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## **Abstract**

Dislocation nucleation is essential to the plastic deformation of small-volume crystalline solids. The free surface may act as an effective source of dislocations to initiate and sustain plastic flow, in conjunction with bulk sources. Here, we develop an atomistic modeling framework to address the probabilistic nature of surface dislocation nucleation. We show the activation volume associated with surface dislocation nucleation is characteristically in the range of  $1-10b^3$ , where  $b$  is the Burgers vector. Such small activation volume leads to sensitive temperature and strain-rate dependence of the nucleation stress, providing an upper bound to the size-strength relation in nanopillar compression experiments.

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## Temperature and Strain-Rate Dependence of Surface Dislocation Nucleation

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Dislocation nucleation is essential to the plastic deformation of small-volume crystalline solids. The free surface may act as an effective source of dislocations to initiate and sustain plastic flow, in conjunction with bulk sources. Here, we develop an atomistic modeling framework to address the probabilistic nature of surface dislocation nucleation. We show the activation volume associated with surface dislocation nucleation is characteristically in the range of  $1-10b^3$ , where  $b$  is the Burgers vector. Such small activation volume leads to sensitive temperature and strain-rate dependence of the nucleation stress, providing an upper bound to the size-strength relation in nanopillar compression experiments.

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Small-volume materials with large surface areas have increasingly become the basic building blocks of modern technology. The mechanical properties of such surface-confined materials are drastically different from their macroscale counterparts. Recent mechanical testing of small-volume metals have measured unusually high strength, at levels of a significant fraction of their ideal strength. For example, uniaxial compression of single-crystal Au pillars with diameter 300 nm [1–3] gave flow strengths  $\sim 800$  MPa. In comparison, the predicted ideal bulk shear strength of Au is only 850 MPa to 1.4 GPa, depending on the mode of loading [4]. Since surface is itself a defect, with significantly miscoordinated atoms compared to the perfect crystal [5], it is natural to ask to what degree the strength of a small-volume material reflects surface properties and surface-mediated processes [6–8], particularly when the sample size is in the range of tens of nm [9].

Dislocation nucleation is expected to be an important factor in the deformation of small-volume materials at low temperature [1,10,11]. In macroscale materials, the density of dislocations increases rapidly once deformation starts, due to double cross slip and other Frank-Read [12] type multiplication processes. In contrast, dislocation multiplication in small-volume samples must contend with dislocation loss from free surfaces, which could lead to dislocation starvation in the bulk. It is also possible that in small-volume materials, the initial configuration does not contain a single dislocation in it [9]. Under these dislocation-starved scenarios, dislocation nucleation from the surface potentially plays a critical role in controlling plastic deformation.

Molecular dynamics (MD) simulations have often been used to probe dislocation nucleation in the bulk crystal and from the surface [13,14]. While MD simulations have revealed rich atomic-scale details of dislocation nucleation processes, they provide less quantitative information regarding plasticity in normal laboratory experiments because of the extreme strain rate ( $\dot{\epsilon} \sim 10^7-10^9/s$ ) applied. A natural question to ask is: to what degree does the MD

result reflect real deformation physics in laboratory experiments where the strain rate is typically  $<1/s$ . To understand the nature of surface nucleation, and to enable quantitative correlations between MD and experimental results, here we take a related but different approach that combines transition state theory and detailed atomistic energy landscape [15]. Such approach allows us to predict the nucleation stress over a large range of temperatures and strain rates, and reveal its statistical nature [16,17] without the limitation of excessive strain rates.

Surface dislocation sources can be characterized by two quantitative measures: athermal strength and activation parameters. The former measures the elastic limit of the surface, at which a dislocation nucleates instantaneously without the aid of thermal fluctuations. The activation parameters, including the activation energy and activation volume, characterize the probabilistic nature of dislocation nucleation by thermal fluctuation when the applied load is below the athermal limit. Specifically, at a given temperature  $T$  and stress  $\sigma$ , the nucleation rate is

$$\nu = N\nu_0 \exp\left(-\frac{Q(\sigma, T)}{k_B T}\right). \quad (1)$$

Here,  $\nu_0$  is the attempt frequency,  $N$  is the number of equivalent surface nucleation sites,  $k_B T$  is the thermal energy, and  $Q$  is the activation free energy [11] whose magnitude is controlled by the local stress  $\sigma$ . The activation volume  $\Omega$ , defined as the derivative of activation free energy with stress, i.e.,  $\Omega(\sigma, T) \equiv -\partial Q/\partial \sigma|_T \approx k_B T \partial \ln(\nu)/\partial \sigma$ , measures the sensitivity of nucleation rate to stress. While the athermal surface strength has received significant attention in recent years [5,6], the activation parameters of surface dislocation source have not been quantitatively studied using the atomistic approach.

