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STEP ORIENTATION, STEP INTERACTIONS AND THEIR DEPENDANCE WITH STEP-STIFFNESS: SIMULATION AND THEORY FOR Cu

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Abstract: Steps on surfaces play a key role in many significant and interesting surface processes. Despite this importance, only few quantitative information about the factors governing step structure are available. In the context of nanostructures, the step stiffness $\tilde{\beta}$ - which describes the resistance of a step to meandering- is one of the key parameters in the widely applicable step continuum [1,2]. Kinetic Monte Carlo (KMC) simulations have been developed to describe all atomic processes occurring during crystal growth and particularly in studying the fluctuations of steps on vicinal (stepped) surfaces. From the spatial correlation functions, we measured the step stiffness and investigate the step-step interactions on Cu(001) surfaces as a function of step orientation at different temperatures.

Using KMC simulation, we study the role of step orientation in equilibrium surface process, the stochastic behavior of steps and the evolution of inter-step on Cu(001)-vicinal surface; in tight connection with the step-stiffness. Our results were compared to theoretical predictions based on the Fokker-Planck formalism [3]. In the first part, we show how this model involving only nearest-neighbor diffusion or the inclusion of the diffusion into next-nearest-neighbor sites leads to relaxation dynamics showing greater fluctuations on a shorter time scale for [110] steps than for the [100] steps. We also extract the interaction strength derived from the fit parameter (ρ) of the generalized Wigner distribution [3,4], which indicates an effective interaction between steps. In the second part, we take into account the next-nearest neighbor interaction. We show how the incorporation of this interaction leads to different steady state configurations as well as different step-stiffness and interaction strength.

Keywords: Surface relaxation, Step dynamics, Step stiffness, Step orientation, Kinetic Monte Carlo simulation, next-nearest neighbor interactions.

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