

femto

The DESY research magazine – Issue 02/16

ZOOM

Will millionths
of a millimetre
be the yardstick
of the future?

The most powerful
accelerator in
the Milky Way

Molecular trick outwits
hospital germs

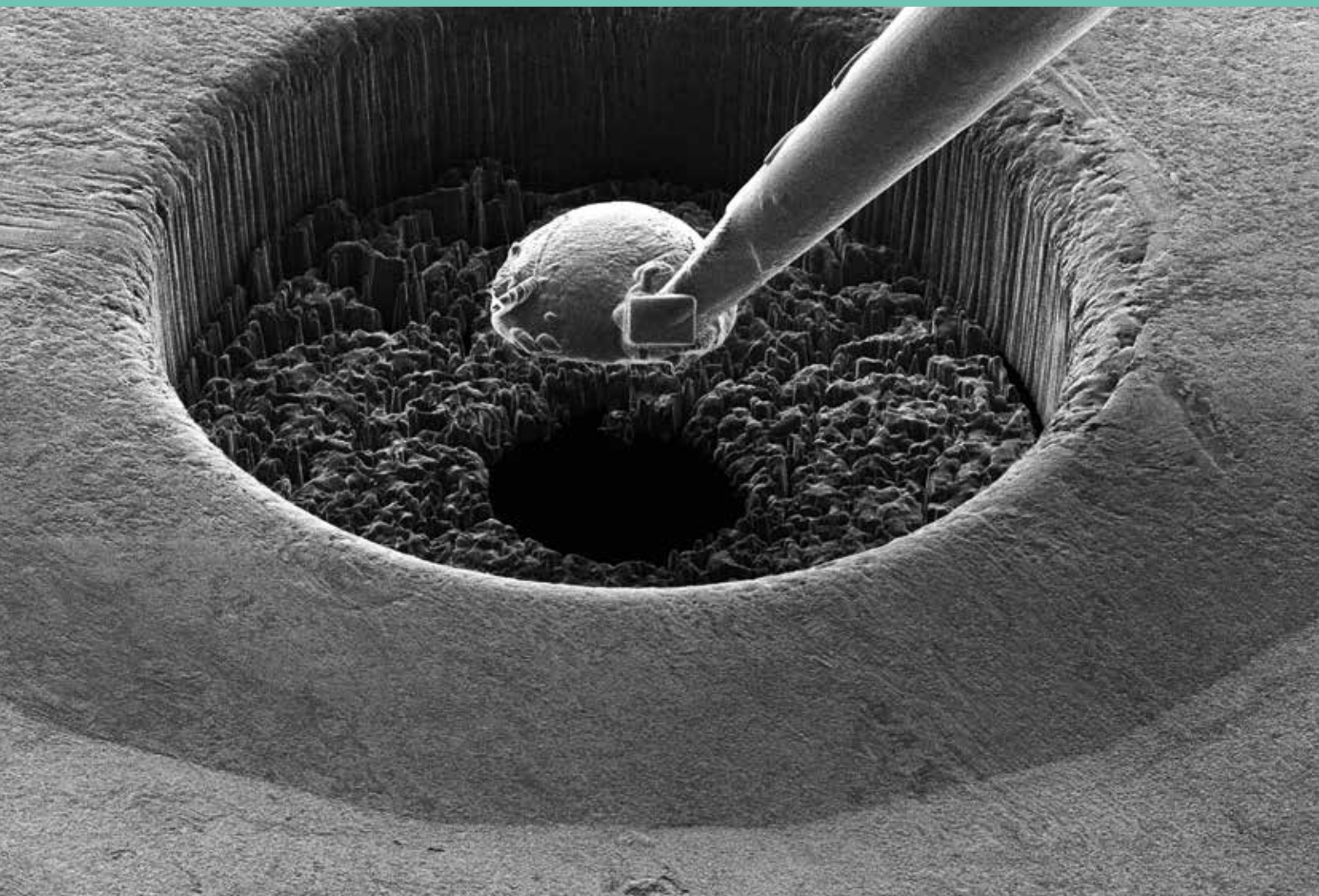
A sign of
a new particle?



femtoscope



Pictures: Leonid Dubrovinsky, University of Bayreuth



Focussed ion beam works materials with nanometre precision

A fine ion beam can be used as a micromilling machine to work materials with tolerances of a few nanometres (millionths of a millimetre). One example of this application is the preparation of the tiny diamond anvils between which samples for ultrahigh-pressure experiments are held. This is done by taking a spherical diamond just a few micrometres (thousandths of a millimetre) in diameter and cutting it in half. The two halves are then turned over and mounted in the pressure cell (photographs). The sample is then placed

between the two inverted hemispheres. Pressures of millions of atmospheres can be created in this way.

In the DESY NanoLab, such a finely focused ion beam is operated jointly with the University of Bayreuth in Germany. The facility can not only be used to trim sample surfaces with nanometre-scale precision, but also to study microscopic defects, cracks or points of corrosion under the surface of materials. The combination with an electron microscope makes it interesting for many areas of application such as nanotechnology, materials sciences and biology.

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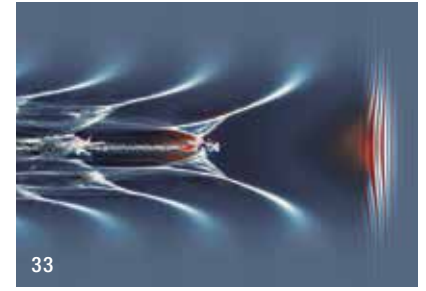
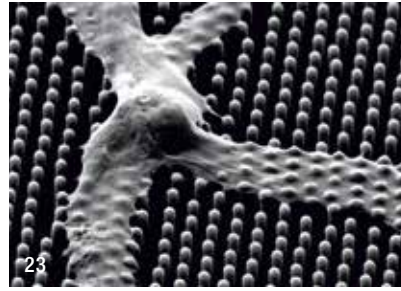
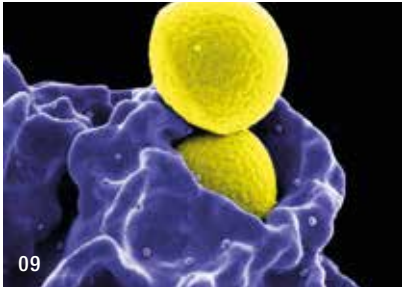
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NANO

Will millionths of a millimetre be the yardstick of the future?

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Nano is a buzzword that almost everyone is familiar with. Moreover, nano is small – very small in fact. One nanometre is one millionth of a millimetre. At the nanoscale, matter has different physical and chemical properties than matter measured in centimetres or metres. At DESY's X-ray radiation sources, researchers can investigate nanomaterials down to the last atom and tailor their properties to different uses.



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Not every bump is an event

The most powerful particle accelerator in the Milky Way

Nature builds the most powerful particle accelerators. From the depths of space, the Earth's atmosphere is bombarded by elementary particles that have one hundred to one hundred thousand times more energy than any terrestrial accelerator could give them. Physicists have been puzzling over the exact origin of this deluge of high-energy particles from outer space – “cosmic radiation” as it's known – ever since the phenomenon was first discovered more than 100 years ago. Various cosmic objects have already been identified as natural particle accelerators. Scientists working with the gamma-ray observatory H.E.S.S. have now located the most powerful accelerator in our own galaxy, the Milky Way.

A huge black hole resides at the centre of the Milky Way. Using the H.E.S.S. (High Energy Stereoscopic System) observatory in Namibia, scientists have discovered intense gamma radiation of extremely high energy around this supermassive object. “We have located an astrophysical accelerator accelerating protons to energies of up to one petaelectronvolt,” says Christian Stegmann, head of DESY in Zeuthen and until recently spokesperson for H.E.S.S.

“We have located an astrophysical accelerator accelerating protons to energies of up to one petaelectronvolt”

Christian Stegmann, DESY

A petaelectronvolt (PeV) is more than 100 times greater than the energy achieved by the largest man-made particle accelerator, the Large Hadron Collider (LHC) at the Geneva particle physics research centre CERN, which also accelerates protons. The discovery marks the first time that scientists have identified a source of cosmic rays with petaelectronvolt energy within the Milky Way. This galactic “pevatron” is most likely the supermassive black hole itself.

Tracking down gamma radiation

For more than 10 years now, H.E.S.S., which is operated by 150 scientists from 12 countries, has been mapping the centre of the Milky Way using highest-energy gamma rays. Cosmic gamma rays are generated by the high-energy protons, electrons and atomic nuclei of cosmic radiation, which are accelerated in various places in the universe. It is not easy to determine where these natural accelerators are located. The problem is that the particles are electrically charged and are therefore deflected from their straight path in interstellar magnetic fields. For this reason, their direction of flight does not point back to their place of origin.

However, the particles of cosmic radiation often encounter interstellar gas or photons (particles of light) close to their source. These collisions produce high-energy gamma rays, which reach the Earth via a straight path because they are not deflected by magnetic fields. >>

The mirror telescopes of the H.E.S.S. observatory in Namibia against the starry backdrop of the Milky Way

> These gamma rays are used by the scientists at the H.E.S.S. observatory to pinpoint the sources of cosmic rays in the sky.

When gamma rays hit the Earth's atmosphere, they produce short bluish flashes of light that can be detected at night by large mirror telescopes with fast light sensors. Using this technique, more than 100 sources of high-energy gamma rays have been discovered in the sky over the past decades. H.E.S.S. is currently the most sensitive tool for their detection.

It was previously known that cosmic radiation with energies of up to about 100 teraelectronvolts (TeV) is generated in the Milky Way by the remains of supernova explosions, for example, or by fast rotating neutron stars, which are known as pulsars. However, theoretical arguments and direct measurements of the cosmic radiation suggest that these particles should be accelerated in our galaxy up to energies of at least 1000 TeV, i.e. one petaelectronvolt (PeV). In recent years, many extragalactic sources that accelerate cosmic rays to multi-TeV energies have been discovered, but the search for accelerators of the highest-energy cosmic rays in our galaxy has remained unsuccessful.

The galactic pevatron

The detailed observations of the centre of the Milky Way carried out using the H.E.S.S. telescopes have now provided the first answers. H.E.S.S. had already detected diffuse highest-energy gamma radiation in the galactic centre during its first years of observation, which started in 2002. The discovery of this diffuse radiation, which covers a volume about 500 light years across, was already a clear indication of a source of cosmic rays in this region, but the scientists were unable to positively identify the source itself at that time. This is where the new studies provide further clues. "The unprecedented amount of observation data and the progress made in analytical methodologies enabled us to simultaneously measure the spatial distribution and the energy of the cosmic rays in the galactic centre," says Aion Viana from the Max Planck Institute for Nuclear Physics in Heidelberg, Germany.

