TWIN-SPACING DEPENDENT YIELD STRENGTH IN THE MATERIALS WITH HIERARCHICAL NANOSTRUCTURES

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Summary The growth nanotwins have been proved both in experiment and MD simulation to strengthen the metallic materials significantly. Inspired by this observation, the hierarchical nanostructures with nanocale twin lamellae can be designed to achieve the higher yield strength in the polycrystalline metals. Here, we propose a mechanism-based theoretical model to predict the yield strength in the hierarchically nanotwinned metals that is related to the thickness of twin lamellae and grain size. The contribution of the partial dislocations is taken into account to describe the softening effect in nanotwinned metals. With decreasing the twin spacing in each layer of twin lamellae, there exits the optical twin spacing to obtain the maximum yield strength in hierarchically nanotwinned metals.

INTRODUCTION

Higher strength in the metallic materials can be expected through various approaches, for example, refining grain size, solid solution alloying and plastic straining. Generating the inner boundaries such as the twin boundaries has been considered as an alternative methodology to strengthen the materials [1]. In the passed ten years, there have been numerous works to be done to give insights into the mechanical performance of nanotwinned metals, including measuring the stress-strain relationship and the failure behaviours [2], performing the atomic simulations to study the deformation mechanisms [3] as well as developing the continuum theoretical models to describe the corresponding mechanical properties [4].

Recently, Liddicoat et al. [5] suggested that the hierarchical nanostructure can be utilized to realize the high strength in the alloys. Meanwhile, experimental studies demonstrated that the hierarchical twins have been observed in the martensitic materials which involved the primary and secondary twin lamellae [6]. In this paper, a dislocation-based plastic model is proposed to describe the constitutive relationship of hierarchically nanotwinned polycrystalline metals and further predict the yield strength varied with the twin spacing and the grain size. The dislocation pileup zones of grain boundaries (GBs) and twin boundaries (TBs), which are related to the strain gradient, are introduced in the proposed model. Numerical results indicate that the flow stresses in these hierarchical structures are sensitive to the twin spacing of the each layer of twin lamellae. The yield strength of the hierarchically nanotwinned metals is greater than the one of the individually nanotwinned metals, and the maximum strength can be obtained by controlling the thickness of the twin spacings for different grain size.

THEORETICAL MODEL

During plastic deformation in the nanotwinned polycrystalline metals, there are plenty of dislocations accumulated along the grain boundaries and twin boundaries. Therefore, the dislocation pileup zones of GBs (GBDPZ) and TBs (TBDPZ) as shown in Fig. 1a are defined in the regions nearby these boundaries, with the thickness of 7-11 times of lattice constant. In these zones, the strain gradient has been observed in experiment, leading to that the strain gradient is addressed to identify the dislocation density of GB/TBDPZ. Suppose that there are only primary and secondary twin lamellae constructed in the nanotwinned polycrystalline metals (Fig. 1b). Due to the existence of the strain gradient nearby the GB/TBs, the strain gradient plastic theory is adopted here to calculate the stress-strain response of the hierarchically nanotwinned metals. Based on the Taylor model (1), the dislocations density should be addressed in the hierarchically twinned metals.

$$\sigma_{flow} = \alpha\mu b\sqrt{\rho} \tag{1}$$

Here, $\rho = \rho_I + \rho_{TB} + \rho_{GB}$ denotes the density of the total dislocations in a unit cell, including the dislocation densities in the TBDPZ of the primary and secondary twin lamellae $\rho_{TB} = \rho_{TB}^1 + \rho_{TB}^2$, the one in the GBDPZ ρ_{GB} and the one in the interior crystal ρ_I. α, μ and b are the empirical constant, the shear modulus and the Burger constant, respectively. The dislocation density in the TBDPZ is written a $\rho_{TB} = k^{TB}\eta^{TB}o / b$, in which $k^{TB} = 12d_{TBDPZ} / \phi^{TB}\pi d_{TB}$, and the local strain gradient in the TBDPZ $\eta^{TB}o$ is expressed as $\eta^{TB}o = \eta_1 d_{TB} + \eta_0 - \eta_P / d_{TB}$ [7]. Here, $\eta_1 = \phi^{TB}N_0 b/(d_{TBDPZ}d_G^2)$ and $\eta_0 = \phi^{TB}n'_p b/(d_{TBDPZ}d_G\sqrt{3})$

