

Self-assembly of aluminum nano-crystals on the decagonal surface of Al-Co-Ni quasicrystal - a low-energy electron diffraction study Y. Weisskopf, M. Erbudak, T. Flückiger, A.R. Kortan, R. Lüscher, M. Mungan^a, *Laboratorium für Festkörperphysik, ETHZ, CH-8093 Zurich, Switzerland*, ^a*Bogaziçi University, Department of Physics, Bebek, 34347 Istanbul, Turkey*

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Periodicity is the unique characteristic of crystalline matter. Quasicrystals lack periodicity, but possess long-range orientational order with fivefold or tenfold point-group symmetries that cannot occur in crystals. Therefore, the structural transition on the atomic scale at the interface where an ordinary crystal and a quasicrystal intersect can potentially disclose structural mysteries of quasicrystalline surfaces and lead to novel surface phenomena. Generally, the equilibrium structure of the crystalline film on a quasicrystalline surface is determined by the relative strengths of epitaxy-imposed ordering versus the stable bulk phase of the film. We have studied the growth morphology of Al on the decagonal surface of $\text{Al}_{70}\text{Co}_{15}\text{Ni}_{15}$ using low-energy electron diffraction. This surface is atomically flat and defect free. Up to roughly a monolayer coverage, there is no measurable change in the observations. Hence, we conclude that epitaxy locks the Al atoms to the strained quasicrystalline lattice. For thicker Al coverages, the strain energy cannot be supported and the structure relaxes to the bulk stable face-centered cubic phase by breaking into multi-twinned domains, each a few nm large and oriented aperiodically, according to the substrate structure. We can follow the growth of Al nano-crystals each having a diameter of about 3 nm and oriented with the [111] crystallographic direction parallel to the surface normal. Each Al island has a particular in-plane orientation enforced by the aperiodic structure of the decagonal surface. This observation on size-selection and self-orientation of Al nano-crystals holds promise in a number of important applications. In order to account for these observations we have performed simulations using both a rigid-lattice atomic model based on an adapted Lennard-Jones potential for the adsorbate-substrate interaction and a molecular-dynamics model with a varying interaction between adatoms. We find that Al nucleation occurs inhomogeneously at specific substrate sites around which the local rotational substrate symmetry is tenfold. Even taking the Al overlayer as a rigid mesh of the (111) surface, we have found that Al grows on the decagonal substrate in a particular size, distribution, and orientational alignment. Furthermore, the observed twinning is reproduced by increasing the interaction between adatoms compared to the adsorbate-substrate interaction.

[1] T. Flückiger, Y. Weisskopf, M. Erbudak, R. Lüscher, and A.R. Kortan, *Nano Lett.* **3**, 1717 (2003).