MS26.25.2

Acta Cryst. (2005). A61, C38

Maximum or Minimum Density Principle Determines the Bulk Terminations of Quasicrystals?

Zorka Papadopolos^a, Gerald Kasner^b, ^aInstitut für Theoretische Physik, Universität Tübingen, Germany. ^bInstitut für Theoretische Physik, Universität Magdeburg, Germany. E-mail: zorka.papadopolos@uni-tuebingen.de

In [1] we announced the "thick layer" concept of the bulk terminations in quasicrystals. We consider a bundle of dense atomic planes in the bulk, not necessarily extremely close together, as a candidate for a termination. We show that only "thick" layers can terminate the bulk of decagonal Al-Cu-Co (d-AlCuCo) in the 2fold directions. Also, the secondary electron images indicate that certain "thick" 5fold and 2fold layers are favoured as terminations of icosahedral Al-Pd-Mn (i-AlPdMn). In particular, the 2fold terrace-like surfaces of i-AlPdMn containing pits are perfectly explained in this framework.

Following a suggestion of Sharma et al. [2], that a gap in the bulk might define a termination, we introduce a minimum density rule on low density "thick" atomic layers as well and show that, in the framework of the model of i-AlPdMn, such a rule does not match the observed step heights on either the 2fold or 5fold surfaces.

[1] Papadopolos Z. et al., *Phys. Rev.* B, 2004, **69**, 224201. [2] Sharma H.R. et al., *Phys. Rev. Lett.*, 2004, **93**, 165502.

Keywords: quasicrystals, surface structure, scanning tunneling microscopy

MS26.25.3

Acta Cryst. (2005). A61, C38

Diffuse Scattering and Phasons in the i-Zn-Mg-Sc Phase and its 1/1 Approximant

<u>Marc de Boissieu</u>^a, T. Ishimasa^b, S. Francoual^{a,c}, ^aLTPCM, UMR CNRS 5614, St Martin d Hères, France, ^bHokkaido University, Sapporo, Japan, ^cILL, Grenoble, France. E-mail: boissieu@ltpcm.inpg.fr

Phasons modes are excitations characteristic of the quasicrystalline sate. In the same way than phonons modes lead to thermal diffuse scattering, phason modes lead to diffuse scattering in the diffraction pattern. This diffuse scattering can be calculated in the framework of the hydrodynamic theory of icosahedral phases.

Diffuse scattering has been extensively studied in the i-AlPdMn phase. It has been shown that most of the observed diffuse scattering is due to phason modes, which are interpreted as pre-transitional fluctuations.

We present an extensive room temperature study of the diffuse scattering in the i-ZnMgSc quasicrystal and its 1/1 periodic approximant. For this purpose, absolute scale measurements of the Xray diffuse scattering have been carried out on the D2AM beam line (ESRF). Whereas the diffuse scattering measured in the 1/1 approximant can be accounted for by the thermal vibrations (TDS), a supplementary contribution to the signal is observed in the quasicrystal. This extra contribution is larger for reflections having a larger Q_{per} component, indicating that it is due to phason modes. This demonstrates that although both phases share the same clusters, phason modes are a characteristic of the quasiperiodic long range order. Using the absolute scale measurement, we find that the amount of diffuse scattering is about for time smaller in the i-ZnMgSc than in the i-AlPdMn phase. This demonstrates the high structural quality of the i-ZnMgSc phase, which is also evidenced by the large number of high Q_{per} reflections observed in the diffraction pattern.

Keywords: quasicrystal, diffuse scattering, phasons

MS26.25.4

Acta Cryst. (2005). A61, C38

A High Pressure High Temperature Study of Co-rich d-Al-Co-Ni <u>Günter Krauss</u>, Qinfen Gu, Sergiy Katrych, Walter Steurer, *Laboratory of Crystallography, ETH Zurich, Switzerland*. E-mail: guenter.krauss@mat.ethz.ch A basic key in the understanding of the stabilization mechanisms of quasicrystals is the knowledge of their stability ranges within the p-T field. In the last decade, the Al-Co-Ni system has become the model system for the study of decagonal quasicrystals [1]. The decagonal phase in this system shows a quite large compositional stability range, going along with changes of the structural disorder and the formation of superstructures as a function of temperature.

