Crystalline Structure: Local and Global Approaches

Nikolai Dolbilin
(Steklov Mathematical Institute of Russian Academy of Sciences;
The International Delone Laboratory of "Discrete and Computational Geometry"
of Yaroslavl State University, Russia) *

Abstract

An appropriate concept for describing an arbitrary discrete atomic structure is the Delone set (or an (r, R)-system). Structures with long-range order such as crystals involve the concept of space group as well.

A mathematical model of an ideal monocrystalline matter is defined now as a Delone set which is invariant with respect to some space group. One should emphasize that under this definition the well-known periodicity of a crystal in all 3 dimensions is not an additional requirement, because full periodicity is implied by the celebrated Schoenflies-Bieberbach theorem, any space group contains a translational subgroup with a finite index.

Thus, a mathematical model of an ideal crystal uses two concepts: a Delone set (which is of local character) and a space group (which is of global character).

Since crystallization is a process which results from mutual interaction of just nearby atoms, it is believed (L. Pauling, R. Feynmann et al) that the long-range order of atomic structures of crystals (and quasi-crystals too) emerges from local rules restricting the arrangement of nearby atoms.

However, there were no whatever rigorous results in this directon until the 1970s, when Delone and his students initiated a local theory of crystals. The main aim of this theory was (and is) the rigorous derivation of the space group symmetry of a crystalline structure from the pair-wise identity of local arrangements around each atoms.

In the talk I will present results on local rules for crystals rules and also a quite opposite approach to the description of crystal.

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*dolbilin@mi.ras.ru