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Growth and ordering of gas films on a decagonal AlNiCo quasicrystal surface W. SETYAWAN, Duke Univ., R.D. DIEHL, Penn State Univ., N. FERRALIS, UC Berkeley, M.W. COLE, Penn State Univ., S. CURTAROLO, Duke Univ. — The growth and ordering of Ne, Ar, Kr, and Xe films on a decagonal surface of $Al_{73}Ni_{10}Co_{13}$ quasicrystal are studied with Grand Canonical Monte Carlo using Lennard-Jones interactions. We observe interesting phenomena that can only be attributed to the quasicrystallinity and/or corrugation of the substrate, including structural evolution of the overlayer films from commensurate pentagonal to incommensurate triangular, substrate-induced alignment of the incommensurate films, and density increase in each layer with the largest one observed in the first layer and in the smallest gas. 2D quasicrystalline epitaxial structures of the overlayer form in all the systems only in the monolayer and at low pressure. The final structure of the films is a triangular lattice with a considerable amount of defects except in Xe/QC. Here a first-order transition occurs in the monolayer resulting in an almost perfect triangular lattice. The next layers of Xe/QC have hexagonal close-packed structures. By simulating fictitious gases, we find that the existence of the transition is correlated with the size mismatch between adsorbate and substrate's characteristic lengths. A simple rule is proposed to predict the phenomenon. We extend the theory to other gases/substrates of technological interest. Research is sponsored by NSF and ACS-PRF.

W. Setyawan
Duke Univ.

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