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Atomistic simulations of melting and solidification using temperature accelerated molecular dynamics TANG-QING YU, Courant Institute of Mathematical Sciences, New York University, AMIT SAMANTA, Program in Applied and Computational Mathematics, Princeton University, WEINAN E, Department of Mathematics and Program in Applied and Computational Mathematics, Princeton University, MARK TUCKERMAN, Department of Chemistry and Courant Institute of Mathematical Sciences, New York University, ERIC VANDEN-EIJNDEN, Courant Institute of Mathematical Sciences, New York University — A detailed understanding of melting/solidification mechanisms in metals remains obscure, though over the years many simulations and experiments have been performed for clarifying it. We have applied the enhanced-sampling method, Temperature-Accelerated Molecular Dynamics, to study the melting/solidification of FCC metals like copper, nickel under the constant temperature and pressure conditions. Free energy surfaces along Steinhardt order parameters and local density are obtained and minimum free energy path (MFEP) between the metastable states are calculated. An analysis of the atomic structure along the MFEP, reveals that an interplay between orientation ordering and positional ordering governs this phase transition.

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