An **eye** for detail

Professor Dr Christoph Koch and **Dr Wouter Van den Broek** of Ulm University's Electron and Ion Microscopy Group bring some of their work advancing the art of microscopy into sharper focus

To begin, how did you become interested in this field of research? What is it about three-dimensional (3D) atomic structures that inspires you?

CK: The properties of any material are determined by the atoms it is made of and how they are arranged. A common approach to understanding materials is thus to run expensive calculations for obtaining equilibrium atom positions for a given composition. Once this equilibrium structure has been obtained, mechanical, electric, magnetic and some other properties can be computed, and simulations of how the material would behave under different environmental conditions, even beyond the capability of any laboratory, can be undertaken.

Having an experimental technique which can image the 3D positions of individual atoms in any kind of material is therefore an enormous step forward for materials science in general. For example, the atomic structure and detailed movement of dislocations responsible for plastic deformation of materials shown in textbooks is purely based on computer simulations, because until now it was impossible to image such details directly. Being able to compare theory and experiment gives us much more confidence in the simulations, may help to improve them and allows us to apply these theories to new problems.

How important is accurate and precise characterisation of nanomaterials to progress in the field?

CK: What makes nanomaterials so special is that a very large part of their volume is comprised of surfaces and interfaces. If we can image the structure of these 'defects' and link that to the macroscopic properties of the material, we will be able to design new materials much more cheaply. X-ray diffraction may give us the atomic structure of perfect crystals, but in nanomaterials it is the deviation from perfect crystallinity that is interesting, and that is exactly what our inversion of dynamical electron scattering (IDES) approach has been developed for.

What advantages do high-resolution transmission electron microscopy (HRTEM) and scanning high-resolution transmission electron microscopy (STEM) have over methods such as 3D atom probe tomography (ATP)?

WVdB: HRTEM and STEM only alter the samples minimally if problems with sample preparation and beam damage can be kept in check. Phenomena like grain boundaries or dislocations can be observed in their natural surroundings at atomic resolution.

ATP attains atomic resolution in much larger samples by peeling off the atoms layer by layer. However, only about 60 per cent of the atoms can currently be detected, and at the freshly peeled surfaces the atoms rearrange themselves in new, slightly different positions. Switching from ATP to TEM therefore trades larger field of view for improved accuracy.

How have you used new mathematical tools, in particular artificial neural network (ANN) theory, in your work?

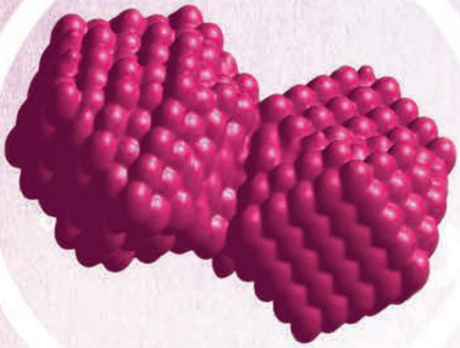
WVdB: In general, the mathematical tools that I use aren't new; for instance, ANNs have been around for decades. But I did use ANNs in a new context and generalised them slightly to apply to complex numbers. This allowed us to set up a mathematical procedure that can retrieve the 3D object from a set of images of this object. Such a technique already exists and is called tomography. What is different in our case though is that the multiple scattering of electrons in a sample is taken into account exactly.

Is your mathematical framework adaptable to working with other technologies? What are your hopes for future applications?

WVdB: Recently, we showed that this framework can describe many different imaging modes. It can handle conventional HRTEM, which uses only one objective lens; scanning confocal electron microscopy, which uses two objective lenses; and coherent diffraction imaging, which uses a series of diffraction patterns. Too often, the microscope must be operated in a state that collects only a small fraction of the electrons so that multiple scattering can be ignored and conventional tomography can be used. With our new technique, it becomes possible to choose the optimal microscope settings, even if they cause severe multiple scattering.

How do you foresee microscopy research progressing in the future?

CK: While the field of microscopy has, for a long time, been pushing the resolution limits by hardware improvement, it now seems time for advanced data analysis techniques to be developed which efficiently take advantage of existing instruments to make new kinds of measurements possible and available even to non-expert users. Quantitative phase microscopy, structured illumination fluorescence microscopy or ptychography are examples of this, and I am convinced that we will see significant developments in these areas, as well as in the field of (transmission) electron microscopy, where quantitative data analysis is still a problem.



Plenty of scope

A German research group has developed an innovative new system for improving the quality of data provided by electron microscopes. This new approach could bring untold benefits to many fields of science

AS THE EYE of science focuses ever more minutely on the world around us, increasingly ingenious ways of observing the tiny particles that make up our world are necessitated. Conventional optical microscopes are a comparatively old technology, having existed in one form or another since the 17th Century. But even when combined with digital technology to produce micrographs and pure digital microscopes, the investigative possibilities of visible light microscopy are no longer sufficient to sustain our interest. In order to progress, we now look to electron microscopes to help us examine the fabric of the Universe. Using techniques such as scanning electron microscopy and transmission electron microscopy (TEM), scientists are able to examine particles and materials that would be impossible to distinguish under conventional light.

TEM is a powerful method to obtain diffraction information from very small volumes of materials. It works by transmitting a beam of electrons through a sample, producing an image from the interaction of those electrons with the constituents of the specimen. This image must then be analysed and interpreted in order to gain information about the sample. TEM yields a more detailed picture than optical microscopy because the de Broglie wavelength of electrons is five orders of magnitude smaller than that of light, and the smaller this measurement is, the more accurate a picture that can be achieved. The technique was first used in the early 1930s, and has been in constant development ever since – it has long been one of the best forms of microscopy for examining materials on a very small scale.

