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Special Seminar

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Probing Mechanical Properties of Nanostructured Materials via Large Scale Molecular Dynamics Simulations

The rapid development of synthesis and characterization of nanostructured materials as well as unprecedented computational power have brought forth a new era of materials research in which experiments, simulation and modeling are performed side by side to probe the unique mechanical properties of nanoscale materials. In this talk, I will discuss our recent study of dislocation nucleation governed softening and maximum strength in nano-twinned metals [1]. In conventional metals, there is plenty of space for dislocations to multiply so that the strength of material is controlled by dislocations interaction with grain boundaries (Hall-Petch strengthening) and other obstacles. For nanostructured materials, in contrast, multiplication and motion of dislocations are severely confined by the nano-scale geometries so that continued plasticity can be expected to be source-controlled. Nano-grained polycrystalline materials were found to be very strong but brittle, owing to the fact that both nucleation and motion of dislocations are effectively suppressed by the nano-scale crystallites. We report a dislocation source controlled mechanism in the newly-developed nano-twinned metals in which there are plenty of dislocation nucleation sites while dislocation motion is not confined. We show that dislocation nucleation plays the governing role in the strength of such materials, resulting in their softening below a critical twin thickness. Ultra-large-scale molecular dynamics simulations and a kinetic theory of dislocation nucleation in nano-twinned metals show that there exists a transition in deformation mechanism, which occurs at a critical twin boundary spacing where the strength is maximized, from the classical Hall-Petch type of strengthening due to dislocation pile-up and cutting through twin planes to a dislocation nucleation governed softening mechanism with nucleation and motion of partial dislocations parallel to the twin planes (twin boundary migration). The simulations indicate that the critical twin boundary spacing for the onset of softening in nano-twinned Cu and the maximum strength depend on the grain size: the smaller the grain size, the smaller the critical twin spacing, and the higher the maximal strength of the material.

Should time permit, I will also discuss a number of other related projects in my research group, including plastic strain recoveries [2] and early Baushinger effect [3] in free standing nanocrystalline films with grain sizes on the order of 50 nm.

[1] X. Li, Y. Wei, L. Lu, K. Lu and H. Gao, 2010, "Dislocation Nucleation Governed Softening and Maximum Strength in Nanotwinned Metals," Nature, Vol. 464, pp. 877-881..
[2] X. Li, Y. Wei, W. Yang and H. Gao, "Competing Grain-Boundary- and Dislocation-Mediated Mechanisms in Plastic Strain Recovery in Nanocrystalline Aluminum," 2009, Proceedings of the National Academy of Sciences of USA, Vol. 106 (38), pp. 16108-16113.
[3] J. Rajagopalan, X. Li, M. T. A. Saif and H. Gao, "Microstructural Heterogeneity can Strongly Influence the Deformation Behavior of Nanocrystalline Metals," work under submission.