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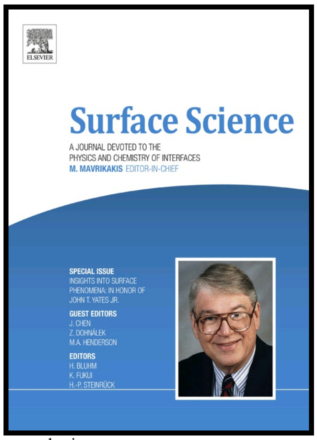

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Role of step stiffness and kinks in the relaxation of vicinal (001) with zigzag [110] steps

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Abstract

We present a kinetic Monte Carlo study of the relaxation dynamics and steady state configurations of <110> steps on a vicinal (001) simple cubic surface. This system is interesting because <110> (fully kinked) steps have different elementary excitation energetics and favor step diffusion more than ⟨100⟩ (nominally straight) steps. In this study we show how this leads to different relaxation dynamics as well as to different steady state configurations, including that 2-bond breaking processes are rate determining for <110> steps in contrast to 3-bond breaking processes for ⟨100⟩–steps found in previous work [Surface Sci. **602**, 3569 (2008)]. The analysis of the terrace-width distribution (TWD) shows a significant role of kink-generation-annihilation processes during the relaxation of steps: the kinetic of relaxation, toward the steady state, is much faster in the case of ⟨110⟩–zigzag steps, with a higher standard deviation of the TWD, in agreement with a decrease of step stiffness due to orientation. We conclude that smaller step stiffness leads inexorably to faster step dynamics towards the steady state. The step-edge anisotropy slows the relaxation of steps and increases the strength of step-step effective interactions.

Graphical Abstract

Step morphology after relaxation for straight-steps (Left) and zigzag-steps (Right).

1. Introduction

Zigzag ⟨110⟩ steps on a vicinal (001) simple cubic lattice with only nearest-neighbor interactions allow step-edge fluctuations (with geometric constraints) which have no energy cost, a situation which does not hold for straight ⟨100⟩ steps [1-3]. This suggests the possibility of different relaxation dynamics and steady state configurations for zigzag steps. A deeper understanding of steps is, of course, relevant to the study of surface nanostructures and is therefore technologically important. Indeed, the physical properties of epitaxial thin films can be manipulated by the understanding of the interfacial strain on the grown material. However, the strain can be controlled by adjusting the miscut angle of the vicinal substrate prior to growth. For example, anisotropic dielectric properties were observed and attributed to different tetragonalities induced by the vicinal substrate (LaAlO3) with miscut orientations along the ⟨100⟩ and ⟨110⟩ directions with different miscut angles [4]. Moreover, different nanostructuring behaviors were obtained depending on the step-orientation [5, 6].

Metropolis Monte Carlo [7-11] was used long ago to study step-edge equilibrium properties as a function of orientation. Subsequent kinetic Monte Carlo (kMC) [12] studies of ⟨100⟩ steps considered the evolution to equilibrium. Here we apply kMC [13] to the study of ⟨110⟩ steps on a vicinal (001) simple cubic surface in order to investigate the change in behavior due to distinctly different step-edge fluctuations.

This study is further motivated by investigations of flexible chains in a 2-D system [14] and interfacial configurations in a 2-D Ising ferromagnet on a square lattice [15], in which the primary observables of interest are interface energy and interface tension as functions of interface orientation. For a 2-D Ising ferromagnet, the