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Strongly correlated breeding of high-speed dislocations

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ABSTRACT

Under very high stresses, dislocations can be accelerated to approach the speed of shear wave over a distance as short as 10^1 nm. Our atomistic simulations demonstrate that dislocations with such high speeds often react in counter-intuitive manners that are beyond textbook descriptions of conventional dislocation behavior. A high-speed dislocation can "rebound" when hitting a free surface rather than simply annihilate. When two high-speed dislocations collide, they can "penetrate" through each other. An individual dislocation can even spontaneously generate multiple dislocations via self-dissociation. These anomalous mechanisms lead to rapid proliferation of dislocations that are strongly correlated both spatially and temporally, and as such may play a role in high-stress and high-strain-rate plastic deformation; a potentially related case is nanoscale pristine single crystals, which often yield via a large strain burst at ultrahigh stresses.

1. Introduction

Following the "smaller is stronger" tenet [1], a nanometer scale metallic single crystal can sustain a sample-wide stress that reaches a significant fraction of the ideal strength ($>10^{-2}$ G, where G is the shear modulus), well into the so-called ultra-strength regime [2]. In these cases, pristine samples of Au [3–5], Al [6], Fe [7], Mo and its alloy [8–10] often exhibit "instantaneous" shape change (e.g., a sudden large strain burst that collapses the sample) once the applied stress reaches the yield point. See Movie 1 through Movie 4 in Supplementary Material for a series of demonstration of the structural collapse of Al nano-pillar [6], Au nano-particle [3], Fe nano-particle [7] and Mo nano-fiber [10], respectively. This kind of cataclysmic plasticity, which is perhaps similar to the electron avalanche in strongly biased insulators during electrical breakdown, is indicative of very strong temporal correlations of a large number of mobile dislocations, but its origin remains poorly understood at present. This example highlights the need to better understand how dislocations behave and multiply, when the driving stresses are very high and the acceleration path is initially clear (obstacle free) for nucleated dislocations. The purpose of this article is to address this issue, and the mechanisms uncovered revealing highly efficient breeding of dislocations may be potentially relevant to the case mentioned above.

Supplementary video related to this article can be found at http://dx.doi.org/10.1016/j.actamat.2016.07.053.

Specifically, we describe strongly correlated plasticity via prolific dislocation multiplication mechanisms arising from dislocations running into free surfaces and into each other at very high speeds. Under an ultra-high shear stress τ, once a dislocation is nucleated, or breaks free from tangling, it may be accelerated rapidly to approach or even exceed the transverse sound speed (c_t), to become so-called "relativistic" dislocation [11] as shown by molecular dynamics (MD) simulations [12–14]. The magnitude of the relativistic acceleration length scale (l_{ra}) can be crudely

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estimated by equating the work done to accelerate the dislocation, $\tau b(1-\eta)l_{ra}$, assuming a certain dissipative loss coefficient η, to the stationary energy E_0 of the dislocation as the excess energy of a relativistic dislocation could be similar to E_0 [11], which is often taken to be $E_0 = Gb^2/2$, where G is the shear modulus and b is the magnitude of Burgers vector. Since in the ultra-strength regime [2] τ is a significant fraction of the ideal strength ($>G/100$), l_{ra} will be of the order of $10^2 b$, or 10^1 nm (see Fig. S1 and associated discussion in online Supplementary Material for the estimation of dissipation coefficient and the acceleration length). A distance of this magnitude for dislocations to accelerate, free of obstacles, is easily available for the first batch of dislocations, after they nucleate from the surface of a pristine nanoscale crystal that often yield at ultrahigh stresses.

Once a high speed of the order of c_t is reached, the stress field, energy, etc. of a dislocation become significantly modified due to the "relativistic" or inertia effects [11,15–19]. Thereupon, anomalous dislocation behaviors and reactions may emerge. In the following, we use MD simulations to systematically illustrate the spectrum of unconventional reactions of high-speed dislocations. We will also briefly comment on their implications on extremely transient but large-amplitude plasticity, for example that seen in nanometer scale pristine single crystals.

2. Simulation methods

A model material based on an empirical potential for Cu [20] was chosen for the current study as an example. This empirical potential of Cu has been successfully applied to a wide range of simulations, including those involving dislocations under high stresses [21–23]. Parallel simulations were performed on Al [24–27], Ni [24] and Au [28] as well, to ensure that the observed phenomena are general and not restricted to a specific metal or a particular interatomic potential. Specifically, we focused on the reactions when a high-speed dislocation hits free surface or other dislocations.