Equation (1) gives the nucleation rate when the system is under constant stress. But in experiments, constant strain rate is more commonly used. Consider a dislocation-free nanowire under constant *elastic* strain rate  $\dot{\epsilon}$ , such that the

stress  $\sigma$  and time  $t$  are directly related by  $\sigma = E\dot{\epsilon}t$ , where  $E$  denotes the apparent Young's modulus of the wire. The probabilistic nature of a thermally activated nucleation process dictates that the nucleation stress is a distribution rather than a constant value when many repeated tests are performed. One can define the (most probable) nucleation stress as the load when the dislocation forms most frequently. An implicit expression [16,17] can be derived for the nucleation stress when the wire is under constant temperature and strain rate [18],

$$\frac{Q(\sigma, T)}{k_B T} = \ln \frac{k_B T N \nu_0}{E \dot{\epsilon} \Omega(\sigma, T)}. \quad (2)$$

In a first approximation of the temperature effect on the activation free energy  $Q(\sigma, T)$  [19], we take  $Q(\sigma, T) = (1 - T/T_m)Q_0(\sigma)$ , where  $T_m$  is the surface disordering temperature, and  $Q_0(\sigma)$  is the activation energy on the zero- $T$  potential energy surface (PES). It follows that the activation volume  $\Omega(\sigma, T) = (1 - T/T_m)\Omega_0(\sigma)$ , where  $\Omega_0 \equiv -dQ_0/d\sigma$ . The prediction of nucleation stress is then reduced to the problem of finding the minimum energy path (MEP) [20] of nucleation on the zero- $T$  PES; namely,  $Q_0(\sigma)$  can be calculated as the energy difference between the saddle point and initial equilibrium state on the MEP, and  $\nu_0$  is vibrational frequency of the normal mode in the MEP reaction coordinate direction at the initial equilibrium state. One can determine the MEP by using, for example, the free-end nudged elastic band (FENEB) method [15], developed recently to efficiently explore strongly driven reactions.

To apply the above atomistically-based, nonlinear theory to predict surface dislocation nucleation, we have studied a model system of a Cu nanowire deformed under uniaxial compression [18]. The wire is initially a perfect crystal with a [001] axis. It has a square cross section and {100} side faces, see Fig. 1(a). We study representative unit processes of the nucleation of a Shockley partial dislocation on one of the {111}<112> slip systems for which the resolved shear stress is maximized. Parenthetically, there are generally three surface nucleation scenarios: (A) a single leading partial dislocation, (B) a full dislocation, with complementary leading and trailing partials, and (C) deformation twinning. The present study focuses on a leading partial dislocation because even in the cases of (B) and (C), nucleation of the first leading partial is usually the most difficult, rate-limiting step [21]. Two representative (competing) nucleation sites are examined: the middle of side surface, which is atomically flat, and the 90° sharp corner, which is an extreme case of heterogeneous surface nucleation. When the wire is under a prescribed compressive stress, e.g., 3.3 GPa (the corresponding compressive strain is 0.085), Fig. 1(b) and 1(c) show, respectively, the saddle-point atomic configurations of nucleation from the side surface and the corner, both of which are identified by the FENEB calculation. The area enclosed by the loop corresponds to the activation area that the dislocation line

