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Diamond will shine brightly for chemistry

Gerhard Materlik, Chief Executive Officer of Diamond Light Source Ltd., describes Diamond, the new generation synchrotron light source set to open at the Rutherford Appleton Laboratory in 2007, and discusses how it will push back the boundaries of what chemists can achieve in many research areas.

Introduction

Diamond is the UK's biggest scientific project for 30 years. It will provide a powerful synchrotron facility for researchers using light in the X-ray and ultraviolet regions, with applications in chemistry, biomedical science, environmental studies and engineering. For chemists, Diamond will offer exciting new opportunities for studying molecular structure, catalysis, high-pressure reactions and rapid reactions. The project is funded jointly by the Council for the Central Laboratory of the Research Councils (86%) and the Wellcome Trust (14%)(Fig. 1).

Diamond takes its place among the 50 or so other synchrotron facilities worldwide; in the UK, the main synchrotron facility is located at Daresbury, Cheshire, and Diamond is intended, eventually, to replace this. It will be a huge boost to the synchrotron radiation research community—reckoned to number 40,000 to 50,000 scientists worldwide. 'The UK is a shareholder of the European Synchrotron Radiation Facility (ESRF) in Grenoble, France. This was the real success story of the 1990s,' explains Professor Materlik. 'It became obvious that a national facility was needed to support the local research infrastructure, for the demand was so much higher than could be met at Grenoble.'

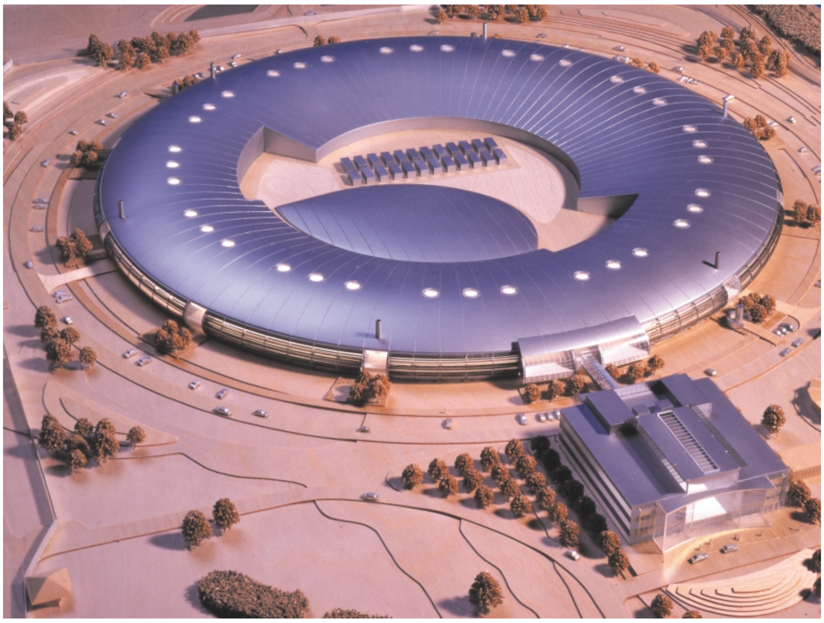

Fig. 1 An artist's impression of the Diamond facility.

Gerhard Materlik was Director of the Hamburg Synchrotron Radiation Laboratory and a member of the DESY (German Electron Synchrotron) Scientific Directorate, before taking up the post as CEO of Diamond in 2001. He began his career in synchrotron science at DESY in 1974, and has also been involved in developing a number of other synchrotron facilities around the world. These include the Cornell High Energy Synchrotron Source in the US, the European Synchrotron Radiation Facility in Grenoble, the Stanford Synchrotron Radiation Laboratory and Advanced Photon Source and Japan's Spring 8 which is currently the world's largest third generation third generation synchrotron radiation facility. His most recent work was on the TESLA XFEL project in Germany, an X-ray free electron laser facility for studying both elementary particles and synchrotron radiation science.

