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.

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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
5 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
10 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
15 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
20 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
25 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
30 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 thermomechanical devices through control of the crystal size and structure.

Due to the particular symmetry of the bcc crystal structure and the complex
35 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
40 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
45 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 [17]) still imply the interesting trend that
50 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
55 response of submiron 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

60 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
65 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
70 dislocation mechanism transition map, influenced by sample size and temperature is then proposed in section 5. Concluding remarks are finally given in section 6.

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
75 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
80 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 field of dislocations in an infinite medium
85 [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,

$$v_m = v_e \cdot w(\theta) + v_s \cdot (1 - w(\theta)) \quad (1)$$

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.

$$v_e = \frac{\tau_{rss}b}{A_eT} \quad (2)$$

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,

$$v_s = \frac{\tau_{rss}b}{A_sT} \exp\left(-\frac{\Delta G}{k_bT}\right) \quad (3)$$

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

$$\Delta G(\sigma, T) = \Delta H(\sigma) - T\Delta S \quad (4)$$

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

90 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 phonon drag dominates, k_b is Boltzmann's constant, ΔH_0 is the activation enthalpy at zero stress. Also, p and q are two constants reflecting the shape of the Peierls potential, which can

be determined by atomistic simulations and experimental data, τ_P is Peierls stress, τ^α is an effective resolved shear stress (rss) , which takes non-Schmid effects into account[33], and is given by:

$$\begin{aligned} \tau^\alpha = & \boldsymbol{\sigma} : \mathbf{m}^\alpha \otimes \mathbf{n}^\alpha + a_1 \boldsymbol{\sigma} : \mathbf{m}^\alpha \otimes \mathbf{n}_1^\alpha + \\ & a_2 \boldsymbol{\sigma} : (\mathbf{n}^\alpha \times \mathbf{m}^\alpha) \otimes \mathbf{n}^\alpha + a_3 \boldsymbol{\sigma} : (\mathbf{n}_1^\alpha \times \mathbf{m}^\alpha) \otimes \mathbf{n}_1^\alpha \end{aligned} \quad (6)$$

where $\boldsymbol{\sigma}$ is the total stress tensor, including the contribution from the Peach-Koehler force, dislocation interaction stress and the image force. $\mathbf{n}^\alpha$ is the slip plane normal vector, $\mathbf{m}^\alpha$ is the slip direction, $\mathbf{n}_1^\alpha$ is the unit normal to the $\{110\}$ plane in the $\mathbf{m}^\alpha$ -zone that makes a 60° angle with the slip plane [33]. The second term on the right hand of Eq. 6 represents the contribution of twinning/anti-twinning asymmetry and the third and fourth terms account for the loading compression/tension asymmetry. a_1 , a_2 and a_3 are non-Schmid material parameters that determine the effects of each non-Schmid stress component on dislocation glide. Their values are determined by atomistic simulations and experiments [27].

In this study, a series of DDD simulations of tension test are performed on W single crystal micropillars with diameters in the range 200-2000 nm. For all studied samples, the aspect ratio of height h to diameter d is fixed to 2. Tensile loading along the $[001]$ direction is applied in order to achieve multi-slip conditions. Only glide on $\{110\}$ slip planes is considered. The sample temperature is varied in the range 150-900 K. W is approximated to be elastically isotropic, and the following materials properties are used: shear modulus $\mu = 161$ GPa, Poisson's ratio $\nu = 0.28$, $p=0.86$, $q=1.69$, $a_1 = 0.938$, $a_2 = 0.71$, $a_3 = 4.43$, $\Delta H_0=1.63\text{eV}$ [34, 35], $\tau_P=960\text{MPa}$, which is obtained by extrapolating the experimental data for high purity W single crystal[36], $A_e = 3.3 \times 10^{-7}(\text{Pa}\cdot\text{s}/\text{K})$, and critical temperature $T_c = 800\text{K}$.

