femto

The DESY research magazine – Issue 01/16

ZOOM

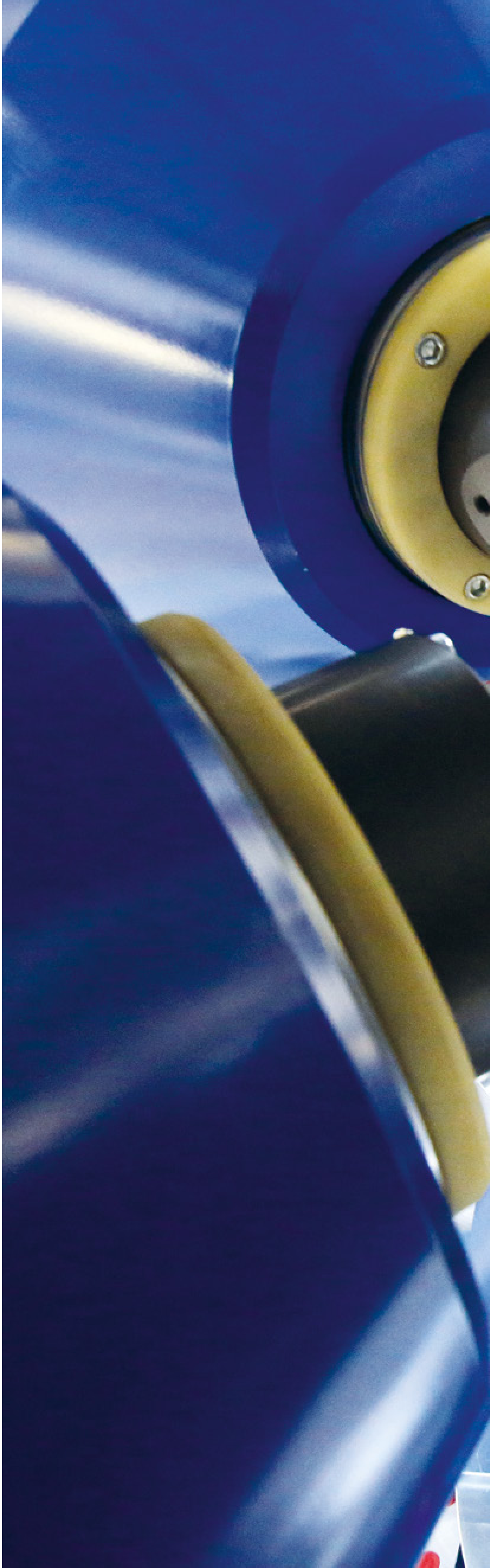
The super X-ray laser

Breakthrough in crystallography

Nanostructures assemble themselves

Why van Gogh's Sunflowers are wilting

DESY



The planet simulator

A new high-pressure press at DESY's X-ray source PETRA III can simulate the interior of planets and synthesise new materials. The Large Volume Press (LVP), which was installed in collaboration with the University of Bayreuth in Germany, can exert a pressure of 500 tonnes on each of its three axes. That corresponds to 300 000 times the atmospheric pressure or the pressure that reigns 900 kilometres under the Earth's surface. The colossal device is 4.5 metres high and weighs 35 tonnes. Depending on the desired pressure, samples with a size of up to one cubic centimetre can be compressed. That's roughly the size of a normal die for board games, and in the field of high-pressure experiments it's very impressive. The LVP is the world's biggest press installed at a synchrotron.

femtoscope

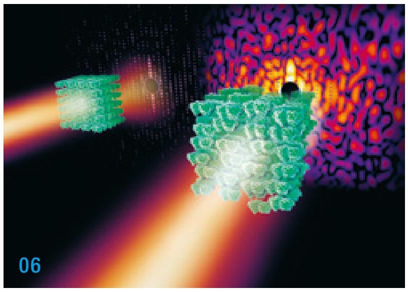
Picture: DESY, Dirk Nölle

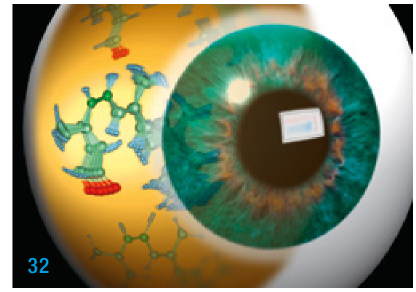
Contents

ZOOM

A superlative X-ray laser

The European XFEL is a high-speed camera, a supermicroscope and a planet simulator rolled into one. Starting in 2017, its intense ultrashort X-ray laser flashes will give researchers from scientific institutes and industry completely new insights into the nanoworld. They'll be able to study the details of viruses at the atomic level, the molecular composition of innovative materials, films of chemical reactions and the characteristics of matter under extreme conditions. DESY is the main shareholder in this engine of discovery.





CAMPUS

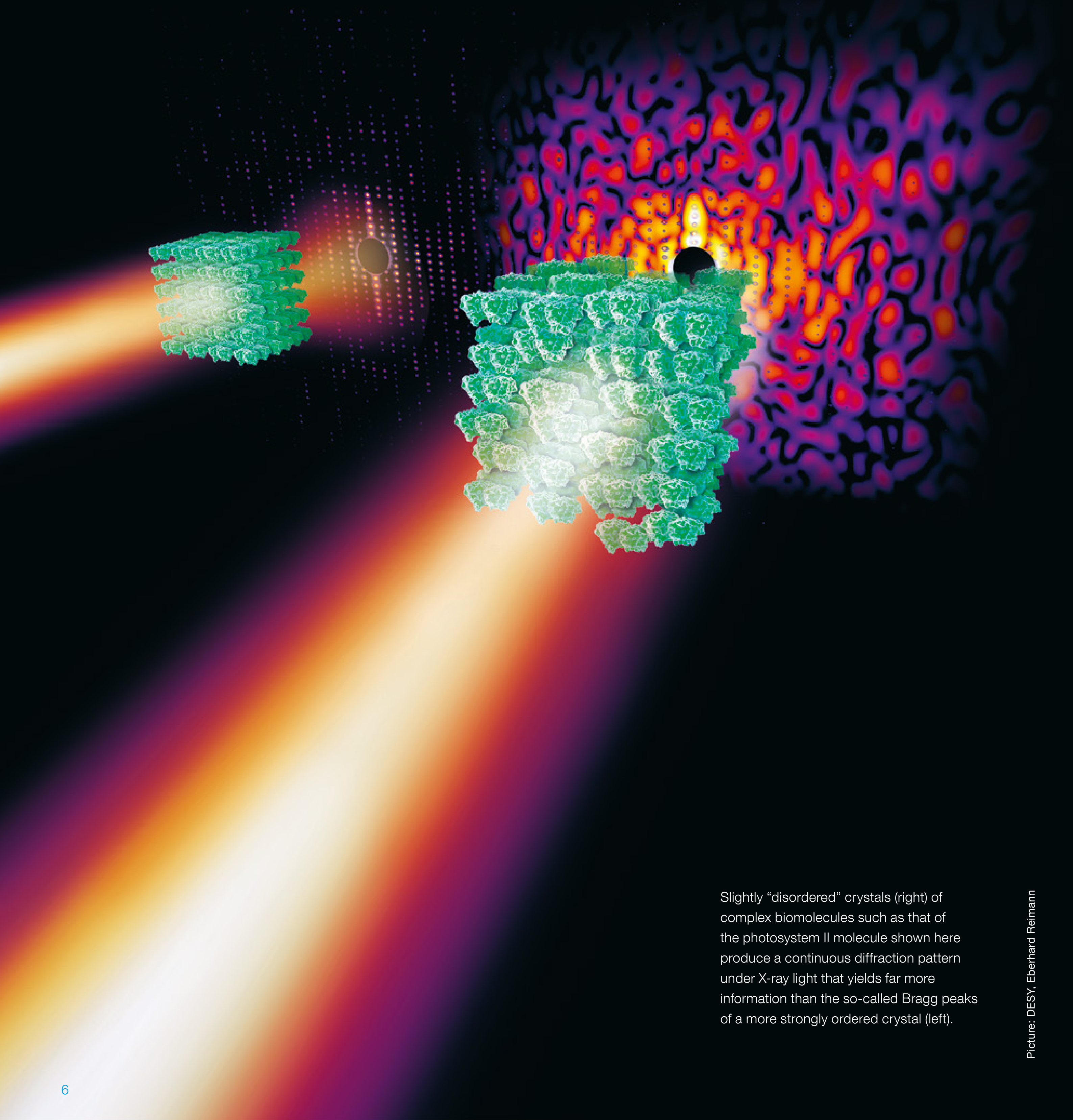
ZOOM

SPECTRUM

SECTIONS

Perfection isn't everything

A pinch of disorder has generated a breakthrough in crystallography



Slightly "disordered" crystals (right) of complex biomolecules such as that of the photosystem II molecule shown here produce a continuous diffraction pattern under X-ray light that yields far more information than the so-called Bragg peaks of a more strongly ordered crystal (left).

Picture: DESY, Eberhard Reimann

Henry Chapman is the head of the Coherent X-ray Imaging division at the Center for Free-Electron Laser Science at DESY.

In science as in real life, being perfect is not always the best option. Sometimes it's the small irregularities that are really interesting. In human terms, this is not a great new insight. Minor character quirks and individual deviations from the norm of a perfect body are generally not regarded as disturbing. Instead, these are the attributes that make an individual lovable and interesting. By contrast, for a precise science such as crystallography, which depends on physical measurement methods and mathematical analyses, this idea has introduced a genuine paradigm shift.

When a crystal is illuminated with X-ray light, a characteristic pattern of bright dots – known as Bragg peaks – appears on the detector. Such diffraction patterns are used to reconstruct the spatial structure of a crystal, right down to the precise atomic structure of the molecules of which the crystal consists. The basic assumption used to be that the more perfectly the molecules were ordered in the interior of the crystal, the better the reconstructed likeness of the molecule would be. However, for biomolecules, which are especially complex and very difficult to crystallise, perfection isn't everything. It's the tiny imperfections of somewhat "disordered" crystals, in which individual molecules are slightly out of kilter, that can provide crucial information for determining the crystal's structure. This information is hidden in the faint continuous diffraction pattern that used to be regarded as a distracting background not worthy of attention.

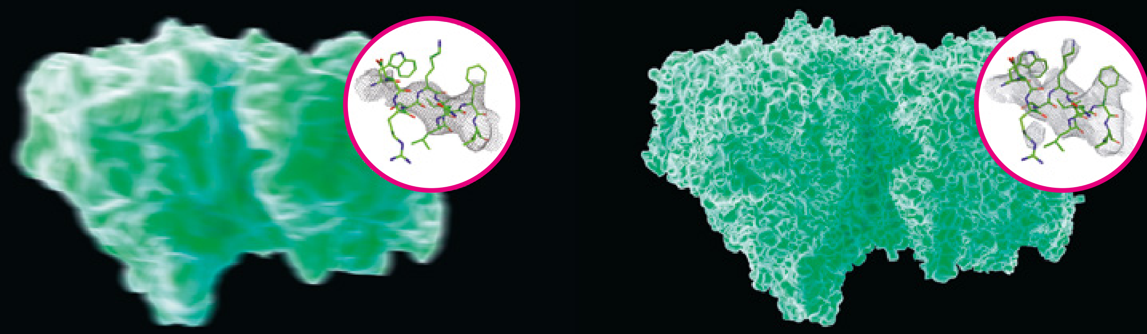
"This discovery has the potential to become a true revolution for the crystallography of complex matter"

Helmut Dosch, DESY

This discovery was made by a team headed by DESY scientist Henry Chapman from the Center for Free-Electron Laser Science (CFEL) in Hamburg. The researchers developed a new method of determining the spatial structures of proteins and other biomolecules that in many cases had not been accessible by means of previous techniques. "Our discovery will allow us to directly view large protein complexes in atomic detail," says Chapman, who is also a professor at the University of Hamburg and a member of the Hamburg Centre for Ultrafast Imaging (CUI). The new method works for less ordered crystals and circumvents the usual need for prior knowledge and chemical insight. "This discovery has the potential to become a true revolution for the crystallography of complex matter," says the Chairman of DESY's Board of Directors, Helmut Dosch. This scientific breakthrough gives researchers access to the blueprints of thousands of molecules of great relevance to medicine and biology. The spatial structure of biomolecules reveals their modes of action and can provide the basis for the development of tailor-made drugs.

"Extreme Sudoku in three dimensions"

But even with a perfect crystal, the Bragg peaks alone are not enough to determine a completely unknown protein structure. "This task is like extreme Sudoku in three dimensions and a million boxes, but with only half the necessary clues," explains Chapman. In crystallography, this complicated puzzle is referred to as the phase problem. Without knowing the phase of the diffracted light waves – the lag of the crests of one wave to another – it is not possible to compute the structure of the molecule from the measured diffraction pattern. But the phases of the individual waves can't be measured. To solve the tricky phase puzzle, more information must therefore be known than just the measured Bragg peaks. This additional information can sometimes be obtained from the known structure of a closely related molecule or through comparison with the diffraction patterns of crystals of chemically modified molecules. This barrier to the determination of the structure is most severe for large protein complexes such as membrane proteins. ››



The analysis of the Bragg peaks alone (left) reveals far less detail of the molecule under study than the additional analysis of the continuous diffraction pattern (right). The magnifying glasses show real data from the study.

Chapman realised that imperfect crystals and the phase problem are linked. The key lies in the weak, continuous diffraction pattern generated by "disordered" crystals. This continuous background is generally thought of as a nuisance and not used for the structural analysis, although it can be useful for providing insights into the vibrations and other dynamics of molecules. But when the disorder consists only of slight displacements of the individual molecules from their ideal positions in the crystal, then the background encodes the full continuous diffraction pattern from the individual "single" molecules in the crystal.

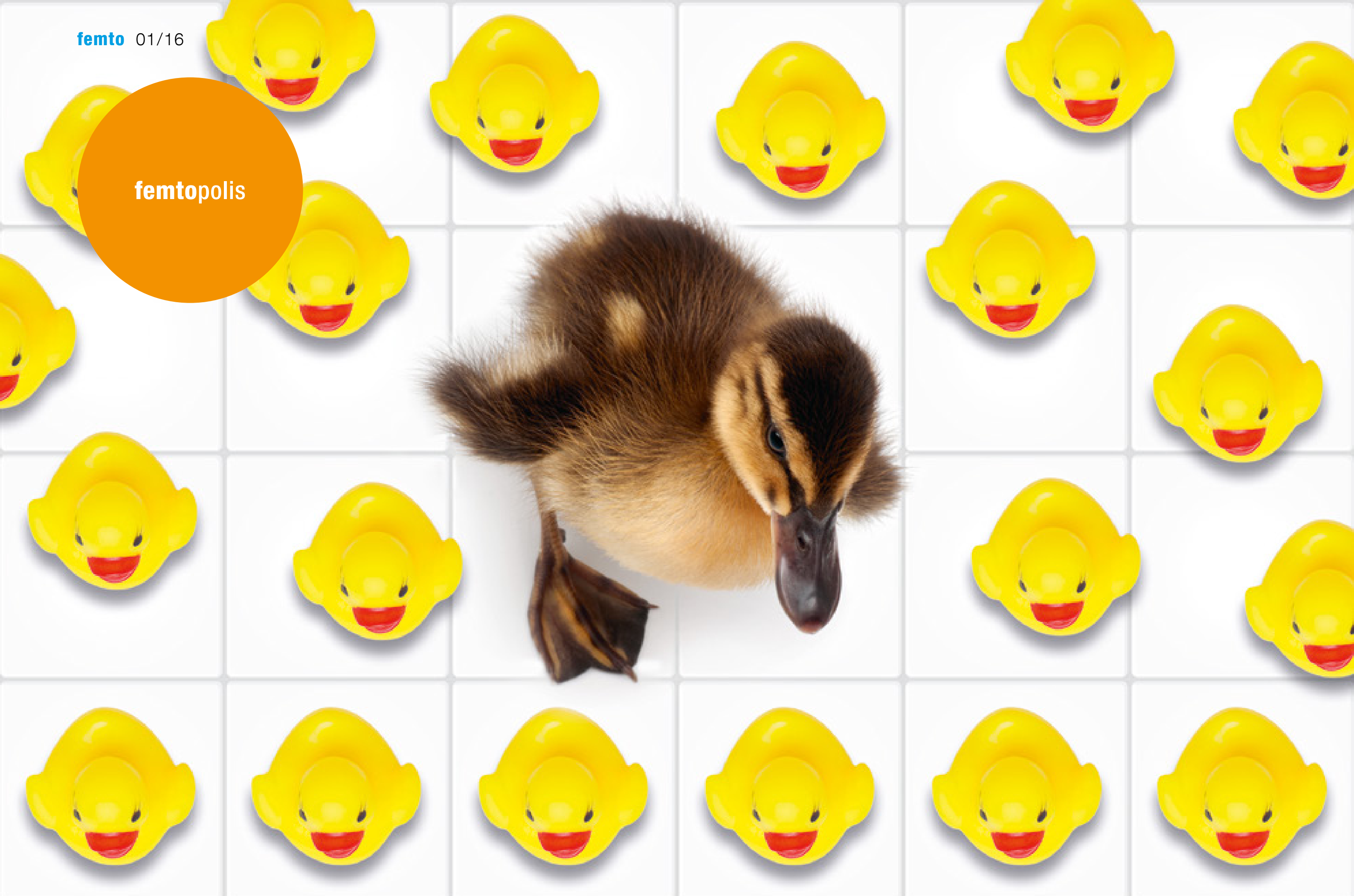
"If you would shoot X-rays on a single molecule, it would produce a continuous diffraction pattern free of any Bragg spots," explains lead author Kartik Ayyer from Chapman's CFEL group. "The pattern would be extremely weak, however, and very difficult to measure. But the 'background' in our crystal analysis is like accumulating many shots from individually aligned single molecules. We essentially just use the crystal as a way to get a lot of single molecules, aligned in common orientations, into the beam." The continuous diffraction pattern provides enough additional information to solve the phase problem directly, without having to resort to other measurements or assumptions. In the analogy with the Sudoku puzzle, the measurements provide enough clues to always arrive at the right answer.

