Department of Civil Engineering and Engineering Mechanics

and

Department of Mechanical Engineering

Columbia University

Atomistic Modeling at Experimental Strain Rates and Time Scales

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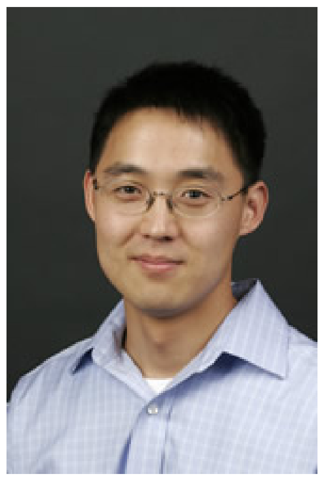

Thursday, October 23, 2014
2:30PM – 3:30PM
303 Mudd

I will present a new computational approach that couples a recently developed potential energy surface exploration technique with applied mechanical loading to study the deformation of atomistic systems at strain rates that are much slower, i.e. experimentally-relevant, as compared to classical molecular dynamics simulations, and at time scales on the order of seconds or longer. I will highlight the capabilities of the new approach via two distinct examples: (1) Providing new insights into the plasticity of amorphous solids, with a particular emphasis on how the shear transformation zone characteristics, which are the amorphous analog to dislocations in crystalline solids, undergo a transition that is strain-rate and temperature-dependent. (2) Uncovering new, mechanical force-induced unfolding pathways for the protein ubiquitin, while also discussing potential differences with experimental data regarding whether ubiquitin unfolds via an intermediate configuration.

Harold S. Park is an Associate Professor of Mechanical Engineering at Boston University. He received his BS, MS and PhD degrees in Mechanical Engineering from Northwestern University in 1999, 2001 and 2004, respectively. He was a postdoctoral researcher at Sandia Labs (California) from 2004-2005. He has over 90 refereed journal publications. He is the recipient of a 2007 NSF CAREER award, a 2008 DARPA Young Faculty Award, the 2009 Gallagher Young Investigator Award from the US Association for Computational Mechanics, and the 2012 ASME Sia Nemat-Nasser Early Career Award in Mechanics of Materials.