Initial equilibrium dislocation configurations are generated through the relaxation of randomly distributed dislocation loops without external loading until further dislocation activity is not noticeable. Dislocation junctions emerge as

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

a natural outcome of dislocation interactions without artificially enforcing pinning points. The initial dislocation density is higher for pillars with smaller diameter. This is designed in order to generate comparable number of initial dislocation junctions in small pillars with that in large pillars. For each sample size, multiple different initial dislocation configurations are used in DDD simulation. Quantitatively, after relaxation, the initial dislocation density and the initial number of dislocation junctions used in the simulations are plotted in Fig. 1, where the points are the averaged values over multiple simulations for the pillar with each diameter, and the error bar is the standard deviation.

The applied strain rate was equal to 10^4 s^{-1} . Even though it is higher than the experimental value, the steady-state flow stresses are found not to be sensitive to the strain rate [14], which is also verified by comparing our simulation results with experimental data as will be discussed below.

3. Temperature and size dependent flow stress

Typical tension test stress-strain curves for various sample sizes of W micropillars at different temperatures are plotted in Fig. 2. For each size, the re-

Figure 2: Stress-strain curves for micropillar tension test under different temperatures with diameter (a) 200 nm, (b) 500 nm, (c) 800 nm and (d) 2000 nm

sults corresponding to the same initial dislocation configuration are presented at different temperatures to avoid the influence of the initial dislocation structure on the results. It is clear from the figure that, regardless of test temperature, all pillars with diameter smaller than 2000 nm exhibit elastic loading followed by significant serrated stress oscillations, which is consistent with experimental observations [7]. In addition, for large sample sizes, significant temperature effects of the flow stress are easily observed, similar to the behavior of bulk specimens. Surprisingly, however, this temperature dependency almost vanishes when the sample size is roughly smaller than 200 nm.

Before disclosing the physical origin of this interesting phenomenon, our simulation results are first compared with available experimental results to validate their effectiveness. Since most experimental investigations focus on the size effect on the flow stress at room temperature, the yield strength for micropillar ($d < 1000$ nm) at room temperature are first evaluated and compared with experiments[6]. This yield strength is defined as the 0.2% offset yield point $\sigma_{0.2}$,

Figure 3: Comparison of the yield strength of W micropillars with experimental data [6] at room temperature. Note the scatter in the data, which is inherent in the plasticity behavior of small size samples.

as is standard in engineering stress-strain relationships of bulk samples. Fig. 3 compares the calculated 0.2% offset yield stress and available experimental data at room temperature, showing generally good agreement. Up till now, systematic experimental studies of the plastic deformation of W micropillars at low and elevated temperatures are not available. However, several experimental studies pointed to the diminished size dependence of the flow stress, as the normalized temperature is decreased[17, 37]. Such inspiring investigations make it possible to reveal the temperature-influenced size effect on the flow stress. This is achieved by directly comparing yield strength data of different BCC metals at room temperature, since the critical temperature is material dependent, and room temperature would correspond to different homologous temperatures. As shown in the logarithmic plot in Fig. 3, the size effect can be expressed as a power law relation, $\sigma_{0.2} = Ad^n$, where d is the pillar diameter, and A and n are fitting parameters. According to the present computer simulation results, the calculated power law exponent n can be plotted in Fig. 4 as a function of the temperature normalized by the critical temperature. This normalized temperature T/T_c actually reflects the extent of how screw dislocations influence

the plastic behavior. When $T/T_c > 1$, namely the temperature is higher than
170 the critical temperature, screw dislocations have similar mobility to edge ones.
This implies that the dislocation behavior in BCC crystals becomes similar to
that of FCC crystals. According to previous studies[5], the power law exponent
for FCC crystals was found to be about -0.6, as indicated by the dotted line
in Fig. 4. As expected, the calculated power law exponent at a temperature
175 900 K ($> T_c$) is -0.59, which is close to -0.6. By contrast, as T/T_c decreases,
the absolute value of the power law exponent decreases. Quantitatively, as T
changes from 600 K to 300 K and further to 150 K, n varies from -0.51, to -0.42
and to -0.09, respectively. This implies that the size effect becomes weaker at
lower normalized temperatures. This is consistent with the experimental results
180 of Schneider and coworkers[17, 38, 39], as plotted in Fig. 4. The deviation of
the simulation and experimental results may be associated with the exact defi-
nition of the yield strength and also variations in the initial dislocation density.
Moreover, the experimental results are corresponding to compression test, while
the simulation are corresponding to tension test. According to Kim et al.’s work
185 [6], the size effect seems stronger for tension test compared with compression
test for W micropillar at room temperature.