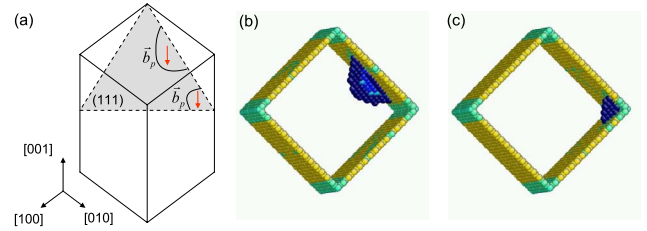


FIG. 1 (color online). Reaction pathway modeling of dislocation nucleation from a Cu nanowire under uniaxial compression. (a) Schematics of a [001] wire showing the Shockley partial dislocation loop (the Burgers vector  $\vec{b}_p = \langle 11\bar{2} \rangle / 6$ ); (b) Saddle-point configuration of an embryonic dislocation loop emanating from the atomically smooth side surface; (c) Saddle-point structure of the loop nucleation from an atomically sharp corner. Atoms are colored by the breaking of local inversion symmetry.

has swept out between the stable (perfect wire without dislocations) and unstable (saddle-point) equilibrium states. Physically, the size of the activation area is proportional to the activation volume, which is to be quantitatively evaluated. We calculate the activation energy  $Q_0$ , and obtain  $Q_0 = 0.64$  eV for nucleation from the side surface and  $Q_0 = 0.1$  eV for corner nucleation. Assuming the same attempt frequency for the two processes, Eq. (1) dictates that the nucleation from corners dominates over competing surface sources such as atomically smooth surface. The favored mode of corner nucleation has been confirmed by our direct MD simulations. We hereafter focus on the corner nucleation, and study the temperature and strain rate dependence of the nucleation stress.

Next, consider the corner dislocation nucleation in a nanowire under constant strain rate. Prediction of nucleation stress based on Eq. (2) requires atomistic input of stress dependent activation energy and activation volume. In Fig. 2(a), we show with circles the calculated activation energies of corner nucleation at different stresses; the solid line is a fitting curve by taking the functional form  $Q_0(\sigma) = A(1 - \sigma/\sigma_{\text{ath}})^\alpha$ , we obtain  $A = 4.8$  eV,  $\sigma_{\text{ath}} = 5.2$  GPa, and  $\alpha = 4.1$ . In Fig. 2(b), we show the activation volume as a function of stress, which is calculated by

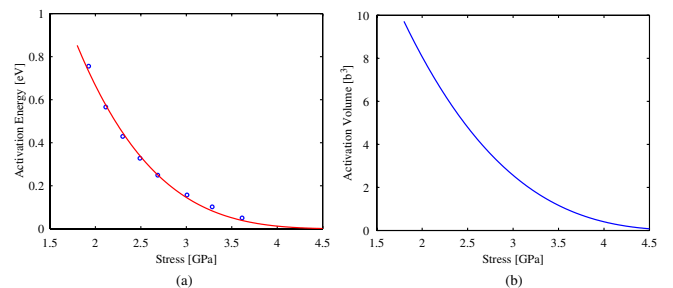


FIG. 2 (color online). Stress-dependent activation parameters for dislocation nucleation from the corner of a Cu nanowire: (a) Circles show the calculated activation energy as a function of stress and the solid line is the fitting curve. (b) The activation volume as a function of stress.

taking the derivative of  $Q_0(\sigma)$  with respect to  $\sigma$ . The magnitude of activation volume is found to be rather small. For example, when  $Q_0 \approx 0.6$  eV, a barrier giving a nucleation rate comparable to typical laboratory experiments (seconds to hours time scale) at room temperature, the corresponding activation volume  $\Omega_0$  is about  $5b^3$ . Moreover, our calculations show that for dislocation nucleation from other types of surface sources, e.g., atomically smooth surface [see Fig. 1(b)], the associated activation volumes are similarly small, about  $10b^3$ . We also change the (100) surface to (111) surface, as well as create surface steps on the (111) surface with and without kinks. We find that when  $Q_0(\sigma) = 0.6$  eV, the corresponding activation volumes are about  $2b^3$ . Altogether, these data show surface dislocation nucleation has activation volumes in the range of  $1\text{--}10b^3$ . The physical significance of such characteristic activation volume will be demonstrated next on the temperature and strain-rate sensitivity of nucleation stress.