The centre of the Milky Way is home to many objects capable of producing high-energy cosmic rays, including a supernova remnant, a pulsar wind nebula and a compact star cluster. "However, the supermassive black hole located at the centre of the galaxy, called Sagittarius A*, is the most plausible source of the PeV protons," says Felix Aharonian from the Heidelberg Max Planck

Institute and the Dublin Institute for Advanced Studies in Ireland.

"Our data show that the observed glow of gamma rays around the galactic centre is symmetrical," says H.E.S.S. researcher Stefan Klepser from DESY. "The gamma rays are of a high energy and concentrated towards the centre, which suggests that they must be the echo of a huge particle accelerator that is located in the centre of this glow. Probably in the galactic centre itself."

Several possible acceleration regions can be considered, either in the immediate vicinity of the black hole, or somewhat further away, where a fraction of the material falling into the black hole is ejected back into space and possibly being accelerated again.

"Our data show that the observed glow of gamma rays around the galactic centre is symmetrical"

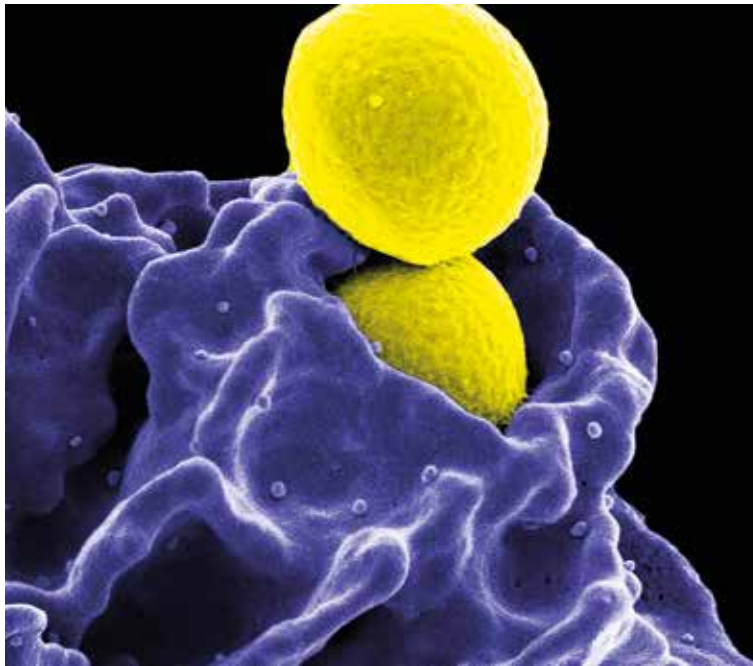
Stefan Klepser, DESY

The observation of gamma rays from the galactic centre provides strong evidence that Sagittarius A* itself is accelerating protons to energies of up to 1 PeV. However, the measurements also show that this source cannot account for the total flux of cosmic rays detected on Earth. "If, however, our central black hole has been more active in the past, then it might actually be responsible for the entire bulk of today's galactic cosmic rays," says H.E.S.S. Deputy Director Christopher van Eldik from the University of Erlangen in Germany. If the researchers' assumption is correct, they will be a big step closer to comprehensively solving the 100-year-old mystery of the origin of cosmic rays.

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Nature, 2016; DOI: 10.1038/nature17147

Custom-made drugs outwit hospital germs

A promising approach in the battle against resistant bacteria



Electron microscope image of antibiotic-resistant *Staphylococcus aureus* bacteria (shown in yellow) in the process of being rendered harmless as they are consumed by a white blood cell (shown in blue)

Picture: National Institute of Allergy and Infectious Diseases (NIAID)

Resistance to antibiotics is a growing problem in the field of healthcare. More and more strains of bacteria are becoming insensitive to certain antibiotics – they learn to adapt to the attacks and are no longer vulnerable to them. As a result, the most important weapon against bacterial infection is in danger of getting dulled. Methicillin-resistant *Staphylococcus aureus* bacteria (MRSA) are often immune to all the usual types of antibiotics and can only be treated using emergency and fall-back drugs. MRSA not only occurs in hospitals, where resistances develop more easily due to the high incidence of germs and

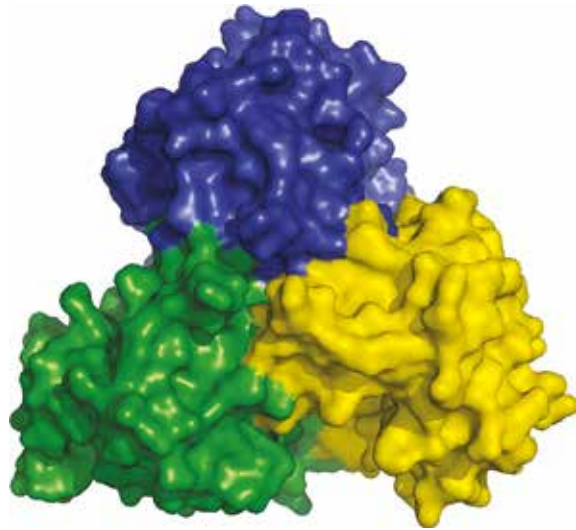
antibiotics; the use of antibiotics in intensive animal farming is also promoting the spread of resistant germs worldwide.

Together with colleagues from Brazil and China, Hamburg scientists working at DESY's X-ray radiation sources have developed a promising approach for outsmarting hospital germs that are resistant to antibiotics. Instead of attacking MRSA bacteria directly, the scientists meddle with a metabolic pathway that is essential to the germs' survival.

"Classical drugs block a particular function of the bacterium," explains Christian Betzel from the University of Hamburg, who conducts research at the Laboratory

for Structural Biology of Infection and Inflammation on the DESY campus. "In such cases, the bacteria can come up with a way of bypassing the blockade, which makes them resistant to that particular drug." Instead, the research group headed by Betzel and Carsten Wrenger from the University of São Paulo cleverly interferes with the vitamin B1 pathway of the staphylococci, without actually blocking it. The bacteria have to manufacture this vital vitamin themselves.

At the beamlines of the European Molecular Biology Laboratory (EMBL) at DESY, the scientists determined the precise >>



The enzyme ThiM is a "trimer", which means that it is composed of three separate ThiM molecules. The active sites are located at the three interfaces of the individual molecules.

atomic structure of the enzymes involved in this process. The scientists then "fed" this enzyme with a custom-made, seemingly useful ingredient for vitamin B1 production. However, this so-called substrate is slightly modified compared with the natural version, so that the form of vitamin B1 produced is in fact useless.

The vitamin trick

"By doing this, we trick the organism," explains Betzel. "We give it something that it believes it needs – but in a slightly modified form so that ultimately it is unable to use it. Ideally, the bacterium won't notice what is wrong, because the vitamin B1 pathway continues to work as it should." The researchers believe that this vitamin is particularly suitable for their approach, for two reasons. "The vitamin B1 pathway is absolutely essential. There are virtually no alternatives," says Markus Perbandt from the University of Hamburg. What's more, "human beings do not have a similar enzyme. That is extremely important in order to avoid cross reactions."

But what must the ideal substrate look like in order for the bacteria to accept it? To find out, the scientists used DESY's X-ray radiation sources to examine the atomic structure of the enzymes

involved. "Six enzymes are involved in the vitamin B1 pathway. Four of them have already been analysed," reports Betzel. "The most interesting of these is an enzyme by the name of ThiM. We only have to alter two atoms in the substrate we 'feed' to this enzyme in order to render it useless." ThiM is a so-called trimer, meaning that it consists of three individual ThiM molecules, which form a complex. "The trimer therefore has three active sites, each located on the interface between the three molecules," explains Betzel.

"It's a bit like offering the bacteria a piece of chocolate next to a piece of dry bread"

Christian Betzel, University of Hamburg

"Once you know the precise structure of the active sites, you can specifically develop a useless substrate," says Perbandt. But the enzyme must not only use the wrong substrate; it should also prefer it to the right one, which is also available. To achieve this, the researchers make their fake substrate more chemically

attractive by attaching certain molecular groups to it. "It's a bit like offering the bacteria a piece of chocolate next to a piece of dry bread," says Betzel. "You can only do this if you know the precise atomic structure of the enzyme you are targeting."

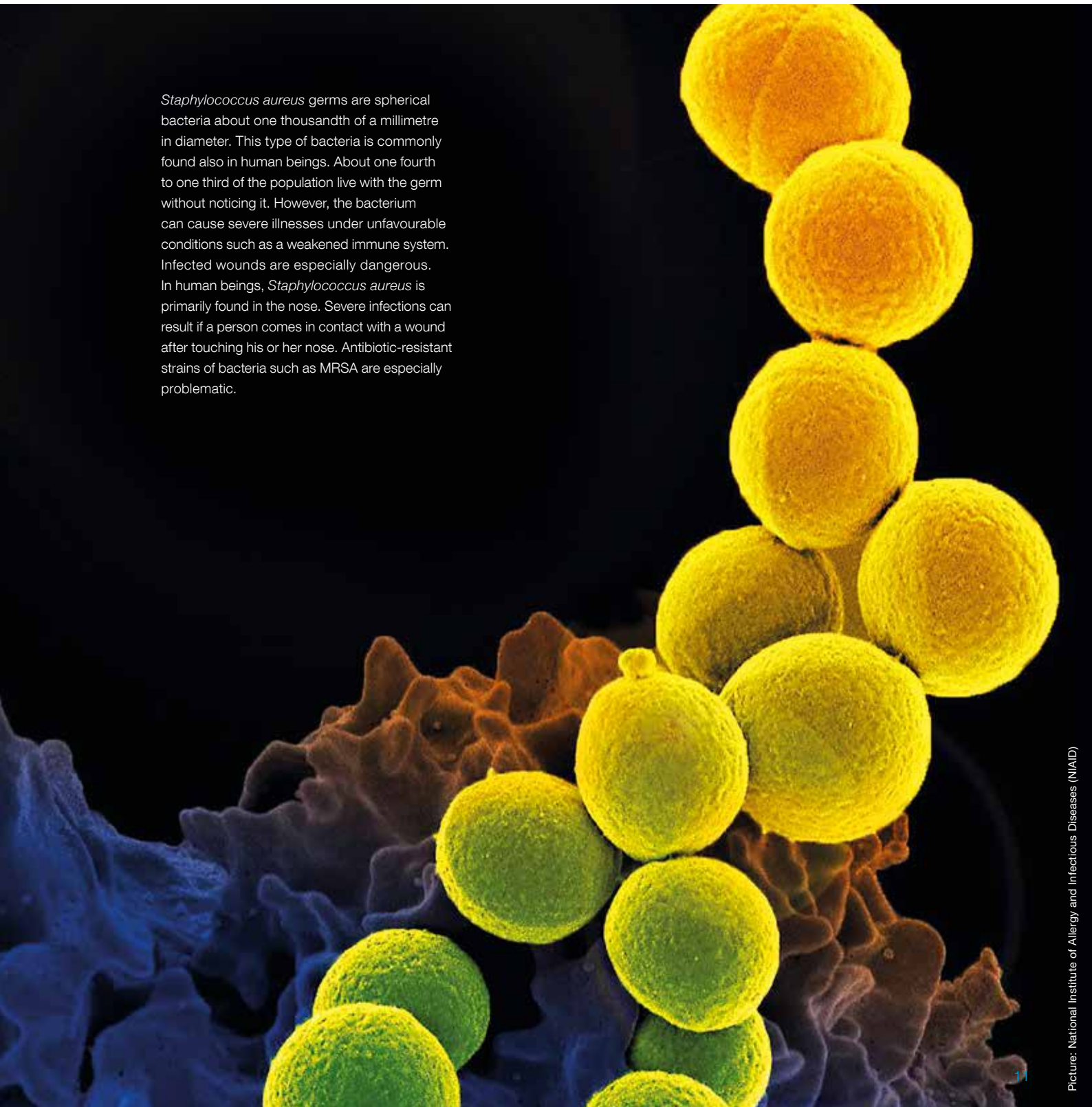
"Of the twelve original candidate drugs, three have proved to be promising," reports Perbandt. "These are now being tested on cell cultures." Whether this will eventually lead to a new treatment is not yet certain, but the approach of custom-designing an active ingredient using knowledge of the precise atomic structure of a biomolecule is not only suitable for medication used for treating MRSA. "This new method of structure-based drug development is a promising means of fighting other pathogens too," says Perbandt. And the method has additional advantages: "Structure-based drug development not only saves money, but also greatly reduces the need for animal testing."

