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Effect of surface energy upon size-dependent yield strength of single-crystalline hollow micro- and nanopillars

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ABSTRACT

The physical nature of the size-dependent yield strength of micro- and nanopillars is still an open issue, where the surface energy may be one factor that influences the size effect of these pillars, especially for hollow pillars. In this study, the influence of the surface energy and surface elasticity upon the size-dependent yield strength of single-crystalline hollow micro- and nanopillars is considered quantitatively. An analytical expression of the size-dependent yield strength is established that considers the surface energy and the inner defects by the principle of minimum potential energy. The predicted yield strength of our model as a function of the pillar size is more precise than that of the well-known single arm source model when comparing the predictions with the experimental results of pillars made of Al or Ni. According to the surface elasticity, the surface energy can be determined by the thickness of the hollow pillars, the surface modulus and the surface strain, where the latter two are related to the external damages.

1. Introduction

Recent investigations show that the yield strength of single-crystalline (SC) micro- or nanopillars presents strong size-dependent characteristics [1–3], where the mechanism of the size effect is dominated by the dimensional pillar size, the surface, and the inner defects. Currently, there are some mechanisms of size-dependent yield strength for such SC materials that are commonly based on the inner defects such as source truncation [4], dislocation starvation [5], or source exhaustion [6]. The stochastic nature of the plastic deformation corresponding to the size-dependent yield strength is explained by low dislocation content or dislocation source number in the microcrystal, so that the usual mean-field conditions for forest hardening are destroyed [5,6]. In these models, the boundary/surface of the micropillars plays a key role in the size effect because it not only determines the dislocation source lengths but also acts as a sink for dislocations. It has been shown that the boundary/surface of the micropillars can significantly affect the measured stiffness values [7]. Moreover, Fan et al. have inserted boundaries inside solid pillars to construct a model of hollow pillars in three-dimensional discrete dislocation dynamics simulations, and the results have shown that the boundary condition affects the strength of the hollow pillars via the wall thickness [8]. Until now, however, there have been almost no experiments conducted on hollow pillars. Recently, the physics of the surface energy has been considered in the description of the surface effect of nanowires and nanosprings [9,10] but, at present, little work has been done to link the size effect of SC micro- and nanopillars to the surface energy, and few studies have been done on hollow pillars.

In this study, an extended single arm source (SAS) model, combined with the surface energy and inner defects to describe the yield strength of hollow micro- and nanopillars, is obtained based on the principle of minimum potential energy. Meanwhile, the analytical form of the surface energy is determined by the thickness of the hollow pillars, the surface modulus and the surface strain according to surface elasticity. The obtained numerical results are then compared with the experimental results, giving proof of the efficiency of the proposed model. The main influences on the size-dependent yield strength are discussed, wherein the surface stress is mainly dominated by the geometries and the surface energy, and the inner defects such as the effective dislocation length and dislocation source number. The relationship between the surface energy and surface strain of the hollow pillars is discussed.

2. Theoretical model

All of the recent experimental and theoretical research on the size effect of micro- and nanopillars show that the critical resolved shear stress (CRSS) results from inner defects, including back

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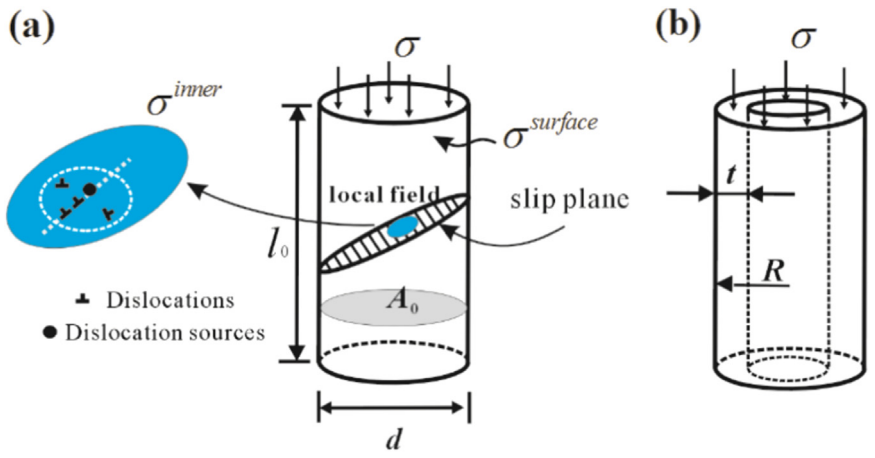

Fig. 1. Schematics of the micro-pillar model. (a) Components of the stress state that considers the effects from both the surface and the inner defects. (b) Cylindrical hollow pillar with diameter d and thickness t.

