

Atomic Level Studies of Step Dynamics in Homogeneous Crystal Growth

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Step dynamics is one of the most important processes that governs atom transport and the resulting growth of a crystal. Our lack of knowledge of such processes is a significant void in our understanding of solid state surface physics. This is not only true from the viewpoint of pure science. The growth of crystalline materials, such as metals, from their vapor is used in numerous technological applications, including the microfabrication of microprocessors, chemical sensors, and biological sensors [1].

Over the last decade technology has pushed microfabrication to the near atomic scale. As technology advances and requires routine manipulation of individual atoms, the ability to benchmark predictive codes against atomic scale surface processes will be necessary. Knowledge of step dynamics in homogeneous systems is the prototypic case. From an atomistic viewpoint, see figure 1, questions arise such as: 1) Does a diffusing adatom descend over the edge of a terrace or does it exchange positions with a step-edge substrate atom?; 2) Can adatom-substrate atom exchange occur during diffusion across a terrace?; 3) Does an atom diffusing along a step edge do so by exchange with atoms in the step edge?; and 4) Does the proximity of other steps influence the answers to the foregoing questions?

Unfortunately, to date all studies seeking answers to questions regarding the atomic scale dynamics at step edges have been conducted in heterogeneous systems, i.e. using an adatom of a different element than the substrate atoms. This is because these studies have been conducted using the field ion microscope (FIM), which, although it provides atomic resolution imaging, can only distinguish the chemical nature of individual atoms for a few particular adatom-substrate combinations. Unusual exchange processes such as those generating an end-state as shown by configuration 3 in fig. 1 have been observed in heterogeneous systems, but never studied in homogeneous systems. The exchange of an adatom with a substrate atom in a homogeneous system cannot be detected using the FIM alone. However, the behavior of individual adatoms on a given substrate can depend significantly on the chemistry of the adatom and thus the results of studies in heterogeneous systems cannot be used to infer atomistic behavior in homogeneous systems [2].

To enable the study of step dynamics in homogeneous systems we employ a new approach - using an adatom that is a stable, relatively rare isotope of the elemental substrate. Thus, the chemistry of adatom-substrate interactions is unaffected. Diffusion is initiated by laser heating the substrate. This process can be observed using the FIM. Figure 2 shows a typical image obtained using the FIM. To distinguish the outcomes of step edge interactions we are using a variant of the FIM known as the atom probe field ion microscope (APFIM), which allows individual atoms to be chosen for time-of-flight mass analysis [3]. An atom at the step edge is removed from the substrate by field desorption and the known isotopic mass of the deposited adatom allows us to determine the outcome of a particular interaction.

We have completed construction of the APFIM. We are currently performing heterodiffusion experiments of tungsten on a rhodium substrate. Rhodium as a substrate is ideal for the calibration of our instrument because it is monoisotopic and provides an excellent reference for many system parameters, such as mass resolution. The results of these experiments are forthcoming. As we move on

to the homogeneous case we will study step dynamics in various low and high-index planes of several body-centered-cubic and face-centered-cubic elements. We will investigate the effect of step spacing and crystallographic orientation on step dynamics. In parallel with the experimental studies we will attempt to explain our observations using new and/or existing theoretical models and extract intrinsic surface parameters involved in possible cooperative exchange diffusion.

References:

- [1] M Giesen, *Progress in Surface Science* **68** (2001), p. 1-154.
 [2] G Antczak and G Ehrlich in “Surface diffusion: metals, metal atoms, and clusters”, (Cambridge University Press, New York).
 [3] M.K. Miller and G.D.W. Smith in “Atom probe microanalysis”, (Materials Research Society, Pittsburgh).

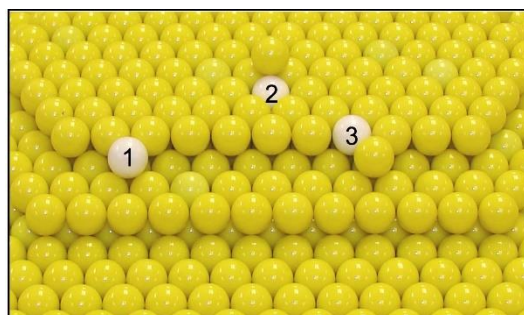


Figure 1. Ball model showing some possible step dynamics at the atomic level on a face-centered-cubic (111) plane with several terraces separated by monatomic steps. The adatom is white and the substrate atoms are yellow. Configuration 1: An adatom has simply descended from the upper terrace to assume a position on the step edge. Configuration 2: An adatom has exchanged with a substrate atom during diffusion across the upper terrace. Configuration 3: The adatom descended from the upper terrace by the coordinated displacement of a step-edge substrate atom.

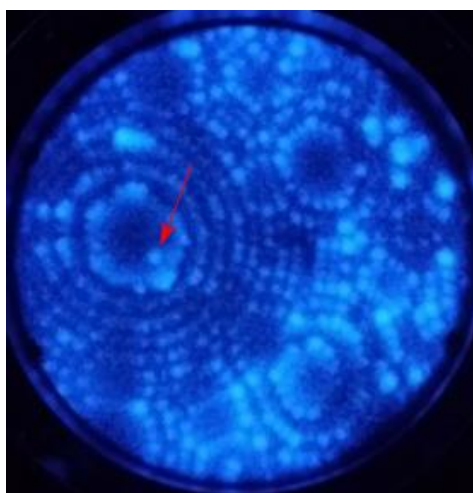


Figure 2. Image of an iridium crystal taken using the field ion microscope. Each bright spot shows the location of an individual atom. An Ir adatom on the $\langle 111 \rangle$ plane near a step edge is highlighted by the red arrow.