Structure of the Pseudodecagonal Al-Co-Ni Approximant PD4

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The similarity of crystalline approximants to the quasicrystals in terms of their compositions, densities and diffraction patterns, makes them very important for determining the structures of quasicrystals. Several crystal structures of these approximants were determined [1–2].

Several periodic pseudodecagonal (PD) structures were found in the Al-Ni-Co system. They are named PD1, PD2 etc. and exhibit diffraction patterns with almost perfect tenfold symmetry and quasiperiodic reflection arrangements [3].

X-ray diffraction data (0.85 Å resolution) from a single crystal of PD4-phase was collected using Oxford XcaliburTM 3 diffractometer. The unit cell parameters for this structure are a = 101.302(9) Å, b = 32.102(2) Å, c = 4.1803(4) Å.

The phase problem for the approximant PD4 was solved by direct methods in the non-centrosymmetric space group *Bbm*2. The refinement of the structure using the deduced model is in progress.

[1] Freiburg C., Grushko B., Wittenberg R., Reichert W., *Mater. Sci. Forum*, 1996, **228-231**, 583-586. [2] Ma X. L., Kuo K. H., *Metall. Trans.*, 1992, **23A**, 1121. [3] Grushko B., Holland-Moritz D., Wittmann R., Wild G., *J. Alloy. Comp.*, 1998, **280**, 215–230.

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