MAR12-2011-005319

Abstract for an Invited Paper
for the MAR12 Meeting of
the American Physical Society

How dislocations and grain boundaries control wear at the nanoscale

IZABELA SZLUFARSKA, University of Wisconsin

Ceramics show outstanding mechanical properties such as high strength and high hardness over a wide range of temperatures and are stable in harsh environments. However, the low fracture toughness of ceramics limits their practical utility for instance as wear-resistance coatings. There have been several reports of improving wear resistance of ceramics by reducing the grain sizes and/or the dimension of the cutting tools to the nanometer regime. Using SiC as a model covalent ceramic, we performed molecular dynamics (MD) simulations of wear for both single crystal and nanocrystalline material. We determined the role of dislocations and grain boundary sliding in improving wear resistance of SiC and we have quantified contributions from these mechanisms to friction and wear. We have discovered instabilities that control sliding of the amorphous-like highly disordered grain boundaries in SiC, in analogy to instabilities and deformation mechanisms that occur in bulk amorphous materials. In this talk we will also present our newly developed analytical model for plowing friction in nanoscale contacts, which model has been validated for both ceramics and metals. In order to isolate the contribution from grain boundary sliding to deformation of nanocrystalline materials, we have performed MD simulations of nanoindentation and uniaxial testing on ultrananocrystalline diamond (UNCD). We have shown that in the absence of dislocation plasticity, hardness and yield strength of nanocrystalline materials scale linearly with the grain boundary shear strength, where the latter property can be controlled by grain boundary doping. Our findings explain the experimental observations that hardness and elastic properties of UNCD decrease with an increasing H content.