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PLASTICITY AND HEAT CONDUCTION IN NANOTWINNED MATERIALS BY ATOMISTIC SIMULATION

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ABSTRACT:

This seminar will present our recent progress in understanding the plasticity, fracture and thermal transport behavior of bulk materials and nanowires strengthened by nanoscale twins using atomistic simulations. The ability of twin boundaries (TBs) in strengthening and maintaining ductility has been well documented; yet most understanding of the origin of these properties relies on perfect-interface assumptions. We will show that as-grown TBs in nanotwinned Cu and Ag-Cu alloys are inherently defective with kink-like steps and curvature, and that these imperfections play a key role in plastic deformation mechanisms. Furthermore, we will show a new type of size effect in the fracture of ultra-thin Au nanowires associated with a ductile-to-brittle transition as the twin size decreases to the angstrom-scale that leads to tensile strengths near the maximum theoretical limit. Also, the fundamental role played by the number, size and orientation of twins in nanoscale heat conduction was studied by molecular dynamics simulation. Thermal conductivity calculations in model silicon materials containing nano-twins oriented either perpendicular or parallel to the transport direction reveal an unusual twin-size dependence related to a change from interface phonon scattering to homogeneous heat conduction due to the intrinsic contribution of the hexagonal TB structure. These results therefore suggest new avenues for structurally designing common crystalline materials with coherent interfaces for high-performance thermoelectric and thermal management applications.

BIOGRAPHY:

Dr. Sansoz earned an engineer diploma in mechanical and aerospace engineering and M.S. in materials science and engineering from the Ecole Nationale Supérieure de Mécanique et Aérotechnique in Poitiers, France (1996) and a Ph.D. with Honors in materials science and engineering from Ecole des Mines de Paris (2000). Before joining the University of Vermont in 2004, Dr. Sansoz was a post-doctoral fellow in mechanical engineering at the University of Rhode Island (2001-2002) and the Johns Hopkins University (2002-2003). Dr. Sansoz is the recipient of a 2008 National Science Foundation CAREER award and the 2009 College of Engineering and Mathematical Sciences Milt Silveira Junior Faculty Award at the University of Vermont.