Three-dimensional kinetic Monte Carlo simulation of prepatterened quantum-dot island growth

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A special prepatterning method is proposed for spatially ordered self-organizing quantum dots on anisotropic semiconductor substrates. Using three-dimensional kinetic Monte Carlo simulations, atoms are deposited with varying intermediate interruption times. We demonstrate the effect of interruption time and long-range anisotropic strain energy on island size uniformity and lateral alignment. © 2007 American Institute of Physics. [DOI: 10.1063/1.2812572]

Self-organized semiconductor quantum dots (QDs) have attracted large interest due to their improved physical properties that may be exploited in devices such as lasers, detectors, and memories. Those grown through the Stranski-Krastanov mode are promising candidates for use in quantum devices because of their defect-free properties and ease of fabrication. However, physical properties are sensitive to the ordering on the surface. Thus, controlling lateral spacing and size distribution of the islands would enable improved device design through indirect control of correlation effects and improved vertical alignment of stacked layers.

Various methods have been proposed recently for patterning the substrate so that uniform lateral ordering and size distribution can be achieved. For instance, surface modification techniques, such as photolithography or nanoindentation, have been used to pattern the substrate where the modifications (using individual atoms, small clusters, or generating mesas or holes) can act as nucleation sites and areas of preferential island formations. However, the dots from lithographic techniques are often too large and not of sufficient spatial density for device application. The most promising quantum structures so far have been fabricated using techniques based on direct crystal growth. Strain-relief patterns are created spontaneously when a material is deposited on a substrate with a different lattice constant. It is also possible to confine growth by using templates or nanocavity arrays. A brief review of various prepatterning methods can also be found in Kirivittaya et al.

Spatial ordering of QD islands can also be improved by employing interlayer strains through vertical stacking or by using high index substrates. It is particularly interesting that uniform spatial distributions of QD chains can also be obtained by adjusting the deposit material coverage and growth interruptions.

In this letter, we present computer simulations based on a three-dimensional (3D) kinetic Monte Carlo (KMC) method for QD island self-organization on prepatterned substrates where the pattern control is achieved by adjusting the growth interruption time. With consideration of the long-range elastic strain energy and under fixed growth parameters, spatially ordered QD island patterns are computationally predicted. Furthermore, correlation between the island pattern and substrate anisotropy (due to different crystalline orientations) is observed.

Our 3D layer-by-layer KMC growth model is developed from the two-dimensional (2D) (x,y)-plane growth model. The 2D hopping probability of an atom from one lattice site to a nearest or next nearest neighbor site in the (x,y) plane is still governed by the Arrhenius law enhanced by the long-range strain energy field.

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p = \nu_0 \exp \left( -\frac{E_s + E_a - E_{ad}(x,y)}{k_BT} \right),
\]

where \(\nu_0\) is the attempt frequency (\(10^{13} \text{s}^{-1}\)), \(T\) the temperature, \(k_B\) the Boltzmann constant, \(E_s\) and \(E_a\) are the binding energies to the surface and to the neighboring atoms, respectively, and \(E_{ad}(x,y)\), which is a function of the plane coordinates \((x,y)\), is the energy correction from the long-range strain field due to the lattice mismatch between the substrate and the deposited material. Furthermore, in order to simulate the 3D adatom diffusion, the surface binding energy is modified to include the effect of the surface geometry. We remark that our model is multiscale based where the continuum long-range strain is considered through the strain energy function in the atomistic KMC simulation. Computer modeling of QD island growth over prepatterned substrates employing pure continuum mechanics was also reported recently.

In simulating the effect of the growth interruption on the QD island distribution, three cases are studied. In case 1, we deposit 1.6 ML InAs atoms to the GaAs substrate and after that, we give the system an interruption time of 250 s (Fig. 1). In case 2, after depositing 0.3 ML InAs atoms to the GaAs substrate, we interrupt growth for 50 s (Fig. 2) after which InAs atoms are deposited until the total coverage reaches 1.6 ML. Finally, we let the system self-assemble for 200 s (Fig. 3), which gives a total interruption time of 250 s.

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system is then annealed for 200 s so that the total position. In other words, after deposition of 0.3 ML followed 100 grid over the isotropic substrate and the GaAs substrate have different crystalline orientations. Here, the prepattern obtained in Fig. 2 is utilized for continuous deposition of atoms in cases 2 and 3. Comparing the spatial distribution in Fig. 4 with those in Figs. 1 and 3, we observe that improved spatial ordering can be achieved with increasing intermediate interruption steps. Comparing the strain energy distribution in the top row with the growth patterns in the bottom row in Fig. 4, we also notice a clear correlation between the growth pattern and substrate anisotropy (or orientation). This result is consistent with other recent reports.20,27

The proposed prepatternning approach cannot only improve the spatial ordering of the QD islands but also make the island size more uniform on a single growth layer. This is shown in Fig. 5 where the histograms for the number of islands versus island size are presented. The first, second, third, and fourth rows are, respectively, the results for the growth over the isotropic, GaAs (001), GaAs (111), and GaAs (113) substrates, while the left, middle, and right columns are, respectively, for cases 1, 2, and 3. Comparing the

stratified that a growth interruption has a smoothing effect on crystal surface,32 and that after the growth interruption, the system exhibits an ordered pattern.33 Therefore, it could be possible to control the QD island pattern by adjusting the growth interruption time. In contrast to the vertical stacking technique20 for improved surface order, this method can be applied to a single growth layer.

We show in Fig. 4 the spatial distribution of the self-organized QD islands on different substrates for case 3 (bottom row for the top-down plan view). Shown in the top row is also the strain energy distribution on the surface of the substrate. The 3D KMC simulation is also on the 100 grid at T=800 K and F=0.1 ML/s, as in cases 1 and 2. However, the deposition is interrupted for 50 s at the end of coverages of 0.3, 0.6, 0.9, 1.2, and 1.6 ML, keeping the total interruption time at 250 s. Comparing the spatial distribution in Fig. 4 with those in Figs. 1 and 3, we observe that improved spatial ordering can be achieved with increasing intermediate interruption steps. Comparing the strain energy distribution in the top row with the growth patterns in the bottom row in Fig. 4, we also notice a clear correlation between the growth pattern and substrate anisotropy (or orientation). This result is consistent with other recent reports.20,27

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