Is there a crystal clear definition of a crystal?

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To clearly define the objects one is working with is a prerequisite for sound scientific work. In particular, a comparison of results is impossible without. In this view, one needs a clear-cut definition of what a crystal is supposed to be. Moreover, in view of the large community of people working with them, it is desirable to even have a well accepted definition. Neither property seems to be satisfied with the present fuzzy definition of a crystal, and the reasons are manifold.

First of all, as several colleagues have pointed out, the present "definition" is not a definition in the mathematical sense, since one has to clarify the meaning of 'essentially discrete'. Neither would the alternative suggested by Ben-Abraham be a definition, because the meaning of 'long-range order' needs further explanation – as it stands, it is as vague as the original one.

Second, for a mathematician, it is not reasonable to use a scheme where a quasicrystal (which should be the more general term) is called a crystal, but not necessarily vice versa. To explain this with an example: Since Harald Bohr, periodic functions form a subclass of the quasiperiodic functions, which, in turn, are a subclass of the almost periodic functions. So, a mathematician would clearly use a scheme where all crystals are quasicrystals, but not all quasicrystals are crystals, and this is in constant use in the mathematical literature on the topic. Moreover, the term 'crystallographic group' is well-established for groups of isometries with compact fundamental domain. In general, the isometry group underlying a quasicrystal is not crystallographic in this sense.

Third, there is the homometry issue, in particular the one with the binary Rudin-Shapiro sequence versus the binary Bernoulli sequence. These two have the same diffraction image, consisting of a Bragg part and an absolutely continuous part, and would be a "crystal" by the present IUCr definition. While the former has a purely deterministic structure, the random structure of the latter is quite far from being deterministic. As an aside, we are not sure what Ben-Abraham's verdict would be: the Rudin-Shapiro is of the same type as the Thue-Morse system, so qualifies for long-range order, but we see no way to decide that for the Bernoulli system on the basis of his suggestion.

Mathematics largely deals with idealizations, thus only perfect structures are considered. From a theoretical point of view, it would be satisfactory to define crystals as structures with pure Bragg spectrum supported on a lattice, and quasicrystals as structures with pure Bragg spectrum on a finitely generated Fourier module (thus including crystals as the special case where this module is a lattice) and then further, more general classes. In theory, no practical difficulty arises from this approach.

In practice, as also pointed out by some, things are more subtle. There is no such thing as an infinite crystal, and neither is there a perfect (or static) arrangement. So, one has to withdraw to a different approach. It seems that most people agree on using the notion of long-range order, in one way or another, to distinguish substances – though the fine line of where to make a cut is a matter of taste and research interest. Nevertheless, the original question now boils down to what long-range order is. This question attracts and deserves attention from several communities.

Now, putting all these problems aside, real world solids are still to be dealt with, and one has to agree on some pragmatic notion of long range order, at least for the time being. Using a spectral approach seems very reasonable, and that is what underlies the present fuzzy definition. We see no principal difficulty with it, except the terminology. We would thus prefer a version where a pure Bragg spectrum with peaks on a lattice (in the strict sense) stands for a crystal, and then a hierarchy of extensions to define a quasicrystal, an almost crystal etc.

For us, the existence of diffuse components provides welcome research problems, but definitely means a deviation from what we would consider to be a crystal.

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