On the Connection between Kinetic Monte Carlo and the Burton-Cabrera-Frank Theory

PAUL PATRONE, University of Maryland, College Park and CNST at NIST Gaithersburg, DIONISIOS MARGETIS, T.L. EINSTEIN, University of Maryland, College Park — In the many years since it was first proposed, the Burton-Cabrera-Frank (BCF) model of step-flow has been experimentally established as one of the cornerstones of surface physics. However, many questions remain regarding the underlying physical processes and theoretical assumptions that give rise to the BCF theory. In this work, we formally derive the BCF theory from an atomistic, kinetic Monte Carlo model of the surface in 1+1 dimensions with one step. Our analysis (i) shows how the BCF theory describes a surface with a low density of adsorbed atoms, and (ii) establishes a set of near-equilibrium conditions ensuring that the theory remains valid for all times.

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