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Temperature and rate sensitivity of melting in Cu AMIT SAMANTA, Applied and Computational Mathematics, Princeton University, Princeton, NJ, USA, TANG-QING YU, Courant Institute of Mathematical Sciences, New York University, New York, USA, WEINAN E, Department of Mathematics and Program in Applied and Computational Mathematics, Princeton University, Princeton, NJ, USA — The nature of melting of a crystal is a long standing topic of interest in materials science. Using advanced simulation techniques such as finite temperature string method and temperature accelerated molecular dynamics, we trace the minimum free energy path (MFEP) for a transition from solid to liquid phase at different temperatures in copper. Analysis of the configurations along the MFEP reveals that the rate determining transition state and the ensuing melting mechanisms are a function of temperature of the system. Close to equilibrium melting temperatures, the saddle point is determined by the critical size of the liquid nucleus, however, at higher temperatures, we find that the saddle structure consists of defect clusters from which the liquid nucleus is formed.

Amit Samanta
Applied and Computational Mathematics,
Princeton University, Princeton, NJ, USA

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