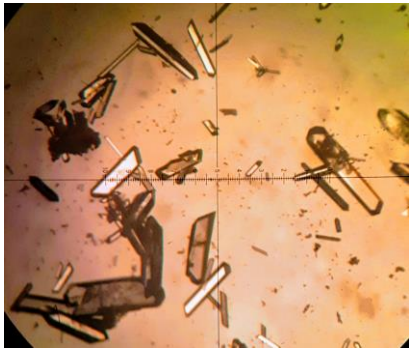
What is a crystal?

- Historically, crystals were first defined in terms of their external morphologies, with the angular and symmetry relationships between their faces.
- This led to a definition based on the three-dimensional translational periodicity inferred from the periodicity of the array of Bragg peaks in the diffraction patterns of most crystals.
- More recently crystals have been discovered for which the array of Bragg peaks is not periodic in three dimensions so that the repeating atomic arrangement lacks translational periodicity in at least one direction.
- The Nobel Prize in Chemistry 2011 was awarded to Dan Shechtman "for the discovery of quasicrystals"



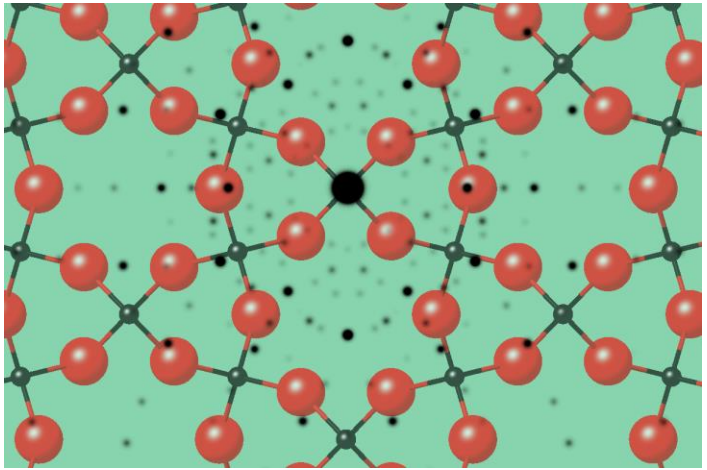
Online Dictionary of Crystallography. ‘Crystal’. https://dictionary.iucr.org/Crystal

What is a crystal?

Direct-space definition:

- A solid is a crystal if its atoms, ions and/or molecules form, on average, a long-range ordered arrangement.

- In most crystals the arrangement is a periodic array that is governed by the rules of translational symmetry. In aperiodic crystals (incommensurate and quasicrystals) the arrangement is not periodic in three dimensions but is nevertheless still fully ordered, where the ordering follows particular mathematical rules.



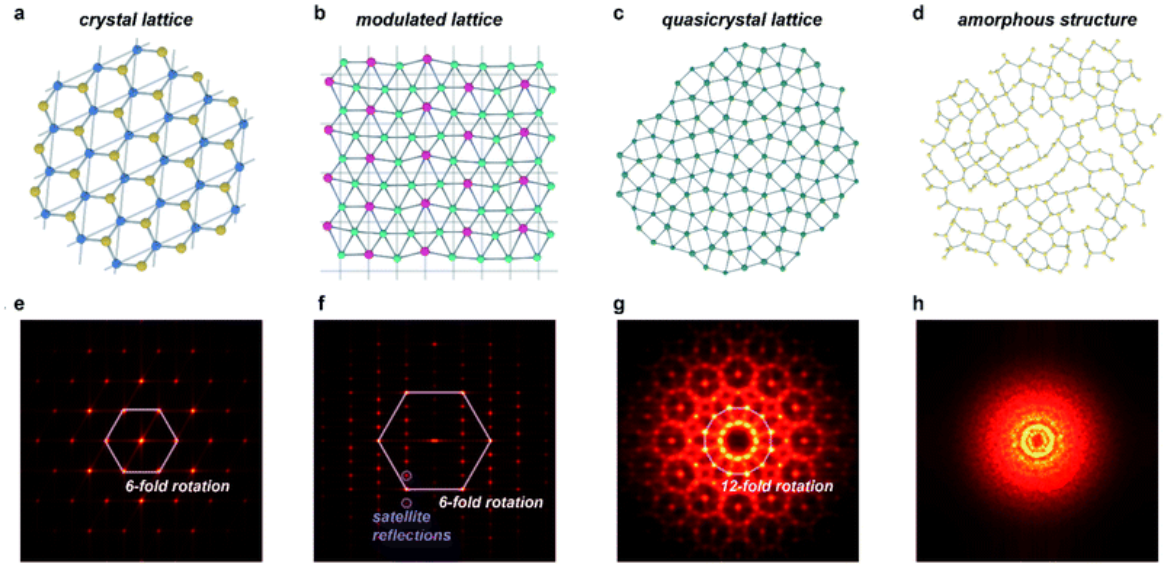
Carolyn P. Brock. Change to the definition of "crystal" in the IUCr Online Dictionalry of Crystallography. *IUCr Newsletter*. **2021**, *29*(2). *https://www.iucr.org/news/newsletter/volume-29/number-2/change-to-the-definition-of-crystal-in-the-iucr-online-dictionary-of-crystallography*

