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Metastability in solid–liquid transitions: the limit of superheating and supercooling[1]

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The inherent free energy barrier to the first-order phase transition may give rise to metastable melting and crystallization, i.e., superheating and supercooling. The limit of superheating and supercooling, a subject of scientific significance, is directly relevant to ultrafast dynamic experiments and molecular dynamics simulations. In the absence of satisfactory first-principles theories for solid–liquid transition and its metastability, we have established the systematics for the maximum superheating and supercooling at a given isobaric heating or cooling rate based on nucleation theory and supercooling experiments. The systematics have been demonstrated to be consistent with molecular dynamics simulations, Landau models and shock wave experiments. The applications of the systematics include, but are not limited to, the interpretation of dynamic experiments and development of the hysteresis method for determining the equilibrium melting temperature and the solid–liquid interfacial energy from superheating or supercooling. In light of superheating and supercooling, we also discuss the effects of defects and heating/cooling rates, the equivalence of temperature and pressure, and the Lindemann melting law.

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