Abstract Submitted
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Atomistic Simulation of Size Effects in Bending a Single Crystal[1] N. SCOTT WEINGARTEN, The Catholic University of America, ROBIN SELINGER, Kent State University — We perform atomistic Monte Carlo simulations of bending a Lennard-Jones single crystal in two dimensions. In examining initial yield, we find an apparent "reverse" size effect. However, when strain rate effects are taken into account, we demonstrate that the size effect disappears. Once geometrically necessary dislocations coalesce to form grain boundaries, we observe a size effect of the usual kind, e.g. smaller samples support a higher scaled bending moment than larger samples. We compare simulation results with recent experiments on bending of highly annealed nanowires [B. Wu et al, Nature Matls 4, 525, 2005.] Finally, we observe a topological instability in the evolution of a grain boundary intersecting a free surface under compressive stress. The grain boundary buckles and nucleates a protruding grain, suggesting a novel mechanism for the formation of a hillock on a compressed metal surface.

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