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Molecular-Dynamics Simulations of Nanowire Growth TOMORR HAXHIMALI, Northwestern University and University of California at Davis, DOREL BUTA, MARK ASTA, University of California at Davis, JEFFREY HOYT, McMaster University — This talk will present results of molecular dynamics simulations investigating the mechanisms of nanowire growth from a liquid. We investigate the model system of elemental Si, modeled with the classical Stillinger-Weber potential. The work aims to investigate the effect of nanowire size on the intrinsic growth mechanisms and the relations between solid-liquid interface velocity, growth direction and driving force. Results will be presented for nanowires with diameters ranging from 5-10 nm, and will be compared with simulations for bulk Si modeled with the same potential. The consequences of these findings for the mechanisms of nanowire growth from liquid catalysts by the vapor-liquid-solid mechanism will be discussed.

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