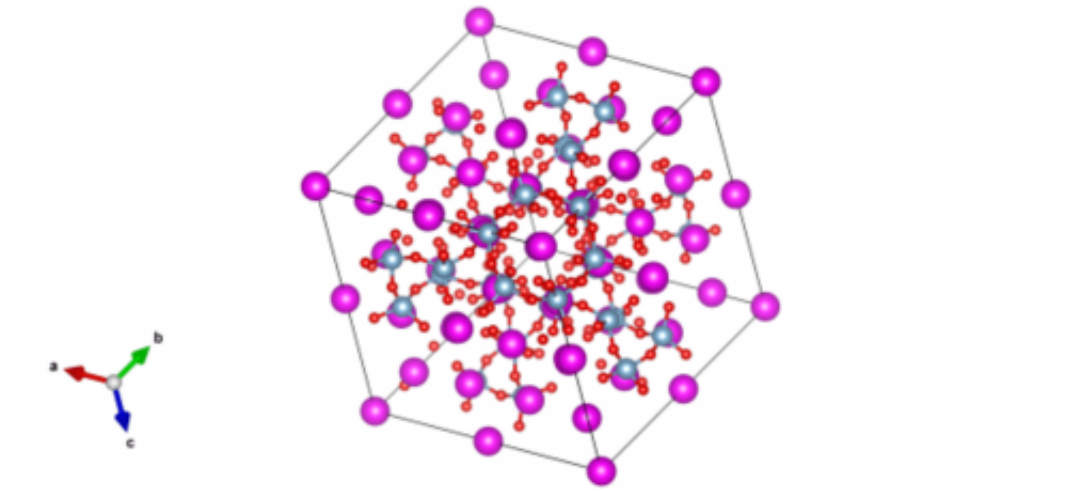
Why I'm proud to be a crystallographer

December 10 2014, by Helen Maynard-Casely



When looked at the right way, even cement can be beautiful. This is the crystal structure of tricalcium aluiminate, a vital mineral in cement.

This year I have learnt more that it is probably healthy to know about crystal structures. I've learnt how you can turn a rabbit green with a protein, read up on French military history and marvelled at how a crystal structure can destroy itself. I've even found cement interesting!

These examples are just the tip of the iceberg, or (to put more appropriately) merely the surface layer of atoms of the science of crystallography and what it has achieved. It's been a pleasure to discover so much about the field this year.

Why? 2014 was sanctioned by the UN to be the International Year of

Crystallography (along with farming and family – or was that family farming?). A definite improvement on last year's 'International year of Quinoa', but as we loll into December I reckon there's a few of you out there still scratching your head as to what it's all about?

Crystallography is the science behind structure, of knowing where your atoms are. There have been some excellent 'explainers' already on The Conversation, and a number of videos explaining it.

To date, across the various databases, there's coming up to 1 million crystal structures that have been determined. That's nearly a million times a researcher has collected a diffraction pattern (like von Laue did to kick off the whole field in 1911) and interpreted how this could be generated from an arrangement of atoms (like Bragg did in 1912). In an effort to highlight just 365 of them, myself and 40 other researchers, have blogged about one every day. I'd urge you to look over the Crystallography 365 project to see the massive diversity of science that crystallography encompasses.

But why be a crystallographer?

I don't usually like giving myself a 'scientific label' – I have a degree in planetary science, a PhD in physics and my first job was in a chemistry department. I promise you (and my parents) that it did all make some sense at the time. But one thread has run through all of these career twists, and that's my use of crystallography.

You'll not find many scientists who call themselves just 'Crystallographers' and that's because (as my career to date shows) it's an inherently interdisciplinary science. Most of us are something else as well, be that geologists, chemists, physicists or biologists. As a scientist starting out, that really appealed to me. I have taken my crystallographic skills, mostly learnt during my PhD in physics, and applied them to

problems in fields diverse as forensics, minerals and explosives. I've even collected a diffraction pattern of cocoa butter!

Then there are the role models. In science, as a rule, there are not usually all that many female role models to look up to. But crystallography smashes that out of the park. From Lonsdale to Hodgkin to Megaw to Franklin, women have been front and centre in some of the biggest leaps in crystallography and the community still retains its healthy gender balance.

It's not just the crystal structure that you can get from these studies, but a very fundamental view of the properties of the material that you are looking at. As a result, crystallography has brought about some of the most famous scientific leaps, 28 Nobel's have been awarded through its application. Knowing where the atoms are in materials brings fundamental insights that have revolutionised our world, from the structure of DNA to giant magneto-resistance.

Crystallography is also often at the forefront of 'movements' in research. For instance, big data is old news in crystallography, with institutions like the Cambridge Crystallography Database Centre (custodian of a database of over 600,000 crystal structures, mostly of molecular compounds) set up to collate molecular structural information and 'mine' that to discover new interactions and even predict how new materials will form.

There's an argument that much of the success of crystallography has been that it is an inherently 'open' science. Most of the software tools that I use day in day out are freeware – developed and maintained by researchers in the field. I'm supremely grateful for their hard work, making tools that are essential to a wide range of scientific projects, with often only citations as reward. Added to this data depositories (such at the Crystallographic Open Database) and standardisation of format have

meant that scientists across disciplines can easily communicate their findings to each other.

So every time I collect a diffraction pattern, I enjoy the fact that I'm part of a collective of people (and one robot on Mars) doing the same thing. It's a fabulous 'clan' to belong to, and that's why I'm proud to be a crystallographer.

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