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Scientific Reports, 2016; DOI: 10.1038/srep22871

“This new method of structure-based drug development is a promising means of fighting other pathogens too”

Markus Perbandt, University of Hamburg

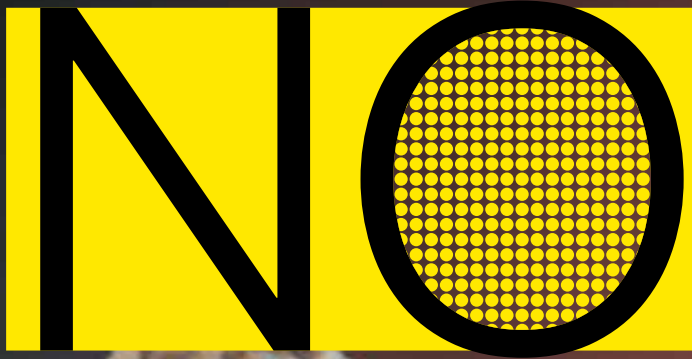
Staphylococcus aureus germs are spherical bacteria about one thousandth of a millimetre in diameter. This type of bacteria is commonly found also in human beings. About one fourth to one third of the population live with the germ without noticing it. However, the bacterium can cause severe illnesses under unfavourable conditions such as a weakened immune system. Infected wounds are especially dangerous. In human beings, *Staphylococcus aureus* is primarily found in the nose. Severe infections can result if a person comes in contact with a wound after touching his or her nose. Antibiotic-resistant strains of bacteria such as MRSA are especially problematic.



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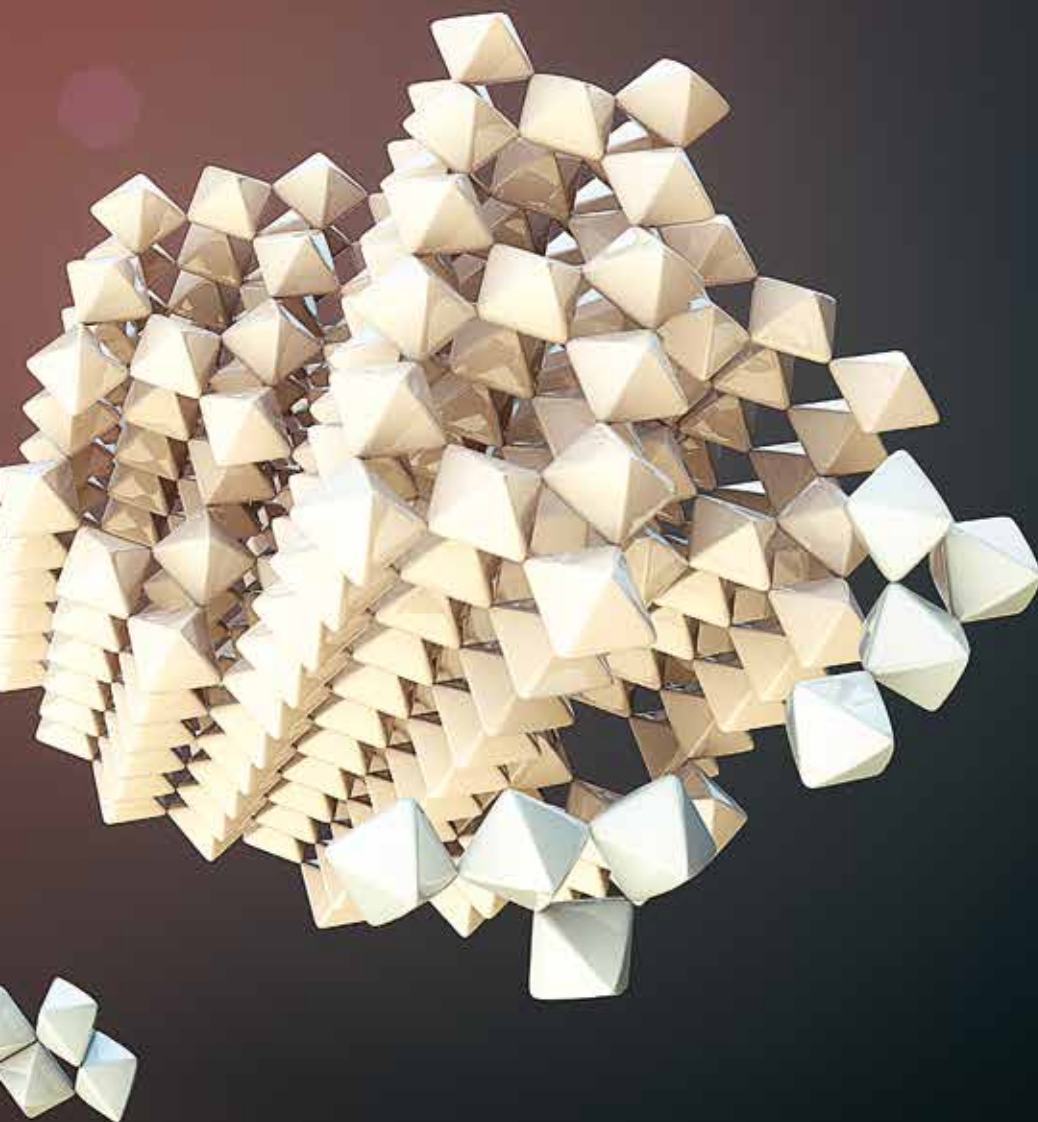


Will a millionth of a millimetre be the yardstick of the future?



Nano is a buzzword that almost everyone is familiar with. Moreover, nano is small – very small in fact. One nanometre is one millionth of a millimetre. At the nanoscale, matter has different physical and chemical properties than matter measured in centimetres or metres. Because nanoparticles are so small, they

have a large surface area relative to their volume. This makes them chemically reactive and interesting for scientists and industry. At DESY's X-ray radiation sources, researchers can investigate nanomaterials down to the last atom and tailor their properties to different uses.



A nanoparticle of tungsten trioxide, which can be used for solar cells and smart windows, for example

NANO hits it big

Why these “dwarfs” are all the rage at DESY



Andreas Stierle heads the DESY NanoLab and is professor of nanosciences at the University of Hamburg.

What do power drills, kitchen pots and garden gnomes have in common? Almost nothing, other than that they all are about 20 to 40 centimetres long. Nobody would think of lumping all of these artificial objects together as “centimetre technology,” writes physicist Christian Meier in his book *Nano*. But that’s precisely what people did with the term “nanotechnology”. “Nano”, which is derived from the Greek word “nanos”, meaning “dwarf”, is used as a prefix to signify a billionth part of a unit of measurement. In the case of nanotechnology, it refers to lengths of a billionth of a metre. There certainly is a reason why this “dwarf” among the units of length is causing a stir, while nobody’s ever heard of “centimetre technology”: Structures and systems that measure less than 100 nanometres demonstrate new functional properties that don’t occur in corresponding macroscopic systems.

This fact has attracted scientists as well as business people and created a whole new field of research and industry aiming to investigate the new phenomena, laws and applications of structures measuring less than 100 nanometres. Nanostructures permit improved or new functionalities for catalysts, data storage systems and sensors, for example. Moreover, nanoscientists are also focusing on the properties of individual nanoparticles. These properties are as diverse as the tiny particles’ areas of application.

A series of scientific breakthroughs made researchers aware of these “dwarfs” in the first place. “Scanning electron microscopes and other techniques let us access ultrascale scales,” explains Andreas Stierle, head of the DESY NanoLab. “Advanced X-ray radiation sources based on electron accelerators open up an especially diverse range of possibilities and can even depict dynamic processes in the nanoworld with atomic resolution.”

“Advanced X-ray radiation sources open up an especially diverse range of possibilities and can even depict dynamic processes in the nanoworld with atomic resolution.”

Andreas Stierle, DESY

At the DESY NanoLab, Stierle and his team combine these radiation sources with a range of analytical equipment and methods in order to investigate materials, nanoparticles, surfaces and processes at the nanoscale, determine their atomic structure and chemical composition, and thus ascertain the nanomaterials’ potential for application. >>



Picture: DESY, Heiner Müller-Eisner

At the DESY NanoLab, scientists can, among other things, use an ultrahigh-vacuum facility to analyse nanosamples with a variety of methods.

femtopolis

Small, smaller, smallest

Mikros” – the Greek word for “small” – serves as the basis for the prefix “micro”, which is the millionth part of a unit of measure. Actually, the millionth part of a metre is already pretty small and a millionth of a second is damned short. However, science today has long left the “micro” stage behind it – small is no longer small enough. Instead, researchers

are now dealing with billionths of a metre in the nanoworld and don’t even recoil from the “femto” scale with its quadrillionths parts of a unit of measure. Whereas “nano” is especially popular when it comes to lengths, because materials demonstrate promising new properties in the nanometre range, “femto” is most appealing to scientists when applied to units of time.

The head of a pin has a diameter of one million nanometres. A human hair is about 80 000 nanometres thick, viruses between 50 and 100 nanometres. Nanotechnology operates at a scale of about 1 to 100 nanometres. And the interplay between the atoms and molecules that nanoscience is investigating occurs at the femtosecond scale.

A femtosecond is one quadrillionth of a second – an unimaginably short amount of time when you consider that human reaction times are about one-tenth of a second. This one-

tenth of a second equals 100 million femtoseconds. Chemical reactions take place at the femtosecond scale, as do the movements of biomolecules. That’s why femtoseconds are so interesting for scientists.

