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

Zorka Papadopolos[a], Gerald Kasner[b], [a]*Institut für Theoretische Physik, Universität Tübingen, Germany.* [b]*Institut 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.

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Keywords: quasicrystals, surface structure, scanning tunneling microscopy

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

Marc de Boissieu[a], T. Ishimasa[b], S. Francoual[a,c], [a]*LTPCM, UMR CNRS 5614, St Martin d Hères, France,* [b]*Hokkaido University, Sapporo, Japan,* [c]*ILL, 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 X-ray 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

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A High Pressure High Temperature Study of Co-rich d-Al-Co-Ni

Günter Krauss, 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.

[1] 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

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Mesoscopic Archimedean Tilings in Polymeric Stars

Yushu Matsushita[a], Wataru Kawashima[a], Atsushi Noro[a], Atsushi Takano[a], Nobuo Tanaka[b], Tomonari Dotera[c], [a]*Department of Applied Chemistry, Japan.* [b]*Ecotopia Science Institute, Nagoya University, Nagoya, Japan.* [c]*Department 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 $S_{1.0}I_{1.0}P_x$. The copolymers exhibit (6^3), (4.8^2) 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

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

Burckhard 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], [a]*Hahn-Meitner-Institut Berlin, Glienicker Str. 100, D-14109 Germany.* [b]*Physikalisches Institut der Universität Heidelberg, Philosophenweg 12, D-69120 Heidelberg, Germany.* [c]*INFM & Dipartimento di Elettronica e Informazione, Politecnico di Milano, Piazza L. da Vinci 32, I-20133Milano, Italy.* [d]*Faculty of Physics and Nucl. Techniques, AGH*

University of Science and Technology, al. Mickiewicza 30, 30-059 Krakow, Poland. [e]*INFM &Dipartimento di Fisica, Universita di Perugia, Via A. Pascoli, I-06123Perugia, Italy.* [f]*Institute of Nuclear Physics, Polish Academy of Sciences, ul. Radzikowskiego 152, 31-342 Krakow, Poland.* E-mail: gebauer@hmi.de

For time- and wavelength-resolved neutron scattering experiments with up to 10^8 n/s per detector module and two-dimensional position resolution of up to 50-100 µm FWHM in the current (2004-2008) EU Joint Research Activity DETNI of NMI3 (http://jra1.neutron-eu.net/jra1) three neutron detector types and a dedicated event-triggered ASIC family are being developed. These high-contrast single-event counting detectors shall replace integrating detectors e.g. in diffraction or radiography and tomography experiments. The ASIC type delivers single micro-strip, pulse-height (energy) and time readout with 2 ns time resolution. The latter is sufficient to suppress chance coincidences between the X- and Y-planes, whilst the energy resolution is used for background suppression and for improving the position resolution by center-of-gravity determination. Except for neutron scattering, e.g. at next generation pulsed spallation neutron sources like ESS, modified versions of two of these detector types and the ASIC family will also be suitable for X-ray detection. These detectors are (i) double-sided silicon micro-strip detectors (Si-MSD) with 51x51 mm^2 size and 80 µm pitch, of which four are combined in one detector module and (ii) hybrid low-pressure micro-strip gas chamber (MSGC) detectors of 254x254 mm^2 sensitive size with columnar CsI converter layers. For thermal neutron detection in both cases ≈3 µm thick ^{157}Gd converters are used, in the MSGC case in composite ^{157}Gd/CsI converters with columnar CsI of <1 µm thickness. For X-ray detection in the MSGC a CsI converter thickness of a few tenths of µm can be used. In this invited talk the detector principles and the present state of development will be reported.

Keywords: neutrons, detectors, very-high rates

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A Direct-conversion Se-based 2D-detector for Protein Crystallography

Jules Hendrix, *Marresearch GmbH, Norderstedt, Germany.* E-mail: jules@marresearch.com

A solid-state detector based on the direct conversion of the absorbed X-rays into charges is described. The conversion takes place in a layer of Selenium as the photoconductor. This concept does not use phosphors and optical elements (e.g. fibre optic tapers), thus avoiding the broadening of reflection spots.

The excellent spatial resolution has two advantages: an excellent spot separation and a significant improvement in signal-to-noise ratio. In addition, the new detector has a low read-out noise level and a high dynamic range.