For corner nucleation, Fig. 3 shows the nucleation stresses (solid lines) predicted by numerically solving Eq. (2) with  $Q_0(\sigma)$  and  $\Omega_0(\sigma)$  as an input [18]. Here, the nucleation stress is plotted as a function of temperature at two characteristic strain rates,  $\dot{\epsilon} = 10^{-3}/\text{s}$  and  $\dot{\epsilon} = 10^8/\text{s}$ , which are typical of laboratory experiments and MD simulations, respectively. To verify theoretical predictions, we have performed direct MD simulations under constant strain rate (about  $10^8/\text{s}$ ) and isothermal conditions. Figure 3 also shows the nucleation stresses (circles) collected from MDs; the scattering of nucleation stresses from MDs is attributed to the effect of thermal uncertainty. Evidently, transition-state-theoretic predictions agree with direct numerical experiments at high strain rates.

The nucleation stresses in Fig. 3 show significant temperature sensitivity. Particularly, we note that under a low strain rate of  $\dot{\epsilon} = 10^{-3}/\text{s}$ , the nucleation stress drops by more than 70% as  $T$  increases from nearly zero to room

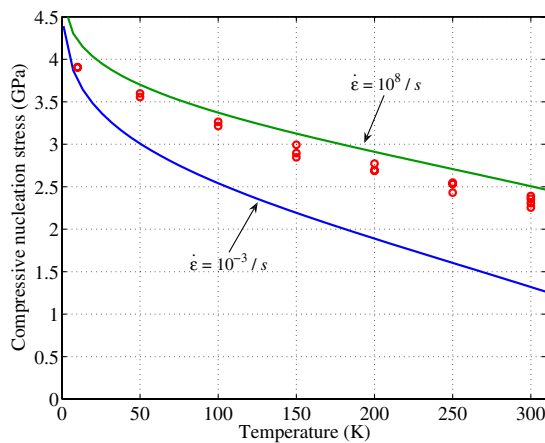


FIG. 3 (color online). Nucleation stress as a function of temperature and strain rate from predictions (solid lines) and direct MD simulations (circles).

temperature. This result clearly underscores the importance of the temperature effect in correlating the zero- $T$  calculations (e.g., ideal surface strength) [5,6] with room-temperature experimental measurements (e.g., compressive strength of nanowires or nanopillars).

The sensitive temperature dependence of nucleation stress arises because of the characteristically small activation volume associated with surface sources. To render this point physically transparent, let us consider a simple case where the activation energy depends linearly on stress. Suppose one knows the activation volume  $\hat{\Omega}$  at a given stress, denoted as  $\hat{\sigma}$ , the activation energy  $Q$  near  $\hat{\sigma}$  can be approximated by a linear relation  $Q(\sigma) = Q(\hat{\sigma}) - \hat{\Omega}(\sigma - \hat{\sigma})$ , or equivalently  $Q(\sigma) = Q^* - \sigma\hat{\Omega}$ , where  $Q^* \equiv Q(\hat{\sigma}) + \hat{\sigma}\hat{\Omega}$  and it corresponds to the nucleation barrier in the absence of applied stress within the linear approximation of stress-dependent activation energy. The nucleation stress given by Eq. (2) is then

$$\sigma = \frac{Q^*}{\hat{\Omega}} - \frac{k_B T}{\hat{\Omega}} \ln \frac{k_B T N \nu_0}{E \dot{\epsilon} \hat{\Omega}}. \quad (3)$$

Here, the first term  $Q^*/\hat{\Omega}$  is the athermal nucleation stress causing instantaneous dislocation nucleation in the linearized model of stress-dependent activation energy. The prefactor of the second term  $k_B T/\hat{\Omega}$  has a stress unit, and it sets the scale of nucleation stress reduction due to thermal fluctuation. In the logarithmic function,  $k_B T N \nu_0$  is the rate of energy exchange of the candidate nucleation sites with the thermal bath, and  $E \dot{\epsilon} \hat{\Omega}$  is the rate of activation energy reduction by the mechanical work. The ratio between the two terms determines the competition of thermal and mechanical effects in mediating the nucleation stress reduction ( $\propto k_B T/\hat{\Omega}$ ) due to thermal fluctuations.

