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A kinetic Monte Carlo method on super-lattices for the study of the defect formation in the growth of close packed structures

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Abstract

A modified Kinetic Lattice Monte Carlo model has been developed to predict growth rate regimes and defect formation in the case of the homo-epitaxial growth of close packed crystalline structures. The model is an improvement over standard Monte Carlo algorithms, which usually retain fixed atom positions and bond partners indicative of perfect crystal lattices. Indeed, we extend the concepts of Monte Carlo growth simulations on super-lattices containing additional sites (defect sites) with respect to those of the reference material. This extension implies a reconsideration of the energetic mapping, which is extensively presented, and allows to describe a complex phenomenology that is out of accessibility of standard stochastic approaches. Results obtained using the Kawasaki and the Bond-Counting rules for the transition probability of the Monte Carlo event are discussed in details. These results demonstrate how the defect types (local or extended), the formation mechanisms and the defect generation regimes can be characterized using our approach.

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1. Introduction

The problematic of the epitaxial crystal growth of materials having close packed crystalline structures is tightly connected to the polytypism (a special case of one-dimensional polymorphism) [1] that such materials usually show. Indeed, close packed crystals can have a high degree of stable crystal configurations with the same chemical composition, a similar content in terms of bulk free energy but a different one-dimensional stacking and different physical and electrical properties. This effect is related to the two possible equivalent sites for the atom sticking on the crystal surface during the deposition process.

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In order to reduce polytype mixing, surface steps can be formed by off-axis cuts of the substrate, thus forcing the epitaxial grown layer to inherit the polytype of the substrate. This technique is known as "step controlled homoepitaxy" [2,3]. This homo-epitaxial step-flow growth contrasts the nucleation and growth of islands of complementary symmetry with respect to that of the substrate which would, eventually, lead to the formation of polycrystalline structures. Island nucleation increases at higher deposition rates; therefore, imposing a low growth rate in the experimental setting is the usual empirical prescription to avoid the polycrystalline growth regime. Indeed, when the time interval between two successive deposition events in the same terrace area is much larger than the average time which the adatom spends in the terrace before encountering the step (diffusion limited regime), an optimal homo-epitaxial growth should occur. Several deposition parameters can influence the quality of the grown crystal (i.e. temperature, off-angle cut, precursor flows, etc.); as a consequence, a deeper understanding of the possible defect formation mechanisms can help to increase the growth rate limit allowing for cheaper epitaxial processes.

In the past the problem of island nucleation and evolution in the homo-epitaxial step-flow growth was studied applying analytical models based on the theory of Burton et al. [4] for the dynamics of the step together with the Avrami nucleation theory [5] or using on-lattice numerical methods (Kinetic Lattice Monte Carlo (KLMC) [6]). Each method has its own advantages and limits. The BCF theory is a continuous theory which correctly accesses the time and length scale of the process (microns and seconds) but it misses the atomic scale description, whereas the limit of standard on-lattice methods is that the kinetic particles (adatoms, terrace atoms and atoms in the bulk) reside in the characteristic lattice sites of the material in study, so that they fail on describing the generation and evolution of defects. On the other hand, off-lattice methods (ab initio [7], molecular dynamics [8] and Monte Carlo [9]), can be successfully used for the study of defects but are unable to reach the time scale of the epitaxial process (seconds). More generally, using standard kinetic schemes, only particular topics of the growth kinetics can be theoretically investigated, since they fail in describing the correlation between the concurrent aspects characterizing the micro-structural evolution of the system (island nucleation, correlation between the evolution of islands with different symmetry, correlation between the island and step evolution, interaction between bulk and surface structures) on the correct time scale of the process.

The goal of this work is to develop an innovative method for the investigation of the growth process kinetics in the case of close packed structures which allow, in principle, to access to the full complexity of the phenomenology in study. The method extends the concepts of the Kinetic Lattice Monte Carlo growth simulation on super-lattices containing additional sites with respect to those of the reference lattice of the material in study [10]. This extension allows to describe the generation and evolution of defects at the atomic level but, also, to overcome the time scale limits typical of the off-lattice methods.

The paper is structured as follows. In Section 2, we introduce the refined lattice used, specifying bonds and neighbors. Section 3 specifies the probability rules used for the adatoms evolution. In Section 4, we discuss the different possible boundary conditions, defining the *Helicoidal Boundary Conditions*. The deposition algorithm, used in the epitaxial process, is specified in Section 5. In Sections 6 and 7, we present the results for the two-dimensional (2D) and three-dimensional (3D) cases, respectively. In Section 8 we, finally, discuss the main results obtained.

2. Numerical methodology

In the *KLMC* method the lattice is represented by a structured mesh which fixes the allowed atom positions and bond partners. In order to achieve the possibility of representing and considering in the evolution algorithm the dynamics of the defective structures we use, as substrate of our *KLMC* model, a refined effective lattice including the real lattice sites of the close packed structure as a sub-lattice. In particular, we use a hexagonal lattice with reduced inter-site distance with respect to the one of the regular lattice. In this refined lattice, second-neighbors are generally associated to the regular relative positions of the close packed structure in study, whereas first-neighbors are associated to defective configurations. Considering a given (0001) layer, this choice allows us to consider all the three possible different adatoms occupation sites (generally called A, B and C) as sites of the hexagonal structure (see Fig. 1), while a single kind of site (A or B or C) is occupied in the regular lattice. The use of a refined lattice implies that: