Z. Kristallogr. **222** (2007) 308–309 / **DOI** 10.1524/zkri.2007.222.6.308

What is a crystal? Introductory remarks to an ongoing discussion

What is a crystal? What a strange question, you may think, because there is a nice definition in the *International Tables for Crystallography, Vol. A.* In chapter 8.1 *Basic concepts*, you will find the following:

> *"Crystals are finite real objects in physical space which may be idealized by infinite three-dimensional periodic crystal structures in point space. Three-dimensional periodicity means that there are translations among the symmetry operations of the object with the translation vectors spanning a three-dimensional space. Extending this concept of crystal structure to more general periodic objects and to n-dimensional space, one obtains the following definition:*
> *Definition: An object in n-dimensional point space E^n is called an n-dimensional crystallographic pattern or, for short, crystal pattern if among its symmetry operations*
> *(i) there are n translations, the translation vectors $\boldsymbol{t}_1, \ldots, \boldsymbol{t}_n$ of which are linearly independent,*
> *(ii) all translation vectors, except the zero vector $\boldsymbol{o}$, have a length of at least $d > 0$.*
> *Condition (i) guarantees the n-dimensional periodicity and thus excludes subperiodic symmetries like layer groups, rod groups and frieze groups. Condition (ii) takes into account the finite size of atoms in actual crystals"*

This concept allows to describe a *real crystal* by comparing it with the model of an *ideal crystal*. In the following I list some terms used for the description of real crystals or their idealized models:

Ideal crystal: infinite mathematical object with an idealized crystal structure; an *ideal crystal* can be *ordered* or *disordered*, if it is *disordered*, it is not *periodic* anymore, however, it has a *periodic average structure*.

Real crystal: single-phase material which can be described referring to an *ideal crystal*.

Perfect crystal: real crystal in thermodynamic equilibrium (only point defects are possible such as thermal vacancies, impurities).

Imperfect crystal: real crystal containing defects that are not in thermodynamic equilibrium as well.

Nanocrystal: real crystal with dimensions on the scale of nanometers; its structure may fundamentally differ from that of larger crystals with the same composition.

Paracrystal: crystal showing string correlated lattice disorder, which is not necessarily bounded.

Metacrystal: crystal consisting of building units other than atoms (ions, molecules), such as *photonic* or *phononic crystals*.

One of the terms missing in this list is *aperiodic crystal* used for incommensurately modulated structures and quasicrystals. Although their structures lack three-dimensional translational periodicity, their Fourier spectra show Bragg peaks only. This property has been used by the IUCr Ad-interim Commission on Aperiodic Crystals to identify *aperiodic crystals* by their '*. . .essentially discrete diffraction diagram. . .*' (Acta Crystallogr. A48 (1992) 928). Consequently, three-dimensional translational periodicity is no more seen as a necessary condition for crystallinity. The reciprocal space definition of a *crystal* by its spectral properties can be much simpler than one based on direct space. Additionally, it has the advantage of being easily accessible experimentally by diffraction methods.

However, so pragmatic this definition may be so fuzzy it is. The term diffraction diagram suggests an experimentally obtained image. How this looks for a *real crystal* cannot be clearly defined. It depends on the kind of radiation used and the quality and size of the crystal studied. A strongly absorbing large and irregularly shaped crystal of poor quality, for instance, would not at all give an *essentially discrete diffraction diagram* even for simple periodic structures. Consequently, the concept of an *aperiodic crystal* should refer to an *ideal aperiodic crystal* of infinite size and to its Fourier spectrum rather than its diffraction diagram.

From time to time some of the members of the *aperiodic-crystals* community feel uneasy and start the discussion on a new definition of *crystals* again. This time, S. Ben Abraham initiated the discussion.

If you think you can contribute to this discussion, please, send me your manuscript.

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