The best crystals are imperfect crystals

This novel concept leads to a paradigm shift in crystallography – the most ordered crystals are no longer the best to analyse with the novel method. Instead, the best crystals are imperfect crystals. "For the first time, we have access to single-molecule diffraction – we have never had this in crystallography before," Chapman explains. "But we have long known how to solve single-molecule diffraction if we could measure it." The field of X-ray coherent diffractive imaging, spurred by the availability of laser-like beams from X-ray free-electron lasers, has developed powerful algorithms to directly solve the phase problem in this case, without having to know anything at all about the molecule. "You don't even have to know chemistry," says Chapman, "but you can learn it by looking at the three-dimensional image you get."

> *"For the first time, we have access to single-molecule diffraction – we have never had this in crystallography before"*
>
> Henry Chapman, DESY

To experimentally demonstrate their novel analysis method, the Chapman group teamed up with the group of Petra Fromme and other colleagues from Arizona State University, the University of Wisconsin, the Greek Foundation for Research and Technology – Hellas FORTH and the SLAC National Accelerator Laboratory in the USA. They used the world's most powerful X-ray laser, LCLS at SLAC, to X-ray imperfect ›› femtopolis



Duck tales

From the bathtub to the research frontier

A rubber duckie that bobs around on the surface of the bathwater is most people's favourite bathtub toy. Scientists have also discovered just how useful it can be. In January 1992, a container load of plastic toys was swept overboard from a Hong Kong-based cargo ship in the eastern Pacific. The toys became part of an unplanned large-scale effort to monitor the spread of plastic rubbish in the oceans. Almost 29 000 rubber ducks and other plastic toys were carried by ocean currents to destinations all over the world. They became sad examples of global material cycles.

A more positive showcase for rubber ducks is in the field of crystallography, where they help scientists analyse the spatial structure of complex biomolecules with the help of intense X-ray light. This analysis is carried out by means of complex calculations known as Fourier transforms – and that's where the ducks come in. They replace the biomolecules in mathematical models, thus serving as test objects whose shape is known and neither too complicated nor too simple. Lots of ducks sitting in a lattice represent a crystal that the researchers have painstakingly grown from biomolecules in order to irradiate it with X-rays and determine the biomolecules' structure from the resulting diffraction pattern. Only if the mathematical models can reconstruct the duck are the models deemed useful for determining the unknown structure of a biomolecule from the corresponding diffraction patterns.

The "Fourier duck" first appeared in a book about optical transforms published by the British crystallographers Charles Alfred Taylor and Henry Solomon Lipson in 1964. Today, it is widely used in educational materials and is familiar to almost every student who takes an introductory course in crystallography.

For decades, it was believed that the more precisely the ducks are arranged on their lattice points, the better. But nature is not always precise. Surprisingly, a lot more can be learned about the ducks – or rather, the molecules they represent – if they are not sitting in overly perfect rows. This insight has resulted in a paradigm shift for crystallographers – and more freedom for the ducks, which are now allowed to swim around their lattice points once in a while.

microcrystals of a membrane protein complex called photosystem II, which is part of the photosynthesis machinery in plants.

Including the continuous diffraction pattern in the analysis immediately improved the spatial resolution – compared to the analysis of the Bragg peaks alone – by around a quarter, from 4.5 ångströms to 3.5 ångströms (an ångström is 0.1 nanometres or billionths of a metre and corresponds roughly to the diameter of a hydrogen atom). The image obtained showed details of molecular features that usually require fitting a chemical model to see. "That is a pretty big deal for biomolecules," explains co-author Anton Barty from DESY. "And we can further improve the resolution if we take more patterns." The team only needed a few hours of measuring time for these experiments, while full-scale measuring campaigns usually last a couple of days.

The scientists hope to obtain even more detailed images of photosystem II and many other macromolecules with their new technique. "This kind of continuous diffraction has actually been seen for a long time from many different poorly diffracting crystals," says Chapman. "It wasn't understood that you can get structural information from it and so analysis techniques suppressed it. We're going to be busy seeing if we can solve structures of molecules from old discarded data."

Nature, 2016; DOI: 10.1038/nature16949

Nano-structures assemble themselves

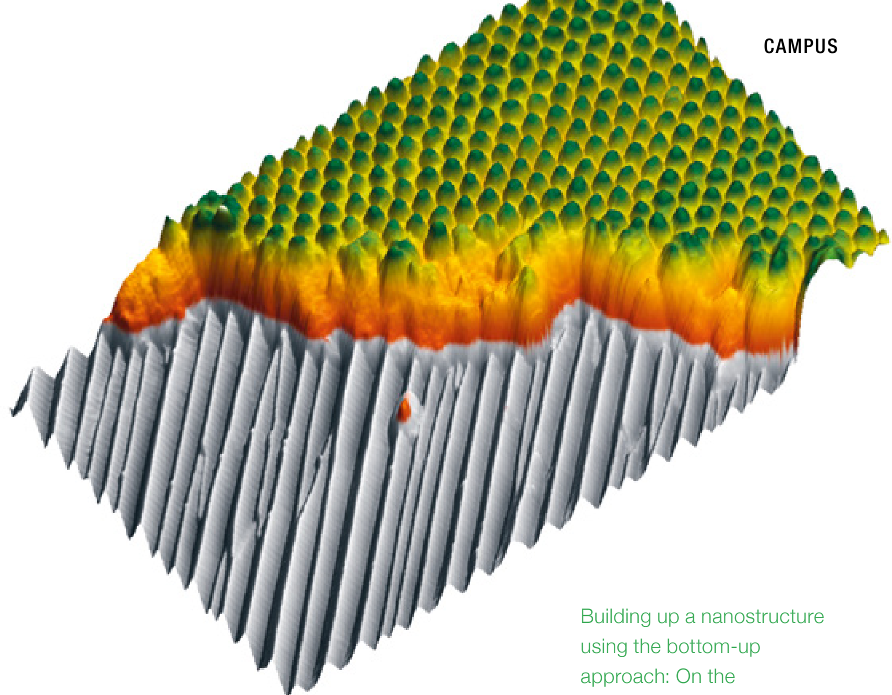
New technique for manufacturing metallic nanosystems

Researchers at DESY have developed a new procedure that enables metallic nanostructures to assemble and line up all by themselves. This so-called bottom-up approach offers a quick and simple alternative to existing procedures, making it interesting for commercial applications as well, in which nanostructures are used more and more often. "Most importantly, the method allows extremely uniform nanostructures to be created in highly regular patterns with comparatively little effort," explains Denise Erb, the lead author of the publication. A special setup, developed by DESY scientist Kai Schlage, enabled the scientists to actually watch the nanostructures as they grew, at DESY's X-ray source PETRA III.

Nanostructures are tiny objects smaller than a thousandth of a millimetre. A nanometre is one millionth of a millimetre. Compared to this, a human hair is huge, having a thickness of almost 40 000 nanometres. For many scientific studies and technological applications, it is essential that the nanostructures repeat in a specific pattern. The size and separation of the individual elements of such patterns can lie anywhere between a few nanometres and several hundred nanometres.

Nanostructures are turning up more and more often in everyday life. "Nanostructures permit improved or new functionalities. In catalytic converters, for example, data storage devices or sensors," says Erb. "The dimensions of the products we normally deal with in our everyday lives are generally of the order of a few centimetres or more. So it would be nice to be able to manufacture materials that incorporate nanostructures on that scale too. And ideally they should be quick and cheap to make as well." However, it is often very challenging to create nanostructures both on large surfaces and with the necessary regularity. This is where the new method comes into its own.

The conventional top-down technique can be compared with sculpting: One begins by coating a surface with the corresponding material. The desired pattern is then gradually carved out of this layer by removing specific areas. This is done bit by bit, which means that the manufacturing time depends directly on the size of the required area. The advantage is that virtually any pattern can be created.



Picture: Denise Erb, DESY

Building up a nanostructure using the bottom-up approach: On the approximately ten nanometre (nm) deep grooves of an aluminium oxide crystal (grey), a 40 nm thick layer of copolymers (brown) is deposited. Metal nanodots (green) then grow on this layer, reaching a height of about 10 nm. The area shown measures 3000 nm by 1800 nm.

"Nanostructures permit improved or new functionalities. In catalytic converters, for example, data storage devices or sensors"

Denise Erb, DESY

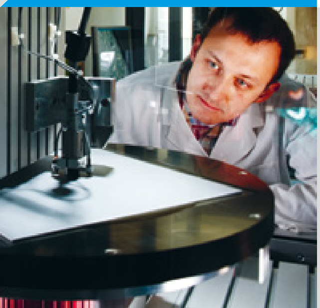
The method used by the researchers at DESY, on the other hand, is based on the so-called bottom-up approach. This makes use of the fact that certain materials have a natural tendency to form nanostructures. "In bottom-up methods, which are also known as self-organising methods, we do not force the material to adopt a certain pattern, as in the top-down method," explains Erb. "Instead, we create conditions that allow the material to self-assemble and form nanostructures. The shape of these nanostructures cannot be chosen arbitrarily, as in top-down procedures – they are dictated by the properties of the material. Nonetheless, the nanostructures that form are extremely interesting to us, and useful." The big advantage is that the nanostructures form over the entire surface at the same time, so that the speed with which the pattern is formed no longer depends on the size of the surface.

To obtain the desired nanostructures using the bottom-up approach, it is also possible to combine several different self-organising materials. The assembly of the nanostructures then takes place in a series of steps, so that the arrangement of the first structure affects the formation of the second structure. Combinations of this kind create particularly uniform patterns. Erb and her colleagues have used this procedure to combine crystals, polymers and metals.

"A particularly exciting aspect, from a scientific point of view, is the possibility of watching the nanostructures form in real time using X-ray diffraction, and observing how they develop their physical properties," says Ralf Röhlsberger, who is in charge of the research group at DESY. At DESY's X-ray light source PETRA III, the scientists watched the process live. Using a special setup, they let the metal nanostructures grow under various conditions directly in the X-ray beam.

With the help of the X-rays, the scientists can see, for example, how the shape and the magnetic properties of the nanostructures evolve. They can thus not only examine the results of their efforts but also study the intermediate stages in detail. As in football, the scientists are not simply interested in the final outcome of the game, but also in how it came about. They would like to know, for example, which parameters played a key role. "Through our research, we hope to establish a method by which nanostructures can be created more easily and quickly," concludes Erb, "but also to develop a better understanding of why these tiny structures behave magnetically, chemically and optically the way they do."

Science Advances, 2015; DOI: 10.1126/sciadv.1500751

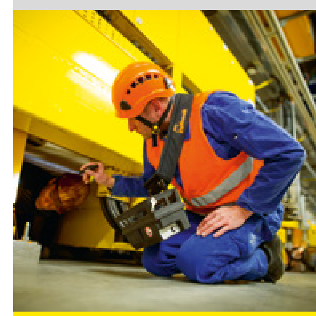


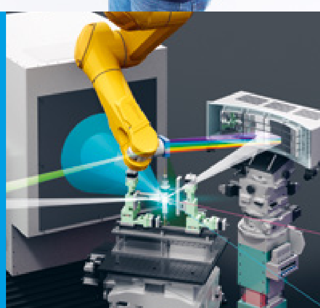
ZOOM

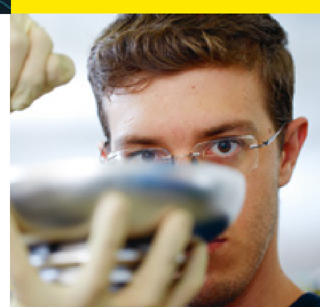
A superlative X-ray laser

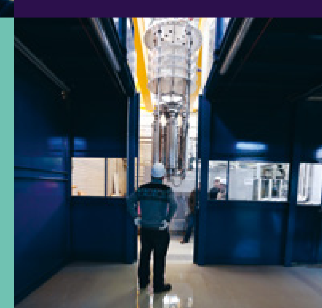
The European XFEL is a high-speed camera, a supermicroscope and a planet simulator rolled into one. Starting in 2017, its intense ultrashort X-ray laser flashes will give researchers from scientific institutes and industry completely new insights into the nanoworld. They'll be able to study the details of viruses at the atomic level, the molecular composition of innovative materials, films of chemical reactions and the characteristics of matter under extreme conditions.

Eleven countries are participating in this joint European project. DESY is the main shareholder and is responsible for the construction and operation of the particle accelerator with its innovative superconducting technology. The European XFEL is mostly located in underground tunnels. The 3.4-kilometre-long facility extends from DESY in Hamburg to the neighbouring town of Schenefeld in the German federal state of Schleswig-Holstein.







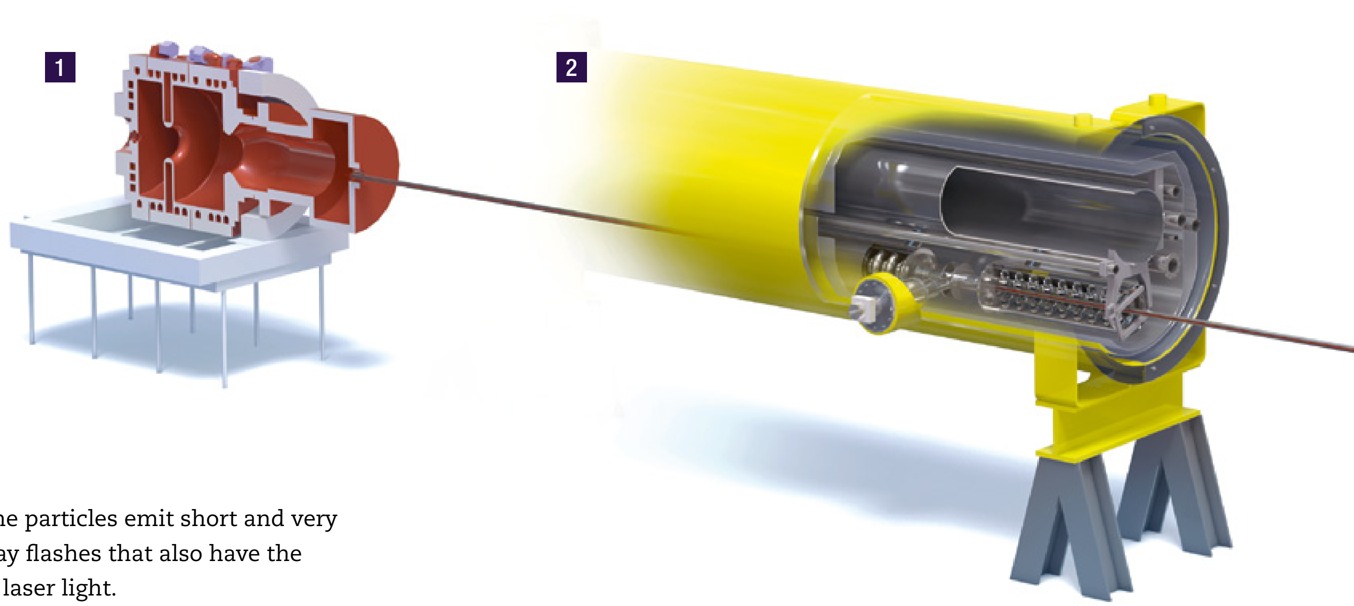


Pictures: European XFEL / DESY

Light for the future

The European XFEL in Hamburg will produce the most intense X-ray laser flashes in the world

The European XFEL stretches for 3.4 kilometres from Hamburg-Bahrenfeld to the town of Schenefeld in Schleswig-Holstein. It's the world's most powerful X-ray laser and one of Europe's biggest scientific facilities. At its heart is a particle accelerator that is close to two kilometres long. It accelerates electrons to almost the speed of light. Special magnet structures called undulators force the speeding electrons to fly along a slalom path.



As a result, the particles emit short and very powerful X-ray flashes that also have the properties of laser light.

