Abstract Submitted
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Phase Transition Plasticity Response in Uniaxially Compressed Silicon Nanospheres[1] TRAIAN DUMITRICA, PAOLO VALENTINI, Department of Mechanical Engineering, University of Minnesota, WILLIAM W. GERBERICH, Department of Chemical Engineering and Materials Science, University of Minnesota — We present a microscopic description for the response of crystalline Si nanospheres up to 10 nm in radius for various uniaxial compression levels. The behavior at low compressions closely resembles the Hertzian predictions. At higher compressions the creation of a new beta-tin phase in the particle core leads to (i) volumetric changes (ii) an increase in elastic moduli, and (iii) significant hardening. Further, (iv) a reversible character of the transformation is obtained with molecular dynamics simulations. The agreement of (i)-(iv) with recent experimental findings [1] challenges the current exclusive view of a dislocation plasticity response in somewhat larger nanoparticles. The phase transition path should dominate in ultrasmall structures, where dislocation activity is prohibited.
[1] W. W. Gerberich et al., J. Mech. Phys. Sol. 51, 979 (2003).
[2] P. Valentini, W. W. Gerberich, and T. Dumitrica, Phys. Rev. Lett. 99, 175701 (2007).

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