Multiscale model of strength in single crystal tungsten under uniaxial and biaxial loading

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ABSTRACT

Understanding and improving the mechanical properties of tungsten as a refractory metal are critical tasks for applications where its very low fracture toughness is a limitation. In this contest, it is important to formulate continuum models capable to provide macroscopic results, based on atomistic results of screw dislocations, the main carriers of plastic deformation in body-centered cubic (bcc) metals.

In this work we present a multiscale model that comprises atomistics and continuum-level crystal plasticity calculations to perform material point simulations and compute the yield strength in single crystal tungsten under different uniaxial and biaxial loading orientations of the standard triangle. Molecular statics calculations are used (i) to study the energetics of kink-pair nucleation as a function of stress for screw dislocation motion, and (ii) to obtain the critical stress deviation from Schmid's law. The atomistic data are used to parameterize the dislocation mobility law, which is embedded as constitutive law into a dislocation-based crystal plasticity framework. The temperature range covered in this work goes from room temperature to 0.5 Tm, where Tm is the melting point.

The results illustrate the importance of the Non-Schmid behavior, the orientation of the crystal and the temperature to determine the yield strength of the material.