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Theory of kinetics of surface evolution: simulations, Langevin, and Fokker-Planck approach[1]

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The study of the the time evolution of morphological features at crystal surfaces has become a topic of great importance, motivated in part by the need of achieving controlled fabrication of nanostructures, and in part by the fundamental statistical mechanics questions that it raises. For the evolution of nanostructure, the control of step dynamics is crucial, since the steps are the fundamental building blocks of crystalline surfaces. Kinetic Monte Carlo (KMC) simulations, coupled to Langevin-type analysis of the scaling properties of step dynamics is a powerful tool for assessing the universal features of surface fluctuations close and far from equilibrium. We discuss the results of KMC simulations of unstable growth of vicinal surfaces, that exhibit anomalous scaling exponents as well as multiscaling. We also discuss a tentative interpretation of the numerics within the Langevin approach, as well as the usefulness of the results in interpreting experimental data. Other theoretical tools, such as the spacing distribution of the eigenvalues of random matrices have been employed, e.g. for investigating the evolution of the terrace width distribution (TWD) on stepped surfaces. We discuss KMC simulations of the relaxation of non equilibrium surface structures towards the equilibrium state. Our results show that relaxation far from equilibrium may be driven by microscopic processes, such as detachment of three-bonded atoms, that differ from those that drive step fluctuations close to equilibrium. Applications of the formalism to out-of-equilibrium states, such as step flow growth, are discussed.

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