Ni-rich decagonal quasicrystals were found to be stable within the applied experimental frameworks $(Al_{72}Co_8Ni_{20}$ up to 70 GPa from powder [2], $Al_{70}Co_{12}Ni_{18}$ up to 10 GPa from single crystal [3], both at ambient temperature). The Co-rich decagonal phase was not yet studied at non-ambient conditions. This phase is neighbored by the recently discovered W-phase [4], which is the highest approximant phase in the Al-Co-Ni system, and therefore the structural behavior of this decagonal phase at non-ambient conditions is of special interest.

The results of an in-situ high pressure high temperature study on $Al_{73}Co_{21}Ni_6$ up to about 16 GPa and 973 K will be discussed.

 Steurer W., Z. Kristallogr., 2004, 219, 391. [2] Hasegawa M., Tsai A.P., Yagi T., Phil. Mag. Lett., 1999, 79, 691. [3] Krauss G., Miletich R., Steurer W., Phil. Mag. Lett., 2003, 83, 525. [4] Sugiyama K., Nishimura S., Hiraga K., J. Alloys Comp., 2002, 342, 65.

Keywords: high pressure, high temperature, quasicrystals

MS26.25.5

Acta Cryst. (2005). A61, C38

Mesoscopic Archimedean Tilings in Polymeric Stars

<u>Yushu Matsushita</u>^a, Wataru Kawashima^a, Atsushi Noro^a, Atsushi Takano^a, Nobuo Tanaka^b, Tomonari Dotera^c, ^aDepartment of Applied Chemistry, Japan. ^bEcotopia Science Institute, Nagoya University, Nagoya, Japan. ^cDepartment of Polymer Chemistry, Kyoto University, Kyoto, Japan. E-mail: yushu@apchem.nagoya-u.ac.jp

Four mesoscopic Archimedean tiling patterns have been observed for the molten ABC star-branched terpolymers composed of polystyrene(S), polyisoprene(I), and poly(2-vinylpyridine)(P) of the type $S_{10}I_{10}P_x$. The copolymers exhibit (6³), (4.8²) and (4.6.12) Archimedean tiling[1] when x are 0.7, 1.2 and 1.9[2], respectively, while the molecule of the type $S_{1,0}I_{1,0}P_{1,3}$ shows more complex $(3^2.4.3.4)$ tiling pattern with mesoscopic length-scale. Namely the side length of the polygons are about 80nm. In this structure the circumstance of a molecule splits into multiple sites and consequently two microdomains with different sizes and shapes are formed for one component. Moreover the experimental results were well explained with the predicted results based on free energy theorem using Monte Carlo method. This pattern has been observed for the other materials on much shorter length-scale, therefore, the experimental fact observed in the present study is demonstrating that the complexity is universal over different hierarchy.

[1] Grunbaum B., Shephard G. C., *Tilings and Patterns*, Freeman, New York, 1986.[2] Takano A., Matsushita Y. et al., *Macromolecules*, 2004, **37**, 9941. Keywords: archimedean tiling, ABC star-branched terpolymer, hierarchy

MS27 DETECTORS: DEVELOPMENTS AND REQUIREMENTS FOR X-RAY, SYNCHROTRON AND NEUTRON SOURCES *Chairpersons*: Naoto Yagi, Christian Broennimann

MS27.25.1

Acta Cryst. (2005). A61, C38-C39

Development of Very-high Rate and Resolution Neutron Detectors in DETNI

Burchhard Gebauer^a, Svyatoslaw S. Alimov^a, Andrea Brogna^b, Siro Buzzetti^c, Wladyslaw Dabrowski^d, Thomasz Fiutowski^d, Martin Klein^b, Caterina Petrillo^e, Francesco Sacchetti^e, Christian J. Schmidt^b, Hans Kristian Soltveit^b, Christian Schulz^a, Robert Szczygiel^f, Ulrich Trunk^b, Clara Turconi^a, Dr. Thomas Wilpert^a, ^aHahn-Meitner-Institut Berlin, Glienicker Str. 100, D-14109 Germany. ^bPhysikalisches Institut der Universität Heidelberg, Philosophenweg 12, D-69120 Heidelberg, Germany. ^cINFM & Dipartimento di Elettronica e Informazione, Politecnico di Milano, Piazza L. da Vinci 32, I-20133Milano, Italy. ^dFaculty of Physics and Nucl. Techniques, AGH