Specifications

Diamond's specifications took into account the requests of potential users, so it has been optimised for operation in the one Ångstrom (0.1 nm) region at an energy of 12 KeV as so many applications are in this region of the X-ray spectrum. The facility has 22 insertion device beamlines leading off a central storage ring. The emittance of the beam—the product of the diameter and the opening angle of the radiation—is at least a factor two times smaller than at the ESRF and the electron beam current is a factor two higher. This ensures that the Diamond light beam will be an order of magnitude

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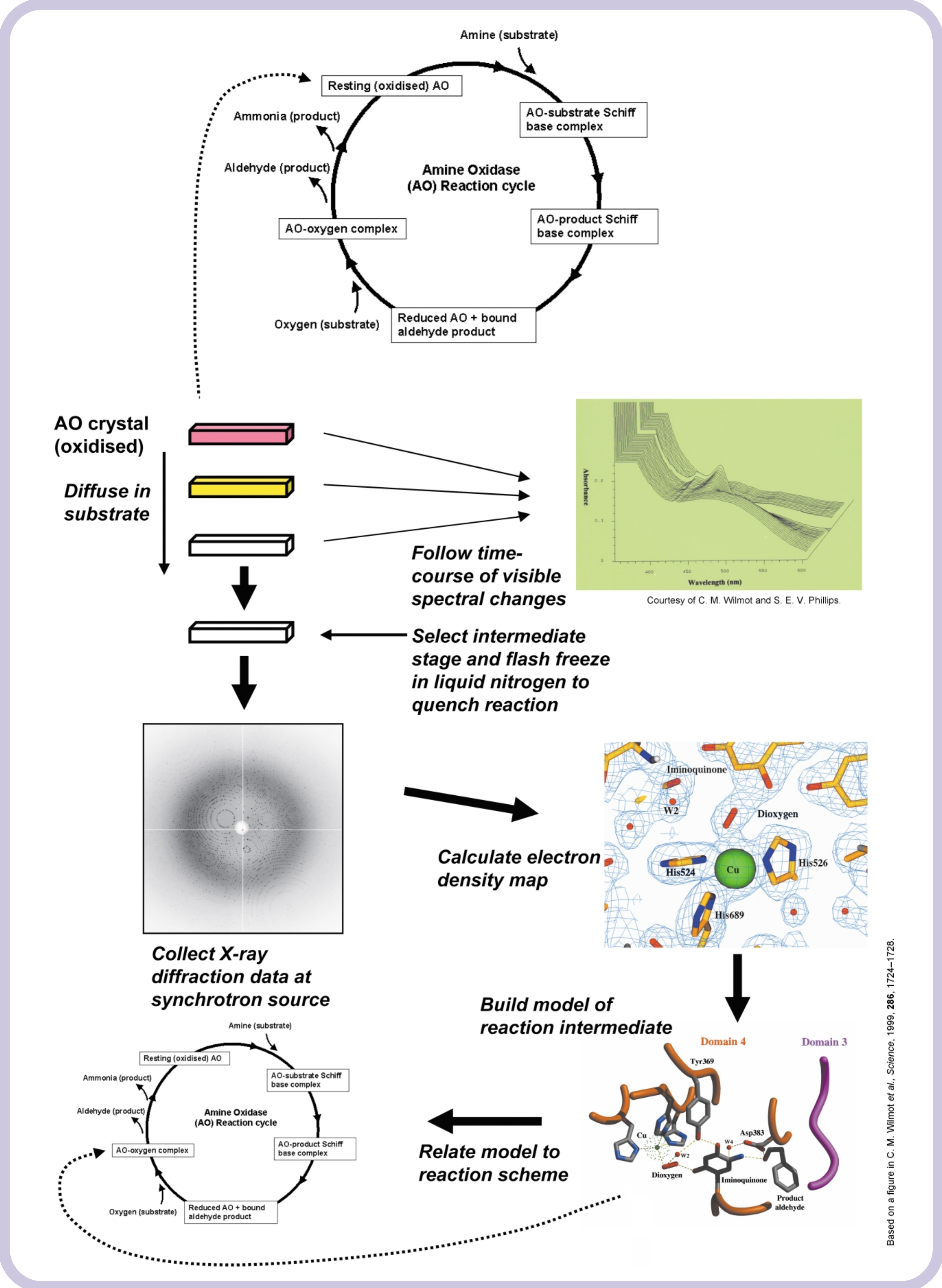

Fig. 2 An example of catalysis that could be studied using synchrotron radiation.

brighter, allowing researchers to work with far smaller samples.

'This is a big step forward,' comments Professor Materlik. 'But in addition to this Diamond is going to be—from early on—aiming to provide a new quality of service to users. So we will try, as much as possible, to make beam operation automatically controlled. The beamlines will be set up for them, whereas at present people have to interact more directly with it. Not everyone wants that—a chemist or biologist is not necessarily an expert on radiation. What they want is to study their process and take the results away.'

