STRUCTURE REFINEMENT OF DECAGONAL QUASICRYSTAL

P. Kuczera [1], B. Kozakowski [1], J. Wolny [1*], and R. Strzałka [1]

[1] *Faculty of Physics and Applied Computer Science, AGH-University of Science ond Technology, al. Mickiewicza 30, 30-059 Kraków, Poland*

Keywords: structure, decagonal quasicrystals

**) e-mail: wolny@novell.ftj.agh.edu.pl*

For the last several years, the structure of basic Ni-rich decagonal Al-Ni-Co quasicrystal has been thoroughly examined by many scientists [1-2]. Their work resulted in some outstanding structural descriptions of this quasicrystal. The majority of published papers focused however on a higher-dimensional approach i.e. the atomic surface modelling method. We present the results of a real space structure refinement of the basic Ni-rich decagonal phase based on a diffraction data set, without referring to the higher-dimensional properties of decagonal quasicrystals.

The structure factor, which was used for the modelling process, was calculated on the basis of a statistical method described briefly in Ref. [3]. Statistical approach allows a purely 3-dimensional, real space optimization of a quasicrystaline structure. The decagonal basic Ni-rich phase is known to consist of aperiodic planes stacked periodically along the quasi-tenfold axis (*c*-axis). There are two planes within one period of the *c* axis. We assumed, that the projection of these two planes along the *c*-axis results in Penrose tiling. The rhombuses of Penrose tiling are divided three times with obedience to the inflation rules. The idealized positions of atoms are the points of subsequent divisions. We also put several atoms in the positions of the fourth division to fulfil the density restriction. There are 71 atoms decorating our structure units. They are divided into groups according to the overlapping rules for kite-clusters [4]. A shift from ideal position, anisotropic Debye-Waller factor, occupation probability and concentration of TM atom are refined. For some groups however some parameters are fixed. We obtained *R*-factor at the level of 12% and R_w-factor of 6%. The resulting structure has the chemical composition, point density and overall density values very close to the experimental ones. The optimization was performed on a set of averaged and corrected 2767 diffraction peaks taken by a four-circle diffractometer at beamline D3 HASYLAB [1].

Acknowledgements: The authors are grateful to Prof. Walter Steurer (ETH Zuerich) for the diffraction data set.

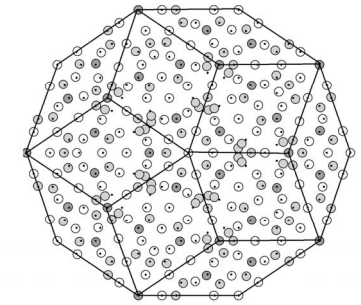

Figure 1. A projection of the refined structure along the periodic axis. Dark grey, light grey and white circles are TM, Al/TM, Al atoms respectively. Black dots indicate ideal Penrose tiling positions.

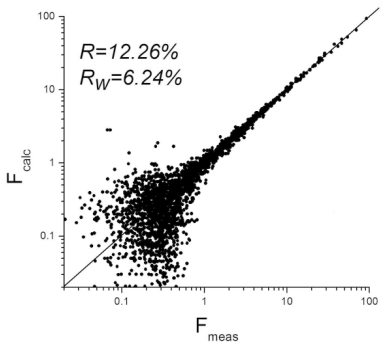

Figure 2. The F_{meas}/F_{calc} plot.

References

[1] A. Cervellino, T. Haibach, W. Steurer, "Structure solution of basic decagonal Al-Co-Ni phase by the atomic surface modelling method", *Acta Cryst. B* **58** (2002) 8–33.

[2] H. Takakura, A.Yamamoto, A.P. Tai, "The structure of Decagonal $Al_{72}Ni_{20}Co_8$ quasicrystal", *Acta Cryst. A* **57** (2001) 576–585.

[3] B. Kozakowski, J. Wolny, "Decorated quasicrystals and their diffraction patterns", *Phil. Mag.* **86** (2006) 549–555.

[4] M. Duda, B. Kozakowski, J. Wolny, "Penrose structures described by different kite-clusters", *J. Non-Cryst. Solids* **353** (2007) 2500–2505.