Although it is intended for synchrotron radiation applications (not only protein crystallography!), it has also been tested successfully on a rotating anode source at 8keV.

Keywords: protein crystallography, X-ray detector, flat panel detector

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Protein Crystallography with the PILATUS 1M Detector

Gregor Huelsen, *SLS Detector Group, Swiss Light Source, Paul Scherrer Institut, Villigen PSI, Switzerland.* E-mail: gregor.huelsen@psi.ch

The PILATUS 1M detector (Pixel Apparatus for the SLS, 1 Million pixels) is a large area X-ray detector, constructed in 2003. X-rays are detected in single photon counting mode leading to excellent and noise free data. The main properties of the device are an energy range of 6 to 30 keV, no leakage current, no readout-noise, a fast read-out time of 6.7 ms and a PSF of one pixel.

Several proteins were measured at the protein crystallography beamline X06SA of the SLS (Swiss Light Source). The properties of the detector enable fine Φ-sliced experiments with continuous sample rotation using the electronic shutter of the camera. This leads to datasets as large as 9000 images. The data are first corrected for flatfield inhomogeneity. The main spatial distortion comes from the tiled assembly of the detector. We have developed a dedicated correction algorithm, which leads to a precision of fraction of a pixel. The corrected data could be processed using a standard crystallographic software package (XDS), leading to reasonable R_{tot}-factors of around 10%. This enabled us to calculate the first refined electron density map ever measured with a pixel detector.

Keywords: data processing, protein crystallography, area detector

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A New High-speed, Photon-counting X-ray Area Detector

Roger Durst, Bruce Becker, Yacouba Diawara, David Khazins, Sergei Medved, Vladisov Sedov, Kingsley Smith, Tim Thorson, Greg Wachter, *Bruker AXS Inc., Madison WI.* E-mail: roger.durst@bruker-axs.com

We describe, for the first time, a powerful new type of imaging detector for X-ray crystallography: the Resistive Micrograp Detector (RMD). This detector is based on new micropattern detector technologies which have been developed for high-energy particle physics experiments [1]. The detector exhibits a number of compelling advantages over the conventional, analog detectors typically used in crystallography experiments (viz., CCDs and image plates). The RMD is a pure digital photon-counter and thus exhibits true single-photon sensitivity with essentially zero intrinsic noise and zero frame readout dead time. This allows it to acquire both very long exposures on weakly diffracting samples without data degradation and also extremely fast exposures for time resolved experiments. It also demonstrates a very high counting rate capability of up to 10^6 X-rays/mm^2-sec with a linear dynamic range of over 9 orders of magnitude (over a thousand times higher than CCD or image plate detectors). With an active area of 20 cm and a spatial resolution better than 100 microns the RMD can resolve over 400 diffraction orders. Also, the RMD is extremely robust, does not require cooling and has no internal dead areas.

[1] Bachman S., Bressan A., Ropelski L., Sauli F., *Nuclear Physics A*, 2000, **663**, 1069C-1072C.

Keywords: X-ray detector technology, area detectors, X-ray imaging

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Dead-time in X-ray Photon Counting Detectors

David Laundy, *CCLRC Daresbury Laboratory, Warrington, Cheshire, WA4 4AD, UK.* E-mail: d.laundy@dl.ac.uk

With modern high flux synchrotron X-ray sources, photon counting detectors must operate at high counting rates where there can be significant non linearity in the detector response caused by the dead-time from overlap of pulses in the counting chain. We have shown that the dead-time not only affects the measured number of counts but also degrades the statistical accuracy obtained from a measurement [1], [2]. This effect can actually cause the statistical accuracy to drop if the source flux is increased beyond a certain value, even though the dead-time correction may still be relatively small.

In addition, we have derived an expression for the dead-time correction that must be used when the source of radiation is time dependent. The use of this correction for pulsed radiation from synchrotron sources operating in single bunch or gapped filling mode is demonstrated.

[1] Laundy D., Collins S. P., *J. Synchrotron Rad.*, 2003, **10**, 214. [2] Laundy D., Tang C .C., Collins S. P., *AIP Conference proceedings*, 2004, **705**, 977.

Keywords: detector properties, synchrotron X-ray instrumentation, X-ray detectors

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