The X-ray flashes make it possible for researchers to image ultrafast processes, because each individual flash is less than 100 quadrillionths of a second long and bright enough to create snapshots. This makes it possible to "film" molecular reactions and thus understand processes that are fundamental to chemical production methods in industry or to the mechanisms of medical effects. In addition, the short-wavelength laser flashes can make the composition of nanomaterials and complex biomolecules visible at the atomic level. On the basis of this knowledge, researchers can go on to develop innovative customised materials and drugs. The X-ray laser also makes it possible to

At the **electron source [1]**, a powerful laser knocks several billion electrons at a time out of a caesium telluride electrode. These electrons are bundled into tiny bunches, which are given a boost in the **accelerator modules [2]**. Powerful radio waves are fed into these modules, and the electrons "ride" the waves like surfers on the ocean. To ensure that the speeding electrons are generate and analyse extreme states of matter – for example, the high pressures and temperatures that exist in the interior of planets. Under such extreme conditions, matter behaves very differently than under "normal" conditions.

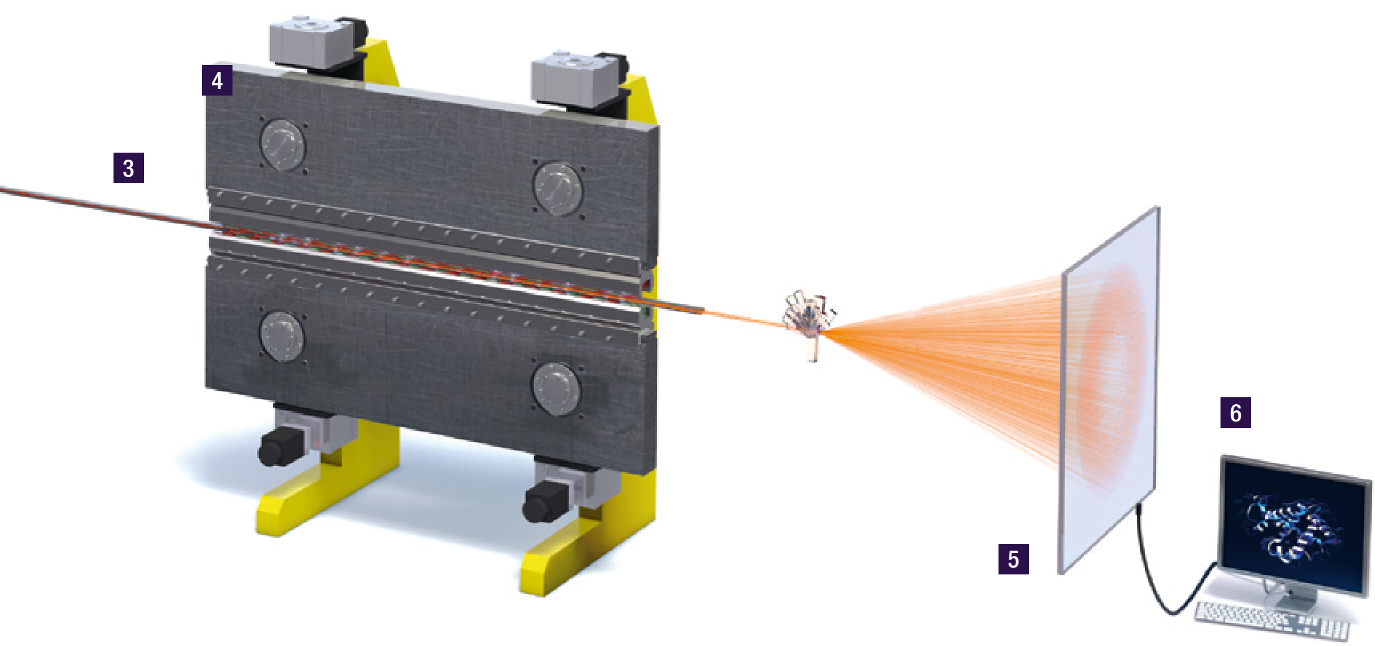
"The European XFEL will open up entirely new opportunities for scientists from research institutes and industry," says Massimo Altarelli, Chairman of the European XFEL Management Board. "Much of this work will be fundamental research. This kind of research develops its biggest effects usually not in the short term and sometimes not in the area that was originally targeted. But without fundamental research, the life we live today would not be conceivable."

A race track for electrons

Eleven countries are participating in this joint European project. DESY is the main shareholder and is responsible for the construction and operation of the particle accelerator with its innovative superconducting technology, which has already been tested at DESY's pioneering X-ray laser facility FLASH. The accelerator modules are massive yellow pipes that are 12 metres long and almost one metre thick.

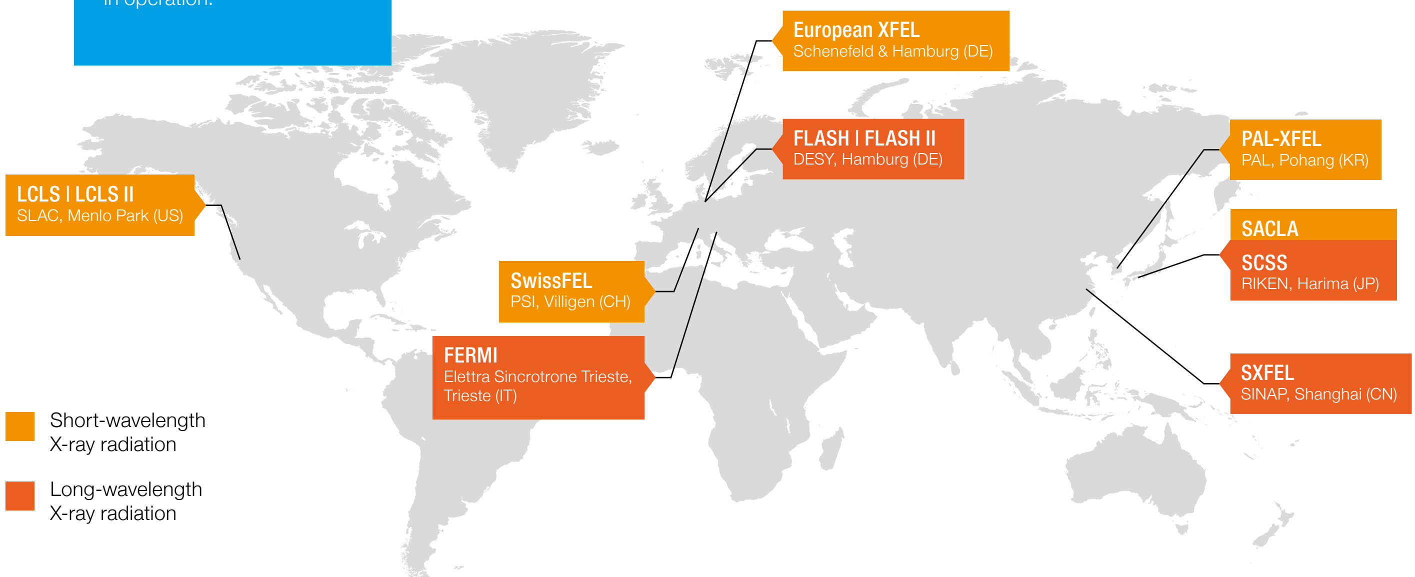
A look at the interior of such a module reveals a complex structure. The electrons fly through a thin pipe from which all the air has been evacuated. Most of the module's components are used for thermal insulation and cooling – various pipes through which liquid helium is pumped in order to reduce the temperature inside the pipe to minus 271 degrees Celsius.

These extreme measures are necessary to ensure that the core components – the cavity resonators – can function properly. These shining silvery components are responsible for the actual acceleration of the electrons. With the help of powerful radio waves, they accelerate the tiny electron bunches to almost the speed of light. Every module is equipped with eight cavities made of the superconducting metal niobium. "Superconducting" means that the metal completely loses its electrical resistance and thus conducts electricity without any loss of energy – when cooled to ultracold temperatures, that is. The advantage of this technology is that it enables considerably more electron bunches to be accelerated and thus more X-ray flashes to be generated per second than conventional, normal-conducting accelerator technology. ››



not slowed down by air, they fly through **vacuum pipes [3]**. Once the electrons have reached their maximum energy, they pass through special magnet structures called **undulators [4]**. The undulators force the electrons to run a slalom course, causing them to emit X-ray flashes. At the end of the undulator section, this radiation has amplified into extremely intense ultrashort X-ray flashes, which are used by researchers at the **measuring stations [5]** to illuminate a variety of samples. The basic principle here is that the atoms of the sample material deflect the X-ray light, and detectors then intercept the deflected radiation. Subsequently, **computers [6]** are used to precisely calculate the spatial structure of the sample, for example, at the atomic level.

X-ray free-electron lasers are being built all over the world. About half of these facilities are already in operation.



A total of 101 superconducting modules will put the electrons through their paces in the two-kilometre-long accelerator tunnel. At certain points, the particles pass through "warm" – that is, uncooled – sections of beam pipe on which various devices are mounted, including magnets that bundle the electron bunches. At the end of the accelerator, the tunnel branches into two tubes. Each of them contains another key component of the facility: the undulators. These are permanent magnets mounted above and below the electron beam pipe, with their north and south poles alternating at four-centimetre intervals. These force the electrons to follow a slalom course.

On a slalom course

The electrons, which are flying at almost the speed of light, emit intense X-ray radiation in each curve. The special feature of the free-electron laser is that it has not just one undulator but 35 of them, arranged one after the other over almost 200 metres. "When the X-ray light emitted by one undulator oscillates in sync with the light of the next one, the light is amplified," explains Tobias Haas, technical coordinator at the European XFEL. "That's the only way I can get the amplification effect I need for a laser." In order to be able to optimally adjust the laser effect, the five-metre-long undulators are separated by intermediate sections called phase shifters.

Past the undulator section, the evacuated beam pipe branches into two. One branch is for the electron bunches, the other for the X-ray laser flashes generated in the undulators. To separate the two beams, bending magnets gently direct the electron beam to the right, into another tunnel. Meanwhile, the X-ray flashes race straight ahead until they hit a special mirror mounted at an obtuse angle. This mirror has been ground to nanometre precision and functions as a distribution station. It either allows the X-ray flashes to go straight on past it into one pipe or deflects them by a tenth of a degree into another pipe. The two pipes run alongside one another for 600 metres, with the distance between them gradually increasing. At the end of the tunnel, after 3.4 kilometres, they are 1.40 metres apart when they penetrate a thick wall of concrete. Directly behind this wall is the big experiment hall with its measuring huts, whose walls contain lead as shielding against the X-ray radiation. The first experiments will be conducted in these huts in 2017. The X-ray flashes will illuminate samples of various kinds, enabling the scientists to study their interior structures and processes.

"We've worked for many years to build this facility," says Haas. "Now we feel as though we can finally see the marathon's finish line." The European XFEL will initially have six measuring stations, but two additional tunnels have already been dug and can be equipped with additional undulators if necessary. In the final configuration, the researchers in the experiment hall will be able to use up to 15 measuring stations.

"Light at the end of the tunnel"

Massimo Altarelli, Chairman of the European XFEL Management Board, is looking forward to the first experiments at the world's biggest X-ray laser facility

Picture: European XFEL

femto: After the six-year construction period, when will research at the European XFEL begin?

Altarelli: I hope we will see the first X-ray laser flashes in February or March 2017. We are currently building the measuring stations in the experiment hall, and the first two of them will start to operate between the spring and summer of 2017. All three undulator sections and six measuring stations should be in operation by the middle of 2018.

femto: What new insights will the facility provide for researchers?

Altarelli: The European XFEL has a number of key advantages compared to existing X-ray sources. Among other things, its flashes are significantly shorter. They're only about ten femtoseconds long. That will make it possible to film molecular processes and chemical reactions. We'll be able to literally see the 'action', just like in an action film. In addition, the flashes have laser properties. In the future, that will enable us to use even samples that cannot be crystallised in order to analyse them in detail at the atomic level. If we succeed in deciphering the structure of individual protein molecules that are of interest to pharmacologists, that would be fantastic! What all these methods have in common is that they enable us to examine previously hidden details and processes in the nanocosmos.

femto: How will society benefit from this research?

Altarelli: The European XFEL will open up entirely new possibilities for scientists from research institutes and industry. Much of this work will be fundamental research. This kind of research develops its biggest effects usually not in the short term and sometimes not in the area that was originally targeted. But without fundamental research, the life we live today would not be conceivable. For example, in the medium and long terms I think there will be great opportunities in medical research – for instance, in the development of drugs and therapies – or in the development of renewable sources of energy and materials for new technologies. And we shouldn't underestimate the fact that the young scientists who come to us will be able to gather experience in a leading global research establishment – experience that they can later apply in the fields of science and industry to develop new products and processes.

femto: The German government gave the European X-ray laser project the green light back in 2003. Why did it take so long to begin construction?

Altarelli: The European XFEL would have been too big and too expensive for a single country to build. That's why it was planned as an international project from the very start. It was easy to get scientists from other countries enthusiastic about the project. But it was more difficult to get the approval of political decision-makers and financial sponsors and to agree on a legal structure. The international agreement was finally signed in September 2009, and at that point the construction could begin.

femto: Did the construction proceed as planned?

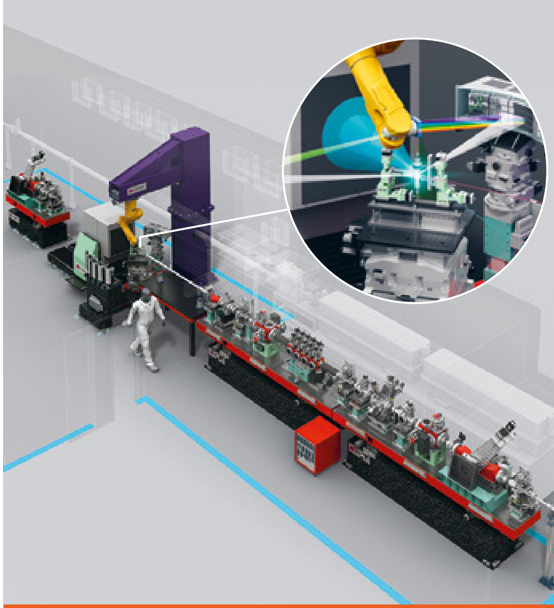
Altarelli: Of course at times I wished it could have gone faster. But after all, we were dealing with a new technology at the boundaries of feasibility, which we had to translate into series production. That was a tremendous challenge. All things considered, the delays were kept within limits, and we can be very satisfied with the result!

femto: How are you and your 280 coworkers feeling at the moment?

Altarelli: We're feeling very good. After a long and complicated planning and construction phase, we're now literally seeing the light at the end of the tunnel – not only for our team but also for researchers all over Europe. Hundreds of experts are already coming to Hamburg for our annual users' meeting. That shows the great interest and the spirit of optimism that scientists are feeling right now.

Experiments at the European XFEL

With its extraordinarily bright, highly energetic and extremely intense X-ray flashes, the European XFEL will yield new insights in a wide range of research fields. It will, for instance, enable scientists to produce images of viruses and biomolecules at atomic resolution, to film chemical reactions in superslow motion and to investigate materials under the extreme conditions that reign deep within giant gas planets. There are many fields of application, ranging from biology, medicine, chemistry and physics to materials science, electronics, nanotechnology and many others. With a total of six measuring stations, the facility offers a wide range of opportunities for scientific investigation. Through their membership in user consortia, among others, numerous institutions participate in various aspects of the experimental activities at the European XFEL. DESY too is involved in such consortia, sometimes in a leading capacity.



Picture: European XFEL, Rey Hori

Planned setup of the FXE measuring station

Investigating the dynamics of the nanoworld

Nanosystems are an increasingly common feature of the everyday world. Examples include metallic nanoparticles in the catalytic converters of cars. An investigation of the properties and the dynamics of such systems not only provides a better understanding of their fundamental nature but also enables an enhancement of everyday products containing nanoparticles. The **MID** (Materials Imaging and Dynamics) measuring station is used for such research. It enables researchers to investigate the nanostructure and dynamics not only of solid materials such as metals but also of soft materials such as polymers and gels and even biological samples. For the investigation of a broad range of samples, various analytic methods are available, which make use of the laser properties of the X-ray free-electron laser radiation, its short pulses and its high intensity.

A 4D supermicroscope in space and time

The principal objects of investigation at the **SPB/SFX** (Single Particles, Clusters, and Biomolecules and Serial Femtosecond Crystallography) measuring station are biomolecules, nanocrystals, virus particles, cell organelles and atom clusters. As a rule, the aim is to determine the two and three-dimensional structure of the object under investigation to an atomic resolution of less than one nanometre (a millionth of a millimetre). However, the 3D microscope is, in fact, a 4D supermicroscope if the high time resolution is taken into account.