Researchers wanting to proceed to the atomic level end up at the Ångström scale. This unit of length, named after the Swedish physicist Anders Jonas Ångström, corresponds to one-tenth of a nanometre. The Ångström is the typical scale for atomic radii, the distances between atoms in crystal structures and the bond lengths in molecules.

The proper time scale for observing the inner workings of atoms is the attosecond, which is a quintillionth of a second – or, to put it another way, the billionth part of a billionth of a second. The electrons in an atomic shell move within a matter of attoseconds. Using ultrashort laser pulses, scientists are conducting research at even this time scale.

> A live view of catalyst deactivation

An example are catalysts, which are materials that speed up chemical reactions or make them possible in the first place, without themselves being consumed. They are indispensable for many industrial processes – from environmental technology and manufacturing processes for fuels to the production of fertiliser for agriculture. The best-known example is undoubtedly the catalytic converter in cars. This device uses a mixture of platinum, rhodium and palladium to convert toxic carbon monoxide and harmful nitrogen oxides into less hazardous compounds. For the first time, Stierle and his team have now observed “live” at the nanoscale how the platinum nanoparticles found in a car’s catalytic converter fuse together during its operation, losing some of their efficiency as a result.

The efficiency of a certain amount of catalyst increases with the size of the exposed area. “A sphere with a diameter of one centimetre has a surface area of just over three square centimetres,” explains Uta Hejral from the DESY NanoLab. “In principle, you could make 1.3 trillion tiny spheres with a diameter of ten nanometres, from the same quantity of material, and these would have a total surface area of 386 square metres – roughly two tennis courts.”

However, the size of the particles can change during operation, and this reduces the performance of the catalytic converter. To study the process, the Hamburg scientists observed platinum and rhodium nanoparticles under controlled conditions similar to the real operating conditions prevailing in an automotive catalytic converter. To this end, they first grew nanoparticles consisting of different mixtures of the two metals on a substrate and then used these samples to convert carbon monoxide (CO) and oxygen (O₂) into carbon dioxide (CO₂) in a reaction chamber at 280 degrees Celsius.

Under these reaction conditions, which are similar to those found in a car’s catalytic converter, the shape of the nanoparticles changed to varying degrees, depending on the ratio of the two metals. “Pure platinum nanoparticles grew appreciably in height, doubling from two to about four nanometres,” reports Hejral. “That came as a real surprise.” Pure rhodium particles on the other hand remained very stable, hardly changing in height. Particles with an equal mixture of platinum and rhodium were almost as stable.

“The study shows that the platinum nanoparticles use the energy released by the

chemical reaction to fuse together,” comments Hejral. “Whereas at the beginning of the experiment, the platinum particles consisted of about 15 000 atoms each, by the end they contained about 23 000. As a result of their agglomeration, the area of the substrate that was coated with platinum nanoparticles dropped from initially 50 percent to about 35 percent.” The researchers believe that the platinum particles strive to adopt a more favourable spherical shape, which is associated with a lower energy level. The manufacturing of nanoparticles with shapes close to the ones that resulted after the agglomeration could reduce the particle rearrangement and hence the drop in efficiency.

Automotive catalytic converters are already largely optimised based on experience, but there are still many open questions concerning the processes that take place on the atomic scale under reaction conditions. These need to be understood to improve the catalyst’s lifetime and efficiency. The new method yields insights into these processes and can be used for applications other than automotive catalytic converters, as Stierle points out. “Our method allows us to determine the optimum mixtures and particle sizes experimentally. This can be used for catalysts in all kinds of different applications, and could open up entirely new possibilities in the chemical industry.”

“Pure platinum nanoparticles grew appreciably in height, doubling from two to about four nanometres”

Uta Hejral, DESY NanoLab

High-speed X-ray technique

At DESY’s PETRA III X-ray radiation source, researchers have also developed a high-speed X-ray technique that enables them to observe catalysts at work in real time. It enables atomic surface structures to be determined so quickly that live recordings can be made of surface reactions like catalysis and corrosion with a time resolution of less than a second. “We can now investigate surface processes that were not observable in real time before and that play a central role in many fields of materials science,” explains Stierle.



Scientist Uta Hejral analysed catalyst nanoparticles at the DESY NanoLab.

The new technique is made possible by the high-energy X-rays of PETRA III, which are scattered into a very small angular range. This lets researchers produce a comparatively compact diffraction pattern that can be recorded at once with a high-end two-dimensional detector. "This approach makes it possible to record data 10 to 100 times faster," explains Stierle. As a consequence, scientists can obtain a full surface structure in less than ten minutes or track individual structural features with a time resolution of less than a second. "We are getting new insights into the kinetics of surface processes, enabling the design of new materials on the atomic level," reports Stierle.

"We can now investigate surface processes that play a central role in materials science."

Andreas Stierle, DESY

Towards the "molecular cinema"

Entire films of the atomic processes on catalytic surfaces can be recorded using the latest generation of X-ray radiation sources – the free-electron lasers. For example, an international team headed by researchers from Hamburg used the X-ray laser LCLS at the US accelerator centre SLAC to observe a catalytic surface in action at the molecular level. For the first time,

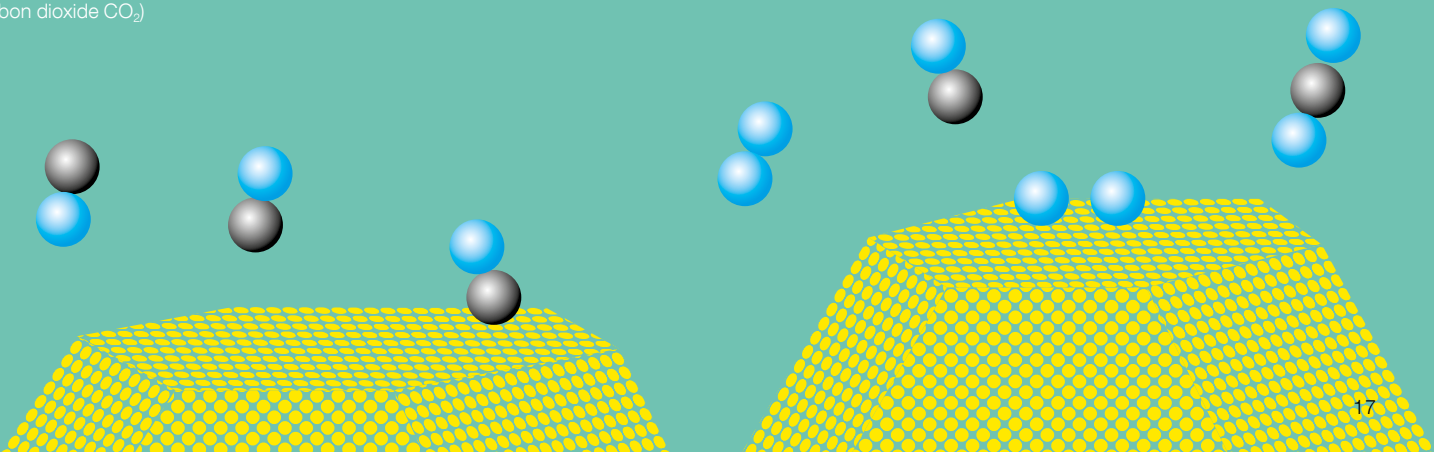
the scientists were able to directly detect a transition state in which the molecules briefly float above the catalyst before they finally fly away. Although more experimental development work will be needed before a complete catalytic reaction on a catalyst in widespread use can be examined with an X-ray laser, the recent observation is an important first step in the investigation of the ultrafast dynamics of surface reactions.

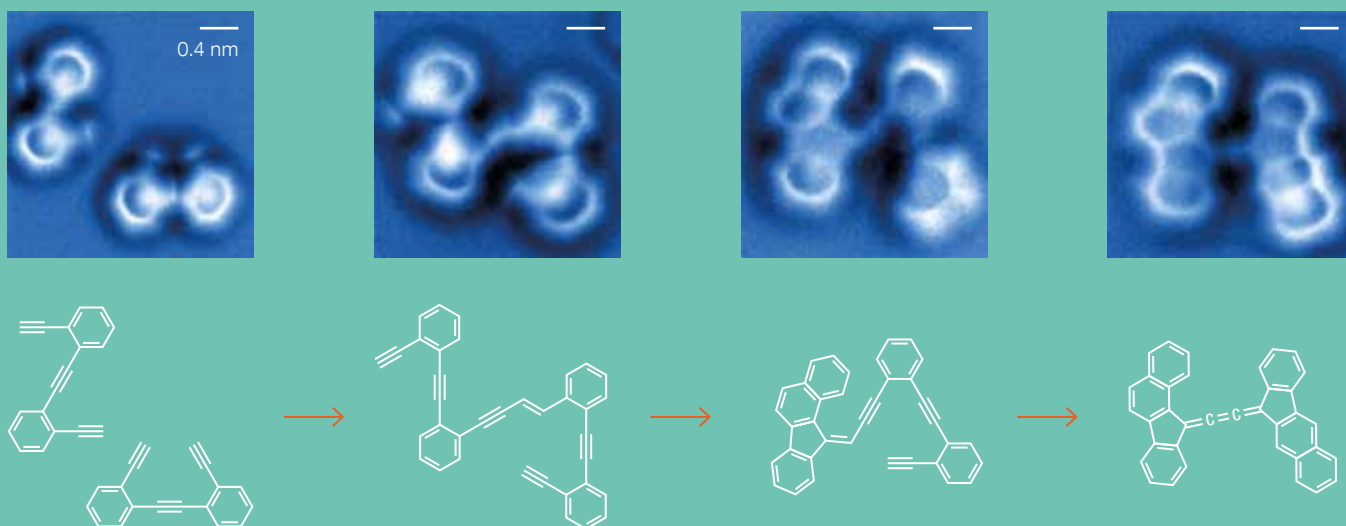
"This investigation showed that it's possible to use X-ray lasers to observe such processes," says Wilfried Wurth, the leading scientist responsible for DESY's free-electron laser FLASH. "It also opens up the possibility of examining much more complex reactions."

In another first, a German-American research team has used FLASH to determine the three-dimensional shape of free-flying nanoparticles of silver. The results show that the tiny particles have a much greater variety of shapes than expected. The functionality of nanoparticles is connected to their geometric shape. This shape can be computed by examining the characteristic way in which the particles scatter X-ray radiation. X-ray sources such as FLASH and the X-ray laser European XFEL, which is currently being built in the Hamburg area, thus serve as a kind of super microscope for the nanoworld.

