Abstract Submitted
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Construction of a kinetics model for liquid-to-solid transitions based on atomistic simulations: Extraction of surface free energies and kinetic coefficients[1] LUIS ZEPEDA-RUIZ, ALEX A. CHERNOV, BABAK SADIGH, TOMAS OPPELSTRUP, AMIT SAMANTA, SEBASTIEN HAMEL, TOMORR HAXHIMALI, LORIN X. BENEDICT, JON L. BELOF, Lawrence Livermore National Laboratory, PLS/WCI TEAM — We discuss work in progress towards a kinetics model for dynamically-driven liquid-solid transitions built from classical MD simulations. Special attention is paid to the growth kinetics of individual solid nuclei at different degrees of undercooling, and a method is presented for extracting solid cluster surface free energies, needed for coarse-grained models of solidification within the framework of an Avrami-like theory. Throughout, the goal of constructing a kinetics model for use in hydrocode simulations is emphasized.

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