Comparison of the computer simulation results with the experimental data
indicates that the simulations are reliable, and that further predictions can be
made based on computations alone. In the following, results of simulations
190 will focus on revealing the interplay between sample size and temperature in
determining the flow stress and post-yield hardening in bcc micropillars. To
quantitatively make this determination, it is valuable to first compare the yield
stress at different temperatures for various pillar sizes. Considering that the
stress-strain curve for submicron crystals displays strong statistical fluctuations
195 (see Fig. 2), and that the yield stress is greatly influenced by the initial dis-
location microstructure, an averaged yield stress is obtained. This is done by
simulations of various realizations for each micropillar size and test temperature,
and then calculating the 0.2 % offset yield stress corresponding to the averaged
stress-strain curve. As shown in Fig. 5, the strong stress oscillations almost

Figure 4: Dependence of the yield strength power law exponent on test temperature. The experimental data are from the work of Schneider et al. [17, 38, 39]. The loading orientation is labeled near the data points

Figure 5: An example showing the method of defining the flow stress of a micropillar with diameter of 200 nm at $T=300\text{K}$. The flow (yield) stress corresponds to the intersection between the dotted line (drawn parallel to the elastic line), and the thick stress-strain curve representing average behavior from several statistical realizations.

Figure 6: The dependence of the flow (yield) stress on temperature for various sample sizes. Note the insensitivity of the flow stress to test temperature when the sample size is small (e.g. 200 nm).

smooth out into a continuous curve. Since the smaller the pillar size, the more significant the stochasticity is, more simulations are carried out to obtain the averaged data for smaller pillars.

The calculated averaged results are summarized in Fig. 6, together with the 0.2 % offset yield stress obtained experimentally for bulk tungsten [2]. Since it is generally accepted that the flow stress is highly orientation dependent [1], the experimental results also correspond to the [001]-orientation tension test, which is the same as the simulation set-up. Figure 6 clearly illustrates the combined temperature and size effects on the yield stress. As the sample size decreases, the temperature sensitivity of the yield stress becomes weaker. For small pillars, the yield stress almost exhibits no temperature dependence. Note that the flow stress for pillars with diameter 2000 nm at 150 K seems somewhat higher. This is on the one hand related to the weak size effect at low temperatures (see Fig.4). On the other hand, a relatively lower initial dislocation density is used when simulating the larger sample (see Fig. 1), in order to generate a comparable number of initial dislocation junctions in pillars with different sizes. This may contribute to the high flow stress.

4. Weak role of screw dislocation at small scale

It is natural to ask what controls the temperature sensitivity. For bulk BCC crystal, the strong temperature sensitivity of flow stress is always attributed to the thermally-activated overcoming of lattice resistance. It directly manifests itself through significantly different screw dislocation mobility at different temperatures. Thus, different stress levels are required to maintain the required plastic flow. Based on this opinion, the weak temperature dependence at small scale implies that the role of screw dislocation becomes less pronounced. The following analysis is aimed at verifying this point of view.

4.1. Limited screw dislocation storage ability

Small sample size generally means higher probability of dislocation surface annihilation. In FCC crystal, this can contribute to significant decrease of dislocation density, even causing mechanical annealing for deep submicron crystal[40, 41]. However, recent experiment and simulation results [6, 42] suggest that it is relative difficult for bcc crystal to reach such kind of dislocation starvation trend. Generally, numbers of dislocations are left after deformation. This feature is also well reproduced by our simulations (see Fig. 7). Then, of special interest is the question whether most of the remaining dislocations are of a screw character similar to that in the bulk bcc crystal. To answer this question, some typical dislocation configurations corresponding to engineering strain 0.4% are given in Fig. 7. The screw dislocation is distinguished from mixed dislocations by using different colors. Here, one dislocation segment is recognized as a screw one, if the angle between its tangent direction and Burgers vector direction is smaller than 15° . Fig. 7 clearly shows how temperature and size influence the structure and amount of screw dislocations. In the case of low temperature and large size, numbers of elongated straight screw dislocations are observed and they dominate the plastic behaviour. In contrast, for small sample or under high temperature, only small amount of short screw dislocations are observed.