Equation (3) explicitly shows the functional dependence of nucleation stress on temperature and strain rate; namely,  $\sigma$  scales, respectively, with  $T \ln T$  and  $\ln \dot{\epsilon}$ . Since  $T$  pre-multiplies the logarithm, the nucleation stress should be most sensitive to temperature, particularly when the activation volume  $\hat{\Omega}$  is small. Recall that in Fig. 2, we show within a range of barrier from 0.1 to 0.6 eV that controls the rate processes in Fig. 3, the activation volume varies, but it remains in a characteristic range of a few  $b^3$ . Such small activation volume causes the sensitive temperature dependence of nucleation stress, as shown in Fig. 3. It is important to note that the activation volume for a typical bulk dislocation source, such as the Frank-Read source, is between  $100\text{--}1000b^3$ , leading to the commonly observed rate-insensitive plastic yield in large crystals at room temperature. This large difference in activation volume between surface and bulk dislocation processes suggests that activation volume can be taken as a kinetic signature of deformation mechanism [22]. Additionally, while the strain rate  $\dot{\epsilon}$  is inside the logarithm in Eq. (3), its effect could be significant on the predicted nucleation stress. For example, if one needs to quantitatively correlate atomistic

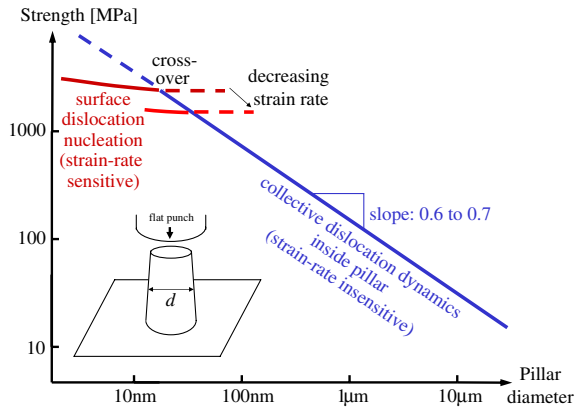


FIG. 4 (color online). Illustration of surface effect on the rate-controlling process: size dependence of yield strength in single-crystal wires or pillars under compression. A power-law scaling was measured in micron-sized pillars [23], where the rate insensitive plastic yield is governed by dislocation dynamics inside the pillar. In very small pillars, surface dislocation nucleation is expected to dominate, giving a logarithmic dependence of yield stress to the pillar size and providing an upper bound to the size-strength relation in nanopillar compression experiments; this upper bound is strain-rate sensitive because of the small activation volume.

calculation results with laboratory experiments, the influence of strain rate could not be ignored, as shown in Fig. 3.

Equation (3) also reveals a size effect on the nucleation stress [16,17] because a change in the wire geometry directly affects the number of equivalent surface nucleation sites  $N$ . Since  $N$  is in the logarithmic function of Eq. (3), the size effect arising from surface nucleation is expected to be weak, compared to that in micropillars showing a power-law scaling with an exponent in the range from  $-0.6$  to  $-0.7$  [3,23]. The latter scaling behavior likely arises from collective dislocation dynamics inside the pillar [23] involving dislocation interactions and multiplications, when the pillar volume is large enough to sustain such a population. Since surface dislocation nucleation likely dominates plastic yielding in the nanoscale samples due to dislocation source starvation in the bulk, one thus expects a transition in the scaling behavior of yield stress on the sample size in an approximate range of tens of nanometers, as illustrated by Fig. 4. Recent experiments on the nanoscale samples show hints of such transition [1–3], but more detailed experimental and modeling studies are needed. Finally, we note that a change in the wire geometry will also affect the activation energy  $Q_0$  and the activation volume  $\Omega_0$  due to the long range elastic interaction associated with the image effects of free surface of the sample, as well as the effect of internal stress of other corners. To evaluate their quantitative influences, we have studied a wire with the side length doubled. When  $Q_0$  varies between 0.24–0.52 eV, the averaged  $\Omega_0$  is about

$4b^3$ , consistent with the previous results that the activation volume of surface dislocation nucleation is in the range of  $1-10b^3$ .

In conclusion, the present work addresses the surface dislocation nucleation aspect of small scale plasticity. We find surface sources have a unique kinetic signature: a small activation volume leading to increased strain-rate and temperature sensitivities of flow stress. A transition in the rate-controlling flow mechanism is predicted from collective dislocation dynamics to single dislocation nucleation for small-volume materials with length scale of tens of nanometers.

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