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Temperature and high strain rate dependence of tensile deformation behavior in single-crystal iron from dislocation dynamics simulations

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Abstract

We conduct dislocation dynamics simulations of Fe periodic single crystals under tensile load at several high strain rates and temperatures. The simulations are connected to the atomistic scale via recently developed, temperature-dependent dislocation mobility relations. We explore strain rates from 10^4 to 10^6 s^{-1} at temperatures of 100, 300 and 600 K. We compute the flow stress as a function of strain rate and temperature, and find very good agreement with experimental data for Fe, suggesting that strain hardening is the dominant materials response mechanism in the range of conditions explored here.

Keywords: Dislocation dynamics; High strain rate deformation; Fe single crystals; Materials strength

1. Introduction

The dependence of the flow stress with strain rate in many materials shows two clearly differentiated regimes, namely a slow increase up to strain rates on the order of 10^7 s^{-1} followed by a sharp upturn at higher rates [1–10]. This shift is believed to be related to a transition in the mechanism of dislocation glide, from thermally activated to viscous drag, which display starkly different stress and temperature dependencies. During deformation at high strain rates, dislocation multiplication and glide may result in high levels of work hardening, often accompanied by twinning at the highest strain rates. This behavior has been confirmed experimentally for a wide number of materials with different underlying microstructures [2,3,7]. The mechanical response in these conditions is characterized by phenomena occurring across several orders of magnitude in length and time scales, and indeed multiscale integrated models that account for the relevant physical processes at each of the scales involved have proven very successful in predicting the material response with strain rate [11,12]. One such scale is that over which dislocation-dislocation interactions dominate the evolution of the strength. To study this regime, methods capable of tracking millions of dislocation segments are needed.

Here, we perform dislocation dynamics (DD) simulations of homogeneous dislocation ensembles in body-centered cubic (bcc) Fe single crystals at different strain rates and temperatures under uniaxial loading. The simulations are conducted to gain insight into the mechanisms governing the flow stress in the strain rate regime thought to be dominated by dislocation glide. A critical aspect for these simulations to be successful is the capability to capture the temperature and strain-rate dependence of single-dislocation motion. In particular, incorporating the dual character of screw dislocation mobility, with clearly distinct thermally activated and viscous regimes, into DD

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simulations has remained a challenge for over two decades, despite its undeniable importance. Several efforts aimed at addressing this shortcoming must be recognized [13,14], albeit only in a preliminary manner. Here we use temperature- and stress-dependent dislocation mobilities derived from the calculations done by Gilbert et al. [15] and Queyreau et al. [16] using molecular dynamics (MD) simulations.

The paper is organized as follows. In the next section, we provide a brief description of the most salient features of DD, provide the simulation conditions and describe the dislocation mobility functions in detail. We then show results from the simulations, including stress–strain curves and dislocation density–strain curves, and compare them with available experimental data. We finish with the discussion section and the conclusions.

2. Computational methods

All of the simulations presented here were carried out using the Parallel Dislocation Simulator [17]. The simulations comprised a cubic cell of size $L = 5$ μm containing a fixed initial network dislocation density ρ_0. To resemble a well-annealed crystal, in all cases we take $\rho_0 = 8.0 \times 10^{12}$ m^{-2}, consisting only of screw dislocations. Furthermore, all four $\frac{1}{2}\langle 1\,1\,1\rangle$ Burgers vectors were populated equally in such a way as to produce zero net Burgers vector in the simulation cell. Network dislocations were made continuous and infinite in space by using periodic boundary conditions, and regenerative sources could only be created by interaction of the initial dislocation network with itself.

A simulation matrix was constructed with temperatures and strain rates of, respectively, 100, 300 and 600 K, and $10^4, 10^5$ and 10^6 s^{-1}. Tensile loading along the [1 0 0] direction was performed in order to achieve multi-slip conditions. Only glide on $\{1\,1\,0\}$ slip planes was considered. Fe is approximated to be an isotropic linear elastic solid and characterized by the values of the shear modulus $\mu = 83$ GPa and Poisson's ratio $\nu = 0.29$.

2.1. Segment mobility

The segment mobilities employed in this work are explained in the following:

Screw mobility. At very high strain rates in the thermally-activated regime, screw dislocation mobility is seen to be independent of its length [18]. This can be rationalized in terms of the competition between kink pair nucleation vs. propagation, which become comparable at these rates. The relationship between stress τ and screw dislocation velocity v in the thermally activated and phonon drag regimes is:

$$\tau_{th}(v;T) = \alpha\tau^*(T)\left\{\left[\frac{v}{C_0(T)} + v_0(T)\right]^{\beta} - v_0(T)^{\beta}\right\} \tag{1}$$

$$\tau_{ph}(v;T) = B(T)(v + v^*(T)) \tag{2}$$

where T is the absolute temperature and the rest of parameters are given in Table 1. The contribution to the material strength from screw dislocations is obtained from the following rule of mixtures:

$$\tau_s = \left(\tau_{th}^n + \tau_{ph}^n\right)^{1/n} \tag{3}$$

Edge dislocations. The edge dislocation mobility is assumed to follow a simple viscous law:

$$\tau_e = \frac{Tv}{A} \tag{4}$$

where A is also given in Table 1.

As a point of reference, with their mobilities described by the above functions, edge dislocations are three orders of magnitude faster than screw dislocations at 100 and two at 300 K, while at 600 K a crossover exists at 300 MPa, with edge velocities being slower than those of their screw counterparts. Fig. 1 illustrates the behavior of the mobility function at the three temperatures of interest.

The above mobility function follows the so-called BCC0 construction [19,20], which keeps edge dislocations confined to their slip plane $\vec{n} \equiv \vec{\xi} \times \vec{b}$ ($\vec{n}$: plane normal; $\vec{\xi}$: line tangent; $\vec{b}$: Burgers vector), while screw segments move on the plane dictated by the maximum resolved shear stress provided that the plane belongs to the $\{1\,1\,0\}$ family. This makes screw dislocations free to cross-slip into any allowed slip plane. Climb is enabled, although with a mobility significantly smaller than that of edge dislocations, and is not expected to play any significant role.

2.2. Numerical challenges

The main numerical challenges are associated with the following aspects of the simulations:

- Time convergence of solution. We use an implicit Newton–Raphson method to integrate the equations of motion. Typically, convergence is achieved after a few iterations, with higher strain rates requiring more iterations.
- High screw/edge mobility asymmetry. At low temperatures and/or strain rates, edge dislocation mobility may be up to several orders of magnitude higher than screw mobility. This sets restrictions on the time step duration, which may get as low as 10^{-11} to 10^{-13} s.

3. Results

3.1. Numerical calculations

Fig. 2 shows the stress–strain curves for the combination of strain rates and temperatures considered in this work. The simulations were run up to the point of generally constant flow stress. This required varying amounts of computational time for each simulation, depending mostly on