

Abstract Submitted  
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**Growth kinetics nano-scale faceted solid-liquid interfaces** TOMORR HAXHIMALI, Northwestern University and University of California, Davis, DOREL BUTA, Department of Chemical Engineering and Material Science, University of California, Davis, JEFFREY HOYT, Department of Material Science and Engineering, McMaster University, Hamilton, Ontario, Canada, MARK ASTA, Department of Chemical Engineering and Material Science, University of California, Davis, PETER VOORHEES, Northwestern University — In this talk we investigate kinetics of a faceted solid-liquid interface during growth of nanowires. To this end we have undertaken Molecular-Dynamics simulations of systems with nanowire-like geometries to probe the kinetics of their solid-liquid interfaces. These simulations has been undertaken for thermally driven systems of elemental material as well as for chemically driven alloys. In both cases the temperature was below the roughening value which assures that the solid-liquid interface remains faceted. However, as these simulations demonstrate the interface can be non-planar, remaining faceted in the middle and bounded by rough parts at the edges of the system. The solid-liquid interface propagates on a layer by layer growth with a growth rate depending on the size of the wire. Based on these insights we develop a kinetic theoretical model for the nucleation of crystal nuclei on the interface. The kinetic theory that we present for nanowire growth is applicable to both pure systems and alloys with non-planar interfaces. The above theoretical model predicts the same form for the dependence of growth velocity on driving force as in MD simulations. In a general context, this study establishes that system size-dependent growth rates are an intrinsic feature of systems with non-planar interfaces.

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