A valence force field-Monte Carlo algorithm for quantum dot growth modeling

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***Abstract*—We present a novel kinetic Monte Carlo version for the atomistic valence force fields algorithm in order to model a self-assembled quantum dot growth process. We show our atomistic model is both computationally favorable and capture more details compared to traditional kinetic Monte Carlo models based on continuum elastic models. We anticipate the model will be useful to experimentalists in understanding better the growth dynamics of quantum dot systems.**

I. Introduction

Self-assembled InAs/GaAs quantum-dot structures (QD) have recently received much attention due to their relevance for optoelectronic devices [1].

Strain caused by the differences of the lattice constants of the QD and substrate (matrix) material is decisive for the so-called self-organized effects, which occur during the growth of strained heterostructures: thermodynamic and kinetic ordering effects which can create a three-dimensional island within a matrix [2].

An important aspect in this context is also the influence of the lattice mismatch induced strain field and its effects on the bandstructure and optoelectronic properties. The strain distribution in crystals is usually treated with the continuum mechanical model [3], or with the valence force field (VFF) model [4], or using density functional techniques [5]. An exhaustive analysis of the VFF and continuum models is presented in Ref. [6].

Heteroepitaxial growth has been simulated with continuum formulations as island dynamics [7], [8], phase field models [9], [10], or sharp interface models [11], [12]. However, recent works showed the importance of using kinetic Monte Carlo (KMC) algorithms [13], [14].

In this work we introduce a new KMC algorithm where the elastic energy is given by the VFF model. Starting from an atomistic configuration which reproduces the experimental deposition of a material with a larger lattice constant than the substrate and with a thickness above the critical thickness of pseudomorphic growth [15], the system is made to evolve toward a thermodynamic equilibrium regulated by constraints given by optimization models of complex systems [16], [17]. To our knowledge this is the first time a model combine atomistic strain calculations with a KMC scheme to describe a QD growth.

II. Theory

A. Valence force fields

Lattice-mismatched zincblende semiconductor alloy ground state configurations have been determined for a group of lattice-mismatched III-V semiconductor alloys, such as GaInN, GaInP, GaInAs, GaInSb, InAsSb, and InPAs [18]. A VFF model for strain energy with two parameters α and β for lattice-mismatched isovalent semiconductor zincblende alloys has been derived in Ref. [19].

B. Kinetic Monte Carlo

Heuristic optimization techniques based on KMC algorithms are used in different fields of science. Among the most used KMC is the simulated annealing (SA), a local search Metropolis algorithm which minimizes the energy of a candidate configuration in a way similar to a real physical system, minimizing its energy under cooling [20]. In this work a new configuration is generated by exchanging cations. The change is always accepted if the energy is lower, or with a probability

$$\exp(-\Delta E/T), \tag{1}$$

if the energy is higher, where ΔE is the change in energy and T is the temperature. In this way, a gradual annealing with decreasing of temperature should help reaching the ground state. However, in a complex systems, i.e. a hard combinatorial problem, SA may be trapped in metastable configurations.

III. Results

In order to check if finding a ground state for the elastic energy was really a hard combinatorial problem, we made some preliminary simulations with an InAs/GaAs zincblende QD, a regular truncated pyramid with base $b = 12\,nm$ hight $h = 5\,nm$. We considered three different In values, i.e., 10%, 30% and 50%, and for each concentration, starting from a random initial configuration of the atoms, we let the system evolve only allowing exchanges between Indium and Gallium atoms that decreased the elastic energy. We considered 20

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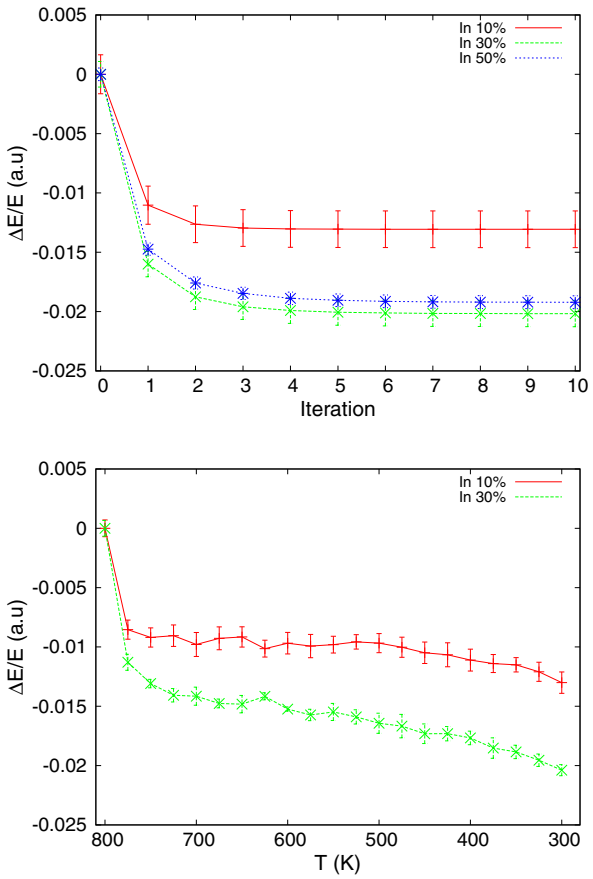

Fig. 1: Top: simple KMC simulations ($\Delta E < 0$) for different In content. Below: SA KMC simulations (one iteration at each temperature). Relative elastic energy axis of ordinates for both plots.

different configurations in order to have a good statistical average. As we can see in Figure 1 (top), the system quickly freezes in a local minimum. Here by 'iteration' we mean a complete sweep of exchanges over all atoms. The final configuration heavily depends on the initial state as evidenced by the large error bars.

In contrast, using an SA algorithm, the system easily reaches a final configuration which is much less dependent on the initial state, as shown in Figure 1 (bottom). Interestingly, the annealing of the QD favors clustering of In atoms. This can be seen in Figure 2, showing a significant increase in the counts of In ions at distances less than 1.5 nm from each other.

We will show an application of our algorithm to a situation that mimics an experimental growth process, using physical parameters derived from real data for growth of InAs/InP QD nucleation. We believe that our model may give interesting indications to the experimentalists particularly about the dependence of the QD size on the growth temperatures.

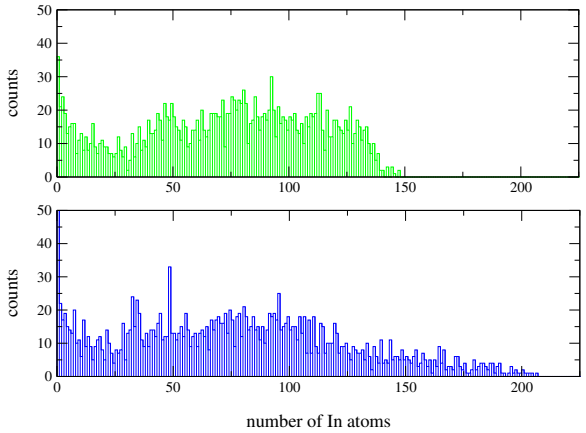

Fig. 2: Statistics showing the counts of the total number of In atoms within spheres of 1.5 nm around each single In atom (50% In content). In other words, there are '*counts*' In atoms which have '*number of In atom*' around within a sphere of 1.5 nm. Original random configuration (Top panel) and after annealing (Bottom panel).

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