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$\eta_P = \sqrt{3}\pi\phi_p b/12d_{TBDPZ}$, n'_p being the number of initial twinning partials in the TBDPZ, N_0 is the maximum number of inclined dislocations in a grain, d_{TB} is the twin spacing, d_{TBDPZ} denotes the thickness of TBDPZ, ϕ_p and ϕ^{TB} is a geometric factor. Therefore, we can derive the dislocation density of TBDPZ in the primary and secondary twin lamellae as follows

$$\rho_{TB}^1 = \frac{12N_0}{\pi d_G^{\,2}} + \frac{12n'_p}{\sqrt{3}\pi d_G}\frac{1}{L_1} - \frac{\sqrt{3}\rho_0}{\pi}\frac{1}{L_1^{\,2}},\quad \rho_{TB}^2 = \frac{12N_0L_1}{\pi d_G^{\,3}} + \frac{12n'_pL_1}{\sqrt{3}\pi d_G^{\,2}}\frac{1}{L_2} - \frac{12\rho_0L_1}{\sqrt{3}\pi d_G}\frac{1}{L_2^{\,2}}, \tag{2}$$

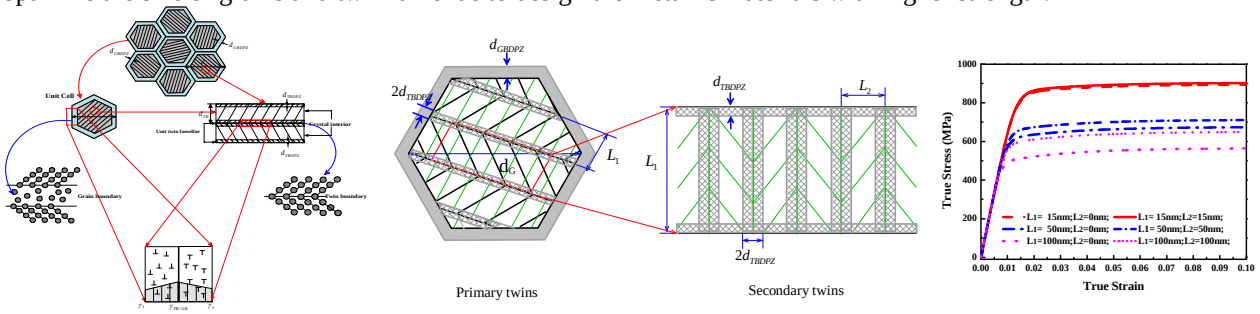
where L_1 and L_2 are the twin spacing in the primary and secondary twin lamellae respectively. The density of dislocations in the GBDPZ can be expressed as $\rho_{GB} = k^{GB}\eta^{GB}/b$ [7], where $k^{GB} = 6d_{GBDPZ}/\phi^{GB}d_G$, ϕ^{GB} is a constant. The density of dislocations in the crystal interior obeys the evolution law with plastic strain according to Kocks and Mecking's model [8]

$$\frac{\partial\rho_I}{\partial\varepsilon^{\mathrm{p}}} = M\left(\frac{k}{d_G} + k_1\sqrt{\rho_I} - k_2\rho_I\right), \tag{3}$$

where M is the Taylor factor, $k = 1/b; k_1 = \psi/b; k_2 = k_{20}(\dot{\varepsilon}/\dot{\varepsilon}_0)^{-1/\mathrm{n}}$, ψ is a proportionality factor, k_{20} and $\dot{\varepsilon}_0$ are the constants, and n is inversely proportional to the temperature. From above derivation, one can note that the flow stress of hierarchically nanotwinned metals is a function of the twin spacings of each layer of twin lamellae and the grain size.

NUMERICAL RESULS AND CONCLUSIONS

Here, we give the polycrystalline copper with hierarchical nanotwins as an example to indentify the proposed model for describing the mechanical behaviours of this kind of hierarchical nanostructure. The parameters are extracted from the literature [7]. Based on the strain gradient plastic theory, we calculated the stress-strain relationship of the hierarchically nanotwinned polycrystalline copper with different twin spacings in the primary and secondary twin lamellae as shown in Fig. 1c. It can be found that the appearance of the secondary twin lamellae can further reinforce the individually nanotwinned copper. The other interesting feature is that the contribution of the secondary twin lamellae on the strength is much more significant for the large primary twin lamellae than the one for the small twin spacing of primary twin lamellae. The further calculation demonstrates that the optimal twin spacings of primary and secondary twin lamellae for the maximum yield strength is 26 nm and 33 nm for d_G=1000nm, and 13 nm and 16.5 nm for d_G=500nm. In summary, we developed a mechanism-based plastic model to describe the plastic deformation of hierarchically nanotwinned metals. Numerical results indicate that the existence of the hierarchical nanotwins can remarkably improve the yield strength of the individually nanotwinned metals. The proposed model can be utilized to optimize the size of grains and twin lamellae to design the metallic materials with higher strength.



(a) (b) (c)

Fig.1 The schematic drawing of hierarchically nanotwinned metals(a.b) and the stress-strain response.

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