A FLAWED SYSTEM

Ingenious and undoubtedly useful as TEM is, there are significant problems with the technique. Perhaps the most prominent that the quantitative interpretation of TEM diffraction data – the image that is the final product of microscopy – has, so far, always been hampered by multiple scattering of the electrons within the object under investigation. This scattering is both the strength and weakness of TEM. The technique works because the sample scatters electrons as they pass through, but if electrons are scattered multiple times problems occur when scientists come to interpret the image. Data taken from TEM are therefore mostly qualitative rather than quantitative, as analysis relies on the interpretation of the observer; this is also an important reason why electron crystallography has not yet been able to take full advantage of its potential.

No comprehensive solution has been developed to resolve this problem, although several experimental methods exist to reduce the effects of dynamical scattering by, for example, averaging over different diffracting conditions. Therefore, what scientists really need in order to advance this kind of microscopy – and the study of virology, oncology, nanotechnology and all the other diverse subjects that use this technology – is a system that can reliably translate TEM data into three-dimensional (3D) arrangements of atoms.

Professor Dr Christoph Koch and Dr Wouter Van den Broek have arrived at just such a system through their research within the Electron and Ion Microscopy (ELIM) group at the University of Ulm in Germany. They believe that they have created a mathematical system that can successfully invert the multiple scattering of electrons, and might also be applied to other mediums such as light as well.

A NOVEL SOLUTION

The researchers have solved the problem of dynamic scattering using a number of mathematical tools: in particular, artificial neural network (ANN) theory and the mathematical framework of compressed sensing. Compressed sensing is a system used for acquiring and reconstructing signals, and applying ANN theory simultaneously gives their method a new degree of reflexiveness and flexibility.

Using the resulting mathematical system, it is possible to once again turn scattering to TEM's advantage – the system helps scientists to reconstruct the electrostatic potential from TEM data, making use of the dynamical scattering as a further set of data. 3D atom positions may be inferred from this reconstructed potential, because at the positions of the atoms the potential has very pronounced peaks.

Other attempts have been made to correct dynamic scattering interference, but they have never been fully satisfactory, either because they gave poorer results or because they were more inefficient than the ANN/compressed sensing system. Two important efforts that should be mentioned, however, are 3D atom probe tomography (ATP) and scanning transmission electron microscopy (STEM) tomography. The new method differs from these techniques in a number of important

What scientists really need is a system that can reliably translate transmission electron microscopy data into accurate three-dimensional arrangements of atoms

ways. In comparison with ATP, for example, which aims to show atomic arrangements in 3D over a large field of view, the new system is far more accurate, albeit over a smaller field of view. ATP evaporates the material of the sample and looks at where the atoms fly, using that information to reconstruct their original positions. Considering that only 60 per cent of the original atoms are accounted for, it is easy to see why this technique cannot provide comprehensive and detailed pictures. The new method is also very different from atomic-resolution STEM tomography, because the latter does not take into account multiple scattering during reconstruction, and also requires a much more complicated experiment.

A RANGE OF POSSIBILITIES

Being a flexible mathematical framework, the combined ANN/compressed sensing system could potentially be used to invert multiple electron scattering in a number of different experimental setups. The ELIM team has already shown it to work with very realistic simulations of high-resolution TEM (HRTEM), ptychography and confocal STEM data. And they are also currently working on applying it to proof-of-concept experiments, also in electron crystallography and light scattering.

Light behaves in a similar way to electrons when passing through a sample such as organic matter – it scatters, and can scatter multiple times en route. The Ulm team hopes to demonstrate that such multiple light scattering can, equally, be inverted using their new technique. If they are successful, this could easily result in a new computer-based 3D holographic imaging technique, which would be a boon to scientists in many fields. For now, however, the team is exploring this concept by simulations.

LOOKING INTO THE FUTURE

The new system obviously has huge potential for advancing the state of the art in microscopy, but most exciting is the advancements that more efficient microscopy will precipitate in other areas. With numerous fields relying on microscopy – such as medicine, nanotechnology, pollution and semiconductor research – the applications are endless. What is more, the potential for discovery in new areas is also very real indeed.

But this is more than an advance with practical applications; Koch and Van den Broek are advancing the reach of science itself, and the way that we see the world at its most basic level. New potential applications, though undoubtedly important, pale in comparison to the potential to see further, deeper and more clearly into the fabric of our Universe than ever before.

INTELLIGENCE

3D ATOMIC-RESOLUTION IMAGING IN THE TRANSMISSION ELECTRON MICROSCOPE

OBJECTIVES

To develop new techniques in quantitative three-dimensional imaging of atom positions and strain with electrons.

GROUP MEMBERS

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FUNDING

Carl Zeiss Foundation

German Research Foundation (DFG)

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PROFESSOR DR CHRISTOPH KOCH received his PhD from Arizona State University in 2002. He then spent nine years as a staff scientist at the Max Planck Institute for Metals Research in Stuttgart before he was appointed Professor at Ulm University in 2011, in a position endowed by the Carl Zeiss Foundation.

DR WOUTER VAN DEN BROEK received his PhD from the University of Antwerp in 2007. He then spent a number of years as a postdoc at EMAT, the institute for electron microscopy for materials science in Antwerp, before he joined Koch's group at Ulm University in 2012.

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