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Computer simulation of quantum dot formation during heteroepitaxial growth of thin films

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Abstract

Influence of mismatch on quantum dot formation during heteroepitaxial growth of thin films with zinc blende structure on GaAs substrate is investigated. A kinetic Monte Carlo model is used for simulation of thin films with different values of lattice mismatch in the range of 4% to 14%. Simulation is performed at a substrate temperature of 700 K and deposition rate of 0.3 ML/s. Also, 'reflection high-energy electron diffraction' (RHEED) intensity of simulated thin films is evaluated during growth. Results of simulation show that at constant temperature and deposition rate, quantum dot size decreases with increasing lattice mismatch, and their distribution function becomes sharp. Simulated RHEED oscillations have a good agreement with morphology of simulated thin films, and results show that growth mode changed from Stranski-Krastanov to Volmer Webber by increasing lattice mismatch.

Keywords: Heteroeiptaxial growth, Monte Carlo, Quantum dots
PACs: 68.00, 68.35, 61.14.

Background

During heteroepitaxial growth of semiconductors, releasing the stress which created due to lattice mismatch of layer and substrate leads to growth of self-assembled nanostructures and nano-patterns with special properties [1-3]. Among these nanostructures, quantum dots can be pointed out [4,5]. Recently, the quantum dots have been investigated widely because of the development of IR lasers, photodiodes, solar cells, and thermophotovoltaic convertors [6-8]. The efficiency of these devices is strongly influenced by different properties of quantum dots (QDs) such as crystal and electronic structure, size and distribution, and also residual stress and defects. Therefore, control of such nanostructural parameters strongly affects the efficiency of devices.

Among semiconductors, GaAs has special properties such as direct bandgap and high electron mobility which have made it a key element in integrated circuits, high-frequency transistors, and light-emitting diodes. Moreover, wide bandgap and high resistivity accompanied with high dielectric constant make it a very good choice for substrate, which causes isolation between the substrate and circuits. Because of this property, GaAs is widely used as a substrate for thin film growth or QD formation [9,10]. An atomistic understanding of the processes which control the quality of interface during growth is very important, and simulation is a suitable tool for understanding strain and stress effects during growth and description of defect formation mechanisms.

Various simulation methods are used for simulation of thin film growth and islands or QD formation. Generally, these methods can be divided into two major groups: continuous and atomistic simulations. The continuous models such as 'phase field model' are based on partial differential equations and have a low computational cost, but they are not appropriate for atomic scale simulation [11]. Molecular dynamic (MD) and Monte Carlo (MC) are the most important models for atomistic scale simulation, while MC involves with a lower computational cost compared to MD method and is suitable for simulation of thin film growth and QD formation [12].

In this study, a kinetic Monte Carlo simulation with valence force field approximation is used for strain energy calculation to describe QD formation during heteroepitaxial growth of a model material with GaAs

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structure. Also, 'reflection high-energy electron diffraction' (RHEED) patterns are simulated by a model.

Simulation model

An 'on-lattice' kinetic Monte Carlo (KMC) method with valence force field approximation is used for simulation of heteroepitaxial growth of thin films and formation of quantum dots. The simulation is performed on an array of 60 × 60 unit cells of GaAs which approximately equals to 30 × 30 nm area of substrate. To consider the effect of mismatch, it is assumed that all physical properties of deposited material such as binding energy and structure are the same as the substrate material except lattice constant. In on-lattice simulation, all suitable points for accommodation or relaxation of deposited atoms are identified at the beginning of simulation, and during simulation, the final points for relaxation are selects based on KMC algorithm [13,14]. Therefore, zinc blende structure is used for identification of both substrate atoms and suitable points for relaxation of deposited atoms, but lattice constant of the region that identifies the layer is different from the substrate in the range of 4% to 14%. After the definition of substrate, the simulation continues as follows:

