Growing Perfectly Uniform and Regular Quantum Dots and Quantum Cellular Automata via Surface Pre-patterning

Uniform and regular quantum dot arrays with precisely controlled positions and sizes may serve as a template for the next generation of nanoelectronic devices: this promise has motivated many researchers to use self-assembled heteroepitaxial growth. Numerous theoretical, modeling and experimental works have shown that unguided self-assembled growth of quantum dots usually fails to realize perfectly ordered dot arrays. Recently more effort has been shifted to use guided self-assembly through pre-patterning. So far several pre-patterning procedures have been reported. It is expected that through pre-patterning, uniform and regular quantum dots can be achieved. In reality, quantum dots have been found to nucleate at different positions even if an ordered pre-patterned substrate is used, often failing to produce the one-to-one relation. Hence how to reliably and reproducibly achieve ordered quantum dot arrays through surface pre-patterning is still an unsolved issue.

We have performed systematic three-dimensional computer simulations to determine the growth windows for achieving ordered quantum dot or ring arrays through pre-patterning substrate surfaces. In the modeled thin film/substrate system, the pre-patterned substrate surface is considered to be fixed. A thin transition layer with a linearly varied mismatch strain covering the pre-patterned substrate surface is introduced to model the wetting effect. Here the focus is on the morphological evolution of the film surface atop the wetting layer through diffusion and deposition.

Our simulations show that for isotropic thin film systems, concave patterning in a squared array may lead to the formation of ordered dots, whereas convex patterning in a squared array may initially lead to the formation of ordered quantum rings, then a transition into quantum dots with further growth. The evolution of the surface chemical potential during growth explains the formation of the ordered surface structures. However, for anisotropic thin film systems, novel surface structures, such as quantum-dot automata arrays, fortress-encoded quantum-dot automata arrays, and ordered quantum dot arrays, can be obtained by controlling the pre-patterning pitch distance and growth rate. In addition, the quantum dot (ring) density, according to the present study, can be significantly higher than the currently experimentally achieved dot densities. For example, for the Ge/Si system, the dot density is predicted to be as high as 400 dots/µm². However, the currently experimentally achieved dot density is only roughly 4–20 dots per µm². Hence, there is still large potential and challenge to increase the dot (ring) density. It is expected that the present work provides a new guideline for controlling the formation and self-assembly of novel surface structures.
Fig. 1: Formation of a quantum ring array initially, and a transition into a quantum dot array.
Fig. 2: Formation of quantum cellular automata.

Contact Person: Assoc Prof Y. W Zhang
Email: zhangyw@ihpc.a-star.edu.sg
Tel: 6516 1542
Fax 6776 3604