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Evaluation of metastable region boundaries for liquid and solid states in MD simulations GENNADY IONOV, VLADIMIR DREMOV, ALEKSEY KARAVAEV, 1. Zababakhin All-Russia Research Institute of Technical Physics, Russian Federal Nuclear Center, SERGEY PROTSENKO, VLADIMIR BAIDAKOV, AZAT TIPEEV, of Thermal Physics, Russian Academy of Sciences, Ural Branch, 106, Amundsen Street — An automatic method based on MD calculations was developed for detecting and tracing the boundaries of metastable states of superheated crystal and supercooled liquid. The main criterion of the detection of early nucleation of new phase is the self-diffusion coefficient temperature dependence. The scanning for nucleation events is performed at continuous temperature change. The set of independent nucleation events at a given pressure allows evaluation of temperature dependence of specific nucleation frequency. The collection of a large number of these calculations allows accurate approximation of the specific nucleation frequency surfaces in the both directions of phase transition. These surfaces provide an opportunity to estimate the behavior of the free energy in the region between overheating and overcooling curves. In addition, dependence of nucleation frequency on pressure and temperature provides an opportunity to integrate the probability of nucleation under dynamic loading and subsequent release and thus to determine the likelihood of the crystallization and melting. The technique was applied to argon, tin and beryllium. Tin is modeled with the EAM potential, well reproducing the properties of BCC phase. Beryllium is modeled with the GEAM/MEAM potential.

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