s9.m31.o5 **A User Interface Toolkit for Small Molecule X-ray Structure Determination and Analysis**. Richard Ian Cooper *Chem Cryst, University of Oxford, Chemistry Research Laboratory, Mansfield Road, Oxford, OX1 3TA, UK. E-mail: richard.cooper@chemical-crystallography.oxford.ac.uk*

Keywords: Validation; User Interface

X-ray crystal structures are routinely determined by researchers with limited crystallographic training. Recent extensions of the tools and facilities available within the CRYSTALS[1] package makes crystallographic analysis accessible to non-expert users.

The tools take the form of interactive dialog boxes which:

- present information in a clear and concise manner (*e.g.* text, plot or 3D model)
- suggest appropriate actions (*i.e.* for guiding the analysis in a standard direction)
- allow selection of actions via standard graphical controls, e.g. menus and buttons

The dialog boxes and their controlling logic can be developed rapidly, and without requiring a compiler, thanks to the development of a cross-platform graphical interface toolkit within CRYSTALS and extensions to the existing macro programming language, 'Scripts'.

An overview of the design and implementation of the toolkit is presented including detailed examples of recently developed tools for guiding structure refinement and graphical analysis of data.

[1] Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout K. & Watkin, D. J. (2003). *J. Appl. Cryst.* **36**, 1487

s10.m32.o1 **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. Mungana, *Laboratorium für Festkörperphysik, ETHZ, CH-8093 Zurich, Switzerland, aBogaziçi University, Department of Physics, Bebek, 34347 Istanbul, Turkey. E-mail: yvesw@phys.ethz.ch*

Keywords: Nanocrystal; Self-Assembly; Electron Diffraction

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. There-fore, 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 phe-nomena. Generally, the equilibrium structure of the crystalline film on a quasicrystalline surface is deter-mined by the relative strengths of epitaxy-imposed or-dering versus the stable bulk phase of the film. We have studied the growth morphology of Al on the decagonal surface of $Al_{70}Co_{15}Ni_{15}$ using low-energy electron dif-fraction. This surface is atomically flat and defect free. Up to roughly a monolayer coverage, there is no meas-urable change in the observations. Hence, we conclude that epitaxy locks the Al atoms to the strained quasi-crystalline 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 struc-ture. 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 orienta-tion 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 num-ber 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 in-teraction and a molecular-dynamics model with a vary-ing interaction between adatoms. We find that Al nu-cleation occurs inhomogeneously at specific substrate sites around which the local rotational substrate symme-try 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, distribu-tion, and orientational alignment. Furthermore, the ob-served twinning is reproduced by increasing the interac-tion 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).