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Temperature insensitivity of the flow stress in body-centered cubic micropillar crystals

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ABSTRACT

Plasticity of body-centered cubic (bcc) crystals is known to have a strong dependence on temperature, as a direct consequence of the thermally-activated process of kink pair nucleation and migration with a high energy (Peierls) barrier. Here we demonstrate that, in the sub-micron size scale, such strong temperature dependence of the flow stress must disappear. We explore the flow stress and hardening behavior of micro-pillar sizes in the range 200–2000 nm at temperatures of 150–900 K. Discrete Dislocation Dynamics (DDD) simulations reveal that the weak temperature sensitivity can be rationalized in terms of the weak role of screw dislocations in controlling plasticity; unique to small crystals of finite size. It is shown that finite, sub-micron samples have limited ability to store screw dislocations. The necessity of applying high stress in sub-micron crystals is demonstrated to greatly enhance the mobility of screw dislocations, rendering it close to that of edge dislocations. This leads to a transition of the dislocation mobility mechanism from being thermal-activated kink dominated to being phonon-drag dominated. Thus, the flow stress gradually becomes not governed by the mobility of screw dislocations (as determined by the critical resolved shear stress), giving rise to the weak temperature sensitivity of the flow stress. A dislocation mechanism map in the temperature-size space is proposed to further illustrate this phenomenon in tungsten micropillars.

1. Introduction

A number of experiments have demonstrated that the flow stress in all body-centered cubic (bcc) crystals decreases sharply as the test temperature is increased. This behavior is observed up to a critical temperature, above which the flow stress becomes *athermal* [1–3]. This phenomenon is generally attributed to a fundamental mechanism that controls dislocation motion in bcc crystals. Kink pairs, at temperatures below a critical value, must be nucleated on the non-planar core structure of screw dislocations by overcoming an energy (Peierls) barrier. Subsequent migration of nucleated kinks leads to overall dislocation motion. In addition to the key influence of the particular symmetric bcc crystal structure, several other factors have been found to affect the extent of the strong temperature dependence. Crystal purity, the polycrystalline nature of large-size samples, and the loading orientation have been shown to influence the temperature dependence of the flow stress. Tungsten, as a prototypical bcc metal, offers great potential for ultra-high temperature applications, such as in magnetic fusion energy devices, plasma-facing components [4], and space electric propulsion. As a representative bcc crystal, the plastic behavior of bulk tungsten is known to be strongly temperature sensitive, and is thus a good candidate for understanding the temperature dependence of the flow stress at sub-micron sizes.

Recent studies on the plasticity of bcc crystals in the micro- and nanometer size range revealed that the limited sample size usually contributes to new features of the plastic behavior. For example, plastic flow becomes size dependent, and the stress–strain relationship exhibits discrete strain bursts instead of the smooth and continuous plastic flow, characteristic of polycrystals [5–7]. An interesting question is whether the temperature will still have the same strong influence on the flow stress in small volumes, as is the case in conventionally large specimens. Coupling effects between temperature and sample size on the plastic deformation and the underlying dislocation mechanisms are thus of great interest. Investigations on these problems will shed light not only on our understanding of submicron plasticity in bcc crystals, but will also provide guidance on improving the mechanical properties of

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thermomechanical devices through control of the crystal size and structure.

Due to the particular symmetry of the bcc crystal structure and the complex dislocation core transformations induced by the applied stress [8,9], the plastic behavior of bcc metals is much more complicated than that of fcc metals. Thus, the deformation mechanisms of bcc crystals are still relatively poorly understood [10,11]. To reveal the plasticity behavior of sub-micron bcc crystals, micropillar compression and tension tests are recently widely used. The focus of such experiments is generally on the size effect, the strain burst behavior, the anomalous slip, the comparison with fcc crystals, and the possibility of mechanical annealing [6,7,12–14]. Some researchers have also investigated the surface orientation effect [15], and the hydrogen embrittlement behavior [16]. Nevertheless, the vast majority of experimental investigations on submicron bcc crystals are carried out at room temperature. Only recently, Schneider et al. compared the size effect of bcc Mo micropillars at room temperature to that at elevated temperatures [17]. Although the influence of external size on the temperature dependence of plasticity is not explicitly studied in that work, the limited experimental results (see Fig. 3(a) in Ref. [17]) still imply the interesting trend that the temperature sensitivity seems to decrease with reduction of the sample size. Till now, little attempt was made to systematically clarify the coupled effects of sample size and temperature on the plasticity of bcc crystals.