Figure 7: Dislocation configurations in micropillars with different sizes at different temperatures when the engineering strain is 0.4% from the top view. Screw dislocations are indicated in red, while mixed dislocations are in blue

To explore it further, the fraction of screw dislocation density among the total dislocation density is calculated. In order to give a sense to the statistic representation, the result for each diameter and temperature in Fig. 8 (a) is the average over several realizations with different initial dislocation configurations. It clearly indicates that decreasing the sample size has the similar influence of increasing the temperature on decreasing the storage ability of screw dislocation. For clarity, the averaged percent value of screw dislocation density during the deformation stage $\epsilon > 0.2\%$ is further evaluated and plotted in Fig. 8 (b). The dash dotted line represents the statistic value of the fraction of screw dislocation density if dislocations randomly orients in the slip plane, which is related to the screw dislocation definition and is calculated as $15^\circ \times 4/360^\circ$ here. Fig. 8 (b) demonstrates that the role of screw dislocation quickly become less important as the external size decreases even at low temperature. Similar phenomenon is also observed experimentally. Cheng et al. find that in nanocrystalline bcc Mo, mixed dislocations gradually becomes the dominated type of dislocation with reducing grain size[43].

This phenomenon can be further understood from two aspects. One is that

Figure 8: (a) Evolution of the percent of screw dislocation density for W micropillar with different sizes at different temperatures. The results are averaged over multiple simulation realizations. (b) Averaged percent of screw dislocation density during the deformation stage $\varepsilon > 0.2\%$

even though the screw dislocation at low temperature has low mobility, its lifetime is still short due to the limited glide free path at small scales. For example, some mixed dislocations may directly glide out of the crystal without forming long screw dislocations, or the screw dislocation is close to a free surface, and is easy to leave the crystal with the aid of the attractive image force. The other is that the mobility of screw dislocation is also strongly influenced by the high flow stress at small scales, which is analysed in detail in the following section.

4.2. High stress enhances screw dislocation mobility

In the case of low temperature, the movement of screw dislocation is always assisted by the thermally-activated kink-pair mechanism. As stress increases, less thermal energy is needed to overcome the Peierls potential [37, 44]. Physically speaking, the increase of yield strength will contribute to the decrease of activation volume V for the thermally activated kink pair nucleation [37, 45],

$$V = bh\lambda^* \quad (7)$$

$$\lambda^* = \left(\frac{\mu b h}{8\pi\tau_a} \right)^{1/2}$$

where b is burgers vector, h is kink height, λ^* is the separated distance of kink pair, τ_a is applied resolved shear stress. The smaller the activation volume,

the less the thermal energy the screw dislocation motion requires. Thus, if
275 the applied stress is high enough, almost no thermal energy is required. The
screw dislocation mobility becomes equal to that of edge dislocation, such as
the atomistic simulation results by Huang et al.[13]. Then, dislocation velocity
will be controlled by dislocation interaction with elastic waves and damping
resulting from momentum loss. The critical stress for this transition at different
280 temperatures can be estimated by the screw dislocation mobility law. From
Eq. 2 and Eq. 3, the critical stress can be calculated by approximately setting
 $\Delta G = 0$. The active glide planes are taken to be the $\{110\}$ family of planes,
resulting in Schmid factors of 0.4082 for $[0\ 0\ 1]$ orientation. If the non-schmid
effect is not taken into account. The calculated stresses are plotted as blue
285 dotted line in Fig. 6. Actually, this is the lower bound of the critical yield stress,
because it actually neglects the dislocation interaction stress and image stress.
For the bulk W, the flow stress is even much lower than this lower bound of
the critical stress. This suggests screw dislocation will control the plastic flow,
which is consistent with the experimental observation that many long screw
290 dislocations are widely observed after yielding [46]. For small micropillars, the
yield stress value can reach a much higher value than this lower bound critical
value. As a result, it is possible that the difference of screw and edge dislocation
mobility almost disappears after yielding, and thus the influence of temperature
on the screw mobility nearly vanishes. This can to some extent explain why
295 the stress-strain curves at $T=600\text{K}$ are close to those at $T=900\text{K}$, and why the
temperature dependence vanishes for small samples (see Fig. 2 and Fig. 6).