The samples are shot laterally through the X-ray beam. Whenever a pulse of the intense radiation hits a crystal of biomolecules, for example, a distinctive X-ray diffraction pattern is generated, which enables the biomolecule's structure to be computed. The spatial structure of a biomolecule provides information about its mode of action and can yield clues for the development of new drugs. Apart from structural biology and cell biology, a host of other fields will benefit from the methods of investigation available at this measuring station, including materials science and nanotechnology.

The exoplanet simulator

The "normal" conditions on the surface of the Earth are the absolute exception for the universe as a whole. Most matter in the universe exists at much higher pressures and temperatures and under more powerful electromagnetic fields. The **HED** (High Energy Density Science) measuring station can simulate the extreme conditions that exist for example in giant gas planets in other solar systems, also known as exoplanets. Various methods are used to generate these extreme conditions, including high-power optical lasers, diamond anvil cells and strong pulsed magnets. The investigation of matter under extreme conditions provides a more complete picture of its material properties beyond the narrow scope of what we call "normal".

An ultrafast quantum film camera

Dynamic processes in the nanocosmos generally occur over an unimaginably short timescale of just a few quadrillionths of a second (femtoseconds). The **FXE** (Femtosecond X-Ray Experiments) measuring station uses the extremely short X-ray flashes from the European XFEL to produce sharp images of extremely rapid processes in solids, liquids and gases. Examples include shock waves propagating, nanoparticles exploding and just about any chemical reaction.

Thanks to the ultrashort exposure times, it is possible to observe processes such as the complex interplay of molecules during a chemical reaction, with the X-ray laser providing previously inaccessible information about the detailed steps. The process under investigation is first triggered by a laser pulse and then, after a precisely defined amount of time, imaged by means of an X-ray flash. The experiment is repeated many times, each time with the moment of exposure at a slightly later point in time. The result is a sequence of stills that can be assembled into a film of the process under investigation.

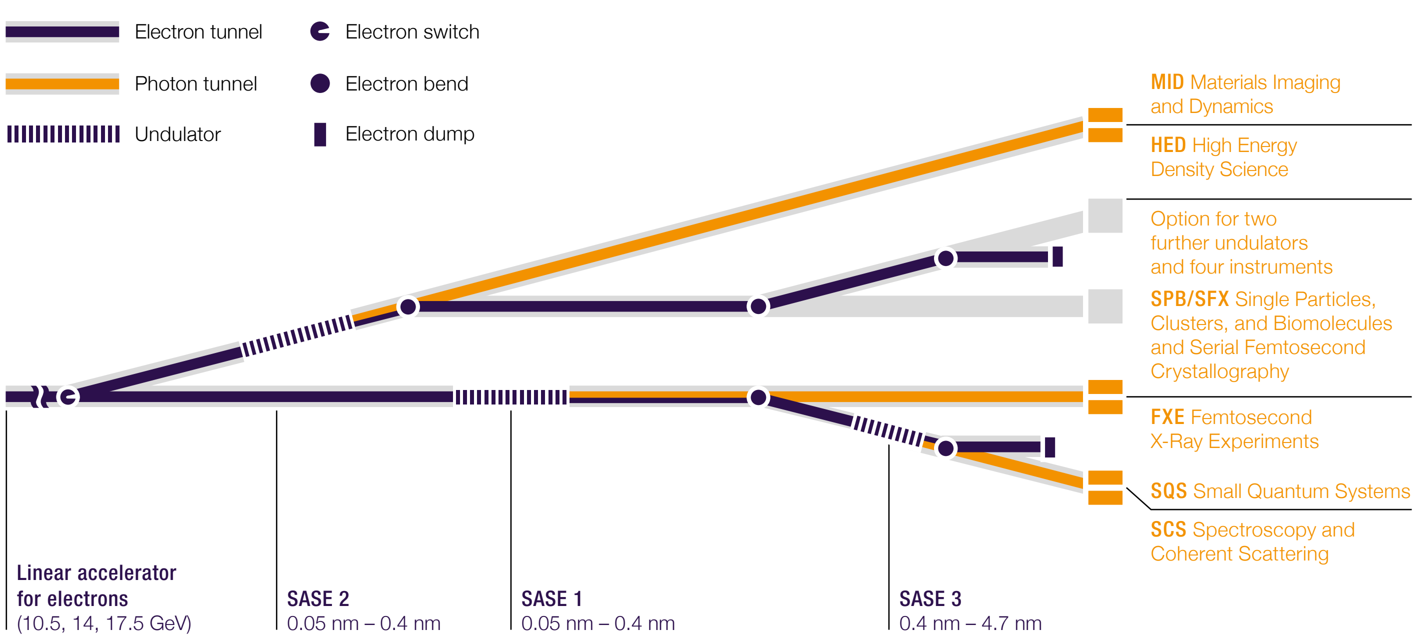
Zooming in on the quantum world

There are many unsolved questions in the realm of atoms and molecules. The **SQS** (Small Quantum Systems) measuring station is used to investigate the behaviour of small quantum systems comprising between one and tens of thousands of atoms. In particular, this multiphoton camera focuses on the interaction between these smallest structural units and the extremely intense X-ray laser flashes. Multiphoton processes often produce lots of electrons and highly charged ions, with molecules breaking up into many separate charged parts. SQS offers researchers a variety of methods with which to investigate these fragments in detail.

The determination of precise atomic data is vital for the development not only of new theoretical models but also of many other experimental methods. Scientists require reliable data in order to support and quantify their results – data that is often lacking even for comparatively simple systems. It is therefore vital to be familiar with the participants of this process – the atoms – in order to understand it as a whole.

The structure and dynamics of complex materials

Researchers who are working with the **SCS** (Spectroscopy and Coherent Scattering) measuring station use what are called “soft” X-rays to investigate the electronic and atomic structure as well as the dynamics of complex and functional materials. Soft X-rays have less energy and a longer wavelength than hard X-rays. They are ideal for investigating, among other things, nanostructured materials and ultrafast magnetisation processes. The potential fields of application for this type of investigation include materials science, surface chemistry and catalysis, nanotechnology and the dynamics of condensed matter.



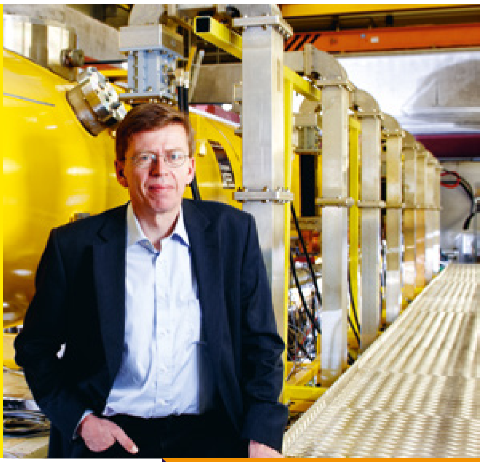
Graphic: European XFEL

Precision from the production line

The production of the superconducting accelerator modules was one of the major challenges in the project to build the European XFEL

There are several accelerator-driven X-ray lasers in operation all over the world. The pioneer was FLASH, which commenced service in 2000 at DESY. For a number of years, LCLS in California and SACLA in Japan have been providing high-intensity X-ray pulses. As documented in numerous publications in the renowned journals *Nature* and *Science*, both facilities have delivered impressive proof of the value of such light sources to the research community. They will be joined at the end of 2016 by the SwissFEL at the Paul Scherrer Institute in Switzerland. The European XFEL has one key advantage over these other facilities: Because it uses superconducting technology, it is able to deliver significantly more X-ray flashes per second than normal-conducting facilities can. This capability is of major benefit for many experiments.

In conventional accelerators, water-cooled cavity resonators made of copper are used to accelerate the electrons to high energies. “But the copper heats up due to its electrical resistance,” explains Reinhard Brinkmann, Director of the Accelerator Division at DESY. “That’s why you can only feed radio waves into the cavities for a tiny fraction of a second; otherwise the material would melt.” This also means that you have to wait a moment for the copper to cool down before applying the next pulse of radio waves. This limits the rate at which the laser can deliver X-ray pulses. Current free-electron lasers can produce a maximum of 120 flashes per second.



Reinhard Brinkmann is Director of the Accelerator Division at DESY.

More flashes thanks to superconductivity

To circumvent this limitation, DESY opted for another approach, namely superconductivity. A superconductor possesses zero electrical resistance. As Brinkmann explains, this means that the radio waves don’t heat up the cavity to any appreciable extent. “As a result, you can switch it on for much longer than a copper cavity.” Thanks to this technology, the European XFEL will be able to produce 27 000 X-ray flashes per second – more than 200 times as many as the number produced by the other facilities.

This means that experiments that take a number of hours to complete at other X-ray laser facilities will require only a few minutes at the European XFEL. It will therefore be possible to conduct more experiments in the same amount of time. Moreover, the higher rate of X-ray flashes from the European XFEL will provide greater temporal resolution, thus enabling even more-detailed investigations of chemical reactions.

However, superconducting accelerators do have one disadvantage: The technology is more expensive and much more complicated than that of conventional accelerators. For example, key components have to be cooled with liquid helium to around minus 271 degrees Celsius. “To a large extent, we were able to use the liquid-helium plant from the former large-scale accelerator HERA,” says DESY scientist Hans Weise, coordinator of the European XFEL Accelerator Consortium. “That meant we didn’t have to build everything from scratch.”

The biggest challenge was to develop and manufacture the superconducting cavities, which are made of niobium rather than copper. DESY produced the initial prototypes in collaboration with a large number of partners based both within Germany and abroad. This was a major breakthrough, but one problem remained: Over 800 superconducting cavities were needed for the three-kilometre-long European XFEL. Some form of series production was therefore required.

High purity for high performance

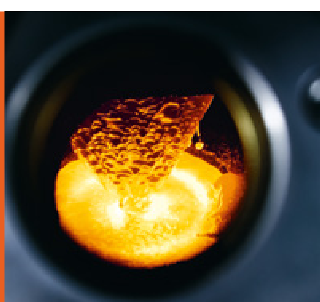
The researchers therefore devised a complex quasi-industrial process that involves numerous partners both in Germany and abroad. Even producing the raw material is an elaborate process. The niobium must be extremely pure, which means it has to be re-melted up to eight times in special furnaces. Each melting process successively reduces the level of impurities, and the final result is ingots of extremely pure niobium, which are then rolled into sheets. In order to check for any remaining impurities, DESY scientists inspected each individual sheet using a special eddy-current testing method. “We scanned all 16 000 niobium sheets,” Brinkmann explains. “Only a few percent had to be rejected.”

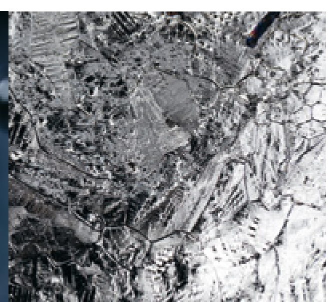
“We scanned all 16 000 niobium sheets; only a few percent had to be rejected.”

Reinhard Brinkmann, DESY

Each sheet that passed scrutiny was then cut and pressed into shape, before being welded into the shape of a cavity – a shiny silver tube, one metre in length and segmented like a caterpillar. “The manufacturing process has to be kept extremely clean,” says Brinkmann. “Even a speck of dust can be enough to stop a cavity working as it should.” For this reason, some of the process stages were conducted in cleanrooms, where the air is scrupulously filtered and particle counters monitor air quality. To prevent components being contaminated, workers wore what looked like surgical gowns, including face masks, hair nets and gloves.

An electron beam was used to weld the niobium sheets. After the welding, the cavities underwent an elaborate cleaning process. They were first dipped into an electrochemical acid bath, then given a high-pressure rinse with specially purified water and finally baked for ››





The niobium (above) is re-melted a number of times (above left) and the rolled sheets (left) are precisely scanned.

Superconducting cavities in the cleanroom several hours at 120 degrees Celsius. “There are processes here which we don’t yet fully understand in all their detail,” Brinkmann explains. “You could almost say that there’s a bit of alchemy to it all.”

Many of the methods that were used were first tested at DESY, then exported to industry and ultimately enhanced in partnership. “It took a while before we could achieve reliable series production; a lot of it was a laborious process of learning and practicing,” says Brinkmann. “But by the end, the whole industrial production process – from the niobium sheets to the finished cavities – ran very smoothly.” The cavities were supplied by an Italian and a German company, with the last one leaving the production line at the beginning of 2016. There were very few rejects. In fact, barely more than a dozen of the more than 800 niobium tubes required subsequent chemical treatment, and the average accelerating gradient proved to be well above the original specification.

Assembly of an accelerator module (right); connecting radio frequency couplers to cavities in the cleanroom (below).

> *“The industrial manufacturing process – from the niobium sheets to the finished cavities – ran very smoothly”*
>
> Reinhard Brinkmann, DESY

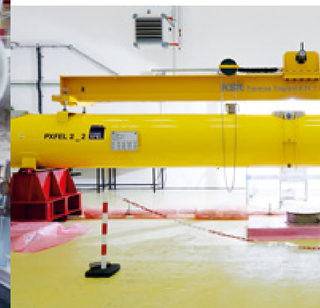
Following production, the cavities were shipped to Saclay near Paris, where they were assembled, in batches of eight, into yellow modules, each with an integrated helium cooling system, just like a large thermos flask. These 101 modules were successively sent back to Hamburg, where they underwent a final series of rigorous tests. Only then could they be installed in the tunnel for the European XFEL.

The construction of the accelerator posed not only technical but also organisational challenges. After all, eight countries were involved in the process. “Some partners are essentially providing financing, while others are contributing components,” explains Riko Wichmann, head of the XFEL Project Office at DESY. “In particular, coordinating the in-kind contributions was not easy and created much more work than we had originally imagined.” A great many institutes and companies were involved in building the accelerator modules. The DESY XFEL project team had to make sure that all the partners delivered their components as punctually as possible. “The late arrival of even a single component would have had a knock-on effect on the whole process, with the danger of a logjam.” A key factor in the success of this enterprise was the close cooperation between DESY, as the leader of the Accelerator Consortium, and European XFEL GmbH, the company responsible for managing the project as a whole.

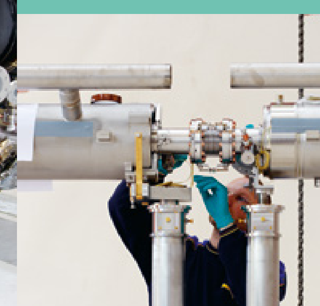
Bunches of billions of electrons

One key component of the facility is the injector. This 50-metre-long part of the facility is responsible for generating the electron bunches, which are then accelerated over a distance of 1.8 kilometres. The injector functions in the following way: At a rate of 27 000 times per second, a laser fires powerful pulses at a pill-shaped piece of metal. Each pulse blasts off a throng of around ten billion electrons. Two superconducting modules pre-accelerate this throng of electrons and shape it into customised bunches. Initially, these bunches are about three millimetres long and one millimetre across. During the acceleration, sophisticated technology ensures that these bunches are further compressed, until finally they are around one thousandth of their original volume. “In order to generate extremely intense X-ray flashes, the electrons have to be concentrated into a minuscule area,” explains Weise.

Another extremely sophisticated technique in use at the European XFEL is the one that ensures



Hans Weise is a leading scientist at DESY and coordinator of the European XFEL Accelerator Consortium.



Testing an accelerator module

precise synchronisation between the ultrashort electron bunches and the X-ray flashes. This synchronisation is required to be able to film chemical reactions, for example. Here, a pulse of light from a conventional laser triggers the reaction. Then, only a brief moment later, an image of the reaction is captured by means of an X-ray flash from the European XFEL. For this process to function, the optical laser and the European XFEL must be precisely coordinated with one another. This is accomplished by a special synchronisation system based on a "laser clock" that ticks in an optical fibre running along the accelerator tunnel. This system measures the exact intervals between

"In order to generate extremely intense X-ray flashes, the electrons have to be concentrated into a minuscule area"

Hans Weise, DESY

the electron bunches and the X-ray flashes – key information for the scientists conducting the experiments.

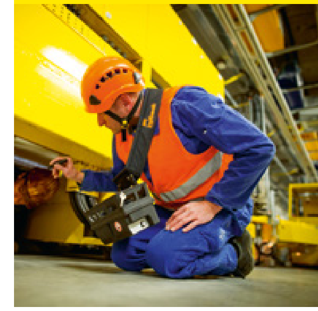
This method was already tested at FLASH, also at DESY. Some 300 metres in length, this X-ray free-electron laser is based on the same superconducting modules used at the European XFEL, but it produces flashes in the soft X-ray and UV ranges. "If you like, FLASH is a 1:10 scale model of the European XFEL," says Reinhard Brinkmann. "Over the years, FLASH has given us countless valuable insights into how to design and build the larger facility." FLASH has been used by scientists from over the world for a decade now. In fact, such is the interest from the research community that DESY is currently doubling the facility's experimentation capacity.

Other research establishments are now also planning to use superconducting accelerator technology in the future. These include SLAC in California, which has been successfully ›› operating the Linac Coherent Light Source (LCLS), an X-ray laser based on a normal-conducting accelerator, since 2009. SLAC is now planning to set up a second light source in the same tunnel. LCLS-II will be 700 metres in length and equipped with 280 superconducting cavities of essentially the same design as those of the European XFEL.

