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Atomistic modeling of epitaxial growth of semiconductor materials

Ignacio Martin-Bragado *, Andrey Sarikov

IMDEA Materials Institute, Calle Eric Kandel, 2, 28906 Getafe, Madrid, Spain

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ABSTRACT

The epitaxial growth of semiconductors is a very important step for the processing of microelectronic devices. Solid Phase Epitaxial Regrowth (SPER) is involved in both the recrystallization of amorphous silicon and germanium areas. Selective epitaxial growth (SEG) is routinely used in manufacturing modern 3D devices like finFETs, raised source/drain transistors, gate-all-around transistors, etc. In this work, lattice kinetic Monte Carlo modeling is used as the main tool for the modeling and simulation of epitaxial growth in IV and III–V based materials. This is done by detecting particular local configurations at the interfaces, and assigning local growth rates depending on such configurations. This simple idea is used to identify recrystallization planes or to compute different formation energies for the trapping, detrapping and migration of atoms. Introduction of defects is also possible by allowing the formation of twins and small defective areas. We will show different cases where our model is used, namely: SPER and defect formation of Si, and we will explain how the models can be extended to simulate the epitaxial growth of III–V materials and to obtain the different facet formation and growth kinetics. All these cases are compared with relevant experimental results from the literature to provide an assessment of their current capabilities but also possible limitations.

1. Introduction

Selected parts of contemporary electronic devices such as source/drain regions of integrated circuit transistors, and devices themselves, are fabricated with a trend to miniaturization down to minimum physically achievable dimensions [1]. For the formation of such miniature regions, advanced technologies of structure growth with high spatial resolution, such as selective area epitaxial growth or localized ion implantation with subsequent recrystallization need to be used [1–3]. Growth in small dimensions leads to the manifestation of specific features such as faceting and preferential growth of low index crystalline planes, formation of local strains, evolution of point and extended defects etc. [4–6]. These features have considerable effects both during the structure growth as well as for the device operation. Therefore, they should be taken into account in the modeling of the kinetics of growth processes to reveal underlying physical mechanisms and to enable a reliable control over the behavior of the structures under study both during their formation and normal work regime of devices.

Small size structures favor the application of the modeling methods that enable to obtain the evolution at atomic level, such as ab initio [7], molecular dynamics (MD) simulations [8,9], and lattice kinetic Monte Carlo (LKMC) modeling [10,11]. As compared to the ab initio and MD simulations, LKMC methods have a higher scaling potential with preservation of reasonable computation efficiency so that the systems of different sizes can be modeled at low cost. LKMC methods are used to simulate the vast variety of solid transformation kinetics such as e.g. shape relaxation of nanoclusters [12], evolution of the defect structure in solid [13] and laser melted Si [14], vacancy mediated interdiffusion in SiGe alloys [15], step flow growth and defect generation of SiC [16,17], hydrogen adatom [18,19] and vacancy defect [20] evolution in graphene, etc. LKMC modeling can be applied to reveal general peculiarities of a particular process. For example, the change of the relaxation mechanism of the fcc nanocluster shape from the surface atom diffusion to the nucleation of two-dimensional islands on a facet upon reducing the temperature below the roughening threshold has been established without the specification of the cluster material [12]. Alternatively, modeling of the behavior of specific material systems requires proper model calibration with respect to the material properties to obtain reliable results. For such calibration, LKMC methods are often combined with the ab initio [18,19] or molecular dynamic [13] simulation methods applied for the smaller scale systems, which provide with the necessary input. In other cases the experimental data sets may be used for the LKMC model calibration. It is also possible that the LKMC results themselves are used for the calibration of macroscopic simulation models such as the kinetics phase field model used to simulate the depth distribution of the vacancy-type

* Corresponding author. Fax: +34 91 550 30 47.
E-mail addresses: ignacio.martin@imdea.org (I. Martin-Bragado), andrey.sarikov@imdea.org (A. Sarikov).

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defects arising from the multishot laser irradiation of a Si substrate [14].

In order to improve the modeling power of the LKMC methods, the extended (augmented) lattices are used, in which additional sites are introduced in the standard lattice [15–17]. In [16], the lattice kinetic Monte Carlo model on the "refined" effective lattice including the real lattice sites of the close packed structure as the sub-lattice has been realized. This model has been used to predict the growth regimes and defect formation of the homoepitaxial growth of close packed crystalline structures. In [17], the application of this model to the epitaxial growth of SiC has enabled to describe the peculiarities of the growth rate behavior and defect structure as the functions of the off-cut angle of substrate and the deposition temperature as well as to suggest a new deposition regime, namely "defective epitaxial regime", between the standard epitaxial step flow and non-epitaxial 2D nucleation regimes. In [15], the LKMC model on the Si lattice augmented with high symmetry sites has been used to simulate the vacancy mediated diffusion in SiGe alloys aimed at the study of the influence of stress and alloy composition on the diffusion mechanism.

This paper presents a brief review of the application of the lattice kinetic Monte Carlo modeling to the study of the kinetics and the peculiarities of the formation of crystalline Si and III–V structures by solid phase epitaxial regrowth (SPER) and metal organic chemical vapor deposition (MOCVD). The algorithms and approaches used to model the defect structures and their evolution during growth, the influence of defects on the growth rate and surface morphology, and the development of preferential faceting are described. In addition, multiscale modeling combining MD, finite-element method (FEM) and LKMC simulations is presented to study the solid phase epitaxial regrowth of amorphized regions in crystalline Si and the formation of their defect structure.

