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COMPETITION BETWEEN LEADING, TRAILING, AND TWINNING PARTIAL DISLOCATION NUCLEATION IN FCC METALS

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Increasing evidence indicates that dislocation nucleation plays a key role in the deformation of nano-structured and nano-dimensioned metals. Yet, our understanding of the nucleation process, whether it is from a free surface, grain boundary, or stress concentration, has remained clouded. For instance, atomic simulations of these materials often show an excessive amount of twin nucleation and/or non-successive partial emission compared to experiment. In this work, we resolve this discrepancy by considering the thermally-activated nature of dislocation nucleation.

We first use a multiscale simulation technique that permits long-time atomic simulations of crack tip behavior and shows that in Al there is a transition from twinning at very short times and high applied loads to dislocation slip at longer times and lower applied loads. Twinning in Al is thus very rare, in agreement with experiments. We then develop an analytic model for the twinning/dislocation-slip competition that predicts dislocation slip to become the preferred mode of deformation with a lower activation energy at lower load levels, corresponding to longer times or slower loading rates, and/or higher temperatures, in agreement with our simulations. Moreover, this transition in mechanism is predicted to occur in all FCC metals, and the difference between materials then lies in the activation energy at which the transition occurs. For Al, Ni, and Pt, the transition occurs at very low activation energies, so that dislocation slip is strongly preferred in these systems except at very low temperatures or extremely high rates. For Ag, Ir, and Pb, the transition occurs at much higher activation energies so that twinning is preferred at room temperature and/or moderate deformation rates. Our ranking of FCC materials with respect to twinnability matches experimental trends, and captures both the temperature and loading-rate dependence that has been absent in prior models.

To study twinning versus dislocation slip via simulation, a multiscale method is essential in overcoming severe computational hurdles. Here, we use the finite-temperature concurrent multiscale Coupled Atomistic Discrete Dislocation (CADD) method to minimize the number of explicit atoms in the computational cell without influencing any physical results and reduce the total CPU time to ~11 CPU years. Second, we use the parallel replica method, running many nominally-identical simulations on independent CPUs and accumulating total simulation time until the first nucleation event of interest occurs in any one of the simulations. Combined, these approaches enable molecular dynamics simulations to access times approaching one microsecond.