stresses from the interactive effect among the dislocations and the activation stress of dislocation sources [6,11–18]. The CRSS that is the main result of inner defects, as reported in the literature [6,18], is usually represented as the inner stress, σ^{inner}. Besides all of the inner defect factors, the surface energy can also play a role in the yield stress of micro- or nanopillars, where the stress induced by the surface energy is expressed as $\sigma^{surface}$ [10], and a schematic of this physical description is shown in Fig. 1. For the case of uniaxial stress state, the total stress σ (σ = CRSS/SF, SF is the Schmid Factor) equal to the external stress is the summation of σ^{inner} and $\sigma^{surface}$. Thus, the total stress can be written as.

$$\sigma = \sigma^{inner} + \sigma^{surface}. \tag{1}$$

If the external stress is equal to zero, $\sigma^{surface}$ can be regarded as the residual stress that influences inner defects. In conventional solid mechanics, the yield strength is determined by the phenomenological theory [10], which doesn't involve the defects inside the pillars. Recently, σ^{inner} has been expressed by the inner defects in the SAS model as [4–6,18].

$$\sigma^{inner} = \left(\frac{\alpha\mu b}{\bar{\lambda}_{\max}} + \tau_0 + 0.5\mu b\sqrt{\rho_0}\right)/SF,\ \alpha = \sqrt{\frac{\pi}{16(1-\nu)}}, \tag{2}$$

where μ is the shear modulus, ν is Poisson's ratio, b is the magnitude of the Burgers vector, τ_0 is the Peierls-Nabarro stress, $\bar{\lambda}_{\max}$ is the longest of the effective average lengths of dislocation sources (λ), and ρ_0 is the initial dislocation density. The SAS model has included the characteristic length of the defects $\bar{\lambda}_{\max}$ inside the pillars, which leads to the size-dependent mechanical properties. This model can be treated as an effective method to explain the size-dependent σ^{inner} in micro-pillars [6,18]. The detailed process used to obtain $\bar{\lambda}_{\max}$ is given in Ref. [18], and the number of pins, n, is related to the sample dimensions and the initial dislocation density [18].

In Fig. 1, the length of the pillar in a longitudinal direction is l_0 and the current length of the deformed configuration is equal to $l_0 + \Delta l$, where Δl is the infinitesimally small elastic deformed increment of the length, and so the engineering strain can be expressed as $\varepsilon = \Delta l/l_0$. As shown in the schematic sketch of the hollow pillars in Fig. 1(b), the tensile rigidity D_0 is considered as follows:

$$D_0 = EA_0 = E\frac{\pi d^2 - \pi(d-2t)^2}{4} = E\pi(2Rt - t^2), \tag{3}$$

where E is the elastic modulus, A_0 is the initial section area, d is the pillar diameter, R ($=d/2$) is the pillar radius and t is the thickness.

The yield stress is the critical stress between the elastic response and the plastic response of a material. Therefore, just before the critical yield condition, the material responses the linear elastic deformation and the strain energy can be written as a quadratic form. The total potential energy is estimated by Π, which is.

$$\Pi = U_e + U_s - W, \tag{4}$$

where U_e is the elastic strain energy, U_s is the surface energy and W is the work done by the external force P. The elastic strain energy is estimated by.

$$U_e = \int_v \int_0^{\varepsilon_{ij}} \sigma_{ij} \mathrm{d}\varepsilon_{ij} \mathrm{d}v = \frac{1}{2} D_0 \varepsilon^2 l_0 \tag{5}$$

where v is the volume of the specimen. And the total surface energy is approximated by.

$$U_s = \gamma S \tag{6}$$

where γ is the surface energy density and S is the surface area. Because the surface area is described by $S = S_0 + O_0\varepsilon l_0(1-\nu)$ under the isotropic assumption, Eq. (6) can be developed as.

$$U_S = \gamma S_0 + \gamma O_0 \varepsilon l_0 (1-\nu) \tag{7}$$

where O_0 is the perimeter of the initial cross-section and S_0 is the initial surface area. The work done by the external force P is given by displacement u.

$$W = Pu = P\varepsilon l_0 \tag{8}$$

By substituting Eqs. (5), (7) and (8) into Eq. (4), the total potential energy can be expressed as.

$$\Pi = \frac{1}{2} D_0 \varepsilon^2 l_0 + \gamma S_0 + \gamma O_0 \varepsilon l_0 (1-\nu) - P\varepsilon l_0. \tag{9}$$

Based on the principle of minimum potential energy, the final equilibrium state is determined by $\partial\Pi/\partial\varepsilon = 0$ with ignoring the high order small term including ε^2. According to the framework of Fig. 1, the strain ε here can be expressed as.

$$\varepsilon = (P - \gamma O_0(1-\nu))/EA_0 = \frac{P}{EA_0} - \frac{\gamma O_0(1-\nu)}{EA_0} \tag{10}$$

If the deformation is elastic, the term (P/A_0) is considered as the total external stress σ, and Eq. (9) can be rewritten as.

$$\varepsilon = \frac{\sigma}{E} - \frac{\gamma O_0(1-\nu)}{EA_0}. \tag{11}$$

If σ=0, the strain in Eq. (11) will be in a compressive state