The possibility of determining the three-dimensional shape of nanoparticles with just one X-ray laser pulse opens up many new fields of research. In future projects, it could for example be possible to directly "film" particle growth in three dimensions. >>

Platinum nanoparticles at the beginning of the experiment (left, in flow of carbon monoxide CO) and after fusing together (right, during the reaction of oxygen O₂ and carbon monoxide CO to form carbon dioxide CO₂)





Chemists have long wished to directly observe how the structure of molecules changes during a chemical reaction. Chemical reactions temporarily create reaction intermediates, which immediately reform into new products. The structure of such reaction intermediates provides detailed insights into the reaction mechanisms, which is of great interest for the chemical industry as well as for other disciplines such as materials science, nanotechnology, biology and medicine. What exactly reacts when with what? Unfortunately, the short lifetimes of reaction intermediates make it particularly difficult to identify and characterise them.

An international research team headed by Felix Fischer, Michael Crommie (University of California, Berkeley, and Lawrence Berkeley National Laboratory) and Angel Rubio (Max Planck Institute for the Structure and Dynamics of Matter at the Centre for Free-Electron Laser Science CFEL in Hamburg as well as University of the Basque Country in San Sebastián) have now observed a complex, technologically relevant catalytic reaction in detail. The images, which were recorded using an atomic-force microscope, show how two organic molecules from the class of enediyne bond at a silver catalyst to create ring-shaped structures and finally produce a new molecule.

> Nanoparticles enhance performance of solar cells

Organic solar cells made of polymers have tremendous potential. They are inexpensive, flexible and extremely versatile. Their drawback compared with the established silicon solar cells is their lower efficiency. Typically, they only convert a few percent of the incident sunlight into electrical power. Nevertheless, organic solar cells are already economically viable in many situations, and scientists are looking for new ways to increase their efficiency.

One promising method is the addition of nanoparticles. It has been shown, for example, that gold nanoparticles absorb additional sunlight, which in turn produces additional electrical charge carriers when the energy is released again by the gold particles. Magnetic nanoparticles too can increase the performance of solar cells made from polymers – provided the right mixture is used. This has been shown in another study at DESY's X-ray source PETRA III. Adding about one percent of such nanoparticles by weight makes the solar cells more efficient, according to the findings of a team of scientists headed by Peter Müller-Buschbaum from the Technical University of Munich in Germany.

“The light creates pairs of charge carriers in the solar cell, consisting of a negatively charged electron and a positively charged hole, which is a site where an electron is missing,” explains Daniel Moseguí González from Müller-Buschbaum's group. “The art of making an organic solar cell is to separate this electron-hole pair before they can recombine. If they did, the charge produced would be lost. We were looking for ways of extending the lifetime of the electron-hole pair, which would allow us to separate more of them and direct them to opposite electrodes.”

Nanoparticles of magnetite (Fe_3O_4) are in fact able to do just that. “In our experiment, adding magnetite nanoparticles to the substrate increased the efficiency of the solar cells by up to 11 percent,” reports Moseguí González. The lifetime of the electron-hole pair is significantly prolonged.

Adding nanoparticles is a routine procedure, which can easily be carried out in the course of the various processes for manufacturing organic solar cells. It is important, however, not to add too many nanoparticles to the solar cell, because the internal structure of organic solar cells is finely adjusted to optimise the distance between the

light-collecting active materials, so that the pairs of charge carriers can be separated as efficiently as possible. These structures lie in the range of 10 to 100 nanometres.

“Adding magnetite nanoparticles to the substrate increased the efficiency of the solar cells by up to 11 percent.”

Daniel Moseguí González, Technical University of Munich

“The X-ray investigation shows that if you mix a large number of nanoparticles into the material used to make the solar cell, you change its structure”, explains DESY physicist Stephan Roth, head of the beamline where the experiments were conducted. “The solar cell we looked at will tolerate magnetite nanoparticle doping levels of up to one percent by mass without changing the structure.”

The scientists observed the largest effect when they doped the substrate with 0.6 percent

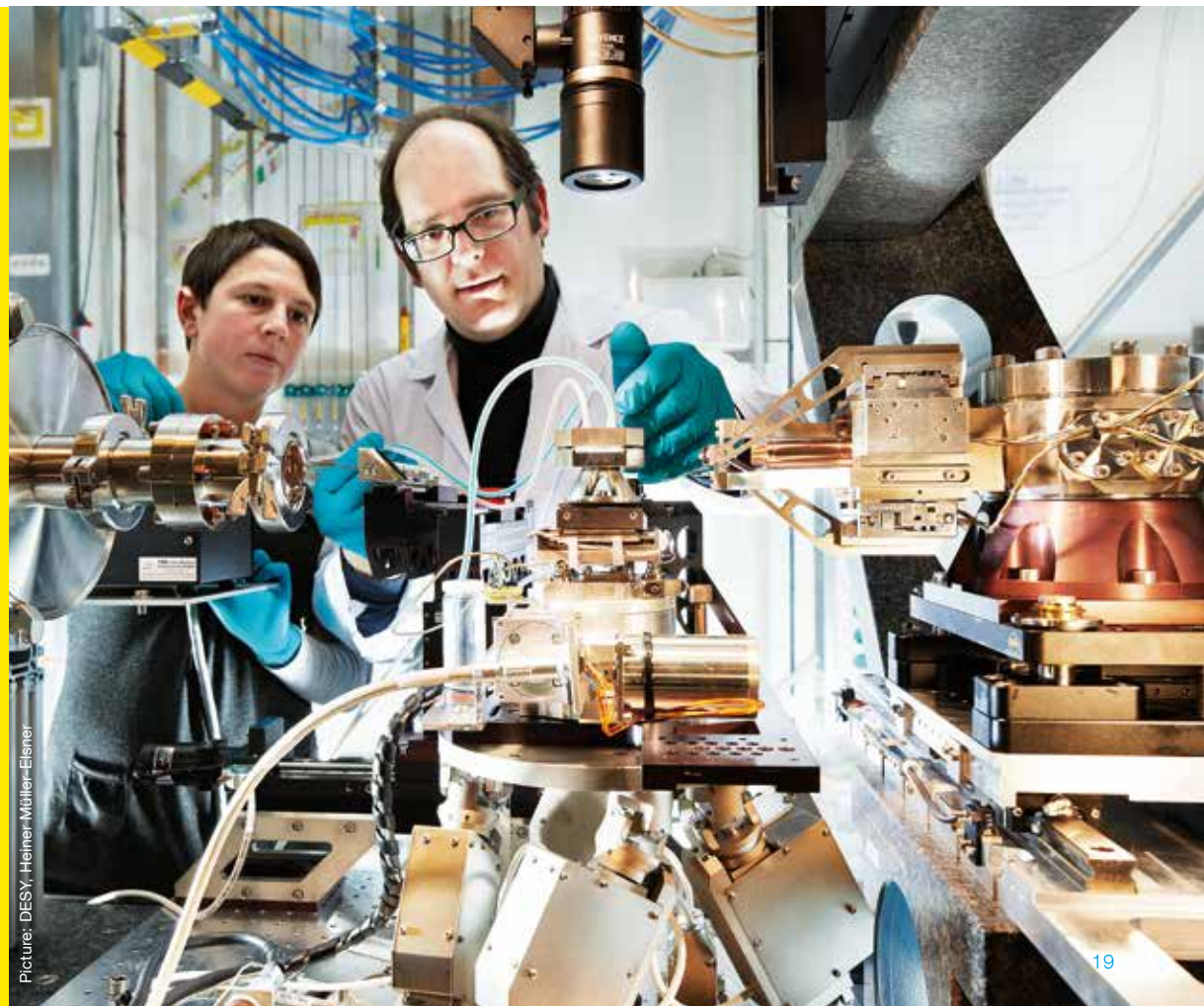
nanoparticles by weight. This caused the efficiency of the examined polymer solar cell to increase from 3.05 to 3.37 percent. “An 11 percent increase in energy yield can be crucial in making a material economically viable for a particular application,” emphasises research leader Müller-Buschbaum.

The researchers believe it will also be possible to increase the efficiency of other polymer solar cells by doping them with nanoparticles. “The combination of high-performance polymers with nanoparticles holds the promise of further increases in the efficiency of organic solar cells in the future. However, without a detailed examination, such as that using the X-rays emitted by a synchrotron, it would be impossible to gain a fundamental understanding of the underlying processes involved,” concludes Müller-Buschbaum.

Innovative tandem solar cells

The trick to creating highly promising tandem solar cells is to use a combination of ultrathin layers. To increase efficiency, a second polymer solar cell is stacked on top of the first one, which absorbs a different part of the solar spectrum. The resulting tandem polymer solar cell converts >>

DESY scientist Stephan Roth analyses various nanomaterials at the X-ray radiation source PETRA III.



Picture: DESY, Heiner Müller-Elsner

more of the incoming sunlight into electric current, thus increasing the energy yield.

But the multilayer coating presents several special challenges, as research leader Jens W. Andreasen from the Technical University of Denmark (DTU) in Roskilde explains: “Lab studies have shown that already coated layers may be dissolved by the solvent from the following layer, causing complete failure of the solar cell.” To prevent redissolution of the first solar cell, the scientists added a carefully composed protective coating between the two tandem solar cell layers. Among other things, the protective coating contains a layer of zinc oxide that is just 40 nanometres thick.

“With 3D ptychography, we were able to image the complete tandem solar cell”

Gerald Falkenberg, DESY

To check the shape and function of the protective coating and the other layers of the tandem solar cell, the scientists used a special X-ray technique at PETRA III. “With 3D ptychography, we were able to image the complete roll-to-roll coated tandem solar cell, showing, among other things, the integrity of the 40-nanometre-thin zinc oxide layer in the protective coating, which successfully preserved the underlying layers from solution damage,” says DESY scientist Gerald Falkenberg, head of the experimental station where the

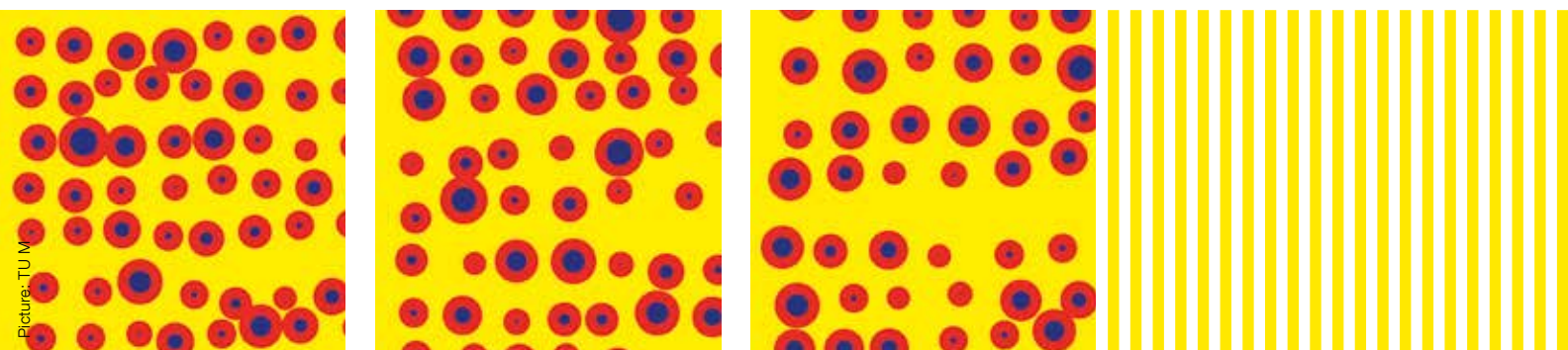
investigations were made. This finding paves the way to a possible industrial application of the technique.

