

s3.m12.p1 **Statistical approach in cluster analysis of 2D quasicrystals.** Aleksandra Dabrowska and Janusz Wolny, Faculty of Physics and Nuclear Techniques, AGH University of Science and Technology, Poland. E-mail: aldabro@poczta.onet.pl

Keywords: Quasicrystals; Clusters; Average unit cell

In quasicrystals, certain characteristic and occurring frequently groups of atoms called clusters can be found.

It is possible to cover the entire structure by some types of them. For instance for Penrose lattice it is the set of atoms lying within regular decagon and called Cartwheel Decagon which covers completely the whole structure. Because some atoms belong to different neighbouring clusters it is important to determine the ways of clusters' overlapping. For the Cartwheel Decagons matching rules were first introduced by Petra Gummelt [1].

In this paper we have calculated the probability distribution of clusters in an average unit cell approach [2]. This probability convoluted with a structure factor for particular cluster what leads to the structure factor for the studied quasicrystal. The analysis was conducted for some characteristic types of clusters' decoration (for example: for non-decorated Penrose lattice). For them we have calculated the formulas for structure factors which we used to obtain the so called enveloped functions connecting all the diffraction peaks. Finally we have discussed applications of the obtained formulas in determination of unknown quasicrystalline structure from measured diffraction pattern.

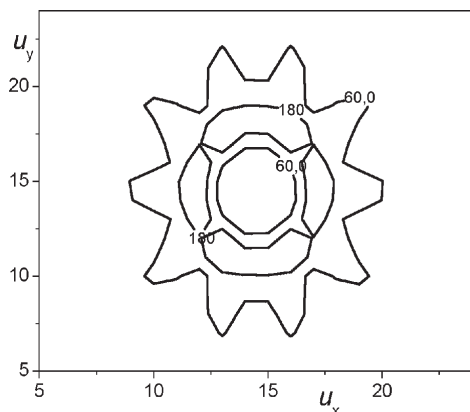


Fig.1. The probability distribution of clusters covering non-decorated Penrose lattice in an average unit cell.

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s3.m12.p2 **Diffraction experiments of decagonal Al-Co-Ni under high-pressure and low-temperature conditions.** Kai H. Hassdenteufel, Günter Krauss, Sergiy Katrych and Walter Steurer, Laboratory of Crystallography, ETH Zurich, CH-8092 Zurich, Switzerland. E-mail: kai.hassdenteufel@mat.ethz.ch

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Until today, the question of the mechanism that stabilizes the quasicrystal's structure is still not answered. Two main possibilities are discussed: entropy stabilization through local/global structural disorder vs. enthalpy stabilization (energetically preferred atomic arrangements, so-called clusters). To find hints about the answer to this question, diffraction experiments under non-ambient conditions are essential. Therefore many experiments were done, starting from different directions (e.g. high-energy ball milling, high-pressure experiments) aiming at the same topic: to induce a low-temperature phase transition of the quasicrystal. Further experiments aiming at this topic are in progress. On the one hand, powder X-ray diffraction measurements are performed, using a ball mill both at room temperature and under liquid nitrogen to induce a phase transition. The phase composition of the sample of the initial decagonal (d)-phase is detected in dependence of varying ball-milling times. This method was successfully used before for the quasiperiodic phase in the system Al-Cu-Co, where a phase transition from the icosahedral phase to a B2-phase was found [1]. *In-situ* low-temperature measurements are also planned, using an N₂-Cryostream between 90 K and 300 K, since a phase transition was detected for the d-phase at 150 K [2]. On the other hand, single-crystal diffraction experiments are performed at low temperature (≥ 20 K) and/or high pressure (≤ 10 GPa) using the ETH diamond anvil cell. The experiments include both *ex-situ* as well as *in-situ* single crystal measurements. Neither X-ray diffraction experiments at low temperature at 20 K nor at high-pressure at 11.5 GPa [3], both performed *in-situ*, did show a phase transition of the Edagawa-phase [4]. This either indicates a high stability of this quasicrystal or a very sluggish kinetics of the phase transition. If the latter is true, we want to overcome it by either high-energy ball milling or non-hydrostatic low-temperature compression.

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