8.6 EFFECTS OF TEMPERATURE ON THE FLOW STRESS AND POST-YIELDING HARDENING OF TUNGSTEN MICROPILLARS — Y.N. Cui, G. Po, N.M. Ghoniem (University of California, Los Angeles)

OBJECTIVE

This work is aimed at developing an effective simulation method to capture the mechanical response and microstructure features of BCC crystals; revealing the underlying dislocation mechanisms of temperature dependent plastic behavior and the small size effects on these mechanisms.

SUMMARY

A powerful simulation method is developed to reveal the BCC crystal plastic deformation mechanisms. The obtained simulation results are shown to be consistent with available experimental results. In addition, a systematic study is carried out to reveal the new features and mechanisms of plastic flow in tungsten micropillars as a function of temperature.

PROGRESS AND STATUS

Introduction

Tungsten offers great potential for applications in magnetic fusion energy devices. As a representative BCC crystal, the plastic behavior of bulk tungsten is strongly temperature sensitive. A number of experiments have demonstrated that the flow stress sharply decreases at high temperatures[1]. At the same time, at submicron scales, limited sample size usually contributes to new features of the plastic behavior, such as the widely observed size effect of flow stress and strain bursts [2]. An interesting question is whether the temperature effect on the flow stress and post-yielding behavior will be influenced by the small sample size. The relationship between size dependence of plastic deformation and the underlying dislocation mechanisms is also of great interest. Investigations on these problems will shed light not only on our understanding BCC submicron plasticity, but will also provide guidance on improving the mechanical properties of tungsten devices through alloying and material processing.

Simulation Set-up

Dislocation Dynamics (DD) simulations, as a powerful approach to reveal the mechanical response and deformation mechanisms, is used here to investigate this problem [3]. An atomistically informed dislocation mobility law for BCC crystal is developed, which can capture both the twinning/anti-twinning and the tension/compression asymmetries. A series of DD simulations are carried out on [001]-oriented W micropillars subjected to uniaxial tension loading under temperatures ranging from 150 K to 900 K.

Results

To validate simulation results, the calculated 0.2% yield strength for W micropillars with diameters ranging from 200 nm to 800 nm at room temperature is first compared with experimental data [2]. Good agreement can be observed, as shown in **Figure 1**. In addition, many experimental observations are well reproduced, such as the tension-compression asymmetry.

Then, a systematic study is carried out to reveal the influence of temperature on the plastic deformation of W micropillars. In the following, only the simulation results for a micropillar with 500 nm diameter are given here as an example. Comprehensive results will be detailed in a separate publication. Figure 2 presents typical engineering stress-strain relationships. For each temperature, the results with three different initial dislocation configurations are given. Even though the results exhibit significant stochastic signature of plastic flow, the temperature effect on the flow stress can still be observed, which is qualitatively similar to that in bulk BCC crystals. Moreover, there is no pronounced strain hardening for the considered strain range.

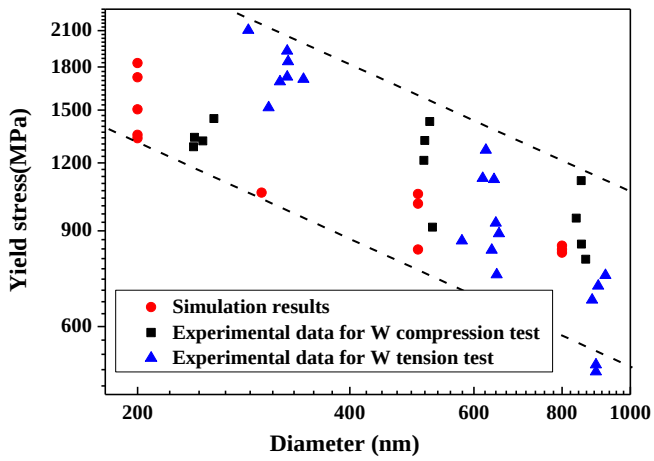

Figure 1. Comparison of the 0.2% offset yield stress for W micropillars between experimental data [2] and the present simulation results at room temperature.