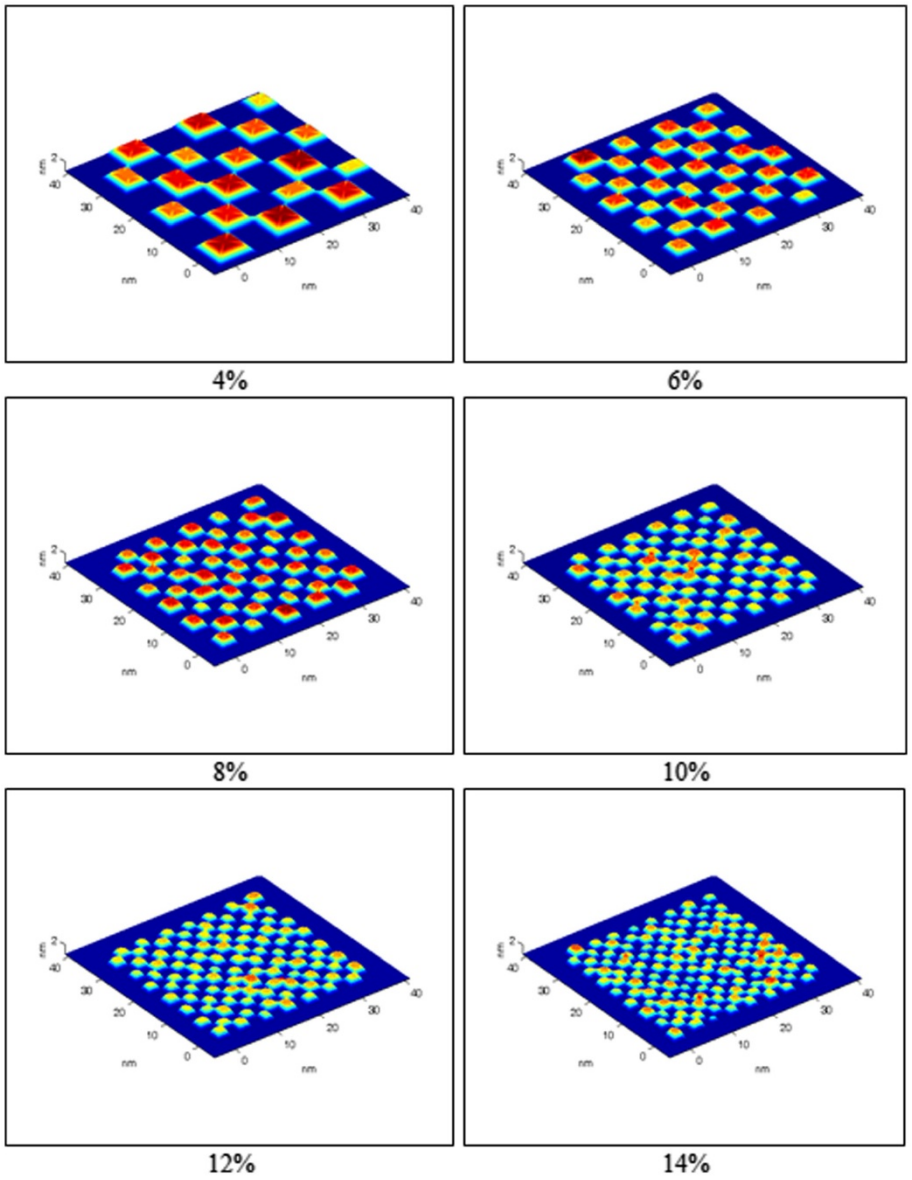

Figure 1 Formation of quantum dots for different values of mismatch. At the substrate temperature of 700 K and deposition rate of 0.3 ML/s.

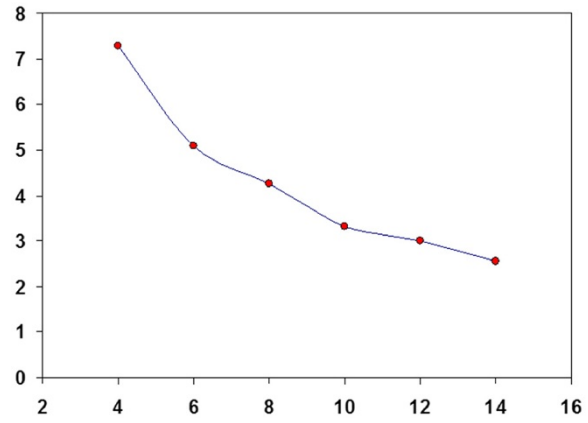

Figure 2 Mean value of QD sizes for different values of mismatch.