Actually, the weak screw dislocation role at small scales also implies weak
strain rate sensitivity. Interestingly, recent experiments find that when the di-
ameter of bcc iron micropillar changes from 1000nm to 200nm, the strain rate
300 sensitivity is indeed reduced by an order [47]. This is also one reason for the
good consistence between experimental data and simulation results using rel-
ative high strain rate. The strain rate sensitivity at submicron scales will be
further investigated in our future work.

5. A dislocation mechanism map

305 The analysis presented above suggests that, at small sample size, even when
the test temperature is lower than the critical value, a mechanism transition
from a kink-pair controlled motion to a phonon drag dominated motion will
occur. This must happen, due to the limited external size and “the smaller
is stronger” trend, as is schematically shown in Fig. 9. In the phonon drag
310 dominated zone, the dislocation behavior is similar to that of FCC crystals.
Accordingly, it is reasonable to propose that, with the reduction of the sam-
ple size, the dominant dislocation mechanism changes from dislocation forest
hardening (with extensive dislocation-dislocation interactions), to a single-arm
source mechanism as a result of surface truncation (see Fig. 7(d)). This is
315 verified by the present simulation results of dislocation configuration evolution.
Meanwhile, simulation results indicate that multiple dislocation sources can
simultaneously operate at the same time in large samples, while only one dislo-
cation source operates intermittently in small samples, leading to the occurrence
of pronounced strain bursts. Note that the role of cross slip is more important
320 in BCC crystals, because of the more available cross slip planes. Thus, many
dislocation loops are formed after multiple cross slip events, as can be seen in
Fig. 7(f) and (h).

In contrast, in the kink dominated regime, plastic deformation is dominated
by the motion of screw dislocations, which is assisted by the formation of kink-
325 pairs. Close examination of the simulation results illustrates several types of
dislocation multiplication mechanisms, as indicated in Fig.10. The detailed
evolution processes for each mechanism are schematically summarized in Fig.11.
In Fig.11 (c), well-known dislocation sources induced by junction formation are
shown, exhibiting a half-track-field-like geometry. The other types of dislocation
330 multiplication mechanisms are assisted by the occurrence of cross-slip. Consid-
ering a long screw dislocation with the indicated Burgers vector, one cross-slip
event occurs via kink pair nucleation on the cross-slip plane. If another kink
pair nucleates on the original slip plane, and they migrate towards each other, a

Figure 9: Dislocation mechanism map of BCC crystals, as a function of sample size and test temperature.

cross-kink forms[12], as shown in Fig.11 (b). In the current simulation, one dis-
 335 location segment is identified as a kink if it has the same Burgers vector and slip
 plane as its connected dislocation lines, but is much shorter than its connected
 long dislocation lines. The minimum length of the kink that can be resolved in
 the simulation is $40b$, where b is the magnitude of burgers vector. Note that the
 atomic sized kink mechanism is indirectly considered in the mobility law. The
 340 two arms of the cross-kink generally have different glide velocities, leading to
 the motion of their intersection point. In the case of low stress and limited size,
 this intersection point may annihilate at the free surface, as indicated in Fig.11
 (d). However, if the stress is high enough, dislocation multiplication occurs due
 to the bowing out of the two arms (see Fig.11 (f)). This is also observed in
 345 previous molecular dynamics simulations [42]. This mechanism is termed "self
 multiplication", and is widely used to explain why dislocation starvation is sel-
 dom observed in small BCC samples [13]. Our simulation results suggest that
 dislocation jogs can also serve as active dislocation sources, and can induce sig-
 nificant dislocation multiplication. This connection between jogs and dislocation
 350 multiplication was also experimentally reported in Nb and Fe over a wide range

