MS22-O2 **The physical space approach to the structure refinement of decagonal quasicrystals. Are three dimensions enough?** Pawel Kuczera,[a,b] Janusz Wolny,[a] Walter Steurer,[b] [a]*AGH – University of Science and Technology, Krakow, Poland.* [b]*Laboratory of Crystallography, ETH, Zurich, Switzerland.*
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The physical space approach to quasicrystal structure refinement [1] will be presented as an alternative to the commonly used higher-dimensional approach. This method allows a purely 3D optimization of a quasicrystalline structure. Its advantages and limitations will be discussed based on three examples of structure refinement of decagonal quasicrystals: Al-Cu-Co, Al-Cu-Rh, Al-Cu-Ir. The synchrotron diffraction experiments were performed at the Swiss – Norwegian beam line at ESRF, Grenoble, France. All three decagonal phases show ~4 Å periodicity (two atomic layers per period). A computer program SUPERFLIP based on the charge-flipping algorithm was used for the initial phasing of the data and obtaining the electron density maps. These maps were used for deriving Rhombic Penrose Tiling (RPT) models with a tiling edge-length of ~17 Å. The atomic decoration of the unit tiles is based on the ~33 Å cluster derived from the HRTEM images of the Al-Cu-Rh and proposed by Hiraga & Oshuna . The decoration of RPT with Hiraga clusters is such, that the cluster centers form the Pentagonal Penrose Tiling of an edge-length of ~20 Å. The Hiraga cluster can be considered as a *supercluster* built of 5 clusters proposed by Deloudi et al. based on the HRTEM images of the Al-Cu-Co phase. Such a structure explains well the strong Patterson maxima of ~12, ~20 and ~33 Å occurring for all three phases and corresponding to the typical inter-cluster distances. Our work shows the first solution of a quasicrystal as a ternary alloy (Rh and Ir phases). The final *R*-values are reasonable, the structure is consistent with the available HRTEM images and the chemical composition agrees well with the EDX measurements. The reconstructions of the atomic surfaces for the refined structures will also be presented and compared to the ones found in the literature for other decagonal quasicrystal refinements.

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MS22-O3 **Diffuse scattering and phason modes in the Zn-Sc icosahedral quasicrystal .** M. de Boissieu [a], T. Yamada [b,a], H. Euchner [c,a], C. Pay Gňmez [d], R. Tamura [b], [a]*SIMaP, Grenoble-INP, CNRS,UJF, Saint Martin d'Hčres Cedex, France,* [b] *Department of Materials .Sci.& Tech., Tokyo Univ. of Science, Noda, Japan.* [c] *ITAP, Universitat Stuttgart, Stuttgart, Germany,* [d] *Ĺngström Lab., Uppsala University, Uppsala,Sweden*
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Recently, a new binary icosahedral quasicrystal Zn-Sc has been obtained by Canfield *et. al*. [1]. It is supposed to be isostructural to the CdYb icosahedral phase [2]. Because of the chemical order and the x-ray contrast between Zn and Sc, this phase offers opportunities for the structure refinement. On the other hand, a large amount of diffuse scattering can be seen on the x-ray diffraction pattern [1]. In this study, we carried out an absolute scale measurement of the x-ray diffuse scattering of i-ZnSc phase to study the possible presence of quenched in phason modes (phason diffuse scattering) and estimate the phason elastic constants K1 and K2. Millimeter size single grains of i-ZnSc have been obtained by slow cooling from the melt. Systematic Q-scans and diffuse scattering maps have been measured on the D2AM beamline (ESRF) using an incoming x-ray energy equal to 9.3 keV.

A large amount of diffuse scattering, with a characteristic shape elongated along directions parallel to 3-fold directions, is observed around the Bragg reflections. The intensity distribution of this diffuse scattering is fully accounted for by the elasticity theory of quasicrystal and long wavelength phason fluctuations [3]. The ratio K2/K1 of the phason elastic constant is found to be close to the three-fold instability limit. Using this single parameter leads to a simulation in perfect agreement with the experiment. The absolute scale intensity measurement allows a direct comparison with the i-ZnMgSc quasicrystal [4]. We find that the amount of diffuse scattering is much larger in the binary Zn-Sc quasicrystal than in the i-ZnMgSc one. As a result, the weak, large Qper, reflections are suppressed in the Zn-Sc diffraction pattern. The consequences of these results on the quasicrystal stability will be discussed.

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