Online Dictionary of Crystallography. 'Crystal'. https://dictionary.iucr.org/Crystal

What is a crystal?

Reciprocal-space definition:

- A material is a crystal if it has essentially a sharp diffraction pattern.
- The word essentially means that most of the intensity of the diffraction is concentrated in relatively sharp Bragg peaks, besides the always present diffuse scattering.



Order in aperiodic crystallography and its manifestation in diffraction. In Oppenheim, J.J.; Skorupskii, G.; Dincă, M. Aperiodic metal–organic frameworks. *Chem. Sci.*, **2020**, *11*, 11094-11103.

Online Dictionary of Crystallography. 'Crystal'. https://dictionary.iucr.org/Crystal

How to grow a crystal?

Recommendations from CCCW25:
Don’t let your supervisor pick at your samples
When working at high temperatures, the key is slow cooling
Use clean glassware
Make sure that where you let your crystals grow, that it is still and quiet
Don’t keep checking on your crystals every five minutes
Try different conditions/set-ups.
If you need to grow crystals in the glovebox….don’t.
Be patient! And avoid vibrations.
Slow cooling
Try lots of DCM and leave it for six months (long time!)
Never submit/bring to the diffractometer your entire sample to the X-ray lab (don’t take all your air sensitive samples to the diffractometer)
In the glovebox, set up your vapor diffusions and leave them alone. Also, the best crystals grow over Christmas!
If vapour diffusion is not working, try other methods, like layering.

How to grow a crystal?

Recommendations from CCCW25:
Always filter your samples before you try to grow crystals.
Set up your crystallizations on Friday, and the weekend works magic
Don’t let yourself get discouraged if it does not work out.
Change the polarity of the solvent (vapour diffusion/layering). Name and respect the crystals.
Do not make eye contact.
For slow evaporation, draw a line on the solvent level, so that you can see how fast it evaporates. And do not let them dry out.
Use a vial with a big surface area, and do not let all the solvent evaporate.
Try a lot!
Benign neglect – if you love your crystals you will leave them alone.
Keep your crystallographer happy with beautiful coloured crystals!
Always filter your solution before putting it aside for crystallization.
Be patient.
Things don’t break if you are nice and slow.

How to grow a crystal?

Recommendations from CCCW25:
Do solubility tests on your compound before using large amounts of solvent.
Especially during the summer, keep your crystal growths in a temperature controlled, cool environment.
Make sure that you have a pure material. Even if the NMR does look messy, that does not mean that you cannot grow crystals; just that pure materials will grow more readily/better.
Ask others for their advice.
Be aware of the chemistry; understand the chemistry of the crystals so that you can grow them.
Heat solutions up, and then cool them very slowly.
You can make a homemade thermos by filling a vessel with vermiculite.
You can buy bulk glass tube stock, score them, and then flame close one end – essentially making very inexpensive NMR tubes (which are great for crystal growth).
Do NOT – The solid material was rapidly heated and then cooled – don't burn the lab down!