The method of Discrete Dislocation Dynamics (DDD) has proven to be a powerful approach for revealing the deformation mechanisms and the mechanical response of submicron crystals [18–22]. It offers the unique advantage that the conditions of the simulation can be controlled very precisely, and can be directly compared to experiments at the same size and length scale. By incorporating the insights gained from atomistic simulations, the specific features of bcc plastic flow have been successfully captured with DDD simulations, such as the non-Schmid effect, the twinning/anti-twinning and the tension/compression asymmetries, etc [23–26]. Therefore, the size effect on the temperature dependent flow stress in small scale bcc crystals is explored in this work using our recently improved atomistically informed DDD model [27].

The paper is organized as follows. In the next section, we provide a brief description of our DDD simulation method. In section 3, the computer simulation results are presented and compared with available experimental data. Then, the combined influence of sample size and temperature on the flow stress is presented. The reason why the small size of micro pillars influences the temperature dependence of the flow stress is analyzed in section 4. A preliminary dislocation mechanism transition map, influenced by sample size and temperature is then proposed in section 5. Concluding remarks are finally given in section 6.

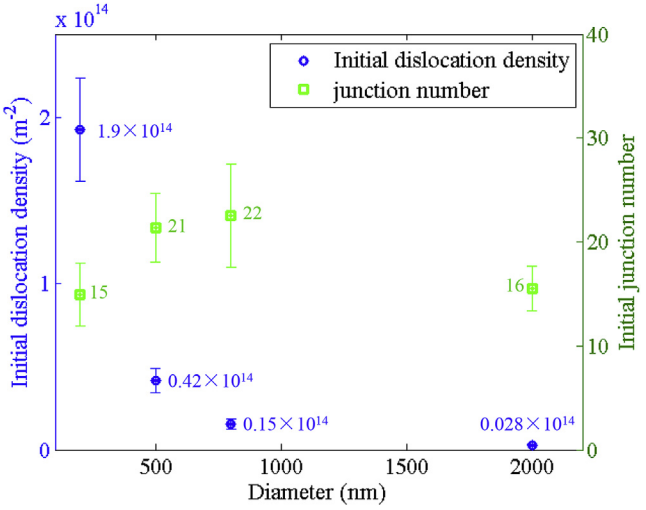

Fig. 1. The initial dislocation density (labeled near the point) and initial number of dislocation junction after relaxation.

2. Computer simulation setup

The DDD method used here has been described in detail in our previous papers [19,28,29]. In this model, dislocation loops of arbitrary shape are split into contiguous curved segments. These, in turn, are discretized into a succession of parametrized cubic splines containing a set of Gauss integration points. The elastic field (stress, strain, and displacements) are all obtained by a fast sum method [28], assuming that dislocations are in an infinite medium. The topology of all dislocations updates every time-step to deal with dislocation junction formation, annihilation, and the occurrence of cross slip. The boundary conditions and image force effects of finite geometry of any shape are considered by utilizing the superposition principle of Eshelby [30]. The finite element method makes boundary corrections to the elastic filed of dislocations in an infinite medium [19]. The resulting computational method is implemented in the open-source C++ computer program: Mechanics Of Defect Evolution Library (MODEL) [31].

An atomistically-informed dislocation mobility law for bcc crystals is used here [27]. Since dislocation mobility is significantly different for screw and edge dislocations, the velocity v_m of an arbitrary mixed dislocation segment is calculated by separating the edge and screw components, and the total velocity is written as,

$$v_m = v_e \cdot w(\theta) + v_s \cdot (1 - w(\theta)) \tag{1}$$

where θ is the angle between the dislocation tangent direction and the Burgers vector direction. $w(\theta)$ is dimensionless weigh function with properties $w(0)=0$, and $w(\pi/2)=1$. Here, $w(\theta)$ is taken as $sin^2\theta$ [27]. Note that the choice of $w(\theta)$ does not qualitatively affect the results presented in the article. The velocity of the edge component, v_e, is determined by the total force acting on it divided by the viscous drag coefficient.

$$v_e = \frac{\tau_{rss} b}{A_e T} \tag{2}$$

where τ_{rss} is the resolved shear stress, which includes the Peach-Koehler (PK) force due to the applied stress and other defects, the self-force, as well as the boundary image force. A_eT is the drag coefficient of an edge dislocation, T is the test temperature, and A_e is a phonon drag constant. For screw dislocations, kink nucleation and motion is taken into account through an Arrhenius-type equation of the form,

$$v_s = \frac{\tau_{rss} b}{A_s T} \exp\left(-\frac{\Delta G}{k_b T}\right) \tag{3}$$

where the Gibbs free energy for kink pair nucleation, ΔG, is given by the phenomenological relations [32],

$$\Delta G(\sigma, T) = \Delta H(\sigma) - T\Delta S \tag{4}$$

$$= \Delta H_0 \left[\left(1 - \left(\frac{\tau^\alpha}{\tau_P}\right)^p\right)^q - \frac{T}{T_c}\right] \tag{5}$$

where v_s is the screw dislocation velocity, T_c is a critical temperature, above which motion is no longer controlled by kink pairs and