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Properties of steps at faceted crystal-melt interfaces from molecular dynamics simulations DOREL BUTA, Northwestern University, MARK ASTA, University of California Davis, JEFFREY HOYT, Sandia National Laboratories — The properties of steps at faceted solid-liquid interfaces are key elements to understanding the anisotropy of interfacial free energies and mobilities, which in turn control the morphology of crystals grown from the melt. We investigate the equilibrium and non-equilibrium dynamics of arrays of steps at vicinal interfaces of Si(111) with molecular dynamics simulations of the Stillinger-Weber model. Step mobilities determined from isothermal crystallization simulations are found to decrease as the density of steps increases. We relate the decrease in step mobility to an increase in the effective stiffness of the interacting steps, manifested by a reduction in the width of equilibrium step fluctuations as the average distance between steps decreases. The analysis of step fluctuations is also instrumental in determining the nature of step-step interactions.

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