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Kinetic Monte Carlo simulations of uniform islands on flat and pillar-like substrates in heteroepitaxial thin film growth

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The fabrication of uniform island nanostructures on heteroepitaxial thin films is a crucial step toward improving the efficiency of optoelectronic and solar cell devices. In this work, we investigate a strained heteroepitaxial thin film system in two dimensions using the kinetic Monte Carlo simulation method. The strain arising from the lattice mismatch is incorporated into the system using an atomistic ball-spring model. Films are grown onto flat and pillar-like substrates. For films on a flat substrate, growth condition dependence of film surface morphology, critical thickness, and island size is presented. For films on pillar-like substrates, uniformity of islands is investigated as a function of patterned substrate parameters. In contrast to the flat substrate, pillar-like substrates provide preferred sites for island formation and enhance island size uniformity. We found three types of island configurations with regular islands located on the top of filled windows, on the top of pillars, and at the bottom of windows. An island configuration diagram as a function of patterned substrate parameters is shown.

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