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A Simple Kinetic Monte Carlo Approach for Epitaxial Submonolayer Growth

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Abstract. Two-component submonolayer growth on triangular lattice is qualitatively studied by kinetic Monte Carlo techniques. The hopping barrier governing surface diffusion of the atoms is estimated using pair interaction potentials. Several degrees of freedoms enhancing the surface diffusion of atoms are also introduced. The main advantages of the presented technique are the reduced number of free parameters and the clear diffusion activated mechanism for the segregation of different types of atoms. The potential of this method is exemplified by reproducing (i) phase-boundary creation and dynamics related to vacancies and stacking faults; (ii) a special co-deposition and segregation process where the segregated atoms of the second component surround the islands formed by the first type of atoms.

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1 Introduction

Simultaneous deposition of different types of atoms is widely encountered in experiments and practical applications [1–8]. It can be used for engineering special coating structures (e.g. nanocomposits by inhibitor additive) [9–13], or for improving the quality

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of the epitaxially grown films by using one component as a kind of surfactant [14,15]. On the other hand impurities (contaminants), operating generally as inhibitors, are always present during the deposition process, and even a minute amount of them can drastically modify both the bulk structure and the surface growth morphology of the films [16–20]. Typical topological features related to inhibitor impurity effects are: (i) irregular shapes of monolayer islands, (ii) bunches of growth steps forming hillocks and dents within the surface of crystals, (iii) truncated and rounded crystal shapes, as well as (iv) deep grain boundary grooves decorated by small crystals in polycrystalline films. Appearance of repeated nucleation and islands on the surface indicates directly that the crystal growth is interrupted by a surface covering layer i.e. the crystals became encapsulated by the impurity phase [1, 18, 19, 21, 22]. This phenomenon was clearly demonstrated by in situ transmission electron microscopy experiments in carbon contaminated indium films [1].

The ideal one-component deposition is thus seldom realized and one always encounters the situation where species of several material components participate in the surface atomic processes. Foreign species can control the course of the fundamental phenomena and the pathway of structure evolution. To understand the effect of surfactant or inhibitor impurities on the structure evolution and the complex atomic processes taking place on the growth surface a consecrated method is to use kinetic Monte Carlo (MC) simulations [23–26]. This computational approach can help researchers in predicting the pathway of structure evolution and the structures that will form at different experimental conditions. By this way one could understand also the effect of the experimentally controllable parameters and engineer structures with desired practical properties.

It is well known that MC simulations are much weaker approximations to reality than the nowadays fashionable ab-initio Molecular Dynamics simulations (for a review see Ref. [27]). By considering kinetic MC simulations several processes are taken into-account only in a phenomenological manner, without a microscopically realistic dynamics. The interaction potentials governing the dynamics of the atoms are either heuristic or determined from ab-initio Density Functional Theory (DFT) calculations [28]. MC simulations offer, however, a great advantage (for a review see Ref. [29]): it is fast and one can study thus larger systems and longer time-scales. Due to this advantage it is also more adaptable for moderate computational resources than Molecular Dynamics methods. Quite reasonable numbers of atoms can be studied on cheap PC type computers. Making MC simulations more realistic is thus an important task. This could help researchers in elaborating powerful codes for predicting, developing structures of thin-films or the topology of auto-organized nano-structures. Here we use a fast and simple kinetic Monte Carlo method for two-component sub-monolayer growths. The presented method can be generalized for several co-deposited components and also for the case of multilayer growth.

This paper is organized as follows. In Sections 2 and 3, the generally used kinetic Monte Carlo techniques are presented and the specific problem considered in the present work is discussed. In Section 4, our simple Monte Carlo approach is described and applied for the targeted problem. The simulation results are presented in Section 5,