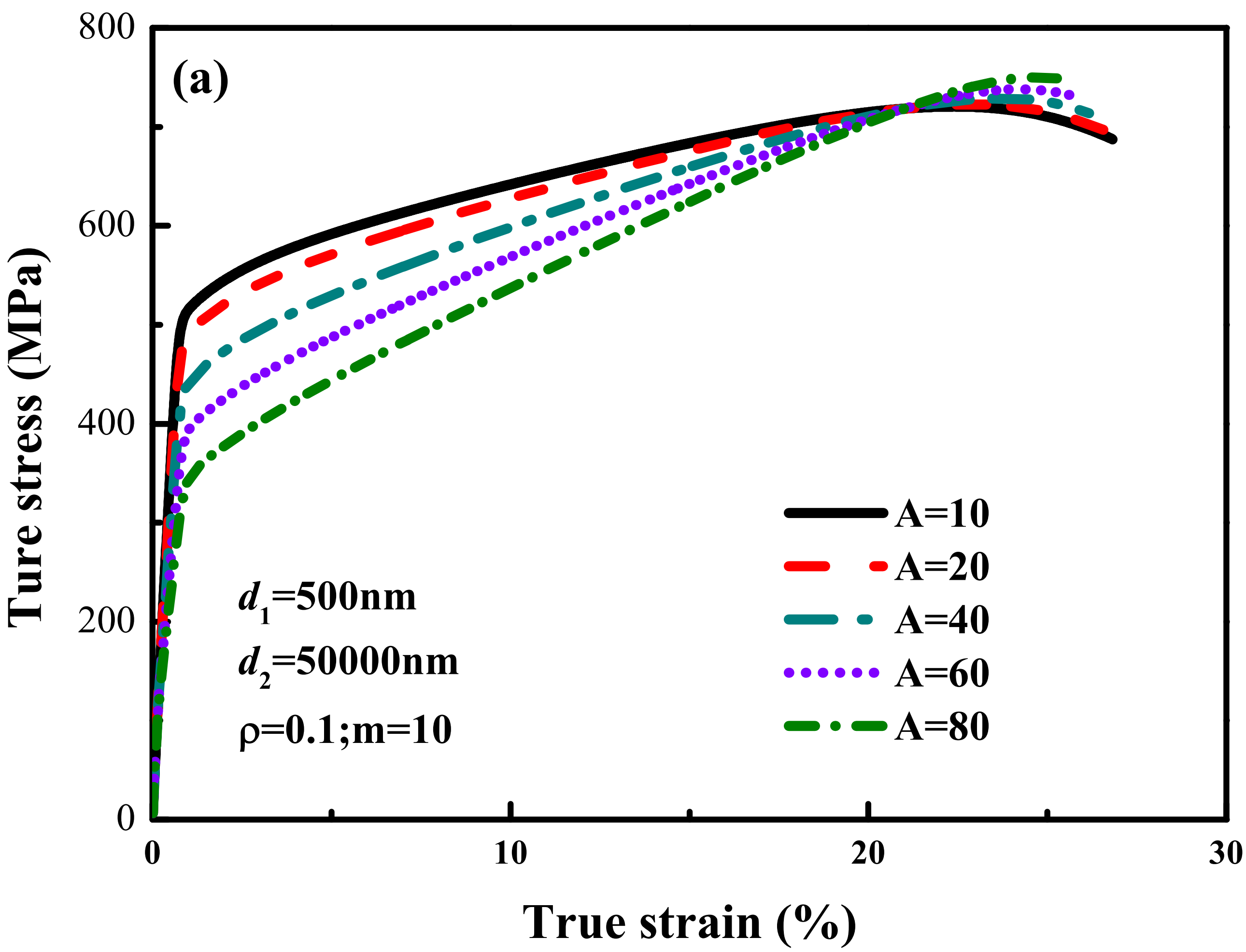
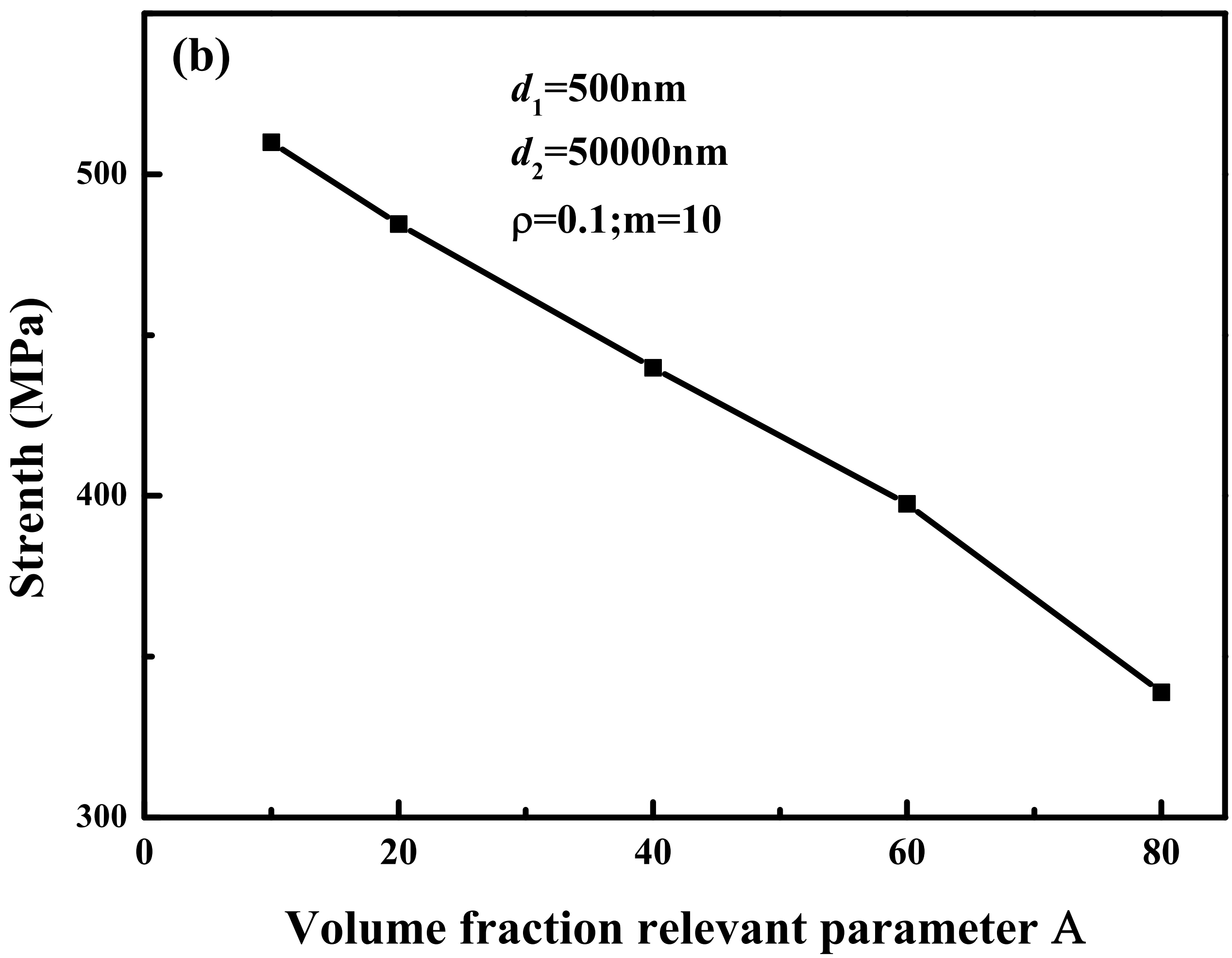
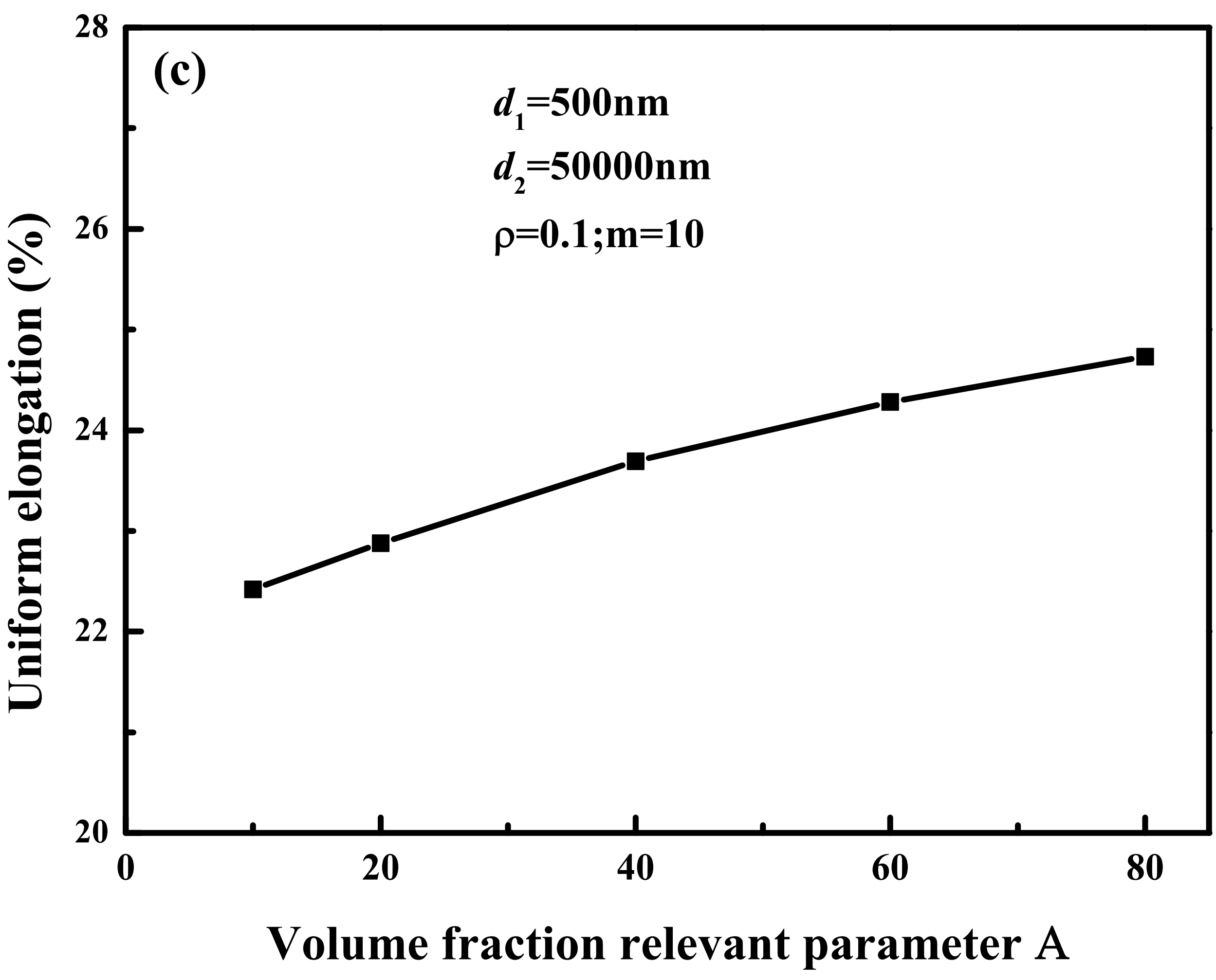

(a)
800
600
400
200
0
0
10
20
30
Ture stress (MPa)
True strain (%)
A=10
A=20
A=40
A=60
A=80
d_1=500nm
d_2=50000nm
ρ=0.1;m=10

Figure5b



(b)
d_1=500nm
d_2=50000nm
ρ=0.1;m=10
Strenth (MPa)
500
400
300
0
20
40
60
80
Volume fraction relevant parameter A

Figure5c


(c)
d_1=500nm
d_2=50000nm
ρ=0.1;m=10
Uniform elongation (%)
Volume fraction relevant parameter A
20
22
24
26
28
0
20
40
60
80