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Accelerated Molecular Dynamics Simulation of the Tensile Behavior of Silver Nanowires on Experimentally Accessible Timescales
DANNY PEREZ, Los Alamos National Laboratory, CHUN-WEI PAO, Academia Sinica, SRIRAM SWAMINARAYAN, ARTHUR F. VOTER, Los Alamos National Laboratory — We present the result of accelerated molecular dynamics simulations of silver [110] nanowires stretched at a fixed velocity. By implementing the parallel-replica dynamics method on the peta-scale Roadrunner super-computer, experimentally-relevant pulling velocities as low as 10^{-6} m/s were directly simulated with full atomistic accuracy in both space and time. Using this tool, we study the tensile behavior of the nanowires as a function of temperature and pulling velocity. We observe that plasticity is initially mediated by the formation of a zig-zag network of stacking faults along various [111] planes. This mechanism is very robust and is observed in almost all of the cases. The next phase of the deformation is however extremely sensitive to external conditions: while fast pulling (on typical molecular dynamics timescales) lead to the accumulation of defects, necking and ultimately failure, slower drives allows for the annihilation of the stacking faults and the formation of thinner, defect-free wires. However, in agreement with experimental observations, this mechanism does not lead to the formation of atomic chains but typically to failure when the thickness of the wires drops below 3 atomic layers.

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