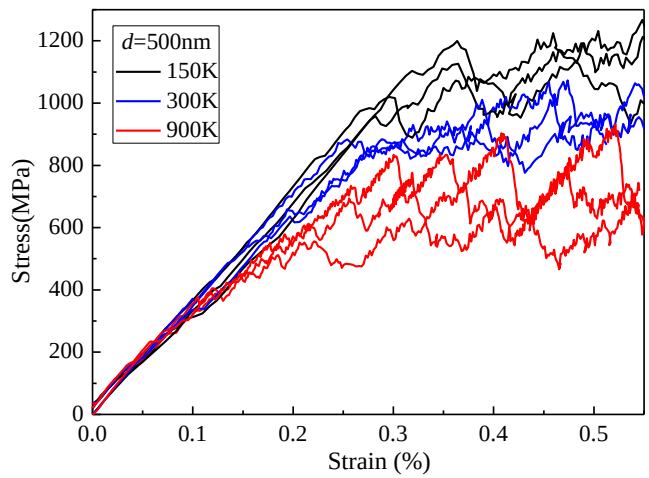

Figure 2. Stress-strain relationships during tension tests of tungsten micropillars with diameter 500 nm at different temperatures.

In order to gain insight into the underlying dislocation mechanisms, close examination of the dislocation configuration evolution is carried out. Two typical dislocation configurations are given in Figure 3. As expected, only at low temperatures, long screw dislocations can be observed due to their low mobility. When the temperature is higher than the athermal temperature (800 K), however, dislocation lines are curved, and mainly have mixed screw-edge character. In addition, single arm sources (SAS) also exhibits different features, as the temperature is raised. At low temperatures, the SAS operates mainly by the bowing out of the mixed part of the dislocation. After it interacts with the free surface, a long screw dislocation will be left inside the pillar. In Figure 4 (d-f), the evolution of the dislocation segment GH reflects this process. This is very similar to the experimental observation in Fe [4]. By way of contrast, in the case of high temperature, the SAS acts similar to half of a Frank-Read source, just like in an FCC micropillar.

The pinning points of these SAS are generally formed by dislocation junctions or jogs. In a BCC crystal, another kind of pinning point is also widely observed. This is the cross kink (see Figure 3) pinning point, which is caused by the cross slip of a screw segment of the dislocation. At low stress, such cross kink has only a short lifetime, because of the quick annihilation at the surface. However, at high stresses, cross kinks can further cause dislocation self-multiplication. As shown in Figure 4 (a-c), a cross kink ABC is first formed with the dislocation segment AB on the (011) slip plane, and segment BC on the slip plane. Under

the combined effects of the applied stress and the dislocation interaction stress, the nearly edge part of the dislocation bows out, as indicated by the arrows in Figure 4(b), until some dislocation segment annihilates from the free surface. Note that the dislocation segment near point B in Figure 4(c) is not very smooth, because cross slip occurs when the dislocation glides close to the free surface. Such kind of surface cross slip is also observed by Rao and Hussein et al. [5, 6] in FCC crystal. Moreover, this self-multiplication process shown in Figure 4(a-c) is also consistent with previous Molecular dynamic and dislocation dynamic simulation results [7].

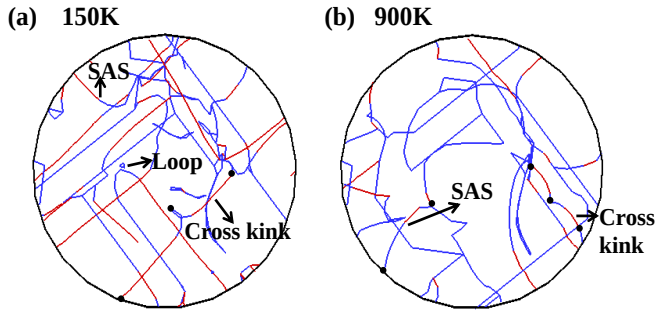

Figure 3. Dislocation configurations at different temperatures: (a) T=150 K and (b) T=900 K, respectively from the top view. Screw dislocations are indicated in red, while mixed dislocations are in blue.