In all our simulations on interactions between high-speed dislocations and free surface or other high-speed dislocations, the samples were first equilibrated under constant stress using Parrinello-Rahman method [29] with an initial temperature that was not controlled by any thermostats thereafter due to the non-equilibrium nature of high-speed dislocation dynamics (a global Nose-Hoover thermostat was also tested and showed negligible difference compared to the results reported here). Initial temperatures ranging from 2 to 400 K were tested to ensure finite temperature has minor effects on the observed high-speed dislocation behaviors (the results with initial temperature of 2 K are shown in the current work). Following the equilibration, a dislocation was introduced from the crystal surface and accelerated by the applied constant stress. Periodic boundary conditions were employed along the dislocation line direction. While some MD simulations on dislocation dynamics also used periodic boundary conditions in the direction of dislocation motion to extend the gliding distance, here we purposely set up free surface in this direction, as free surfaces are generally the terminus of dislocations in nanoscale single crystal metals. The atomistic configurations of dislocations were identified by the common neighbor analysis [30,31] and the dislocation extraction algorithm [32] and visualized using AtomEye [33]. Dislocation speeds were computed by identifying the dislocation positions at different time. All dislocation speeds used are the instantaneous speeds right before dislocation reactions. A time step of 1 fs was used throughout all simulations which were carried out with the LAMMPS package [34]. Further details on the MD simulations can be found in Supplementary Material.

3. Results and discussion

3.1. Speed-dependent reactions of dislocation with free surface

Interfaces such as grain boundaries, phase boundaries has been extensively studied as they often play an important role in materials' mechanical properties via dislocation-interface interactions. However, when materials scale down to nanometer dimensions and become single crystals that are free of pre-existing dislocations, dislocation-free surface interactions have been largely overlooked as one often expects that dislocation should simply annihilate at free surfaces, as shown in Fig. 1(a): here a relatively slowly moving (instantaneous speed before annihilation is $v \sim 0.56c_t$, where $c_t = 2920$ m/s is the shear wave speed) screw dislocation (screw dislocations are thought to be easily nucleated than edge or mixed dislocation in nanoscale single crystals [22,35]) simply annihilates at the free surface of a slab configuration which is subject to a shear stress of 0.4 GPa and an initial temperature of 2 K. This annihilation process reduces the number of active dislocations (n_d) from 1 to 0, as often discussed in the dislocation starvation model [36]. However, when the dislocation speed becomes sufficiently high, the incident dislocation often does not simply disappear. Instead, it can "bounce back" from the free surface. As shown in Fig. 1(b), when the instantaneous speed before hitting a surface is increased to $v \sim 0.66c_t$ (by applying a higher shear stress 1.0 GPa), a new partial dislocation is immediately generated (31.0 ps) and accelerated to glide back (40.0 ps) upon its annihilation at free surface (25.0 ps–28.0 ps). This annihilation-regeneration process, which occurs within only a few picoseconds, appears as if the incident dislocation partially rebounded from the free surface. As a result, n_d is kept constant after the reaction ($1 \rightarrow 1$). Additionally, a small atomic step was created on the surface as the rebounded partial dislocation is of mixed character. Also due to the stacking fault ribbon of the incident dislocation, the rebounded partial dislocation (with opposite Burgers vector as to the leading partial of the incident dislocation) generally does not appear on exactly the same slip plane (otherwise atoms on the two oppositely shifted atomic planes will sit on top of each other) as that of the incident dislocation but appear one slip plane above. If the speed further approaches c_t, an incident dislocation could even rebound into multiple new dislocations. As shown in Fig. 1(c), for instantaneous speed $v \sim 0.78c_t$ (the applied shear stress now is 1.8 GPa) before hitting a surface, the dislocation core becomes wider (the dislocation now enters the so-called "breathing mode" [37–39] in which the separation between leading and trailing partials varies quasi-periodically in time) before hitting free surface such that the leading partial and trailing partial are obviously separated and rebound one after the other. The leading partial first rebounds into a new partial dislocation, before the trailing partial hits the free surface (22.6 ps). Then the trailing partial hits the free surface and annihilates (24.4 ps), upon which three new partials are immediately generated (27.0 ps). One of them is a trailing partial that complements the first rebounded partial to form a full dislocation, and the other two are leading partials running on other neighboring slip planes. Consequently, n_d is tripled after the reaction ($1 \rightarrow 3$).

For convenience, we use the following convention to name the rebound events: $b^{reb}/b^{inc}<1 \rightarrow$ partial-rebound, $b^{reb}/b^{inc} = 1 \rightarrow$ full-rebound, $n_d^{reb}/n_d^{inc} = 1 \rightarrow$ single rebound, $n_d^{reb}/n_d^{inc} = 2 \rightarrow$ double rebound and $n_d^{reb}/n_d^{inc} \geq 3 \rightarrow$ multiple rebound, where b^{reb} and b^{inc} are the magnitude of Burgers vectors of rebounding and incident dislocations, and n_d^{reb} and n_d^{inc} are the number of rebounded dislocations and the number of incident dislocations, respectively. Such a scheme is also used to describe other reactions that will be discussed later. More detailed illustrations about the above

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