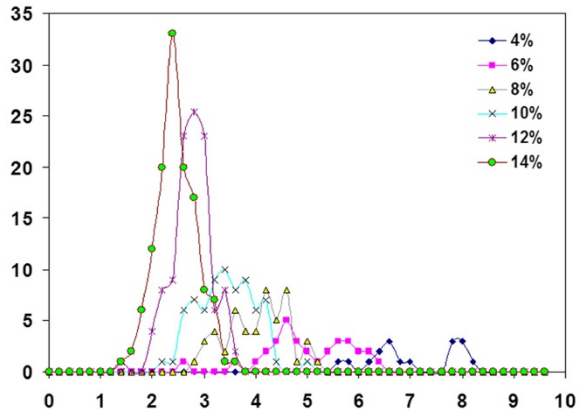

Figure 4 QD size distribution for different values of mismatch.

1. Atoms of Ga and As with equal rates accommodated on the substrate randomly.
2. An adatom on the substrate is selected randomly, and all transition states and related probabilities $w_{i \rightarrow j}$ are evaluated:

$$w_{i \rightarrow j} = \nu \exp(-\Delta E / k_B T) \quad \Delta E = E_j - E_i. \tag{1}$$

In this stage, surface diffusion and also interlayer migration are considered. For interlayer migration, the model introduced by Fazouan et al. [15] is used. In this model, each adatom in the N layer is allowed to migrate to a proper position two atomic layers above or below the N layer. The energy of adatoms in each position is evaluated using the following:

$$E_i = \sum_{j=1}^{m} \phi_{ij} + E_s, \tag{2}$$

where m is the number of nearest neighbors; ϕ_{ij}, the binding energy; and E_s, the energy of strain resulting from the mismatch. In GaAs structure, the normal bond angle of Ga-As-Ga is 109.47°, but at the interface of layer and substrate because of mismatch, bond angles vary from this value and result to an additional term in energy. In valence force field approximation [16],

$$E_s = \frac{9}{8} k_\theta \sum_{\text{bond angles}} \left(\frac{1}{3} + \cos\theta \right)^2, \tag{3}$$

where θ is the bond angle and k_θ is a constant.

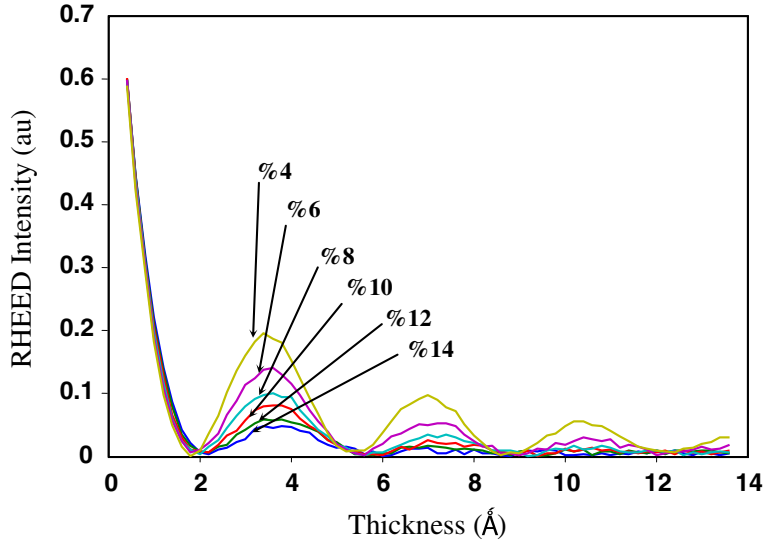

Figure 3 RHEED intensity versus thickness of model GaAs thin film. On GaAs substrate for different values of mismatch.

