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Modeling of Polycrystalline and Wurtzite Si Nanowires with Symmetry-Adapted Objective Molecular Dynamics TRAIAN DUMITRICA, Department of Mechanical Engineering, University of Minnesota, DONG-BO ZHANG, Department of Chemical Engineering and Materials Science, University of Minnesota, MING HUA, Department of Mechanical Engineering, University of Minnesota — The stability and properties of the most promising ground state candidate Si nanowires with less than 10 nm in diameter is comparatively studied with molecular dynamics coupled with non-orthogonal tight-binding and classical potential models. The computationally-expensive tight-binding treatment becomes tractable due to the substantial simplification in the number of atoms introduced by the presented symmetry-adapted objective molecular dynamics scheme. It indicates that the achiral polycrystalline of five-fold symmetry and the wurtzite wires of three-fold symmetry are the most favorable quasi one-dimensional Si arrangements. Quantitative differences with the classical model description are noted over the whole diameter range. Using a Wulff energy decomposition approach it is revealed that these differences are caused by the inability of the classical potential to accurately describe the interaction of Si atoms on surfaces and strained morphologies.

Traian Dumitrica
Department of Mechanical Engineering, University of Minnesota

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