

Quasicrystal Structure Analysis. The State of the Art

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The quasicrystal is an aperiodic solid showing Bragg peaks with noncrystallographic symmetry. It is recently clarified that the structure of quasicrystals can be analyzed by using a newly developed direct method and a structure refinement which is based on a higher-dimensional cluster model. They are equally applicable to decagonal and icosahedral quasicrystals since all quasicrystals seem to consist of some atom clusters (or building units)[1].

For the initial model building, the low-density elimination method (LDEM) is efficient [2]. This gives rough shape and size of occupation domains (OD) of a quasicrystal, which specify the location of atoms in a higher-dimensional space.

An initial model for the structure refinement is obtained from the rough ODs determined by LDEM by considering atom clusters, which are included in its crystal approximants. The distribution of atom clusters can not, however, be determined uniquely because of the existence of random phason strain, which is seen in all quasicrystals. This is usually inferred from high-resolution electron microscopy images or simply assumed based on a quasiperiodic tiling. The random phason is taken into account as the phason displacement parameter in the refinement. The paper demonstrates structure determination of quasicrystals in the light of recently developed techniques.

[1] Yamamoto A., Takakura H., *Ferroelectrics*, 2004, **305**, 223. [2] Takakura H., Shiono M., Sato T. J., Yamamoto A., Tsai A. P., *Phys. Rev. Lett.*, 2001, **86**, 236.

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