of temperatures [48–50]. Such jogs are generally formed by multiple cross slip events (see Fig.11 (e)). The fate of dislocation segments around a jog depends on the jog length y [51]. If the difference between the applied resolved shear stress τ_a and lattice friction stress τ_f is lower than the interaction stress between segments separated a distance y , namely: $\tau_a - \tau_f < 0.25\mu b / [2\pi(1 - \nu)y]$, these
 355 dislocation segments cannot pass each other. Then, dislocation dipoles form, as illustrated in Fig.11 (g). Otherwise, they operate independently, similar to single arm sources (SAS, see Fig.11 (i)). On the other hand, the occurrence of
 360 another cross-slip event will cause recombination between the two arms, giving rise to a closed prismatic loop. Therein, and as shown in Fig.11 (j) and (k), small loops are left in the sample as debris, while larger loops may expand as a new multiplication source driven by the applied stress.

Figure 10: Typical dislocation configurations at 150 K when the applied stress is 1.1 ~ 1.2 GPa for W micropillars with (a) $d=200$ nm, (b) $d=500$ nm, (c) $d=800$ nm and (d) $d=2000$ nm. Salient dislocation mechanisms are marked by letters, including (C) pinning on a dislocation tangle, (F) cross kink multiplication, (I) pinning on super-jogs, (K) loop expansion, (G) dislocation dipole, and (J) debris loops. Different colors in the figure are used to represent different Burgers vectors, grey= (111) , purple= $(1\bar{1}1)$, orange= $(11\bar{1})$, red= $(1\bar{1}\bar{1})$. Some of the blue numbers in (b) and (c) indicate the slip planes.

In all simulated micropillars, such as those typically shown in Fig.10, when

Figure 11: Schematic showing the mechanisms of dislocation multiplication, debris formation, and dipole formation in BCC crystals at low temperature. The black dislocation lines are in plane 1 and the blue ones are in plane 2

the diameter is less than 200 nm, the most frequent observed multiplication
 365 mechanism is the single arm source around a dislocation junction. According
 to Fig. 1, even though the initial dislocation density in the pillar with diameter
 200 nm is much higher than that in larger pillar, the initial dislocation junction
 number is still relatively small. Thus, the reason that the dislocation junction
 mechanism is widely observed in small samples should not be artificially induced
 370 by the initial dislocation configuration. It can be understood in terms of the
 limited space available for multiple cross slip events to occur, which means lower
 possibility of forming and activating the source of cross kink and super-jogs. For
 larger diameters of 500 nm and 800 nm, however, the cross kink multiplication
 and jog-induced multiplication mechanisms are also widely observed. This is on
 375 the one hand related to the pronounced surface-induced image force, which can
 promote the occurrence of cross slip and the formation of cross kinks[42], and
 on the other hand related to the high stress levels and relative large space that
 can accomodate dislocation multiplication. For larger samples with diameter
 2000 nm, during the initial deformation stage, the dominant dislocation sources
 380 are double-pinned half-loop dislocations, such as those schematically shown in
 Fig. 9. After many long screw dislocations are left inside the pillar due to their
 slow mobility, both multiple available cross slip planes and complex dislocation

Figure 12: (a) Schematic showing the common source in BCC crystals at low temperatures. The pinning point can originate from a junction, cross-kink, or a jog; (b) The critical length of the source that can be activated in bulk BCC crystals at different temperatures; (c) Schematic illustrating the influence of sample size at different temperatures in a logarithmic manner.

interactions favor the occurrence of cross slip, leading to the formation of a large density of superjogs. Thus, the jogged screw dislocation is widely observed in the following plastic flow stage, as is evidenced in Fig.10(d). In addition, even for larger samples, the flow stress at relatively low temperatures is also high, which can easily reach the criterion for dislocation multiplication around jogs. Therefore, the most frequently observed multiplication mechanism becomes the jog-induced multiplication process. This observation is also consistent with previous DDD simulation results [52], and with experimental observations [50]. Dislocation multiplication induced by loop expansion leaving plenty of dislocation debris is also observed in our simulations (such as Fig.10 and Fig. 7(c),(e))

and (g)). For larger micropillars, the motion of jogged screw dislocations results in a high density of dislocation debris, which explains why plenty of prismatic debris loops are observed in bulk W crystals[53].

