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Calculation of entropy in classical and first-principles molecular dynamics simulation DMITRY MINAKOV, Moscow Institute of Physics and Technology (State University), PAVEL LEVASHOV, Joint Institute for High Temperatures RAS — Theoretical determination of solid-liquid phase boundaries is a longstanding problem in physics. Direct reconstruction of melting curves based on the equality of Gibbs energy for both phases sets a complicated task of entropy calculation, that remains the major impediment of this method. We present a detailed analysis of entropy reconstruction from a velocity autocorrelation function in molecular dynamics simulation for solid and liquid states. The reconstruction is based on the vibrational density of states (VDOS) and for the liquid phase is known as a two-phase thermodynamic (2PT) model. We compare this method with more complicated technique of thermodynamic integration and the Widoms particle insertion method. We also present results of *ab initio* calculations of melting curve and release isentropes using 2PT model for various metals.

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