2. Lattice kinetic Monte Carlo modeling of solid phase epitaxial regrowth of Si

2.1. Anisotropic planar Si regrowth

The kinetics of the solid phase epitaxial regrowth of Si using the lattice kinetic Monte Carlo method is modeled on the ideal Si lattice introduced for the whole system consisting of amorphous and crystalline Si phases with an initially perfect interface between them. The distinction between the Si atoms in both phases is established by assigning the "amorphous" or "crystalline" atoms tags depending on the phase the Si atoms belong. Si atoms have a probability to transfer from the amorphous to the crystalline phase at the amorphous/crystalline interface, which is achieved by changing the respective atom tag. The probability of such transition depends on the orientation of the growing plane of crystalline Si phase, which is a consequence of the geometry of Si atoms incorporation shown schematically in Fig. 1 for {100}, {110} and {111} plane orientations. Following the qualitative model proposed by Drosd and Washburn [21], it is assumed that each atom in the amorphous phase needs to form two undistorted bonds with the crystal to transfer in the crystalline state. This is naturally achieved for {100} oriented surfaces. However, for {110} surfaces a cluster of two adjacent atoms in the amorphous phase is necessary for each Si atom to complete two undistorted bonds, while a cluster of three atoms should form for {111} surfaces, respectively. A coordination number n is thus associated with each configuration of Si atoms incorporated in the lattice, characterizing the number of simultaneously crystallized Si atoms ($n=1$, 2 and 3 for {100}, {110} and {111} planes orientations, respectively).

The recrystallization kinetics is modeled as a series of consecutive events of a transition of a Si atom from the amorphous in

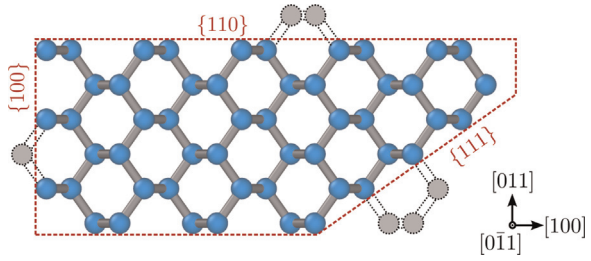

Fig. 1. Atomistic configurations for {100}, {011} and {111} local recrystallizations. Si atoms in the crystalline phase are shown inside the contoured geometrical figure, while outside it the sites to be occupied by atoms from the amorphous Si phase are indicated.

the crystalline Si state with the frequency of an event f calculated as follows [10]:

$$f = K(\text{site}) \times \exp\left(-\frac{E_{activation}}{kT}\right) \quad (1)$$

using the single activation energy of amorphous-to-crystalline transition $E_{activation}$ and three pre-exponential factors characterizing the growth rates of three basic orientations, $K(100)$, $K(110)$, and $K(111)$, respectively. The values of the parameters in Formula (1) are obtained by model calibration to the available experimental data on the kinetics of the recrystallization of amorphous layers on the top of crystalline Si. Using three pre-exponential factors $K(100)$, $K(110)$, and $K(111)$, the different recrystallization rates for the three mentioned basic plane orientations are obtained as well as the formation of faceted structures during recrystallization (see Fig. 2) [10], in agreement with the results of experimental observations [22]. In addition, the effect of the strain appearing as a result of ~2% volume mismatch between amorphous and crystalline Si [23] and leading to the retardation of recrystallization is successfully accounted for by modifying the value of $E_{activation}$ with strain related components as further described in Section 2.3.

The LKMC model described in this section is further modified to include the formation of the twin defects during amorphous Si epitaxial regrowth [24]. These defects are known to influence on the SPER rate and structure, including the shape and the interface roughness between the amorphous and crystalline Si phases. To model the formation of twin defects during the SPER process, the Si atoms in the lattice sites after the recrystallization event are assigned one of the following two tags, namely: *normal* for the sites sharing the substrate configurations, and *defective* for the sites that are assumed not to bond properly to their neighbors but to form twin defects similar to those observed in MD simulations [9,25]. New defective sites are produced by either of the two mechanisms: (i) {111} sites (and thus related with the $K(111)$ pre-exponential factor) have a probability $P_{def}^{\{111\}}$ of becoming defective,

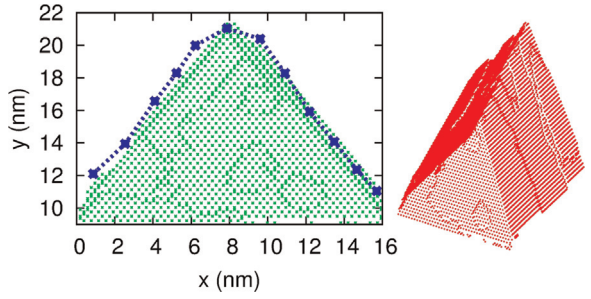

Fig. 2. Left: arrow tip formation during SPER of a thin Si fin (16×50 nm^2). Simulation results (symbols) and experimental amorphous/crystalline regrowth (line, taken from [22]) after a 60 s, 600 °C annealing are presented. Right: 3D view of the same simulation.

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