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3D Simulation of the Growth of Alloy Semiconductor Quantum Dots Considering Morphological and Compositional Coupling JUNYAN GUO, YONG-WEI ZHANG, SRIDHAR NARAYANASWAMY, IHPC, Singapore — Fabrication of quantum dots (QDs) with high density may be realized by self-assembly via heteroepitaxial growth of thin films. Since the electronic and optoelectronic properties of QDs are sensitive to size, morphology, strain and especially composition, it is of great importance to control their composition profiles and morphology, and engineer the strain in them. Since the growth is a dynamic process, which carries out via surface diffusion driven primarily by strain relaxation and entropy change due to chemical intermixing, a strong coupling between morphological and composition evolutions during this process leads to a rather complex dynamics, which has not been fully understood. In this work, a 3-D finite element model is developed, which is capable of modeling the formation, self-assembly and coarsening of hetero-epitaxial alloy islands by considering the coupling of morphological and compositional evolution. Several interesting experimental observations, such as fast coarsening kinetics; asymmetries in composition profile and island shape; lateral motion of alloy islands have been observed in our simulations. Our model predictions have painted a rather complete picture for the entire dynamic evolution during the growth of nanoscale heteroepitaxial islands.



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