Structure of the 10-fold d-Al-Ni-Co Quasicrystal Surface

N. Ferralis[a], K. Pussi[b], E.J. Cox[c], M. Gierer[d], J. Ledieu[c],
I. R. Fisher[e], C. J. Jenks[e], M. Lindroos[b] [1], R. McGrath[c], R. D. Diehl[a]

[a] Department of Physics & Materials Research Institute, Penn State University, University Park, PA 16802

[b] Institute of Physics, Tampere University of Technology, P.O.Box 692, Tampere, Finland.

[c] Department of Physics & Surface Science Centre, University of Liverpool, Liverpool, L69 3BX, UK

[d] Institute for Crystallography and Applied Mineralogy, Theresienstr. 41, 80333 München, Germany.

[e] Ames Laboratory and Department of Chemistry, Iowa State University, Ames, IA 50011, USA.

The structure of the 10-fold surface of decagonal Al-Ni-Co was studied using low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM).

The LEED calculations were performed using the LEED program of Moritz [1], which was modified for quasicrystalline structures [2]. The agreement between the calculated and experimental spectra was tested using the Pendry R-factor [3]. The absence of a repeating unit cell parallel to the quasicrystal surface means that the number of atoms with different scattering properties is infinite. Therefore, some approximations have been applied to make the calculation tractable. These approximations [2] are the Average Neighbor Approximation (ANA), the Diagonal Dominance Approximation and the Average T-Matrix Approximation (ATA).

The STM data were compared to the LEED structure by superposition of the top layer of the LEED structure model and the STM data. A 75 Å $\times$ 75 Å patch of the STM data was chosen and a match was sought between the protrusions and the atomic model.

The surface region is a relaxed truncated bulk structure, having the same composition as the bulk. The outermost layer spacing is contracted by 10% relative to the bulk interlayer spacing, while the next layer spacing is expanded by 5%. A small degree of intralayer rumpling was observed within each layer (see Fig. 1). There is a one-to-one correspondence between protrusions observed in the STM images and transition metal atoms in the model structure (see Fig. 2), indicating that in-plane reconstruction is minimal. Pendry r-factor for the best-fit structure is 0.32.

A unique and important feature of this study is that the positions and types (Al or TM) of all surface atoms have been identified. Unlike the icosahedral surfaces, the decagonal surface structure is wholly determined because there is effectively only one type of termination (two terminations related to each other by a rotation symmetry). This result provides a definite model for the surface structure, which can be used in the interpretation of other studies of this surface, as a basis for the interpretation of adsorption and growth on this surface, and for first principles calculations of surface geometric, electronic and dynamical properties.

[1] Tel. +358-3-3115 2417, Fax. +358-3-3115 2600, E-mail: matti.lindroos@tut.fi

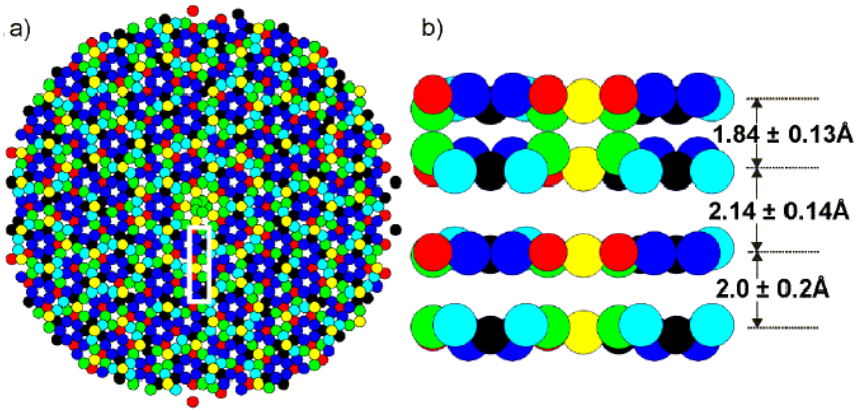

Figure 1: (a) One layer of the quasicrystal slab, having a diameter of about 90 Å. (b) Side view (viewing white box in (a) from the left) showing the surface relaxations and rumpling for the top four layers. The rumpling is exaggerated for clarity. Red and black correspond to transition metal atoms and green, blue, cyan and yellow correspond to aluminium atoms.

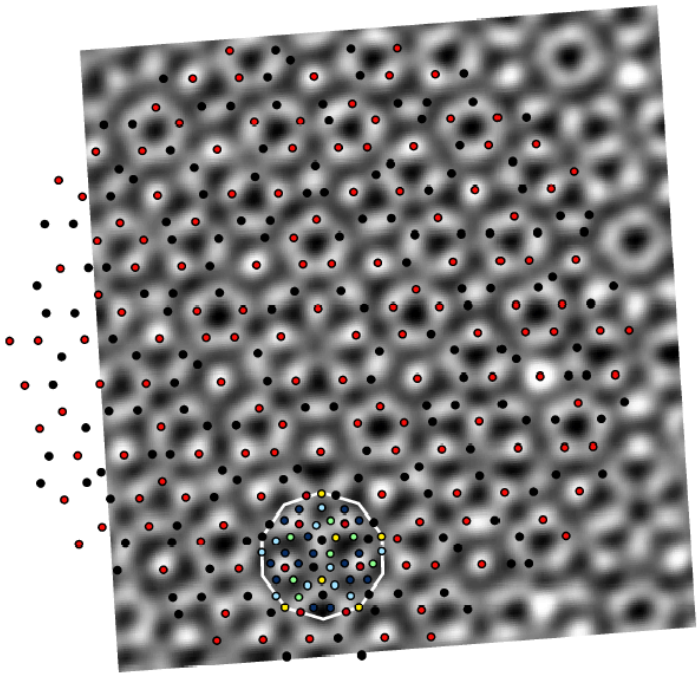

Figure 2: Superposition of the atom positions from the LEED result onto the STM image. The color coding of atoms is the same as that shown in Fig. 1. The protrusions corresponding to red atoms are generally brighter, consistent with them being closer to the surface. The decagon denotes the quasi-unit-cell identified in bulk structure studies.

1 W. Moritz, J. Phys.: C 13, 353 (1984).
2 M. Gierer, M. A. Van Hove, A. I. Goldman, et al., Phys. Rev. B 57, 7628 (1998).
3 J. B. Pendry, J. Phys.: C 13, 937 (1980).