MD Study of the Nucleation and Growth of Deformation Twins in Polycrystalline Tantalum

LUIS SANDOVAL, DAVID RICHARDS, Condensed Matter and Materials, Lawrence Livermore National Laboratory, Livermore, California 94550, USA — Recovered samples from high strain rate experiments clearly show that twin formation serves as an important plasticity mechanism in Tantalum. Despite years of study however, the nucleation and growth mechanisms of twining are still poorly understood, especially in bcc metals. Twins are typically thought to nucleate at grain boundaries via a cooperative emission of partials after a critical value of shear stress. We have used molecular dynamics (MD) simulation to observe the nucleation and growth of twin domains from grain boundaries and grain boundary junctions in polycrystalline cells, which have been prepared as arrangements of hexagon-columnar grains. Using a Finnis-Sinclair potential, we have examined the role of strain rate, temperature and hydrostatic pressure on the kinetic phenomena, in particular the twinning threshold and twin growth rates. We discuss how kinetic parameters extracted from MD simulations help inform a multiscale strength model for Tantalum that includes both twinning and slip as deformation mechanisms in the regime of high strain rates.

1This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 (LLNL-ABS-461533).