The ambitious goal is to build a laser at SLAC that, from 2019 onwards, will be capable of producing one million flashes per second, albeit at longer wavelengths and therefore not with the same high resolution as the archetype in Hamburg. “DESY has given us a lot of support for our planning,” says project leader John Galayda. “Having access to DESY’s knowledge and experience is the reason why we’ve made such rapid progress.” This was particularly true when it came to designing the highly complex accelerator modules and the superconducting niobium cavities. “We’re buying them from the same two companies that supplied the European XFEL,” Galayda explains. “For us, it’s a great advantage that there are already manufacturers with such extensive experience in building these cavities.”

“Having access to DESY’s knowledge and experience is the reason why we’ve made such rapid progress”

John Galayda, SLAC



The accelerator modules were transported and installed within the tunnel using the special electric vehicle “Mullewupp” (bottom left).

"A triumph for DESY"

DESY is the main shareholder of the European XFEL. Helmut Dosch, the Chairman of the DESY Board of Directors, talks about the research centre's expectations concerning the European X-ray laser.

femto: What does the European XFEL mean for DESY?

Dosch: The European XFEL is one of the world's most revolutionary large-scale research projects. It brings together a completely novel particle accelerator technology, which was developed by DESY, with the tremendous potential for discovery that the unique experimentation opportunities will offer to scientists coming from all over the world. DESY designed this major facility and established the theoretical and technical foundations for its realisation. Last but not least, DESY built FLASH, the pioneering facility for X-ray lasers of this kind. I am therefore convinced that the European XFEL will become a great triumph for DESY.

femto: What perspectives does this open up for Hamburg as a centre of science?

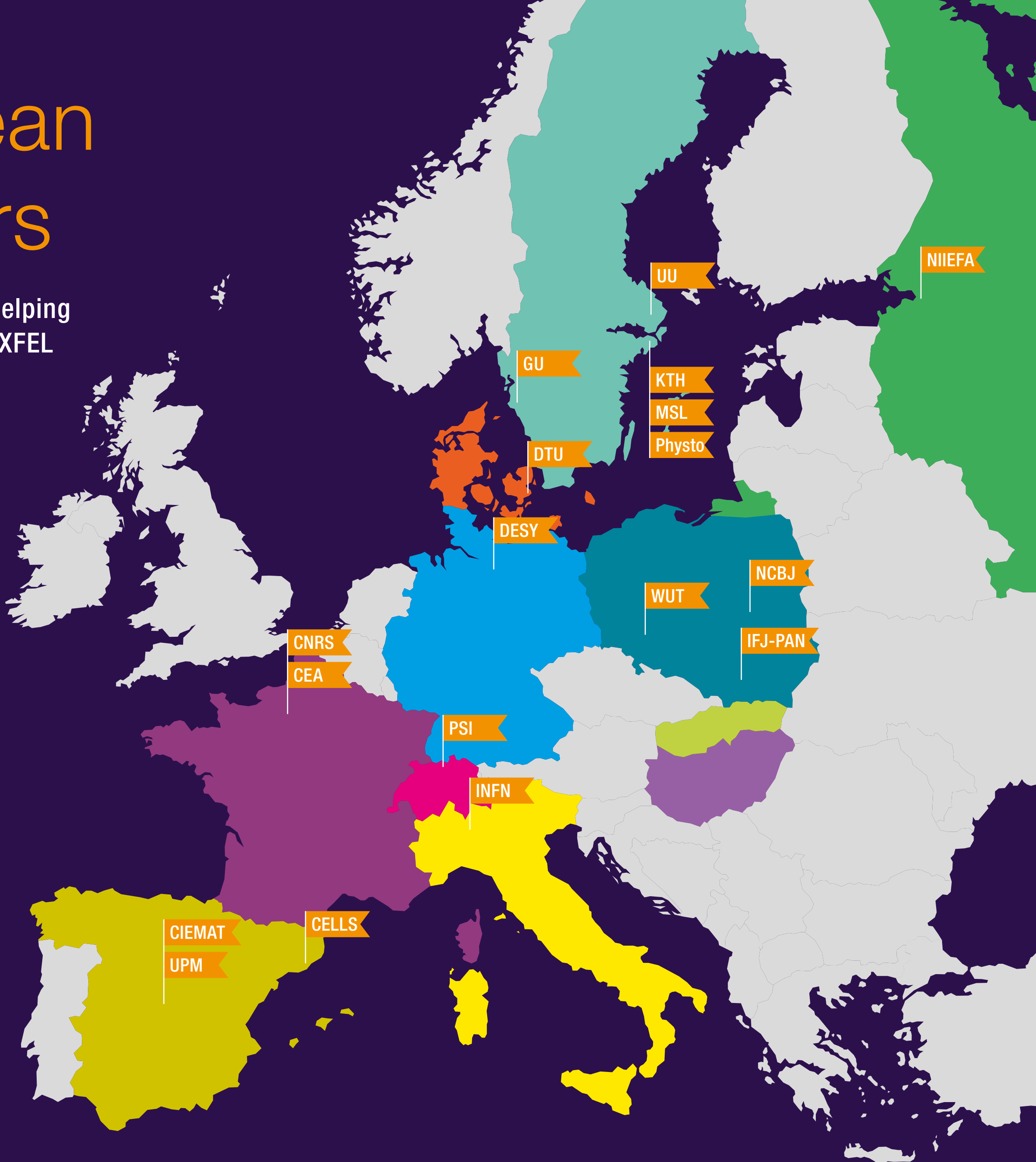
Dosch: With the European X-ray laser facility – in synergy with the outstanding X-ray light sources PETRA III and FLASH that already exist at DESY – a worldwide unique research infrastructure is being created in the Hamburg metropolitan region. Pioneering interdisciplinary research partnerships have already developed around these facilities in recent years – for example the Center for Free-Electron Laser Science (CFEL) and the Centre for Structural Systems Biology (CSSB), which is currently under construction. This development is attracting the best scientists to Hamburg, and it's also offering high-tech companies a highly attractive environment where they can develop new ideas and technologies whose impact goes far beyond the research environment. In these ways, DESY and its cooperation partners are making a sustained contribution to a new culture of innovation in the Hamburg metropolitan region.

femto: What are the outstanding features of the European XFEL in addition to the scientific aspects?

Dosch: The European X-ray laser is already a beacon of highly professional project management. According to our present state of knowledge, the European XFEL will fulfil all of its projected design parameters, including the project costs. This once again demonstrates DESY's expertise regarding the design and construction of highly complex particle accelerator facilities. The technologies that will be used at the European XFEL have already pushed back the boundaries of technical feasibility. That applies especially to the two-kilometre-long superconducting accelerator – a DESY technology. To make the European XFEL a beacon of science as well, we will have to make some pioneering scientific discoveries in the years ahead. But I have no doubt whatsoever in this respect – our top scientists are already raring to go.

European partners

Eleven countries are helping to build the European XFEL



Institutions and selected in-kind contributions

The complete detailed list is available at: http://www.xfel.eu/project/in_kind_contributions/

DTU Technical University of Denmark, Copenhagen (Denmark)

- High-tech components for scientific instruments

CNRS Centre National de la Recherche Scientifique, Orsay (France)

- Production of radio frequency couplers for the superconducting linear accelerator

CEA Commissariat à l'Energie Atomique et aux Energies Alternatives, Saclay (France)

- Assembly of modules consisting of eight superconducting cavities each
- Construction of the 103 accelerator modules (including two prototypes)

DESY Deutsches Elektronen-Synchrotron, Hamburg (Germany)

- Design, manufacturing support and testing of the superconducting cavities
- Design, manufacturing support and testing of the accelerator modules
- Cryogenics for the accelerator complex
- Radio frequency provision
- Construction and operation of the injector
- Construction and operation of the main accelerator
- Construction and operation of the beamlines
- Safety monitoring
- Contributions to the facility and IT infrastructure
- Coordination of the entire facility
- Awarding and monitoring of contracts
- Commissioning of the European XFEL

INFN Istituto Nazionale di Fisica Nucleare, Milan (Italy)

- Production, testing and delivery of superconducting cavities
- Cryostats
- 3.9 GHz accelerator module for the injector

NCBJ National Centre for Nuclear Research, Świerk (Poland)

- Production, testing and delivery of HOM couplers and absorbers for the accelerator
- Programmable logic controllers for scientific instruments

WUT Wrocław University of Technology, Wrocław (Poland)

- Production, testing and installation of vertical test stands for the cavity test

- Production, testing and installation of the XATL1 transfer line
- Vertical cryostats

IFJ-PAN Henryk Niewodniczański Institute of Nuclear Physics of the Polish Academy of Sciences, Kraków (Poland)

- Testing of all superconducting cavities, magnets and accelerator modules

JINR Joint Institute for Nuclear Research, Dubna (Russia)

- Design, production, testing and delivery of three MCP-based detectors

IHEP Institute for High Energy Physics, Protvino (Russia)

- Design, production and installation of cryogenic systems for the accelerator
- Design, production and installation of the beam stops

NIIEFA D.V. Efremov Institute of Electro-physical Apparatus, St. Petersburg (Russia)

- Design, production and delivery of normal-conducting magnets

BINP Budker Institute of Nuclear Physics, Novosibirsk (Russia)

- Design, production and testing of magnets, vacuum components and power supply
- Design, production and construction of test stands for superconducting accelerator modules
- Cryogenic equipment
- Power supply

INR Institute for Nuclear Research at the Russian Academy of Sciences, Moscow (Russia)

- Design, production and delivery of transverse deflecting structures and electron beam diagnostics

CELLS Consortium for the Exploitation of the Synchrotron Light Laboratory, Barcelona (Spain)

- Seven mechanical support systems for undulators

CIEMAT Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas, Madrid (Spain)

- Design, production, testing and delivery of undulator intersections
- Design and production of superconducting beamline magnets

UPM Universidad Politécnica de Madrid, Madrid (Spain)

- Design, production, testing and delivery of the power supply for superconducting magnets

KTH Royal Institute of Technology, Stockholm (Sweden)

- Investigation of X-ray lenses and cooling systems

GU University of Gothenburg, Gothenburg (Sweden)

- Magnetic bottle electron spectrometer

MSL Manne Siegbahn Laboratory of Stockholm University, Stockholm (Sweden)

- Measurement of magnets
- Design, construction and delivery of temperature sensors for the undulators

Physto Department of Physics of Stockholm University, Stockholm (Sweden)

- Configuration, validation and delivery of the timing and synchronisation system

UU Uppsala University, Uppsala (Sweden)

- Design, production and delivery of a laser-controlled sample injector, including laser heating
- Secondment of physicists for equipping the structural biology measuring station

PSI Paul Scherrer Institute, Villigen (Switzerland)

- Design, production and installation of the beam position monitors and intra-bunchtrain feedback systems

The in-kind contributions are the result of cooperations between institutes, and there is some overlap in activities between the partners.

A bike ride through the X-ray laser

Two schoolboys explore the European XFEL

Friday, 19 February, is a grey day. But at least it's not raining as we set out on our bike ride down the road from Hamburg-Sülldorf to Bahrenfeld. Our destination is a long tunnel for a research facility that is expected to generate 27 000 X-ray flashes per second. At this point, we can't really imagine it. We're looking forward to the experience, a bit excited, though also exhausted from the past week at school.

We arrive at Albert-Einstein-Ring and the office buildings of European XFEL GmbH, where we have an appointment with Frank Poppe from the PR group. He's going to ride through the tunnel with us and explain the X-ray laser that is being constructed inside it. But there's no tunnel in sight. First of all, we're given our equipment and a lecture on safety. Each of us gets an access card and a pair of rubber boots with steel caps, because there's still a construction site at the end of the tunnel and safety shoes are mandatory. We also have to wear helmets, in case we bump our heads against the technical equipment in the tunnel or something falls on our heads. When we arrive at the entrance building of the X-ray laser on the DESY campus, each of us also gets a "self-rescuer". It's a self-contained breathing apparatus that looks like a snorkel with a bag, and it enables you to go on breathing for half an hour if a fire should break out in the tunnel. We also get goggles to protect our eyes from smoke. Frank demonstrates the equipment, a bit like a flight attendant showing you how to use the oxygen masks in a plane.

Finally, our tour begins. In the entrance hall is a shaft that's almost 40 metres deep and is securely protected by a railing. A huge indoor crane hanging from the ceiling is used to transport heavy loads down the shaft. This crane is very important, because all the components for the particle accelerator that is being built down there have to go down this shaft and be loaded directly on a special transport vehicle. This includes the yellow pipes weighing several tonnes that contain the components of the accelerator itself. Later on, we see this special vehicle in the tunnel. It's called the Mullewupp (which means "mole" in the local dialect) and it looks like a yellow mining locomotive. On its 360 degree tyres it can move in any direction from a standing position. That's an important skill when it has to manoeuvre inside the narrow tunnel. In addition, it can not only

transport loads weighing several tonnes but also jack them up, because the accelerator hangs from the ceiling of the tunnel. To do all that, the Mullewupp needs lots of power, so it has gigantic batteries – using a petrol engine would be too hazardous inside the tunnel.

So, down we go – into the tunnel. Using our access cards, we pass through the safety barrier and push our bikes into the lift, which takes us down seven stories. The accelerator tunnel is built like an underground train tunnel. It's a round concrete pipe with a floor, completely straight, and it's so

long that you can't see the end of it. Yellow accelerator modules are hanging from the ceiling of the right half of the tunnel. The electrons could already start flying here – but they wouldn't get very far, because construction is still in full swing. The temperature in the modules is minus 271 degrees Celsius so the electricity can flow without any resistance. In addition, the electrons fly through a vacuum so that they don't bounce against anything and can be accelerated to almost the speed of light – 300 000 kilometres per second. That's very hard to imagine.

In the left half of the tunnel, there's a path for the Mullewupp and for our bikes. We've got to be careful to travel in a really straight line and not bump into anything. Riding through the tunnel is a weird and exciting experience! To our right are the yellow modules and lots of extremely large magnets. Frank explains that these magnets will help to bundle the electron beam. Two bright blue "dipole" magnets are larger than the others. They come from St. Petersburg and cost 57 000 euros each. They are part of the Russian contribution to the European XFEL. The programme's partner countries don't just contribute money to build the X-ray laser; they also provide important components such as these magnets.

After travelling the first two kilometres through the accelerator tunnel, we reach a plywood door. At that point, we are in a bleak-looking operations building located directly under the Osdorfer Born housing estate. This is where the tunnel divides into two branches, and from here on the electrons will be used to generate the X-ray laser flashes that the researchers are interested in.

We ride our bikes into the tunnel on the right. A few of the yellow structures in which the light flashes will be generated are already standing here. It's hard to remember what they're called. Demulators? Odolators? Emulators? No, these are undulators. Inside them, alternating magnets force the electrons to travel along a slalom course and radiate X-ray flashes. Undulators are strong magnets that can't be turned off, so your watch may get stuck on one of them if you bring it too close.

The yellow-orange undulators are produced in Germany and Spain. There's also another undulator that really stands out because of its neon yellow-green colour. It comes from China, and it works really well, but the Chinese somehow got the colour wrong. It really looks weird!

Then we come to yet another place where the tunnel divides into several branches. The two original tunnels branch into five tunnels in all, and each of these tunnels leads to various measuring stations. Our tunnel eventually becomes very narrow and warm, and we have to ride our bikes very carefully. There are no more undulators here. To our right is only the beam pipe, through which the X-ray laser radiation flies, and lots of testing devices that are used to monitor the light to see if it fulfils all the quality requirements. At last, we come to the end of the tunnel and to another door. We push our bikes through it, out of the tunnel and into the underground experiment hall. This hall is as big as a football field, and several measuring huts are now being built inside it. This is where the researchers will be looking at atoms and filming chemical reactions. In one of these huts, which has thick concrete walls, they will conduct experiments under extremely high pressure and at high temperatures – that is, under the same conditions that exist in the interiors of planets.

We push our bikes into the lift and it takes us back to the surface, where they are building labs and offices at the moment. We ride our bikes to the exit, give back our helmets, rubber boots and self-rescuers, and find ourselves standing in the town of Schenefeld, right next to a big tennis complex. By now it's dark outside. We say goodbye to Frank and ride our bikes home. It's been an exciting trip, but it's also been very tiring. We've seen a lot and learned a lot. And someday we'd like to go back down into the tunnel – this time with our skateboards.

Vincent van Beusekom and Louis Wild are sixth-formers at their secondary school, the Marion Dönhoff Gymnasium in Hamburg-Blankenese. When they're not outdoors on their bikes or longboards, they like to play Minecraft. They're planning to make a film about the X-ray laser facility using the images they recorded with their GoPro cameras.