Nanomaterials with new properties

Classical materials such as ceramics, metals and polymers have their typical mechanical properties. They are hard, soft, strong, flexible or stiff. Scientists from the Hamburg University of Technology (TUHH), the University of Hamburg, Helmholtz-Zentrum Geesthacht and DESY have now synthesised a nanomaterial that unites several different properties and could thereby open the way to new applications in medical engineering and manufacturing. The innovative material is at the same time strong, hard and very stiff. On the smallest scale, its structure resembles that of biological hard tissue, such as mother of pearl and dental enamel. It consists of uniformly sized iron oxide nanoparticles, which are coated with organic oleic acid.

By applying a controlled thermal treatment and other means, scientists have managed to create a very strong bond between the oleic acid molecules, thereby markedly improving the mechanical properties of the nanocomposite. This new class of material could, for example, be suitable for filling dental cavities or manufacturing watch cases. The materials used in applications like these need to be both hard and damage-tolerant.

The bonding properties of the oleic acid, which serves as an adhesive, were examined spectroscopically by the staff of the DESY NanoLab. “Our measurements showed that the oleic acid molecules survive the thermal



Schematic depiction of the active layer of an organic solar cell: The orange dots represent the active domains, where light is converted into charge carriers. Researchers at the Technical University of Munich used DESY's PETRA III X-ray radiation source to observe the degradation of these solar cells in real time. During operation, the domains increase in diameter and become more widely spaced.

treatment and form additional crosslinks during the process,” reports NanoLab director Stierle. “This important finding can serve as the basis for successfully modelling the mechanical properties of this novel material.” Since oleic acid is very often used when processing other nanoparticles too, this method could potentially improve the mechanical properties of a great many other nanomaterials as well.

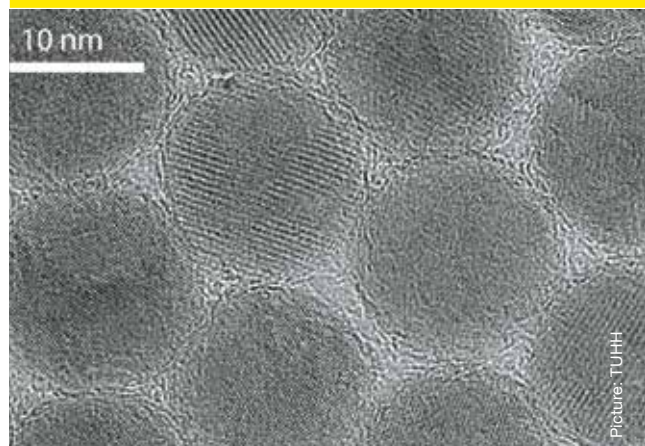
Self-organisation in the nanoworld

Researchers at DESY have also developed a new procedure that allows metallic nanostructures to simultaneously 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 too, in which nanostructures are used more and more often. For many scientific questions and technological applications, it is essential that the nanostructures repeat in an ordered pattern. The size and separation of the individual elements of such patterns can lie anywhere between a few nanometres and several hundred nanometres. 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 method allows extremely uniform nanostructures to be created in highly regular patterns”

Denise Erb, DESY

“Most importantly, the method allows extremely uniform nanostructures to be created in highly regular patterns with comparatively little effort,” explains Denise Erb from Ralf Röhlsberger’s research group at DESY. A special setup allowed the scientists to use the X-ray radiation source PETRA III to actually watch the nanostructures as they grew. “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 big advantage of this approach is that the



High-resolution electron micrograph of nanoparticles of iron oxide surrounded by oleic acid molecules

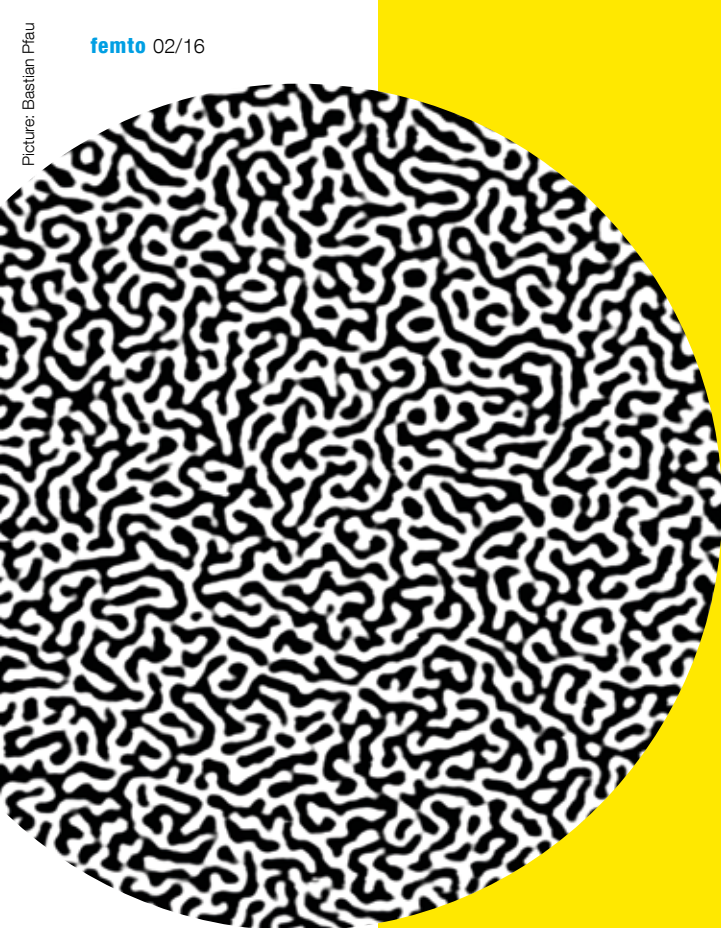
Picture: TUHH

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 structures and 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 Röhlsberger.

The miniaturisation of data storage devices

Nanostructures also open up new possibilities for developing increasingly smaller and faster magnetic data storage systems. In order to understand the processes that underlie magnetisation in detail, scientists are using facilities such as the free-electron laser FLASH. “The ultrashort X-ray flashes enable FLASH to determine even the tiniest temporal and spatial changes in the size and properties of magnetic domains,” explains DESY leading scientist Gerhard Grübel, whose group uses X-ray laser light to analyse magnetic materials and other substances. >>



The magnetic-force microscope image shows the magnetic domains' labyrinthine structure.

> Iron and other ferromagnetic materials are often divided into nanometre-sized magnetic domains. At FLASH, an international research team headed by Grübel and Stefan Eisebitt from Berlin Technical University in Germany has discovered that electrons can move very quickly back and forth between areas with different magnetisation and thereby influence the demagnetisation of the material. This effect could play a crucial role in the miniaturisation of magnetic storage systems.

The researchers first used a short laser pulse to induce the demagnetisation of the sample, which they afterwards analysed with the X-ray laser light. "Optical demagnetisation is by far the quickest process for locally changing magnetisation, and this in turn is the basis for magnetic data storage," explains Eisebitt. "Optical processes could therefore help make magnetic storage systems faster in the future."

Supermicroscopes for nanoscience

Because short-wave X-ray light is ideal for making atoms and molecules visible, there is a correspondingly big demand for such radiation among nanoscientists. "DESY's X-ray sources FLASH and PETRA III are ideal supermicroscopes for observing and understanding structures

and processes in the nanoworld," states DESY Research Director Edgar Weckert. "At our Hamburg campus, we work together with various institutions and partners to conduct interdisciplinary research on materials and substances at the nanoscale."

In the field of materials research, DESY cooperates closely with Helmholtz-Zentrum Geesthacht in Germany. It also works together with the University of Hamburg, which operates several institutes in the vicinity of DESY and is currently setting up the Center for Hybrid Nanostructures, which specialises in the combination of nanoelectronic and biological materials.

"DESY's X-ray sources FLASH and PETRA III are ideal supermicroscopes for observing and understanding structures and processes in the nanoworld"

Edgar Weckert, DESY

"The nanosciences have huge potential," says Weckert. "Nanoscientists are developing materials with completely new properties as well as innovative applications for areas such as healthcare, mobility and future energy supplies."



Edgar Weckert is Director in charge of Photon Science at DESY.

The MIXTURE

matters

Many researchers are convinced that combining a variety of materials at the nanolevel opens up huge possibilities. To research such materials, the University of Hamburg is currently building the Center for Hybrid Nanostructures (CHyN) on the DESY campus in Hamburg. The centre will be completed later this year and go into operation in 2017. Its first director is Robert Blick, head of the Institute of Nanostructure and Solid-State Physics (INF) at the University of Hamburg.

femto: Mr. Blick, what are hybrid nanostructures?

Blick: Hybrid nanostructures primarily involve the mixing of different materials at the nanometre level. These structures combine semiconductors with magnetic metals, for example, or semiconductors with biological materials. Such mixing can create completely new functions. These arise from the material mix or from the fact that many materials gain entirely new properties at the nanoscale.

femto: What can these structures be used for?

Blick: A great example is our current partnership with Lund University in Sweden. In this cooperation, we are combining nanowires with living nerve cells. The colleagues from Lund have installed a kind of solar cell in these wires, which are up to 50 nanometres thick and a few micrometres long. When light shines on this structure, it creates a voltage that can be used to activate a cell's function. For example, we are using this method to experiment with ways of triggering the action potential of nerve cells from mice. That could be the first step towards the creation of a retinal implant, for example.

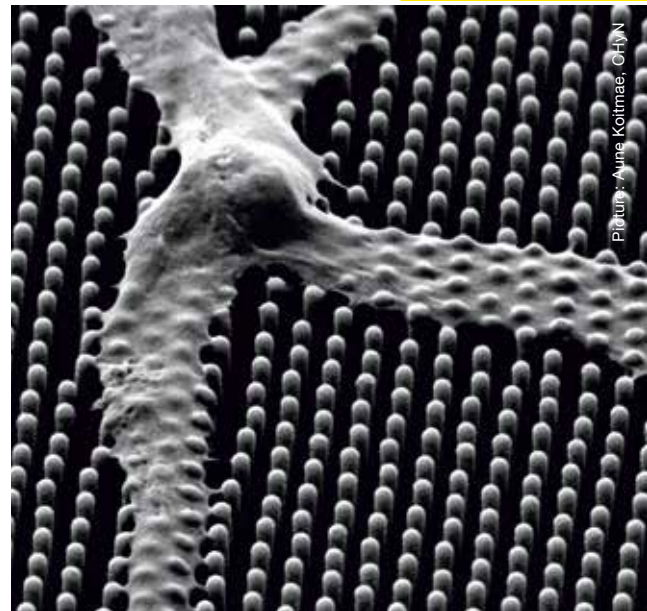
femto: That sounds futuristic.