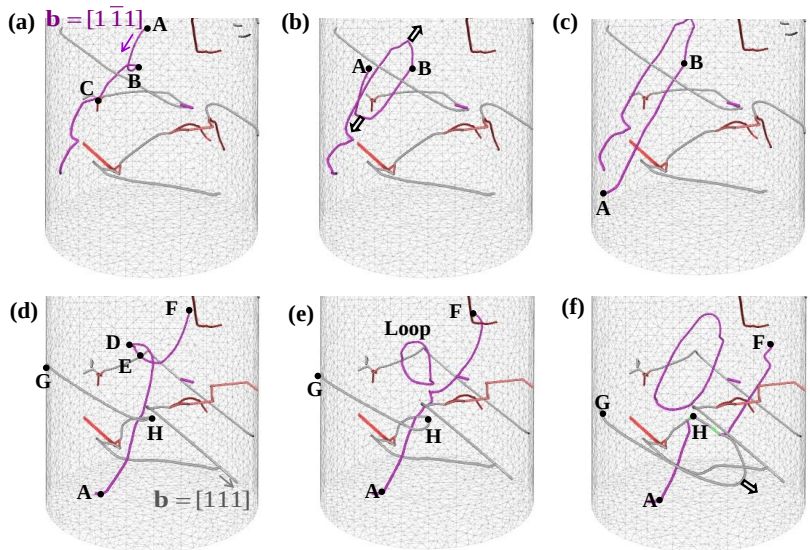

Figure 4. Snapshots of dislocation configurations showing the dislocation self-multiplication process in a W micropillar at 150 K, when the engineering strain is between 0.42% and 0.47%. Hollow arrows indicate the dislocation motion direction. Different colors in the figure are used to represent different burgers vectors, grey=(111), purple= $(1\bar{1}1)$, orange= $(11\bar{1})$, red= $(1\bar{1}\bar{1})$

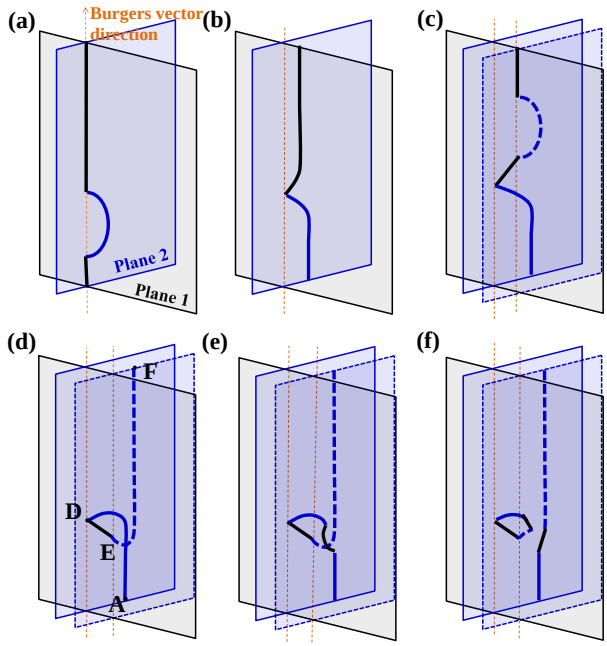

Figure 5. Schematic showing the dislocation loop formation mechanism by multiple crosses slip. The thick lines represent dislocation lines, whose colors indicate their slip planes as indicated in (a).

Interestingly, a new kind of self-multiplication mechanism is also revealed in our simulations as shown in Figure 4(d-f). The dislocation multiplies through forming a large dislocation loop. Figure 5 further schematically shows the formation process of the dislocation loop. After some amount of deformation, many relatively long screw dislocations are left in the BCC crystal. After one dislocation segment cross slips, a cross kink can be formed as shown in Figure 5(b). Then, another cross slip occurs because of the complex internal stress field induced by other dislocations. The upper-side mixed part of the dislocation in Figure 5(c) quickly bows out and forms the dislocation configuration, as shown in Figure 5(d), which exactly corresponds to the dislocation segment ADEF in Figure 4(d). Here, the dislocation segments DE and AD belong to two parallel slip planes, while segment DE belongs to the (011) slip plane. After another cross slip occurs, as shown in Figure 5(e), a dislocation loop is generated. Note that when the formed dislocation loop is small, it does not expand under the instantaneous stress level, as shown in Figure 3(b). This dislocation loop formation mechanism can also explain the reason why many dislocation loops and debris are experimentally observed in deformed BCC crystal.

References

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