Picture: J.M. Harms, MPSD

The alkali fulleride K_3C_{60}, which contains football-like molecules comprising 60 carbon atoms, can be induced to lose its electrical resistance at a temperature as high as minus 170 degrees Celsius by subjecting it to intense laser flashes.

Footballs with no resistance

Signs of light-induced superconductivity in buckminsterfullerenes

When illuminated with an intense infrared laser, tiny metallic, football-like molecules lose their electrical resistance at comparatively elevated temperatures. This was discovered by a team of physicists led by Daniele Nicoletti from the Max Planck Institute for the Structure and Dynamics of Matter at the DESY campus in Hamburg. Such experiments should enable a more precise understanding of the phenomenon of superconductivity.

At present, superconductors are mostly used in special applications. Even the best of these materials have to be cooled to minus 70 degrees Celsius before they lose their electrical resistance, so their use is restricted to specialised areas such as the magnets for MRI scanners, fusion plants or particle accelerators. The Max Planck physicists from the group of institute director Andrea Cavalleri investigated the fulleride K_3C_{60}, a metal compound incorporating football-shaped fullerenes, which normally becomes superconductive at a temperature of around minus 250 degrees Celsius. However, when the material was illuminated with the infrared laser, it became superconductive for a brief moment at minus 170 degrees Celsius.

Back in 2013, researchers of the institute had shown that a certain ceramic, when subjected to infrared laser pulses, became superconductive for a fraction of a second even at room temperature. Given that fullerenes have a relatively simple chemical composition, the scientists hope that these new experiments will enable them to better understand the phenomenon of light-induced, short-term superconductivity at relatively high temperatures. Such insights could help scientists develop a material able to conduct electricity without loss at room temperature without any optical excitation.

Nature, 2016; DOI: 10.1038/nature16522

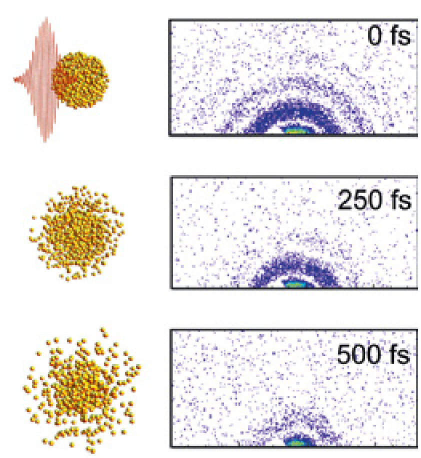
Exploding nanoparticles

Scientists film nanocosmos with unprecedented spatial and temporal resolution

Using an X-ray supermicroscope, a German–US team of scientists led by Tais Gorkhover from Berlin Technical University and Christoph Bostedt from Argonne National Laboratory has filmed the explosion of individual nanoparticles in ultraslow motion. In the process, they were able for the first time ever to achieve a spatial resolution better than eight nanometres combined with a temporal resolution of 100 femtoseconds. A nanometre is one millionth of a metre, a femtosecond one quadrillionth of a second.

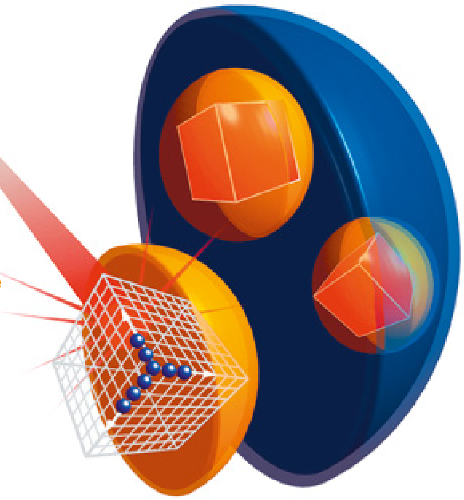
The research team used the LCLS X-ray laser at SLAC National Accelerator Laboratory in California to investigate exploding nanoparticles of frozen xenon. The minuscule particles had a diameter of some 40 nanometres, around 1000 times thinner than a single human hair. “The nanoparticles were superheated by means of intense radiation from an infrared laser and made to explode in a vacuum chamber,” explains DESY researcher Jochen Küpper from the team. The X-ray flashes were precisely timed to capture images of various stages of the explosion. The experiment was repeated over and over, each time with a new nanoparticle and a slightly greater delay before the X-ray flash. These temporally staggered snapshots were then assembled to make a film of the explosion.

Nature Photonics, 2016; DOI: 10.1038/NPHOTON.2015.264



Picture: Tais Gorkhover, SLAC

Three stages of the explosion of a xenon nanoparticle, captured as diffraction images (right) by means of an X-ray laser. The state of the sample (left) can be calculated from the diffraction patterns.



Picture: Thomas Seine, EMBL/CFEL

Schematic representation of the beam from a free-electron laser hitting a protein crystal in the peroxisome of a yeast cell

Scientists X-ray protein crystals inside cells

New approach could make it easier to determine the structure of biomolecules

Scientists from the European Molecular Biology Laboratory (EMBL) have teamed up with researchers from DESY and the SLAC National Accelerator Laboratory in California to X-ray naturally produced protein crystals in biological cells. The study, which was carried out using the LCLS X-ray laser at SLAC, shows that these natural crystals can be used to determine the spatial structure of the proteins.

Crystallography enables scientists to study the atomic structure of proteins. First, however, they need to produce a crystal from the biomolecule under investigation. “Producing protein crystals in the lab for crystallography experiments is not always easy,” says EMBL researcher Daniel Passon. “So imagine if we could get cells to do this for us: a tiny crystal factory in a cell!”

For a structural biologist, growing protein crystals is all part of the job. Less well known is the fact that certain organisms naturally produce crystals within their cells. In certain yeast cells, for example, cell organelles known as peroxisomes pack alcohol oxidase molecules tightly together to form crystals. It was this natural crystal production that enabled the researchers to determine the structure of the alcohol oxidase molecule. Furthermore, results were better when the crystal was left within the cell rather than being removed beforehand for X-raying. The researchers now hope to be able to harness the natural ability of the peroxisome in order to induce it to produce crystals of other proteins.

International Union of Crystallography Journal, 2016; DOI: 10.1107/S2052252515022927

A new nanomaterial

A nanocomposite with medical and product applications

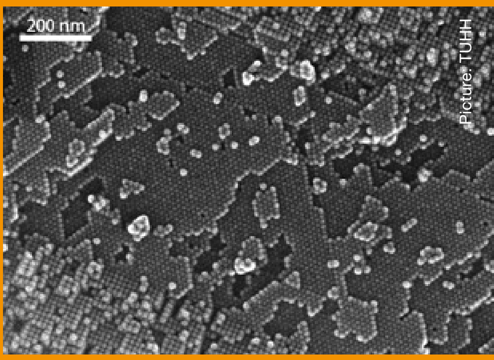
Hamburg researchers have developed a new nanomaterial that combines a number of desirable properties and thereby offers potential applications in the fields of medical technology and manufacturing. On the smallest scale, the structure of the new material resembles that of biological hard tissue, such as mother of pearl and dental enamel. It consists of uniformly sized iron oxide nanoparticles with a coating of oleic acid.

In previous work with this material, the bonds between the oleic acid molecules were very weak and based on Van der Waals forces. By means of drying, hot-pressing and controlled heat treatment, the scientists have now managed to create a much stronger bond between the oleic acid molecules, thereby decisively improving the nanocomposite’s mechanical properties. This new class of material might be suitable for filling dental cavities, for example, or manufacturing watch cases – applications requiring a material that is both hard and non-breakable.

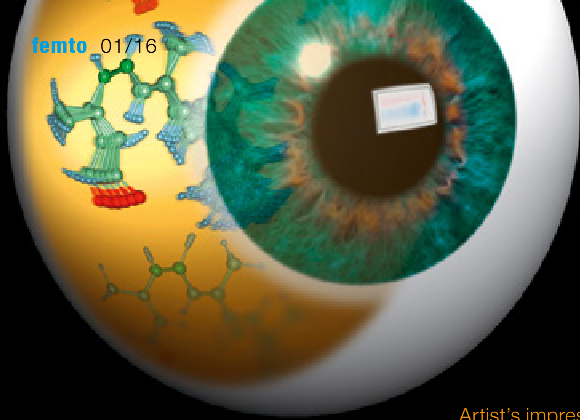
The scientists from the Hamburg University of Technology (TUHH), the University of Hamburg, the Helmholtz Centre Geesthacht and DESY presented their novel nanocomposite in the journal *Nature Materials*. As oleic acid is frequently used when processing other nanoparticles, this new method could potentially improve the mechanical properties of a great many other nanocomposites as well.

Nature Materials, 2016; DOI: 10.1038/NMAT4553

The new material under a scanning electron microscope. It is made up of uniformly sized iron oxide nanoparticles.



Picture: J.M. Harms, MPSD



Artist's impression of the molecular motion of the light-sensitive part of rhodopsin

Molecular breakdance

Our sense of vision is based on highly choreographed, ultrafast molecular motions

The visual process is based on the detection of light by a pigment in the retina called rhodopsin or, alternatively, visual purple. Investigations by a team of scientists led by R. J. Dwayne Miller from the Max Planck Institute for the Structure and Dynamics of Matter and the University of Toronto in Canada have shown that the primary photochemical step of this process operates at a much faster speed than previously thought.

Rhodopsin gets its light sensitivity from a repeating chain of single- and double-bonded carbon atoms. The absorption of a photon causes an extremely short, momentary weakening of a specific double bond, resulting in a rotation about that bond. Until recently, scientists were unable to precisely determine the speed of this so-called isomerisation. With the advent of femtosecond lasers, however, it was shown that the process takes place within at most 200 femtoseconds. A femtosecond is one quadrillionth of a second.

Using a highly sensitive technique from the field of ultrafast spectroscopy, the team under Max Planck Director Miller and Oliver P. Ernst from the University of Toronto looked again at the isomerisation reaction of bovine rhodopsin and showed that the process occurs over a timescale of 30 femtoseconds. “It turns out that the primary step of vision is nearly ten times faster than anyone thought,” says Miller, “and that the atomic motions are all perfectly choreographed by the protein.” Temporal analysis of the experimental data revealed a molecular breakdance comprising localised stretching, wagging and torsional motions.

Nature Chemistry, 2015; DOI: 10.1038/nchem.2398

An optical funnel for nanoparticles

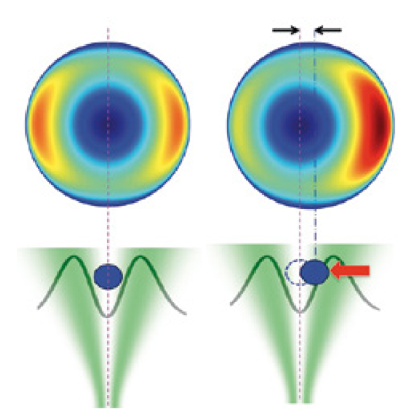
New method promises more precise delivery of biological samples into X-ray laser beams

Researchers have constructed an optical funnel that can precisely deliver a stream of proteins, viruses or other nanoparticles into the tightly collimated beam of an X-ray laser for analysis. The funnel consists of a specially modified light beam with a helical wavefront. This produces a dark region at the centre of the beam, where the light intensity falls to zero. An optical lens gives the beam its funnel-like shape.

In contrast to conventional optical traps, the funnel uses thermal forces to control the particles. Whenever a particle gets too close to the wall of the optical funnel, it heats up on the side closest to the wall. Air molecules colliding with the particle on the warm side are repelled with greater momentum than those on the cold side. This momentum imbalance results in a so-called photophoretic force, which pushes the particle from the hot to the cold side and thus toward regions of lower light intensity.

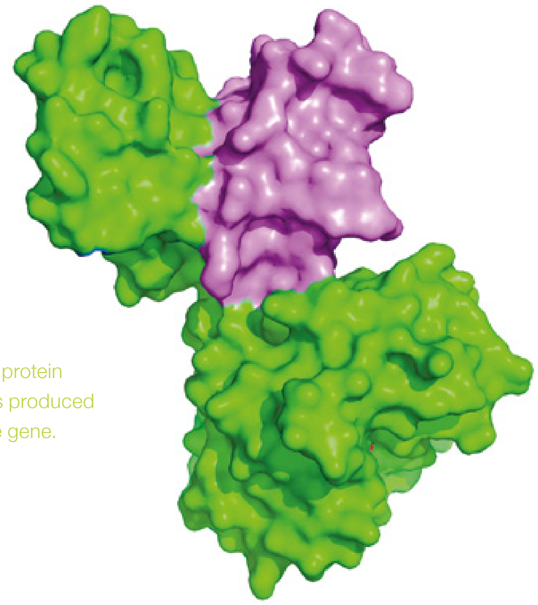
The team, which was led by Andrei Rode from the Australian National University in Canberra and included DESY researchers from the Center for Free-Electron Laser Science (CFEL) and the Centre for Ultrafast Imaging (CUI), tested their concept with tiny graphite beads between 12 and 20 micrometres in diameter. The advantage of this method is that the photophoretic forces can be much stronger than the direct optical forces in conventional optical traps. Moreover, particles spend most of the time in the dark region of the funnel, which prevents them from the potentially damaging effects of heating up.

Physical Review Applied, 2015; DOI: 10.1103/PhysRevApplied.4.064001



Particles inside the optical funnel are heated on the sides and thereby directed into the dark central area.

Picture: N. Eckerskorn et al., Phys. Rev. Applied



Picture: Rob Meijers, EMBL

The entire protein complex is produced by a single gene.

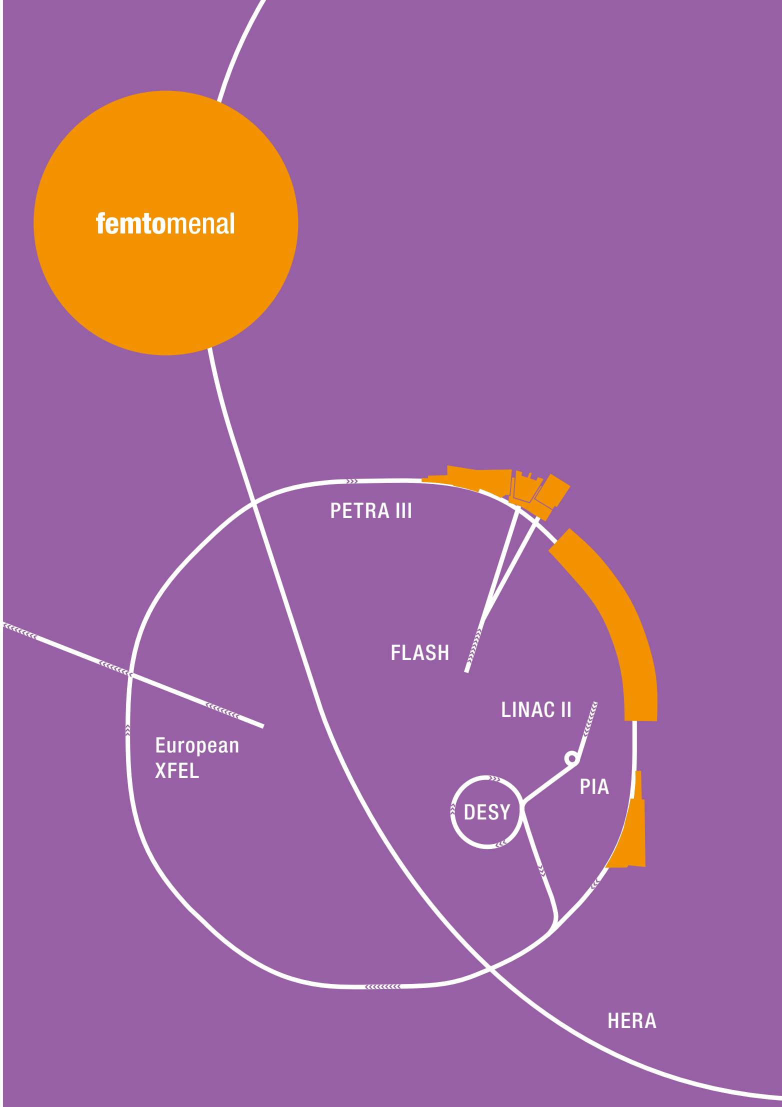
One gene, two proteins, one complex

Normally, a gene produces exactly one protein. Occasionally, it may produce two. But, as Rob Meijers, group leader at the Hamburg outstation of the European Molecular Biology Laboratory (EMBL) on the DESY campus, points out, to see two proteins produced from the same gene that then bind together to form a complex – that is truly unique. Meijers and his team were investigating viral enzymes that degrade the cell walls of *Clostridium* bacteria. They discovered that there is both a short and a long variant of the enzyme, each produced by the same gene. This is because the gene has two different starting points and can therefore produce proteins of different lengths. “This study shows how two such proteins from the same gene form a complex, and how the shorter protein regulates the full-length protein,” says Meijers. “To our knowledge, that has never been seen before.”

