Shells, silicon & neighbourly atoms

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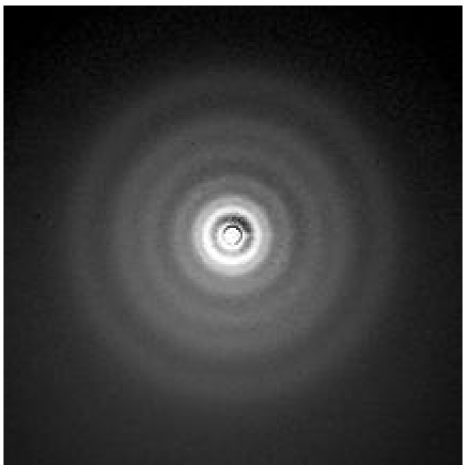

Ring-like pattern observed using crystallographic techniques, in this example silicon has been used.

What do shells, solar panels and DVDs have in common? At the atomic scale they are 'amorphous', that is -- unlike crystals -- they are built from irregular arrangements of atoms.

As Andrew Goodwin of Oxford University’s Department of Chemistry explains this irregularity is important: it’s what allows shells to grow their curved edges and gives silicon its incredibly useful electronic properties.

But for scientists this irregularity also makes such materials tricky.

‘Our main technique for establishing what materials look like on the atomic scale is crystallography,’ Andrew tells me, ‘and this relies explicitly on the existence of a repeating arrangement of atoms in order to work. So the problem of studying amorphous materials with their seemingly-random arrangements of atoms has remained just that: a problem.'

Now, Andrew, and colleagues from Cambridge and Ohio, report in this week's [Physical Review Letters](#) how tantalising crystallographic clues could offer a new approach to understanding amorphous materials.

'For decades we've known that the ring-like patterns amorphous materials produce in crystallographic experiments contain limited information about the surrounding environment of each atom,' Andrew comments, 'but the big question has always been how to use this to create a coherent picture of the structure of a material.'

He explains that the new approach comes from the 'neighbourly behaviour' of atoms which means that similar atoms should experience a similar environment.

'The spacing of the rings in the 'ring-like pattern' is related to the distances between atoms in the material, and the intensity of the rings is essentially related to how many neighbours each atom has,' Andrew tells me.

'So, using silicon as an example, a typical analysis of its corresponding crystallographic pattern would have told us that the distance between silicon atoms is about 235 trillionths of a metre [picometres], and that on average each silicon atom has four neighbours.'

Yet this information alone isn't enough to build reliable models of what the atomic structure of a material such as silicon actually looks like.

Such models fail because they rely on the average 'neighbourly behaviour' of the atoms which means in these models some silicon atoms can have three neighbours if others have five - something other techniques such as spectroscopy show is incorrect.

The new insight relates to the fact that such experiments are sensitive to the number of neighbours each atom has, so an atom with three neighbours would appear as a different 'type' of atom to one with five neighbours.

'Because there is only one 'type' of atom observed for silicon we know that not only is the average number of neighbours equal to four, but that each silicon atom must have exactly four neighbours,' Andrew adds.

'If we incorporate this extra information when building a model, the answer seems to fall out almost straight away. We simply tell our program how many different types of atom there are, and in what proportions, and this is enough to produce a realistic model from the ring-like patterns.'

The findings suggest that crystallography might, after all, be able to unlock the structural secrets of some of Nature's most irregular materials: opening the way for new kinds of science and powerful new technologies.

More information: Paper: prl.aps.org/abstract/PRL/v104/i12/e125501

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