

Simulation of Disorder Phenomena in Decagonal Quasicrystals, Miroslav Kobas, Thomas Weber and Walter Steurer, *Laboratory for Crystallography, ETH Zurich, Switzerland*, E-mail: miroslav.kobas@mat.ethz.ch

Keywords: Quasicrystal; Disorder; Simulation

The decagonal quasicrystal with nominal composition $\text{Al}_{70}\text{Co}_{12}\text{Ni}_{18}$, the so-called Edagawa-phase [1], features an extraordinary richness of complex scattering. The view perpendicular to the tenfold axis shows alternating 'Bragg layers' and 'diffuse interlayers'. Bragg layers contain both Bragg reflections and diffuse scattering, while diffuse interlayers contain diffuse scattering only. In the present study, the focus lies on the diffuse scattering inside the Bragg layers. To understand the origin of these diffuse features, simulations of disorder phenomena on different scales and in different dimensions have been performed. In a first approach, the 'cluster' form factors of about 6 Å-sized sub-clusters are calculated. The goal of this approach is to identify essential structural building units of the quasicrystal structure. Good agreement with experimental observations are obtained with sub-clusters reported by Saitoh et al. [2]. In a second approach, disorder phenomena of 20-32 Å sized clusters reported in literature [3-6] are simulated. The goal of this approach is to determine local disorder phenomena in the quasicrystal structure. Best agreement with experimental results is achieved with a fivefold orientational disorder of the Abe-cluster [3]. These results are discussed in the framework of electron microscopy studies done by other groups. Especially, links between cluster-models showing m symmetry and $5m$ symmetry are discussed with regard to plausible disorder phenomena. Furthermore, the influence of some disorder phenomena on the formation of quasicrystalline order is pointed out. In a third approach, disorder related to thermal diffuse scattering (TDS) and phasonic diffuse scattering (PDS) of the Edagawa-phase is calculated [7]. With this technique it is possible to describe complex disorder in three-dimensional space by just a few parameters in five-dimensional space. The goal of this approach is to evaluate the importance of TDS and PDS for the Edagawa-phase. Good agreement with experimental data is achieved and it can be concluded that TDS and PDS constitute the major part of the experimentally observed diffuse scattering inside the Bragg layers. In a next step, the results from these five-dimensional simulations need to be translated into three-dimensional structural information. Combining the results of all approaches will provide insight into the disordered, real structure of the Edagawa-phase. This will be another piece in the puzzle to the comprehension of a real quasicrystal structure.

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