The interaction between these two proteins plays a key role in how the viral enzymes, known as endolysines, destroy the cell wall of the *Clostridium* bacteria. The species of the genus *Clostridium* include some dangerous pathogens. Viruses that attack bacteria – so-called bacteriophages – could provide a new weapon in the fight to combat bacterial infections. This makes them, and particularly their enzymes, very interesting objects of research.

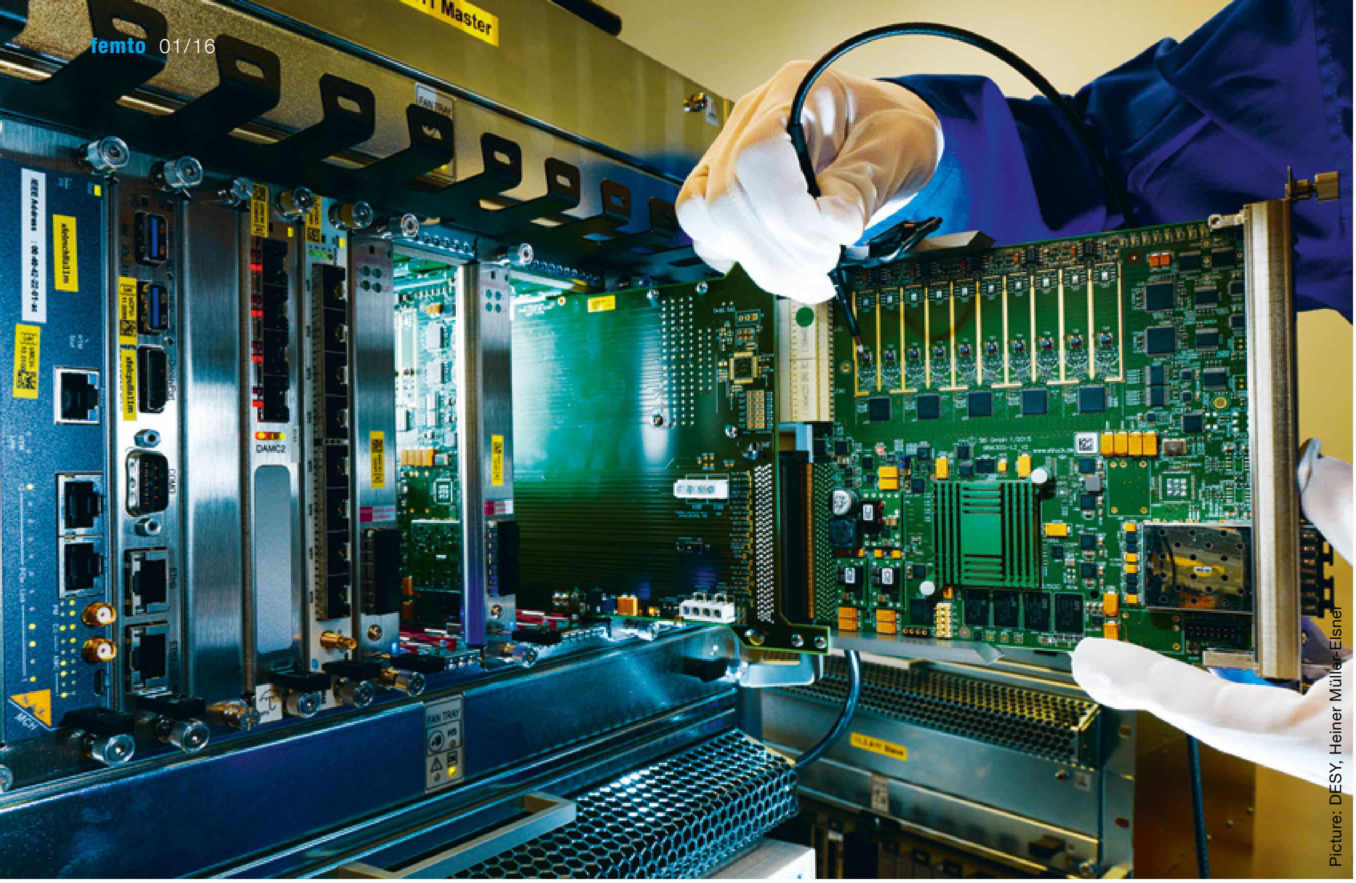
Journal of Biological Chemistry, 2015; DOI: 10.1074/jbc.M115.671172

femtomenal



16 288 metres of tunnels

The accelerator tunnels on the DESY campus and in the surrounding area add up to precisely 16 kilometres and 288 metres in length. Many of them are linked together to form an underground network through which ultrafast particles must be guided with the utmost precision. For example, electrons destined for the PETRA III storage ring pass through a cascade of three accelerators and need to be delivered from one to the next with an accuracy of 50 picoseconds – a picosecond is a millionth of a millionth of a second. All in all, the tunnels that these electrons fly through measure 3.5 kilometres in length. While a high-speed train moving at 230 km/h would need 54 seconds to travel this distance, the particles are about four million times faster. Travelling at almost the speed of light, they could cover this distance in just 12 microseconds (millionths of a second) – if they weren’t forced to take multiple turns in the pre-accelerators before entering PETRA III.



Picture: DESY, Heiner Müller-Elsner

The fast DESY control technology also has big potential for industrial applications.

Licensed to measure

A new electronic standard conquers the market

Particle accelerators are highly complex facilities, often several kilometres in length and packed with high technology. It takes very fast and extremely precise systems to control these particle race tracks – systems that are capable of processing many datasets in parallel. Such systems must run problem-free for at least ten years, 24 hours a day. Even if a power supply unit fails, everything else must continue to function without interruption. Various electronic standards have been established in recent decades to facilitate the development of systems capable of meeting such specifications. These electronic standards provide a uniform description on the basis of which such systems can be constructed with components either bought in or produced in-house.

According to DESY accelerator expert Holger Schlarb, three of the already existing standards would, in principle, have been suitable for operating a particle accelerator. There was only one problem: "Ultimately, none of them was suitable for DESY's future development." This development includes the 3.4-kilometre-long European XFEL X-ray laser, currently under construction in western Hamburg. For this reason, Schlarb and his team helped to developed a new industry standard and took it to marketability together with the DESY Technology Transfer (TT) group. For the last three years, the physicists and DESY-TT have been pushing its commercialisation and its use in industry. It was a new departure not only for the researchers but also for DESY.

The team first looked at the standard that most closely approximated their requirements: MicroTCA (Micro Telecommunications Computing Architecture). "This is a very common industry standard," Schlarb explains. "It comes from the telecoms sector and does everything we want, except for one thing: recording extremely high-quality analogue data." Unfortunately, that is absolutely essential for research with particle accelerators. The DESY physicists therefore collaborated with other institutes and industrial partners to add this missing function – the ability to carry out analogue measurements.

A new industry standard was established – MicroTCA.4 – and on this basis, the DESY team then developed a system of control boards capable of processing both analogue and digital signals. With this setup, over 100 parameters can be read out in real time several hundred million times a second. Thanks to an integrated management system, everything can be operated and maintained remotely. What's more, the system is scalable across a range of applications, i.e. it is suitable for small units all the way up to highly complex, large-scale facilities.

"We want to establish MicroTCA.4 in the scientific community and in industrial markets"

Holger Schlarb, DESY

This makes the new standard an interesting proposition not only for the scientific community but also for industry, where there are many potential fields of application. These include telecommunications, online inspection, aviation, medical technology and precision metrology. For this reason, the Helmholtz Association, DESY and industrial partners put up four million euros in 2012 to promote its commercialisation and use in industrial companies. It was unfamiliar territory for the researchers, who since then have been attending trade fairs, giving workshops and acting as consultants. "We want to establish MicroTCA.4 in the scientific community and in industrial markets," says Schlarb. "The new standard impressively shows how science and industry can benefit from the innovative power of research," adds Katja Kroschewski, the head of DESY-TT.

With one patent and 18 licensing agreements based on this development work, the investment in the new standard is already paying off. "This way, we generate income and have the opportunity to develop things further," says Michael Fenner, a development engineer at DESY. And even if the process is progressing too slowly for the researchers themselves, industry expert Heiko Körte predicts a highly promising future. "We're already using MicroTCA.4 as the basic standard for a whole range of projects," says Körte, Director of Sales & Marketing at the systems manufacturer N.A.T. in Bonn, Germany. This includes traffic management systems and various wireless applications for fixed and mobile networks. The standard also looks set to play a growing role in the fields of medical technology and disaster management.

"We're already using MicroTCA.4 as the basic standard for a whole range of projects"

Heiko Körte, N.A.T.

"This standard is ideal in a situation after an earthquake, for example, when you need to set up base stations for mobile communications, or for setting up mobile-network transmission stations in areas around the world with little or no infrastructure," says Körte. "The MicroTCA standard has been a remarkable success over the past

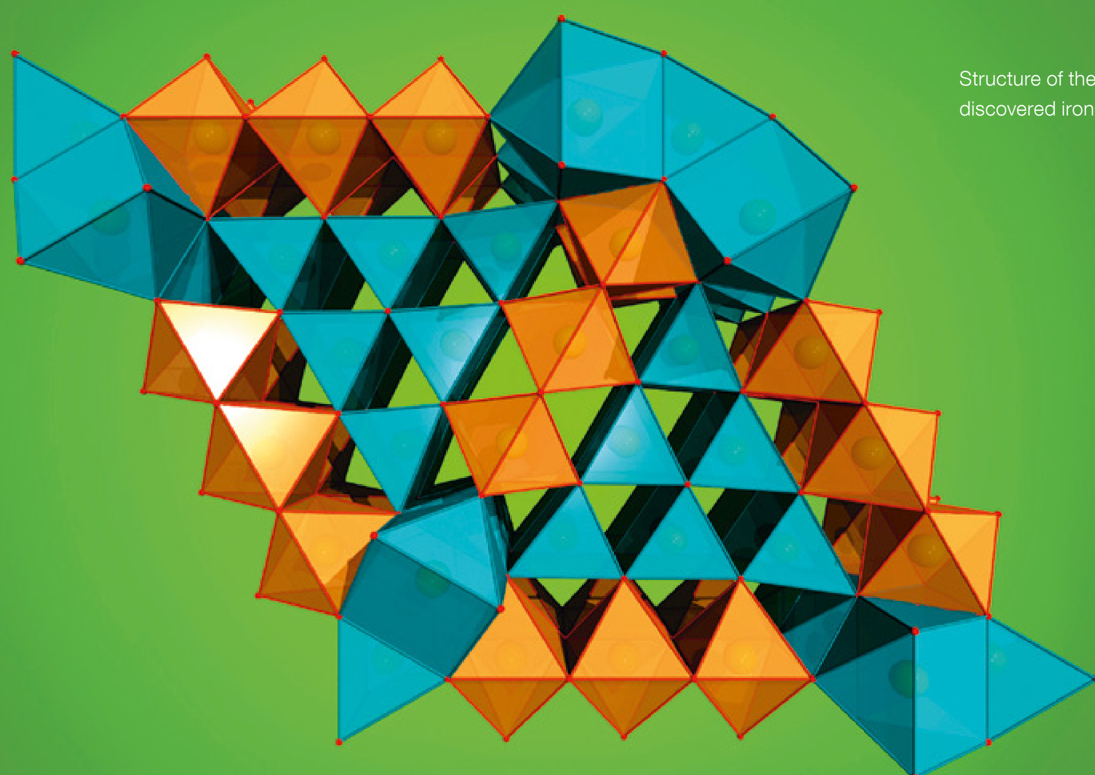
DESY scientist Holger Schlarb was extensively involved in the development of the MicroTCA.4 standard.

eight years." Compared to the VME, Compact PCI and VPX standards, Körte estimates that MicroTCA now has a market share, with respect to new applications, of between 30 and 35 percent. A market study from 2014 put annual growth at nine percent. MicroTCA.4 is part of this story.

N.A.T. was a key partner in the development of MicroTCA and has meanwhile switched to this standard for 85 percent of its products. Of that, 12 percent are based on MicroTCA.4 – a figure that is set to increase in future. Körte is optimistic that the new standard will establish itself on the market. Companies need a bit of time to become familiar with the new standard and its possible applications, he explains: "But that's a transitional process. It will take a few years yet, but less than ten."

An unknown oxygen source in the Earth's mantle

Discovery of new iron oxides provides decisive clues



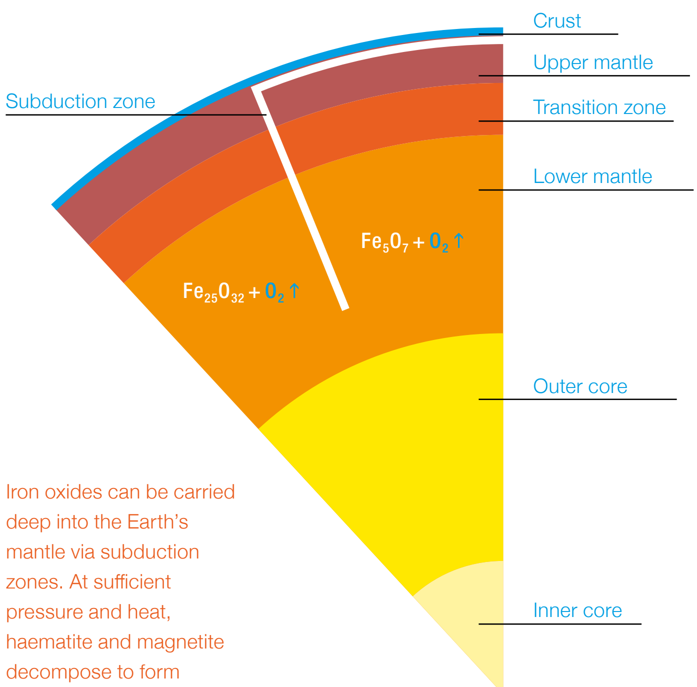
Structure of the newly discovered iron oxide $Fe_{25}O_{32}$

Picture: Elena Bykova, University of Bayreuth

Experiments using special high-pressure cells have revealed the existence of two new iron oxides. The discovery by Elena Bykova from the University of Bayreuth in Germany and her team points to the existence of a large and hitherto unknown source of oxygen in the Earth's lower mantle, raising a number of interesting questions. What happens to the oxygen, for example? Does it react with the surrounding rock? Or does it rise towards the surface? And how does it affect geochemical processes within the Earth system?

Iron oxides in nature take on different forms. "The most common iron oxide is haematite, Fe_2O_3, which is the end product of many geological processes and the main source of iron for our civilisation," explains Bykova. During the past five years, however, scientists have discovered other iron oxides that form at high pressures and temperatures. To further investigate the behaviour of haematite and magnetite (Fe_3O_4), Bykova and her colleagues used a special pressure cell at DESY's X-ray light source PETRA III.

"In this so-called diamond anvil cell, a minute sample can be compressed between two diamonds to several hundred thousand times the atmospheric pressure while a meticulously



Iron oxides can be carried deep into the Earth's mantle via subduction zones. At sufficient pressure and heat, haematite and magnetite decompose to form new iron oxides, thereby releasing large quantities of oxygen. The fate of this oxygen has yet to be explored.

aligned laser can also heat the sample to several thousand degrees Celsius through the transparent diamond anvils," explains DESY scientist Hanns-Peter Liermann. At the same time, the exceptionally bright and fine X-ray beam of PETRA III can track structural changes in the sample. Similar measurements were also made at the European Synchrotron Radiation Source (ESRF) in Grenoble, France, and at the Advanced Photon Source (APS) in Chicago, USA.

"In this so-called diamond anvil cell, a minute sample can be compressed between two diamonds to several hundred thousand times the atmospheric pressure"

Hanns-Peter Liermann, DESY

When the scientists applied a pressure of more than 67 gigapascals (about 670 000 times the standard atmospheric pressure) to their haematite samples and heated them to more than 2400 degrees Celsius, Fe_2O_3 decomposed and formed Fe_5O_7, a new iron oxide that had not been seen before. These pressure and temperature conditions correspond to those in a depth of roughly 1500 kilometres below the surface of the Earth. At an even higher pressure of 70 gigapascals, corresponding to about 1670 kilometres below the surface, magnetite decomposed and another new iron oxide with the formula $Fe_{25}O_{32}$ formed. The formation of both of these previously unknown compounds leads to the release of oxygen.

Although iron oxides do not normally exist in the bulk of the Earth's lower mantle, they can be transported there via subduction zones, where one tectonic plate dives under another. Haematite and magnetite are major components of so-called banded iron formations and ironstones, huge sedimentary rock formations occurring on all continents. These formations may be up to several hundred metres thick and hundreds of kilometres long. Deposited in the world's oceans about two billion years ago, banded iron formations form part of the ocean floor and are recycled into the Earth's interior by subduction processes, which can carry them to great depths, possibly even as far as the core–mantle boundary region.

As the team observed, at conditions corresponding to the middle of the Earth's lower mantle, haematite and magnetite decompose, releasing huge amounts of oxygen-rich fluid (oxygen is usually liquid under these conditions). "We estimate that this source so far provided an amount of oxygen equivalent to eight to ten times the mass of oxygen in the atmosphere," says Bykova. "That's a surprise, and it is not quite clear what happens with the oxygen down there."