3. The values of Q_n are evaluated as follows:

$$\begin{aligned} \mathrm{Q}_1 &= 0 \\ \mathrm{Q}_2 &= \sum_{j=1}^{1} w_{i\to \mathrm{j}} = w_{i\to 1} \\ \mathrm{Q}_3 &= \sum_{j=1}^{2} w_{i\to \mathrm{j}} = w_{i\to 1} + w_{i\to 2} \\ \mathrm{Q}_\mathrm{N} &= \sum_{j=1}^{N-1} w_{i\to \mathrm{j}} = w_{i\to 1} + w_{i\to 2} + \ldots + \ldots w_{i\to \mathrm{N}-1}. \end{aligned} \tag{4}$$

4. A random number ($0 < R < 1$) has to be generated, and in case of $Q_n < R < Q_{n+1}$, the state of $n + 1$ accepts and the system transits to state of $n + 1$.
5. Another random number $0 < U < 1$ have to be generated in relation to simulation time, and the simulation time increases by $\Delta \mathrm{t} = -\frac{\ln(U)}{Q_N}$.
6. If the mean value of Δt is greater than the average time interval between arrival of two atoms, then the algorithm returns to stage 1, otherwise it goes to stage 2. During simulation of thin film growth and formation of QD RHEED intensity of thin films was also simulated using the following [17]:

$$I = \left| \sum_{n=0}^{\infty} (\theta_n - \theta_{n+1}) e^{-in\pi} \right|^2, \tag{5}$$

where θ_n is the coverage of n_{th} layer.

Results and discussion

For GaAs system, the interaction energies are $\phi_{\mathrm{Ga\text{-}As}}$ = 0.75 eV, $\phi_{\mathrm{Ga\text{-}Ga}}$ = 0.17 eV, and $\phi_{\mathrm{As\text{-}As}}$ = 0.2 eV and k_θ = 1.1 eV [15]. Results of simulation for growth of four layers of model GaAs thin films for different values of mismatch in the range of 4% to 14% at a substrate temperature of 700 K and deposition rate of 0.3 ML/s are shown in Figure 1. Results show that simulated thin films consist of pyramid and dome-shaped islands (QDs). The pyramid and dome-shaped islands are experimentally observed during heteroepitaxial growth of thin films such as Ge/Si system [1]. Considering that the melting point of GaAs is 1,535 K, the reduced temperature for our simulated film is about 0.5 which is at the lower part of zone III in structural zone model (SZM) [18-20]. In the case of homoepitaxial growth, formation of a smooth surface is expected in zone III of SZM, but in heteroepitaxial growth due to relaxation of misfit energy, the structure of thin film is changed to dome-shaped islands. Mean value of islands sizes (QDs) for different values of mismatch is shown in Figure 2. Results in Figures 1 and 2 show reduction in the size of QDs by increasing the value of mismatch. RHEED intensities of simulated thin films are also evaluated using Equation 5, and results are shown in Figure 3. Results in this figure show that increasing of the mismatch results in a faster damping of RHEED oscillations. Results also show that by increasing the mismatch, the growth mode slowly switches from Stranski-Krastanov to Volmer Webber [15].

Size distribution of QDs is shown in Figure 4. This figure shows an approximately normal (or Gaussian) distribution which its width decreases by increasing the mismatch while its maximum shifts towards smaller values. Results are in agreement with Ratstc et al.'s simulation work [21].

Conclusion

In this paper, influence of lattice mismatch on island growth and QD formation of a model GaAs thin film is investigated. Results show that the size of QDs is decreased by increasing the mismatch while the size distribution becomes sharper. Results also show that by increasing the mismatch value, the growth mode is changed from Stranski-Krastanov to Volmer Webber.

Competing interests

The authors declare that they have no competing interests.

Authors' contributions

MGS and EE both carried out the simulations. All authors read and approved the final manuscript.

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