Comment on “Lattice Resistance to Dislocation Motion at the Nanoscale”

In a recent Letter [1], Dutta et al. showed that dislocations move faster in thin films than in the bulk and that this is caused by a reduction in lattice resistance at the nanoscale. In this Comment, I show that the results presented in [1] do not agree with previously published results and are not reproducible. Furthermore, I am able to show their explanation of lattice resistance is not supported by Peierls stress calculations.

The results presented by Dutta et al. show that dislocation velocity increases from ~728 to ~1050 m/s as the film thickness decreases from 75 to 8.5 nm. They conclude that the bulk velocity of an edge dislocation in molybdenum is 728 m/s at 300 K under and applied shear stress of 250 MPa. Using the same potential and full periodic boundary conditions with a special dipole configuration, Chang [2] determined the drag coefficient to be $B = 6.0 \times 10^{-5}$ Pa·s for small stresses. Using this value, or interpreting from his Fig. 5-11, one obtains velocities around 1000–1100 m/s, significantly higher than the bulk value reported by Dutta et al. and more representative of the value obtained for their thinnest film studied. In addition, the thin film configuration has been used extensively in the past with face-centered-cubic (fcc) metals to determine dislocation mobility in the bulk (for example, see [3] and references therein). In these prior studies, converged bulk mobility values were obtained using film thickness of order 10 nm, significantly smaller than the 75 nm reported by Dutta et al. While the material studied by Dutta is body-centered-cubic (bcc), one does not expect to see significant differences between edge dislocations in bcc and fcc metals.

To verify the thickness dependence, I repeated the simulations using the same interatomic potential and simulation methodology. Figure 1 shows my results for the same temperature and applied shear stress. The velocity is plotted as a function of film thickness, and we do not see significant size dependence. We also note that these simulations show a converged velocity of around 1070 m/s, in agreement with Chang’s results for bulk simulations. These simulations create stress waves that move through the film and a steady state velocity is not achieved until several reflections of the wave have occurred. It is, therefore, essential to run the simulation long enough to obtain time converged velocity values, which can be several hundred picoseconds for thick (~100 nm) films.

Finally, I would like to point out that lattice friction should not contribute to the drag and cannot explain their results. The Peierls stress is a standard measure of lattice friction and this has been measured for the interatomic potential used by Dutta et al. to be ~25 MPa [2]. For the simulated conditions of Dutta et al. (250 MPa, 300 K), the stress is 1 order of magnitude larger than the Peierls stress, suggesting that lattice friction is not contributing significantly to the drag. However, it is worthwhile to check the thickness dependence of the Peierls stress to eliminate lattice friction as a contributor to size dependence. I computed the Peierls stress to ±1 MPa in a thin film as shown in Fig. 1. The Peierls stress for large thicknesses converges to around 20 MPa, in good agreement with Chang’s result. However, below about 8 nm the Peierls stress rises, in direct contrast to that predicted by Dutta et al. This discussion and the data I have presented bring the results and conclusions presented in [1] into question.

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