Blick: Yes, that's more or less something for the far future. However, we are also creating things that are already being used. For example, we are working with a company in California to develop a high-throughput device for genome analysis. In such systems, the DNA base pairs move through nanopores and are optically read out. To date, you have to reduce the speed of the base pairs because the analysis methods aren't fast enough. In our new approach, we can accelerate the process tenfold by implementing an electric radio frequency setup around the nanopore.

femto: Where do these materials have great potential?

Blick: We are pursuing a completely new approach. We are creating materials at the interface between traditional solid-state physics and quantum mechanics. When you bring physics, biology and chemistry together at this scale, you create something completely new. This can go into any direction whatsoever. We can create and use properties and functions that aren't available at other levels. I think this is clearly the wave of the future.

<http://www.chyn.de/>



Mouse nerve cell growing on a matrix of nanowires

The BOOM in NANO RESEARCH

The potential offered by nanotechnology is vast – and largely still awaiting research and application. All around the world, science and industry are busy working on ways of using nanomaterials. Potential applications range from batteries and displays to textiles, packaging and medical technology.

Although they are invisible even under a conventional microscope, a glance at the label of numerous products tells you they are there: nanoparticles, which have long since left the laboratory to become a feature of everyday life. In sunblock, for example, minuscule particles of titanium dioxide protect our skin against ultraviolet radiation. Likewise, nanoparticles of silver help to neutralise the smell of sweat in T-shirts and to make plasters antiseptic. The electronic switching elements in computer chips exploit nanotechnology, as do self-cleaning coatings for cars and roof tiles. Yet this is only the beginning: Experts predict many more applications for nanoparticles. In the future, they could well help in the fight against cancer and other diseases as well as secure our energy supplies and neutralise pollution.

And although it is still early days, nanotechnology is more than just a fancy name for a developing research field with a considerable number of everyday applications. The truly exciting thing about this technology is that it becomes possible to manipulate structures that are smaller than 100 millionths of a millimetre, i.e. 100 nanometres. It's only recently that researchers have started to understand and, most importantly, exploit such effects.

Football-like fullerenes

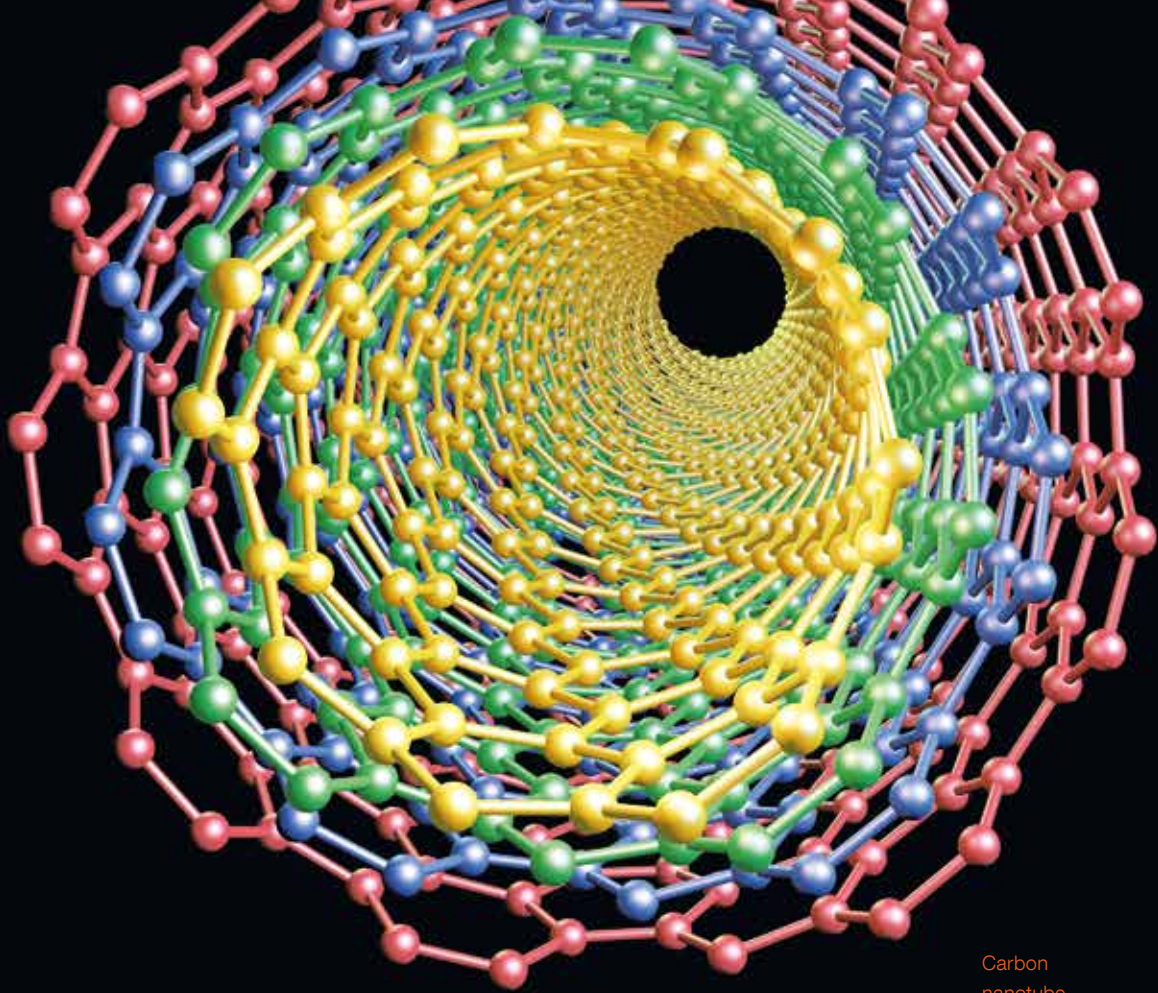
In 1981, the scanning tunnelling microscope was unveiled. This was the first instrument to provide a reasonably three-dimensional view of structures in the nanoworld. In the following years, scientists discovered a number

of nanoparticles with spectacular properties. The first big hype was sparked by so-called fullerenes – carbon molecules that look like tiny footballs. Researchers had been close to a breakthrough for quite some time, but it was not until 1985 that the chemists Harold Kroto, Robert Curl and Richard Smalley first described the fullerenes in the scientific journal *Nature*. A fullerene consists of 60 carbon atoms. Its surface is made up of 12 pentagons and 20 hexagons – just like an association football. At the time, experts were convinced that the discovery of fullerenes would launch a whole new chemistry. In 1996, the scientists who made the discovery were awarded the Nobel Prize in Chemistry.

“Back then, folks were predicting a big future for fullerenes,” says Karl-Heinz Haas, Managing Director of the Fraunhofer Nanotechnology Alliance, which focuses on research into nanomaterials and their application. “But to date, their uses have remained limited.” For example, fullerenes are found in anti-aging crèmes on account of their high electron affinity, which makes them good free-radical scavengers. But that's not the new chemistry that experts were dreaming of. “In the future, fullerenes may turn out to have a useful role to play in medicine and photovoltaics,” says Haas.

In the early 1990s, the Japanese researcher Sumio Iijima discovered another highly promising nanomaterial: so-called carbon nanotubes, cylindrical molecules of carbon with a specific strength way in excess of steel. Nanotubes are incredibly robust and conduct electrical current and heat better than any other known material. Their discovery prompted many a flight of fancy among materials scientists, ranging from the development of high-resolution displays with extremely low energy consumption to ultratensile fibres that engineers could use to build elevators all the way up to satellites in orbit. Nanotubes are currently found in batteries, displays and sporting equipment. The problem is, however, that they remain very expensive to produce. “At present, efforts are focused on trying to reduce production costs,” says Haas.

The most recent discovery of another carbon nanomaterial was also rewarded with the Nobel Prize in 2010: graphene, a two-dimensional lattice of carbon atoms. The two physicists Andre Geim and Konstantin Novoselov first demonstrated its existence in 2004. Using adhesive tape, they painstakingly stripped layer after layer from a piece of graphite until only a single layer, one atom in thickness, remained. They had produced graphene.

Carbon
nanotube

Researchers are fascinated in particular by the excellent electrical conductivity of graphene, which makes it a candidate for a host of applications. “It’s almost transparent, which means it is interesting for flexible applications such as touchscreens,” says Haas. Scientists hope soon to be able to build graphene transistors, which will be much faster than conventional silicon ones. Indeed, the IT company IBM has recently unveiled a prototype.

“Our task is to do the spadework and show that we can convert this know-how and these discoveries into products that bring a tangible benefit”

Karl-Heinz Haas, Fraunhofer Nanotechnology Alliance

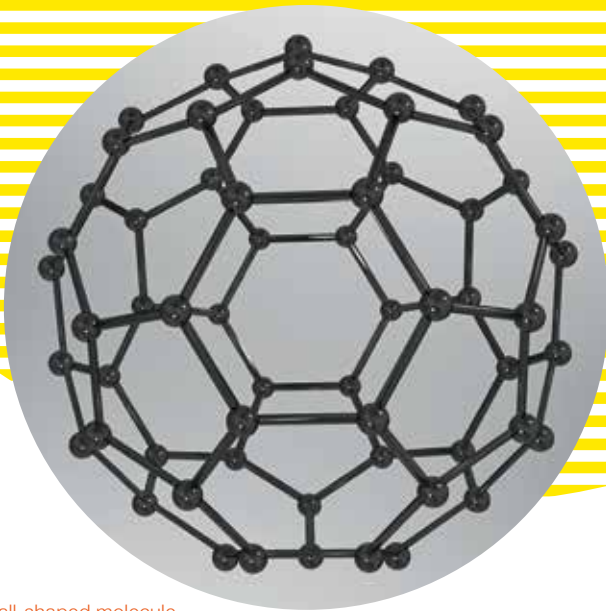
Industrial nanomaterials

Aside from carbon nanoparticles, industry produces quite a number of other nanomaterials. These are used in a wide range of technical areas

as well in consumer products such as paint, cosmetics, textiles and packaging materials. Such materials include nanosilver, titanium dioxide and nanoclay.

