A COMPUTATIONAL STUDY ON OVERALL MECHANICAL BEHAVIOR OF NANO-CRYSTALLINE AND ULTRA-FINE POLYCRYSTALLINE METALS

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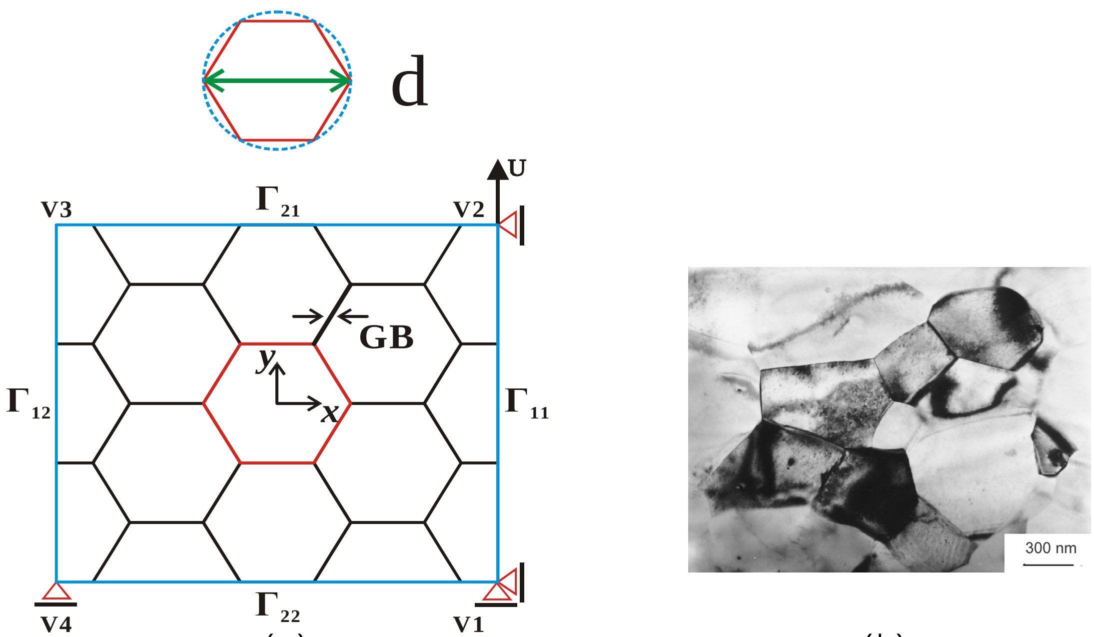
Summary Investigation on the mechanical behavior of nanocrystalline and ultra-fine polycrystalline metals accompanying by intergranular fracture has been performed. Both the finite element method which is based on the conventional theory of mechanism-based strain gradient plasticity accounting for the size effects and the mixed-mode cohesive interface model are used. A systematical studies on the overall strength and ductility of polycrystalline aggregates which depend on both grain interiors and grain boundaries for different grain sizes and different interface properties are carried out. The results have shown that the overall strength and ductility of polycrystalline aggregates with nanoscale and ultra-fine grains strongly depend on the properties of the grain boundaries, and about the ductility of the nanocrystalline and ultra-fine polycrystalline metals, there is a competition of grain boundary deformation with that of grain interiors.

INTRODUCTION

Investigations on the mechanical behaviors of polycrystalline materials with grain sizes typically less than 100 nm (nanocrystalline (nc) metals) or within 100-1000 nm (ultra-fine crystalline (ufc) metals) have been the key subjects worldwide over the past two decades [1]. The nc/ufc metals exhibit the higher yield strength, tensile strength, and hardness, but the lower tensile ductility relative to their bulk counterparts. In the present research, the strain gradient plasticity theory [2] is used to describe the size effects of the inelastic deformation in grain interiors, and a cohesive interface model is used to describe both the grain-boundary separation and the intergranular fracture process. Particular attention is focused on the influence of both grain interiors and grain boundary properties on the overall strength and ductility of the nc/ufc metals.

MODEL AND DESCRIPTIONS

To particularly study the mechanical behaviors of the nc/ufc materials, and to investigate how the competition of grain-boundary deformation with that of grain interior determines the observed overall stress-strain response and the overall ductility of polycrystalline aggregates by various properties of grain boundary and grain interiors, a regular quasi-three-dimensional representative volume element with taking into account of three dimensional effects is presented here. Fig. 1 shows the schematic figure of representative calculation model. The calculation model is consisted of twelve regular hexagon grains. The diameter of grain, d is the diameter of the circumcircle of regular hexagon.