The oxygen-rich fluid could either locally oxidise surrounding rocks or migrate to the transition zone, or even to the upper mantle. "This remains to be explored," says co-author Maxim Bykov of the University of Bayreuth. "For now, we can only say that there is a huge source of oxygen in the mantle that can significantly affect geochemical processes by changing oxidation states and mobilising trace elements. This will open a large new field of modelling."

The discovery of the new iron oxides thus not only adds to the knowledge about the fundamental characteristics of these substances, underlines Bykov. "Our work shows that we maybe miss significant parts of the processes in the Earth. Subducted slabs can apparently produce unexpected things. The effects on Earth's global dynamics, including climate variations, have to be investigated."

Nature Communications, 2016; DOI: 10.1038/NCOMMS10661

A particle accelerator on a microchip

Innovative development is expected to facilitate access to accelerator technology

In a new development that would have been barely conceivable only a short time ago, scientists are now working on a miniature particle accelerator the size of a microchip. The international project is being funded by a grant of 13.5 million US dollars (12.6 million euros) from the Gordon and Betty Moore Foundation. DESY and the University of Hamburg are among the partners involved in this international project, headed by Robert Byer of Stanford University (USA) and Peter Hommelhoff of the University of Erlangen-Nürnberg (Germany). Within five years, they hope to produce a working prototype of an "accelerator on a chip".

"The impact of shrinking accelerators can be compared to the evolution of computers that once occupied entire rooms and can now be worn around your wrist," says Hommelhoff. Large-scale facilities will remain essential for many purposes, at least in the short term. However, this advance could mean that accelerators will become available in areas that have previously had no access to such technologies.

"This prototype could set the stage for a new generation of 'tabletop' accelerators, with unanticipated discoveries in biology and materials science and potential applications in security scanning, medical therapy and X-ray imaging," explains Byer.

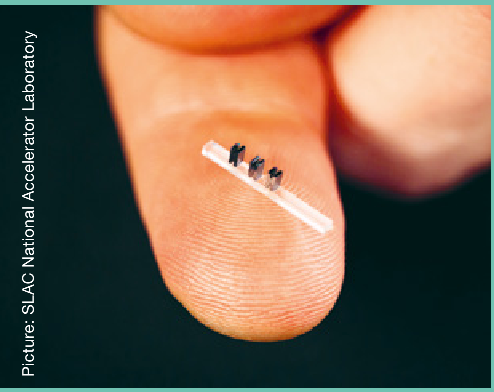
The project is based on advances in nanophotonics, the art of creating and using nanostructures to generate and manipulate light. A laser producing visible or infrared light is used to accelerate the electrically charged elementary particles, rather than the radio frequency (RF) waves currently used. The wavelength of this laser radiation is some ten thousand to one hundred thousand times shorter than that of the radio waves. "The advantage is that everything is up to fifty times smaller," explains DESY scientist Franz Kärtner, who is also a professor at the University of Hamburg and the Massachusetts Institute of Technology (MIT) in the USA and a member of Hamburg's Centre for Ultrafast Imaging (CUI).

"The typical transverse dimensions of an accelerator cell shrink from ten centimetres to one micrometre," adds Ingmar Hartl, head of the laser group in DESY's Photon Science Division. At the moment, the material of choice for the miniature accelerator modules is silicon. "The advantage is that we can draw on the highly advanced production technologies that are already available for silicon microchips," explains Hartl.

DESY will bring its vast know-how as an international leader in laser technology to the project, which has already paid off in other collaborations involving the University of Erlangen-Nürnberg. There, Hommelhoff's group showed that, for slow electrons, a microstructured accelerator module is able to achieve higher accelerating gradients than RF technology. Byer's group had independently demonstrated the same effect for fast, relativistic electrons.

However, it is still a long way from an experimental setup in a laboratory to a working prototype. Individual components of the system will have to be developed from scratch. Among other things, DESY is working on a high-precision electron source to feed the elementary particles into the accelerator modules, a powerful laser for accelerating them, and an electron undulator for generating X-ray radiation. The interaction between the miniature components is also not yet a routine matter, especially when it comes to joining up several accelerator modules.

The SINBAD (Short Innovative Bunches and Accelerators at DESY) accelerator development lab that is currently being set up at DESY will provide the ideal testing environment for the miniature accelerator modules. "SINBAD will allow us to feed high-quality electron beams into the modules, to test the quality of the beams and to work out an efficient way of coupling the laser. DESY offers unique opportunities in this respect," explains DESY accelerator expert Ralph Aßmann.



Picture: SLAC National Accelerator Laboratory

Three "accelerators on a chip" made of silicon are mounted on a clear base.

Why van Gogh's Sunflowers are wilting

X-ray investigation shows how chrome yellow darkens

The colour of Vincent van Gogh's famous *Sunflowers* is changing over time, because of the mixture of pigments used by the Dutch master. Evidence for the process comes from a detailed X-ray investigation of the *Sunflowers* version at the Van Gogh Museum in Amsterdam. A group of scientists headed by Letizia Monico from the Institute of Molecular Science and Technology (CNR-ISTM) of Perugia, the University of Perugia in Italy and the University of Antwerp in the Netherlands shone X-rays from DESY's light source PETRA III through tiny particles of paint taken from the painting. The study identifies areas of the painting that should be monitored particularly closely for any changes.

Vincent van Gogh (1853–1890) is famous for his use of bright yellow colours. The Dutch painter used chrome yellows, a class of compounds consisting of lead, chromium and oxygen. "There are different shades of the pigment, and not all of them are photochemically stable over time," explains Monico. "Lighter chrome yellow has sulphur mixed into it and is susceptible to chemical degradation when exposed to light, which leads to a darkening of the pigment."

The scientists examined the *Sunflowers* painting, which dates back to 1889, to determine whether van Gogh had used different types of chrome yellow when painting it. He produced three versions of the painting, one of which is on display at the National Gallery in London, one at the Seji Togo Memorial Sompo Japan Nipponkoa Museum of Art in Tokyo and one at the Van Gogh Museum in Amsterdam. Two small paint samples, measuring less than one millimetre each, were taken from the painting in Amsterdam and examined using DESY's X-ray source PETRA III. "The analysis shows that the orange-yellow hues mainly contain the light-fast version of chrome yellow, whereas the light-sensitive type is mainly found in the pale yellow areas," reports Gerald Falkenberg, who is in charge of the beamline where the X-ray diffraction measurements were carried out.

"This study also has broader implications for assessing the colours of other works of art"

Koen Janssens, University of Antwerp

At the European Synchrotron Radiation Facility (ESRF) in Grenoble, the team examined the chemical state of the paint samples. When light-sensitive chrome yellow darkens, the chromium is reduced from its highest oxidation state Cr^{VI} to Cr^{III}. The scientists were indeed able to detect a relative proportion of 35 percent Cr^{III} on the surface of the paint. "At least at the two sites from which the paint samples were taken, a colour change has occurred in *Sunflowers* as a result of the reduction of chrome yellow," says Monico. This suggests that the painting *Sunflowers* may originally have looked different from what we see today.

Credit: Van Gogh Museum, Amsterdam (Vincent van Gogh Foundation)

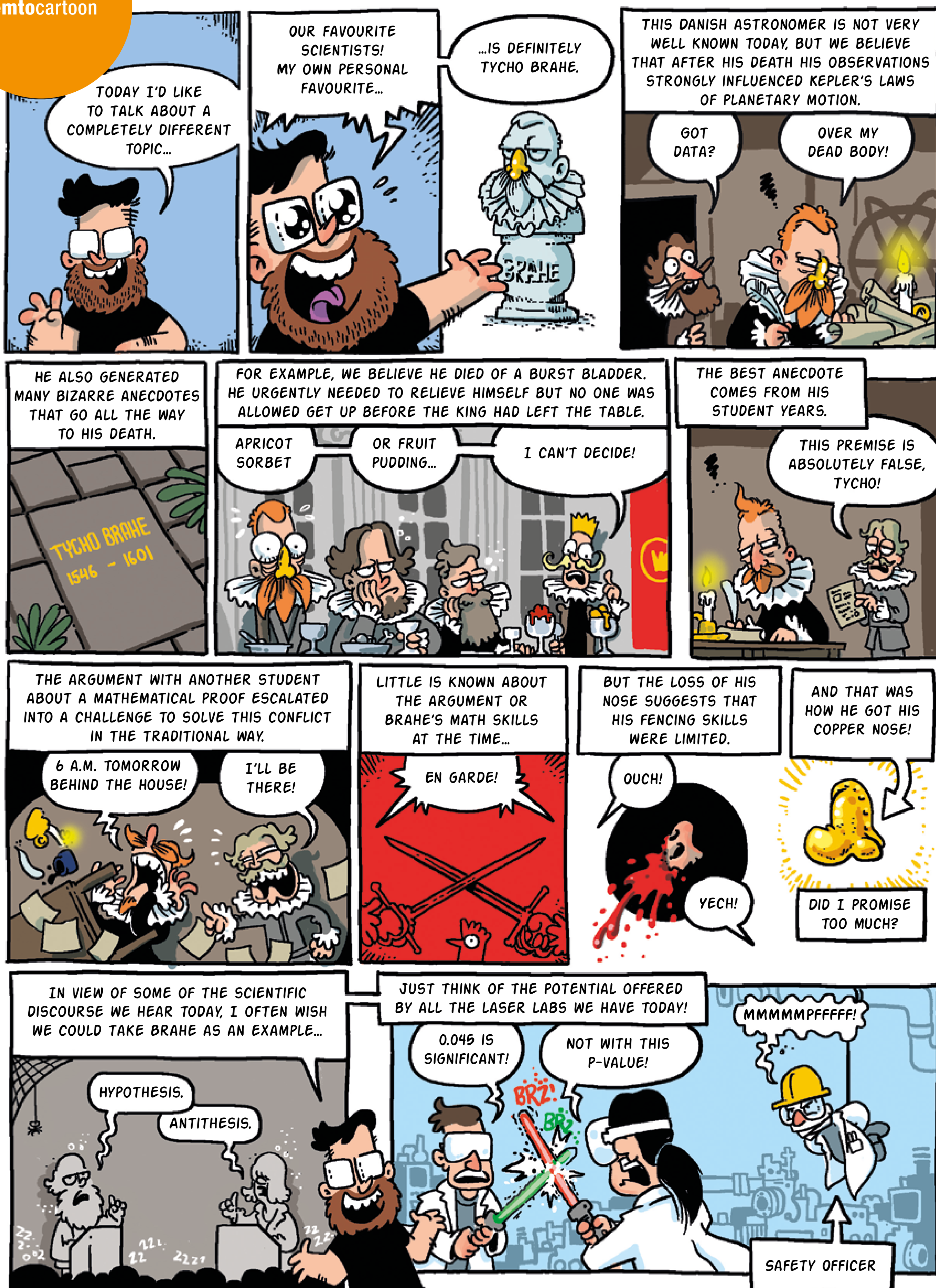
Sunflowers, 1889,
Vincent van Gogh (1853–1890)

The scientists used a mobile scanner to identify those parts of the painting which ought to be monitored particularly closely for possible changes. "Since chrome yellow pigments were widely used by late 19th-century painters, this study also has broader implications for assessing the colours of other works of art," emphasises Koen Janssens from the University of Antwerp, who was extensively involved in the study.

Angewandte Chemie, 2015; DOI: 10.1002/ange.201505840

femtocartoon

By Johannes Kretzschmar



Imprint

femto is published by
Deutsches Elektronen-Synchrotron DESY,
a research centre of the Helmholtz Association

Editorial board address
Notkestraße 85, 22607 Hamburg, Germany
Tel.: +49 40 8998-3613, fax: +49 40 8998-4307
e-mail: femto@desy.de
Internet: www.desy.de/femto
ISSN 2199-5192

Editorial board
Till Mundzeck (responsible under press law)
Ute Wilhelmsen

Contributors to this issue
Frank Grotelüschen, Kristin Hüttmann

Design and production
Diana von Ilsemann

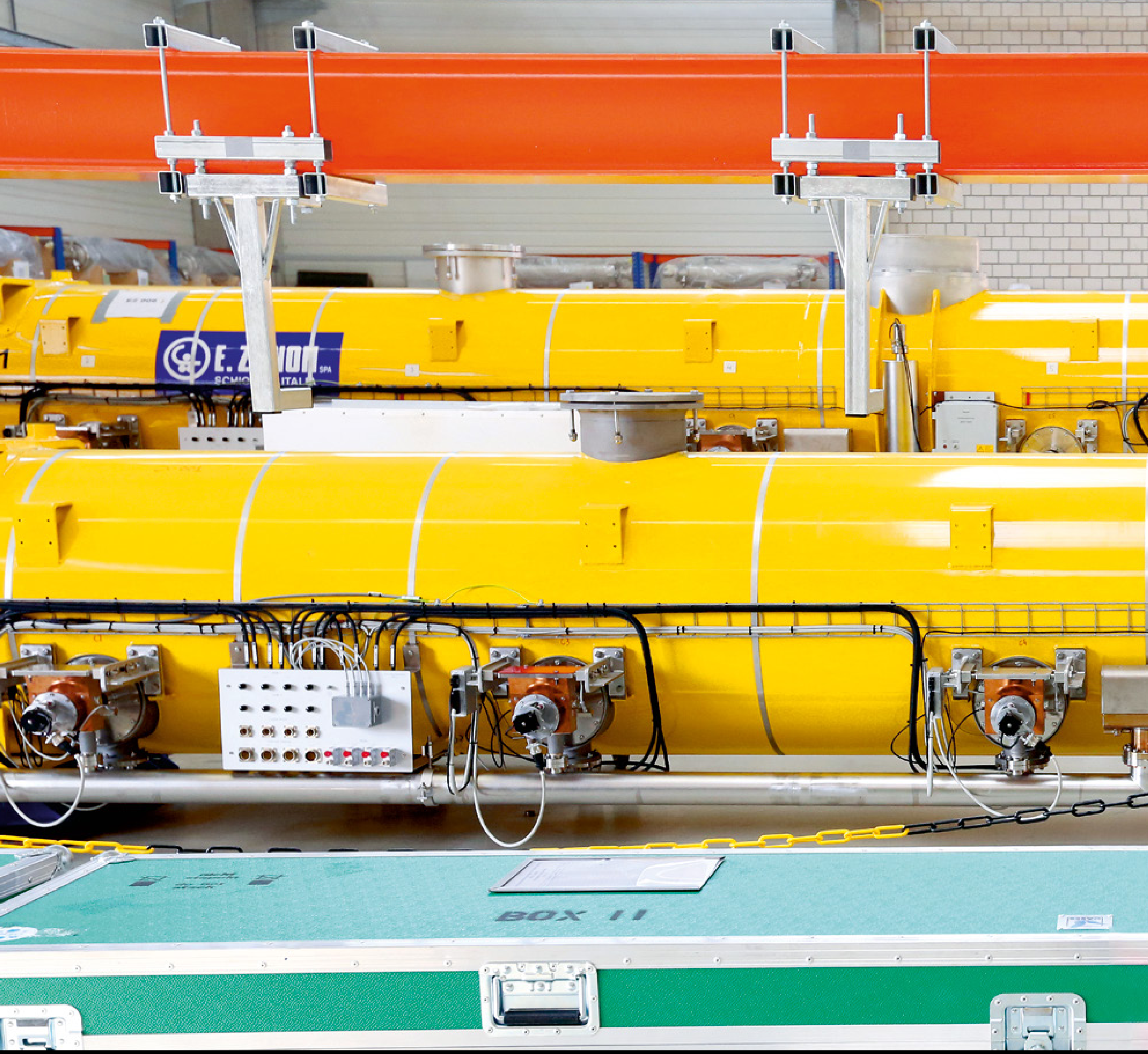
Translation
TransForm GmbH, Cologne
Ilka Flegel

Cover picture
Dirk Nölle, DESY

Printing and image processing
Heigener Europrint GmbH

Copy deadline
March 2016

Cover picture
In the new European XFEL X-ray laser, electrons are accelerated to almost the speed of light and then made to generate intense ultrashort X-ray flashes. The accelerator elements are housed in yellow pipes that are 12 metres long and almost one metre thick. In a test hall at DESY, the complex components are carefully checked before they are installed in the X-ray laser facility's accelerator tunnel.



The DESY research centre

DESY is one of the world's leading particle accelerator centres. Researchers use the large-scale facilities at DESY to explore the microcosm in all its variety – ranging from the interaction of tiny elementary particles to the behaviour of innovative nanomaterials and the vital processes that take place between biomolecules. The accelerators and detectors that DESY develops and builds at its locations in Hamburg and Zeuthen are unique research tools. The DESY facilities generate the most intense X-ray radiation in the world, accelerate particles to record energies and open up completely new windows onto the universe.

DESY is a member of the Helmholtz Association,
Germany's largest scientific organisation.

HELMHOLTZ
ASSOCIATION

DESY