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Epitaxial orientations and temperature dependence of the 5- to 6-fold ordering transition STEFANO CURTAROLO, WAHYU SETYAWAN, Duke University, NICOLA FERRALIS, MILTON W. COLE, RENEE DIEHL, Penn State University — The ordering of Xe films on an $Al_{73}Ni_{10}Co_{17}$ quasicrystalline surface is studied using grand canonical Monte Carlo simulations with an empirical adsorption potential based on Lennard-Jones interatomic potentials. At all temperatures studied (20-140K), there is a continuous 5- to 6-fold ordering transition in the monolayer [1]. The ordering transition shows interesting temperature-dependent phenomena [2]. At intermediate T (40K$< T <$130K), the transition occurs before the second layer forms. Moreover, this T-dependent transition shows a non-monotonic dependence on coverage, completing earliest at $T \sim$70K. At low T (<40K), the transition does not complete, whereas at high T (>130K), the transition completes by the transfer of atoms from the second layer to the first layer. At all temperatures, after the transition completes, the orientations of the monolayer domains are along the 5-fold axes of the quasicrystal. The existence of pentagonal defects gives rise to domains that are rotated by n*60°/5 with n = 1, 2, 3, 4, or 5. The defect density increases with T, suggesting that entropy plays the major role in defect formation [2]. Research sponsored by NSF. [1] S. Curtarolo et al., Phys. Rev. Lett. **95**, 136104 (2005). [2] W. Setyawan, N. Ferralis, R. D. Diehl, M. W. Cole, and S. Curtarolo, *Xe films on a decagonal Al-Ni-Co quasicrystal surface*, (2005).

Stefano Curtarolo
Duke University

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