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What is a crystal?

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In April 1991 the Commission on Aperiodic Crystals [1] adopted the following definition of a crystal:

> *"[In the following]* ***by 'crystal' we mean any solid having an essentially discrete diffraction diagram****, [and by 'aperiodic crystal' we mean any crystal in which three-dimensional lattice periodicity can be considered to be absent.]"*

This definition has, in my opinion, two flaws. (1) It explicitly depends on diffraction, hence on a specific method, albeit important and widespread. (2) More importantly, and in part as a consequence of (1), it is not general enough. To show this one simple example should be sufficient.

Consider the Thue-Morse substitution sequence. It can be generated by the deceivingly simple algorithm

$$\begin{aligned} a &\rightarrow ab, \\ b &\rightarrow ba. \end{aligned} \tag{1}$$

This sequence is, of course, perfectly deterministic. In other words, it possesses long range positional order. Nevertheless, it is by no means periodic, and not even quasiperiodic. Its spectrum is singular continuous; it has no discrete part. Its physical realization has been achieved almost two decades ago [2]. Somewhat later, Axel and Terauchi [3] reported high-resolution X-ray diffraction spectra of Thue-Morse GaAs-AlAs heterostructures produced by molecular beam epitaxy. The spectra showed the essential features of singular continuous measures.

Thus we have an example of a solid with deterministic positional long range order and no essentially discrete (*i.e.* Bragg-type) diffraction pattern. Nevertheless, I am rather sure that most of us would consider this solid structure to be a crystal. It is possible to produce many more structures based on substitution series that are neither periodic nor quasiperiodic and hence do not have a Bragg-type diffraction pattern.

It is true that all such structures would be artificially fabricated. But that is true of most anorganic crystalline phases we deal with nowadays.

After having discussed the matter with some colleagues I suggest to adopt the following definition of a crystal:

> **By crystal we mean a solid that has long-range positional order.**

This is concise and clear cut. Thus it can serve the scientist in the lab as well as the teacher in the classroom. On the other hand, as many scientific definitions, it may need an appendix of commentaries and remarks. Thus, one might elucidate what long-range order means in terms of correlation functions. There might be recommendations concerning ways to determine the existence of long-range order. Perhaps there should be a remark about structured diffuse scattering.

Mainly, one should state **what is not a crystal**. I have in mind soft condensed matter possessing various degrees of order, such as mesophases (liquid crystals), ordered structures of colloidal particles and other analogs of crystals. All these may, of course, well be studied by crystallographic methods but, in my opinion, they should not be called crystals.

I hope by this note to revive the discussion on this subject and eventually arrive to a consensus in our community.

References

[1] IUCr: Report of the Executive Committee for 1991. Acta Crystallogr. A**48** (1992) 922–946; p. 928.
[2] Merlin, R.; Bajema, K.; Nagle, J.; Ploog, K.: Raman scattering by acoustic phonons and structural properties of Fibonacci, Thue-Morse, and random superlattices. J. Phys. (Paris), Colloq. **48** (1987) C5-503–C5-532.
[3] Axel, F.; Terauchi, H.: High-resolution X-ray diffraction of Thue-Morse GaAs–AlAs heterostructures: Towards a novel description of disorder. Phys. Rev. Lett. **66** (1991) 2223–2226.

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