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Free energy of steps using atomistic simulations[1] RODRIGO FREITAS, TIMOFEY FROLOV, MARK ASTA, Department of Materials Science and Engineering, University of California, Berkeley — The properties of solid-liquid interfaces are known to play critical roles in solidification processes. Particularly special importance is given to thermodynamic quantities that describe the equilibrium state of these surfaces. For example, on the solid-liquid-vapor heteroepitaxial growth of semiconductor nanowires the crystal nucleation process on the faceted solid-liquid interface is influenced by the solid-liquid and vapor-solid interfacial free energies, and also by the free energies of associated steps at these faceted interfaces. Crystal-growth theories and mesoscale simulation methods depend on quantitative information about these properties, which are often poorly characterized from experimental measurements. In this work we propose an extension of the capillary fluctuation method for calculation of the free energy of steps on faceted crystal surfaces. From equilibrium atomistic simulations of steps on (111) surfaces of Copper we computed accurately the step free energy for different step orientations. We show that the step free energy remains finite at all temperature up to the melting point and that the results obtained agree with the more well established method of thermodynamic integration if finite size effects are taken into account.

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Rodrigo Moura Freitas
University of California, Berkeley

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