Multiscale Modeling of Ductile Materials

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We present a modeling approach to bridge the atomistic with macroscopic scales in crystalline materials. We show that the meticulous application of this paradigm renders truly predictive models of the mechanical behavior of complex systems. In particular we predict the hardening of Ta single crystal and its dependency for a wide range of temperatures, strain rates. The feat of this approach is that predictions from these atomistically informed models recover most of the macroscopic characteristic features of the available experimental data, without a priori knowledge of such experimental tests. This approach provides a procedure to forecast the mechanical behavior of material in extreme conditions where experimental data is simply not available or very difficult to collect.

The present methodology combines identification and modeling of the controlling unit processes at microscopic level with the direct atomistic determination of fundamental material properties. This modeling paradigm is used to describe the mechanical behavior of Ta single crystals at *high-strain* rate. In formulating the model we specifically consider the following unit processes: double-kink formation and thermally activated motion of kinks (Wang, Strachan, Cagin and Goddard, 2002); the close-range interactions between primary and forest dislocations, leading to the formation of jogs; the percolation motion of dislocations through a random array of forest dislocations introducing short-range obstacles of different strengths; dislocation multiplication due to breeding by double cross-slip; and dislocation pair annihilation.

The resulting atmostically-informed model is then used to predict the macroscopic response of structural solids subjected to complex loading scenarios by resorting large-scale massive parallel computations. The considerable computing effort is distributed among processors *via* a parallel implementation based on mesh partitioning and message passing (Radovitzky, Meiron and Samtaney, 2001).