Based on the analysis above, a dislocation mechanism map is presented in Fig. 9, summarizing the interplay between the sample size and its temperature in determining the source operative mechanism. The map clearly shows that both temperature and size cooperate to induce transitions between dominant dislocation mechanisms. To understand the contribution of a given mechanism transition on the extent of its temperature dependence, we consider the following argument. For a specific temperature, the size effect can be attributed to its influence on the dislocation source operation, which can be mainly understood from two aspects. One is the truncation effect on the source length, and the other is the limited available number of dislocation sources. In the following, analysis is first given from these two perspectives to show that the size effect is indeed weaker in the low temperature regime.

First, in the kink dominated regime, even though multiple dislocation mechanisms may exist, a common dislocation source character can be observed for different characteristic sizes, as plotted in Fig.12(a). Here, the pinning point may originate from a junction, cross kink, or a jog. Irrespective of these differences, the operation stress of such kind of source can be roughly estimated according to the line tension model, namely $\tau_a - \tau_f = \mu b / \lambda$, where λ is its critical length, as indicated in Fig.12 (a). Since the flow stress in bulk bcc is high at low temperatures, the critical source length can reach a small value. Fig. 12 (b) give a crude estimation of the source length that can be activated in bulk W sample, according to the fitted experimental flow stress data given by the black solid line in Fig. 6. It can be seen that when the temperature is lower than room temperature, even the bulk flow stress can activate sources with length smaller than 174 nm. Therefore, for the considered size regime in this investigation, the truncation effect induced by the external size on the source length is weaker at lower temperature.

Second, the number of pinning points is generally limited in small samples.

However, at low temperatures, in addition to pinning points induced by junctions, both cross-kinks and jogs can supply pinning points. Thus, the dislocation source density is larger in this case. The present analysis is the first to clearly establish an understanding of the experimental observations that the influence of sample size on plastic flow in BCC crystals is weak at low temperatures [17] from the viewpoint of dislocation mechanism. The trend in this anomalous size dependence of the flow stress on temperature is schematically illustrated in Fig.12 (c). Considering that the power law trend is always observed for size dependence, the two straight lines are plotted in the logarithmic schematic diagram. Fig.12 (c) clearly shows that the weaker size dependence at lower temperatures can exactly explain the weaker temperature effect at smaller scales.

6. Summary and Conclusions

Atomistically informed dislocation dynamics simulations of the tension tests of W single-crystal micropillars have been systematically carried out. The aim was to map out the combined influence of sample size and test temperature on the flow stress and operative dislocation mechanisms. The simulation results show general good agreement with available experimental data on the flow stress dependence on size and temperature, and with the experimental observations of dislocation microstructures in W. Contrary to the popular notion that bcc crystals generally have strong temperature dependence of the flow stress, in the present work we show a gradual vanishing temperature sensitivity of the flow stress as the sample size decreases. Careful analysis of the simulation results suggests that this is related to the weak role of screw dislocations at small scales, and the inability of small samples to store them. The fraction of screw dislocations decreases sharply with the reduction of sample size, even at low temperatures. At the same time, the very high flow stress in small scale bcc crystals, together with the image force effect, can greatly enhance the mobility of screw dislocations. This suggests that the mixed dislocations control the plastic response in bcc metals in the very small scale regime as against bulk

specimens. These can further result in a transition of the dislocation mobility mechanism from kink-pair dominated to phonon-drag dominated, even when the temperature is lower than the traditional critical temperature. The critical temperature for this mobility mechanism transition has been found to depend on sample size, decreasing as the size gets smaller. In addition, various dislocation multiplication mechanisms in submicron bcc crystals have been discovered. At low temperatures and small sample size, the dominant mechanisms have been found to be junction formation, cross-kink formation, and jog formation. As the size increases further, still at low temperatures, dislocation loop expansion and tangles become dominant. At temperatures above the critical value, the cross-slip mechanism participates in small sizes together with junctions, transitioning to dislocation tangles and interaction dominated behavior at larger sample sizes.

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Graphical Abstract