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MS25-P4 A complex pseudo-decagonal quasicrystal approximant solved by the strong reflections approach and refined against Rotation Electron Diffraction (RED) data

Sven Hovmöller[1], Devinder Singh[1], Benjamin Grushko[2], Wei Wan[1], Yifeng Yun[1], Xiaodong Zou[1]

1. Department of Materials and Environmental Chemistry, Stockholm University, SE 10691 Stockholm, Sweden
2. PGI-5, Forschungszentrum Jülich, 52425 Jülich, Germany

email: sven.hovmoller@mmk.su.se

The strong-reflections approach is valid on structures that contain similar atomic clusters and electron diffraction patterns with similar intensity distribution of reflections. It is based on the fact that the strongest reflections largely determine the atomic positions in a structure and represent the main structure features of a crystal. Thus, this approach can be used for structure solution. In the present study, the structure of the complex pseudo-decagonal (PD) quasicrystal approximant PD1 in the Al-Co-Ni alloy system was solved by phasing the strong reflections from rotation electron diffraction [1] (RED) data using the known PD2 structure [2]. The PD1 crystal is primitive and orthorhombic *Pnam*, with unit cell parameters *a*=37.7, *b*=39.7, *c*=4.1 Å. Electron diffraction studies show that in reciprocal space, the positions of the strongest reflections and their intensity distributions are similar for both approximants. The high-resolution transmission electron microscopy (HRTEM) image after image processing with CRISP (crystallographic image processing program) shows that PD1 and PD2 intergrow with each other. The orientation relationship between PD1 and PD2 was found by comparing the Fourier transforms, calculated from the two regions in the HRTEM image. By applying the strong-reflections approach, the structure factor amplitudes and phases of PD1 were deduced from those of the known PD2 structure. The structure of PD1 contains 115 unique atoms (31 Co/Ni and 84 Al). They were located from a density map calculated from only the 15 (!) strongest unique reflections. As with other approximants in the PD series, PD1 is built of characteristic 2 nm wheel clusters with 5-fold rotational symmetry [3], which agrees with results from HRTEM images.

References

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