(a) (b)

Fig. 1 Representative cell model (a) for nano- or ultra-fine polycrystalline metal (b)[1] with periodic boundary conditions of *xy* plane and *z* direction

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As displayed in Fig. 1, periodic boundary conditions are enforced along the four sides in *xy* coordinate plane [3]:

$$\vec{\mathbf{u}}_{12} - \vec{\mathbf{u}}_{V4} = \vec{\mathbf{u}}_{11} - \vec{\mathbf{u}}_{V1} \tag{1}$$

$$\vec{\mathbf{u}}_{22} - \vec{\mathbf{u}}_{V1} = \vec{\mathbf{u}}_{21} - \vec{\mathbf{u}}_{V2} \tag{2}$$

$$\vec{\mathbf{u}}_{V3} - \vec{\mathbf{u}}_{V2} = \vec{\mathbf{u}}_{V4} - \vec{\mathbf{u}}_{V1} \tag{3}$$

where $\vec{\mathbf{u}}_{ij}$ is the displacement vector for any material point on the corresponding boundary $\boldsymbol{\Gamma}_{ij}$, and $\vec{\mathbf{u}}_{Vi}$ is the displacement vector for each vertex Vi.

The intergranular fracture process of grains is described by the cohesive zone (CZ) model.

A comparative parameter study for overall strength and ductility of polycrystalline aggregates affected by the material parameters of grain boundaries and grain interiors with different grain sizes is performed. The overall stress-strain relation of the nanostructured materials with parameter dependence normalized by the initial yield stress σ_Y and intrinsic material length l can be expressed as follows

$$\frac{\sigma}{\sigma_Y} = f\left(\underbrace{\frac{E}{\sigma_Y},\ \nu,\ N,\ \frac{d}{l}}_{\text{intragranular parameters}},\ \underbrace{\frac{T_1}{\sigma_Y},\ \frac{T_S}{T_1},\ \frac{G_{IC}}{\sigma_Y l},\ \frac{G_{SC}}{G_{IC}},\ \frac{K_c}{\sigma_Y}}_{\text{interfacial parameters}},\ \varepsilon\right) \tag{4}$$

where the intragranular parameters are Young modulus E, Poisson's ratio ν, initial yield stress σ_Y, strain hardening exponent N, grain diameter d, respectively. The interfacial parameters of grain boundary are maximum separation strength T_1 and T_S, mode I and shear mode fracture toughness G_{IC} and G_{SC}, effective initial separation modulus $K_c = T_1/\left(\delta_m^0/l\right)$ in CZ model.

RESULTS AND BRIEF DISCUSSIONS

A typical computational result for overall stress-strain relations of the nc/ufc metal related to a series of values of grain boundary separation strength T_1/σ_Y is shown in Fig.2. From Fig.2, the overall stress-strain relations are closely dominated by the properties of grain boundary, and the maximum strengths of the overall materials are also dominated by the properties of grain boundary for each case. The failure characteristic is a catastrophic process at strength point.

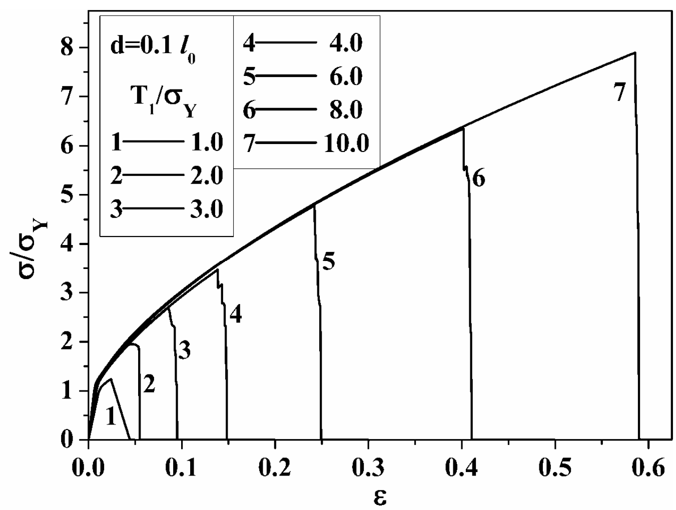

Fig. 2. Overall stress–strain curves related to the grain boundary separation strength T_1/σ_Y

References

[1] Wei YG, Shu SQ, Du Y, Zhu C. International Journal of Plasticity **21**(11):2089-2106, 2005.

[2] Huang Y, Qu S, Hwang KC, Li M, Gao H. International Journal of Plasticity **20**(4-5):753-782, 2004.

[3] van der Sluis O, Schreurs PJG, Meijer HEH. Mechanics of Materials **33**(9):499-522,2001.