

Follow-up contribution to the discussion on “What is a crystal?”

About crystals and their definition

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“Die Hauptsache ist, dass die Hauptsache die Hauptsache bleibt.”
(H. Dürbeck)

A look back into history tells us that crystallography was developed without a definition of a crystal, or more precise: the definition has grown with the knowledge about an only vaguely described object. This is painful for mathematicians but not for physicists. Physicists can show the material they deal with, it exists as soon as they have shown, named and described it, mathematicians have to define it: it does not exist as long as it is not defined.

Thus there are at least two ways of approaching towards this topic, and any mixing of the approaches will cause confusion.

The extreme point of view is perhaps: for a physicist it would be sufficient to have an IUCr-commission to where he sends his material and which from case to case decides if it is crystalline or not. This commission would soon try to reduce its work and publish a list of criteria for materials that are definitely non-crystalline or definitely crystalline and which people should **not** send to the commission. In principle physicists could work with such a system – surely, not all of them were lucky with it. OK, it is **an extreme point of view**. After some years the IUCr-commission would publish a report on its experience with the material they had tested. Then they also will give a list of positive criteria and this list will contain all the procedures the busy people in the commission have applied to test the solids and powders and even liquids they got. Surely this list would tell something about Bragg peaks under diffraction by X-rays, neutrons and electrons, on reflections and satellites etc. And this report would be a helpful thing for physicists and for some years the commission could close its doors until somebody finds a material, the crystalline nature of which could not to be decided by means of the list. Then a new session of the commission will be necessary. So far, this is a possible procedure for physicists, chemists, mineralogists and biologists.

From a less extreme point of view the wish of S. Ben Abraham to have a short comprehensive definition of the scientific object, we deal with, is well founded. It could be found ‘boiling down’ (as J. D. H. Donnay used to say) the virtual list mentioned above. In the proposals I read up to now (S. Ben Abraham, T. Janssen, M. Senechal & L. W. Kahn, M. Baake & D. Frettlöh, R. Lifshitz) a lot of good ideas for such a formulation are given (in far better English than I could offer).

Thus I will give no further proposal but only remind you of two aspects, one of which W. Steurer already has mentioned: **Don’t mix mathematics and physics**. The diffraction diagram has no place in a mathematical definition of the object and it doesn’t need to have, as all properties which are to be respected, can be formulated by means of Fourier-transforms.

The second aspect is: Keep in your mind that **you must be able to teach the topic**. It is hard enough to talk about crystals, the symmetry group of which is a space group (in any dimension). For many students a space group is a picture and a page in the *International Tables*. But imagine a student who has to learn in the beginning: the symmetry group of the ‘generalized’ crystal is a groupoid with some extra properties and the space groups are discussed only later as a special case in a corollary. The result will be that students get texts they do not really understand and they will help themselves with some oversimplified pictures (– there are enough physicists who believe that the 14 Bravais lattices are the final result of crystallography). Thinking in this direction may result in retaining the actual state of the art, namely to have a definition for a proper (‘eigentlichen’) crystal, surrounded by a list of extensions.

Mathematicians cannot be lucky with a procedure which decides from case to case, what a crystal is. They really need a definition. No, they need a series of definitions. And these definitions must include the classical definition which comes from the ideas of Sohncke, Fedorov, Schoenflies, Bieberbach *et al.* This definition should respect that a crystal can be described either by a function or by a discrete point set which obey the symmetry of a space group. Any mathematical definition must be independent of the question if the ‘crystal’ will ever see an X-ray or not. But especially mathematicians should think about the problem that their products have to find the way into a student’s brain (and often even worse: into a colleague’s brain). Perhaps, from this point of view the definition of the *International Tables of Crystallography*, vol. A, followed by a list of modifications, is not so bad at all.

Finally, I would like to give a remark with respect to the very interesting and thoroughly worked out paper by RON LIFSHITZ. The definition he gives in section 6 is a possible solution of the problem, but I am not completely glad with it (– this is no question of ‘right’ or ‘wrong’). The reason is that, as discussed in his section 2, he turns from the commonly well formalized term “symmetry” to

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the not well-defined term “order”. The complexity of the problem is shifted from the question “**What is a crystal?**” to the question “**What is order?**” Thus it is not surprising that the sections 3, 4 and 5 of his paper try to analyze the meaning of the Fourier-space definition of ‘long-range positional order’ in direct space. Mathematicians can live with the definition of section 6 (if Bragg peaks do not refer to X-rays), but I fear that the content of the sections 3, 4 and 5 will be reduced to very simplified pictures in textbooks for physicists. Although I see that the paper of Ron Lifshitz gives an excellent analysis of the problem, I doubt if I would begin a textbook on crystallography with his definition, as the hurdle which must be leaped over, to enter crystallography becomes higher compared to the classical way.

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References

The papers of this discussion, see this issue pp. 310–317.