The next step, continues Professor Materlik, is to put as much data as possible from Diamond into a grid database system to be made available to the scientific community. They will also try to make the beamlines, where possible, remotely accessible, so that the whole research team does not need to come to the facility. Instead, the experiment could be run remotely from a computer in the research lab, a groundbreaking advance that could change the whole culture of this kind of research. This full automation represents the next generation of synchrotron facility, beyond the current 'third generation' where the emphasis when built has been very much on improving source brightness and on learning how to get insertion device beamline operating.

Diamond's impact on chemistry

The range of potential applications for Diamond are very broad. 'It's light, and we use light for everything—to make things happen, as a production tool, as a cutting tool, to study and see things,' says Professor Materlik. 'The Diamond light will be used in the same way. Since we have the whole spectrum, we can study over a wide range of sample sizes, but the emphasis is to be on the one angstrom range, because there are so many problems to be explored—in protein crystallography, for instance.'

For chemistry, Diamond will offer several techniques for studying the dynamics of catalysis (Fig. 2). Currently, diffraction or microscopy is used to study structure. Electronic behaviour within materials is typically investigated with spectroscopy. With Diamond, both methods will be available on the beamlines and, on some, they will be 'married' together. This will mean that during a catalytic reaction, binding changes can be seen, by looking at electronic levels, and also distance changes between atoms, and how these are related. 'If you were to push this very far, you could even ask questions about timescale,' says Professor Materlik. 'You could study chemistry in real time, taking a molecular crystal and triggering it with an optical laser, then look with the synchrotron beam at how the structure and electronic levels had changed. This is going to have a big impact on chemistry.'

Diamond will also make possible new research in high-pressure chemistry. Sample cross-sections can be made very small, owing to the intensity of the beam, and so can be exposed to very high pressure. This can be applied to catalytic studies—to see how a catalyst changes its properties under pressure, for instance. There will also be a beamline dedicated to engineering studies, looking at high pressure reactions in liquids used in industry, or at how welding joints develop in real time or when they are put under strain.

Other application areas

Another important application area for Diamond will be environmental studies. The synchrotron beam will allow detailed analysis of rock and soil samples from polluted areas. Previously, research has shown that *Alyssum lesbiacum*, a plant native to the island of Lesbos in Greece, has the surprising ability to absorb large amounts of nickel. A potential project for Diamond might be to identify and study the plant proteins responsible for this detoxification process.

Biomedical science, of course, is going to be one of the major applications for Diamond, thanks to the involvement of the Wellcome Trust. Three of the first seven beamlines to be commissioned will be dedicated to biology and, of the next phase, one of four beamlines will also be for biological studies (the plan is to bring four new beamlines onstream each year, till all 22 are in operation). The focus on biology is a reflection of UK interest in the human genome project and in related issues, such as protein structure and function. The new synchrotron will allow data to be collected in minutes, rather than days, representing a significant time saving in producing structures of complex biomolecules. Synchrotron radiation can also be used in medical diagnosis—to detect individual cancer cells within biopsy samples, for example. The new beams will be able to improve the quality of such images and provide them in a much shorter time.

Looking to the future

In the future, Diamond could be complemented by other technologies for carrying out similar work, such as free electron lasers which use a linear driver/accelerator rather than a storage ring. This would represent a new area of research, allowing investigation at the femtosecond level. 'Currently our pulses are 30 picoseconds long, so you cannot quite 'see' an electron changing its orbit. For that you need to go below the femtosecond level,' explains Professor Materlik. 'That's what the free electron lasers do, they may allow you to watch reactions on orbital scale. At the picosecond level, it's only possible to study movements and vibrations of atoms themselves.' There are already proposals for such free electron laser facilities around the world. For instance, the Daresbury laboratory is currently proposing to build such a 'fourth generation' light source for low-energy photons. No-one knows exactly what will emerge from Diamond and other advanced light facilities—but this exciting new range of tools is sure to push the study of chemical structures and reactions way beyond its current limits.

For more information

See the diamond website http://www.diamond.ac.uk, including the newsletter on http://www.diamond.ac.uk/Activity/ACTIVITY=Newsletter

Professor Materlik was talking to Susan Aldridge.