“There’s a lot here that is more than just a vision,” says Haas. “There are already lots of applications.” Experts are beginning to realise just what this technology can do. But it all takes time and patience. “Our task is to do the spadework and show that we can convert this know-how and these discoveries into products that bring a tangible benefit.” That’s what researchers and industry are now doing worldwide. According to the German Federal Ministry of Education and Research (BMBF), in Germany alone there are over 2000 institutions involved in work with nanotechnology, including around 200 research institutes and 600 academic research organisations.

The range of research interests is extremely diverse – not surprisingly, given the wide scope of applications for nanotechnology. According to the latest *Nano Report* from the BMBF, the most common research topic is nanomaterials, followed by nanocoatings, nanoanalytics and nanobiotechnology. Applications in the field of nanomaterials are the most successful. >>



Football-shaped molecule (fullerene) made up of 60 carbon atoms

> Uses in medicine

The *Nano Report* shows that experts are particularly pinning their hopes on developments in the medical field. The research institutes canvassed in the report predict that in the coming years, it will be the areas of medicine, pharmaceuticals and energy technology that profit most from the achievements of nanotechnology. They have thus displaced electronics, where, as Haas explains, nanotechnology is already standard. “Over the last five or ten years, micro-electronics has effectively become nano-electronics. All the structures are smaller than 100 nanometres.”

In the field of medicine too, there have been a number of advances in recent years. Scientists have developed a variety of nanoscale systems for transporting pharmaceutical substances and delivering them to precise parts of the body. “Drug-delivery systems is an area where there are more and more applications of nanotechnology,” says Wolfgang Luther from the department for Innovation Mentoring and Consultation at the Technology Centre of the Association of German Engineers (VDI) in Düsseldorf. Polysaccharides or polymers in nanoparticle form are used not only to deliver drugs to a specific part of the body but also to release them at a specific time.

“There’s a lot of hope being pinned on the use of nanotechnology in personalised medicine,” explains Luther. Further advances in high-throughput analysis will enable medical scientists to determine, with ever greater speed and precision, specific characteristics in the genetic makeup and metabolism of individual

patients. And this will provide the basis for developing customised prevention and therapy.

There are also plans to produce spare body parts from nanomaterials using 3D printers. “We’re not talking about complete limbs here,” says Haas from the Fraunhofer Nanotechnology Alliance. “But it’s already possible to make ear ossicles and small dental parts.” That’s a beginning.

Meanwhile, more and more advances are being made in the fields of environmental and energy technology. “It’s already possible to break down atmospheric pollutants using nanomaterials,” says Luther. “It’s their large surface area that makes them so effective, and there’s potential for further progress here.” Research into groundwater remediation is testing nanomaterials made of minuscule particles of iron and active charcoal. It is hoped that these will accelerate the decomposition of chlorinated hydrocarbons in polluted groundwater.

“Energy is one of the focal areas of nanotechnology research in Germany”

Wolfgang Luther, VDI Technology Centre, Düsseldorf

The use of nanomaterials in solar cells and energy storage systems could help to promote the development of renewable energy and cut energy consumption. “Energy is one of the focal areas of nanotechnology research in Germany,” say Luther. A lot of research funding is currently going into the development of battery technology. “High-performance batteries are crucial for putting electric vehicles on the roads. That’s where Germany wants to catch up with the competition from Asia.” Another key component of electric motors are magnets. The raw materials for these are rare earth metals, which are limited in availability. Scientists and engineers therefore hope to develop magnets made of materials free of rare earth metals, such as hard ferrites. These materials could also be used in the generators of wind turbines.

Risks and side effects

The widespread use of these minuscule particles also carries a variety of risks, however. “The problem is that we still know too little about how a lot of nanomaterials and nanoparticles actually work in order to be able to make

a sound assessment in this area,” says Peter Laux, head of the Unit Product Research and Nanotechnology at the Federal Institute for Risk Assessment (BfR) in Berlin. This would require suitable analytical methods in order to trace these minute particles. “But these methods are still under development.”

“The problem is that we still know too little about how a lot of nano-materials actually work”

Peter Laux, BfR Berlin

Scientists are already investigating, for example, how nanoparticles behave in the product life cycle and to what extent they enter water and soil. The washing of laundry, for example, releases silver nanoparticles into the wastewater. Treatment plants are unable to remove these tiny particles completely, with the result that they could accumulate in the water and soil. According to experts, there is risk that in the course of time microorganisms will ingest the silver and be harmed by it.

Work is therefore under way to draw up design criteria for sustainable nanomaterials. For this purpose, scientists are investigating how nanoparticles behave in water, soil and sediments, and whether and how they accumulate in the soil as well as in plants and animals.

Experts from the BfR strongly welcome the EU regulation on cosmetics, which entered into force in July 2013. This requires manufacturers to register with the EU Commission any cosmetic products containing nanomaterials and to indicate on the packaging the presence of such materials by means of the word “nano”. As of December 2004, another regulation on packaging and other materials in contact with foodstuffs stipulates that these may not contain any substances that endanger public health or might change the foodstuffs in any way. This also applies to nanomaterials.

BfR experts recognise a need for more research in the area of textiles. A recent study indicates that nanoparticles embedded in fibres are not released as quickly as those in surface coatings for materials used in a jacket or T-shirt. But a lot of questions remain. It is still unclear, for example, how silver nanoparticles that are released from fabrics behave – whether, for instance, they might penetrate healthy skin and

accumulate in certain types of tissue. All this is currently under investigation.

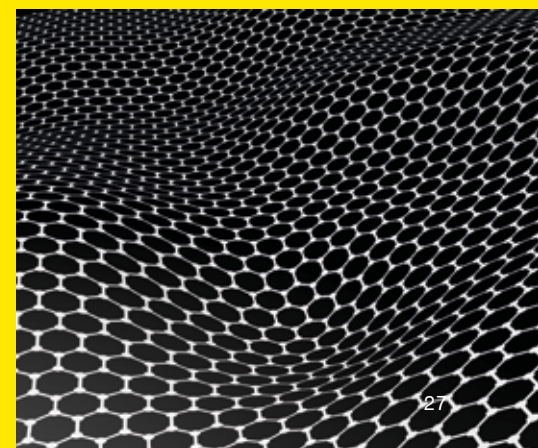
On the other hand, experts are confident that nanoparticles firmly embedded in tennis racquets or computer screens, for example, will stay put. “I’ve got no qualms about using a computer that’s been produced using nanotechnology,” says Fraunhofer researcher Haas. More problematic are nanoparticles that can be inhaled: “It’s still not clear whether nanoparticles can cross the air–blood barrier or other barriers in the body and whether they can then accumulate in the organs or tissue.” For this reason, the BfR advises against the use of sprays that release nanoparticles.

Leading role

Germany, the USA and Japan are the three top countries for cutting-edge research in the field of nanotechnology. “Germany leads the way within Europe,” Haas confirms. When it comes to implementing that technology, however, there’s still scope for improvement. The emphasis in the future will therefore be on turning visions into practicable applications. The job of research will be to determine which applications can be made better and more sustainable by the use of nanotechnology. At the same time, production costs must also come down further.

For the people engaged in basic research, the search continues. “The key question,” says Haas, “is what new materials are still to be found.” Who knows what scientists working with adhesive tape and high-resolution supermicroscopes might yet discover?

Structure of graphene



BRILLIANT RING for NANO RESEARCH

DESY operates one of the world's best X-ray radiation sources: PETRA III. Research groups from around the world use its intense X-ray radiation for a host of experiments, ranging from medical research to nanotechnology. Yet the 2300-metre-long PETRA ring accelerator holds even greater potential. As Christian Schroer, leading scientist at PETRA III, explains, the facility could be extended to create an extremely focused, high-resolution 3D X-ray microscope.

femto: PETRA III is one of the world's top X-ray sources. Why the upgrade to PETRA IV?

Schroer: There's still a long way to go before we reach the limits of X-ray physics. Rebuilding the storage ring will give us an even more tightly focused X-ray beam. The advantage of such a beam is that everything we already do with PETRA III can then be investigated using microscopy techniques – that is, X-ray analysis combined with microscopy.

femto: What does this mean in practice?

Schroer: It means that in future we will be able to investigate samples – and their interior as well – with a spatial resolution in the nanometre range. Most samples are heterogeneous, and their properties display local variation. The only way to determine these variations is with an extremely focused X-ray beam, which will enable us to measure these properties with pinpoint precision.

The very best X-ray microscopes currently available have a maximum spatial resolution of around 10 nanometres. At the atomic level, i.e. on a scale at least 10 times smaller, we can gain insights using diffraction experiments or spectroscopic

methods. PETRA IV will enable us to precisely investigate the gap in between, which is a very interesting area because it's right in this length range that we encounter nanoparticles responsible for processes such as catalysis.

“There's still a long way to go before we reach the limits of X-ray physics”

femto: How will PETRA IV fill this gap?

Schroer: The trick is to focus the beam of X-rays so finely that all the light hits one point. It's only by making the beam as small as possible that we can make use of all the radiation from the source. To date, we can use only one percent of the radiation for X-ray microscopy. The remaining 99 percent is wasted, because the beam is not focused enough for this method.

In the accelerator ring, magnets are used to hold the electrons on their circular path. These magnets have to be arranged so that the

electrons are guided as smoothly as possible around the bend while also remaining tightly collimated on an extremely fine orbit. The larger the storage ring, the better this works. With a circumference of 2300 metres, PETRA is the world's largest storage ring for the production of X-ray radiation. This gives us the option of producing the most tightly collimated beam worldwide. But this goal can only be achieved with novel, very special accelerator technologies, which we plan to use for PETRA IV.

femto: What will this mean for the nanosciences?

Schroer: PETRA IV really will enable us to view individual nanoparticles. Today's experiments often involve a blanket investigation of a large number of nanoparticles. This yields a mean result that doesn't necessarily correspond to the true picture, not least when the particles are all highly dissimilar. That's why we want to take a look at individual nanoparticles under an X-ray microscope.

Ultimately, almost all the methods that we are using today with synchrotron radiation will also be available for spatially resolved use at PETRA IV. This will of course be crucial for the nanosciences, but also for materials research in terms of the analysis and development of nanostructured materials.

femto: Which applications are we talking about here?

Schroer: Important fields include catalysis, battery research, energy generation and also microelectronics. There, for example, you will be able to see the conductors and the transistors in detail. PETRA IV can also make important contributions to the life sciences, environmental sciences and Earth sciences.



Christian Schroer is leading scientist at DESY's X-ray radiation source PETRA III (pictured, rear) and a professor at the University of Hamburg.

In catalysis research, for example, PETRA IV will allow us to observe individual nanoparticles during a reaction. And we'll be doing that practically under normal operating conditions in a real chemical reactor. In other words, we will be able to follow, right down to the atomic level, all the chemical and physical processes that are taking place in a sample.

femto: Will that benefit industry?

Schroer: These new experimental opportunities will help industry lay the foundations for the development of new materials and production processes, which will enable the development of improved catalysts, batteries and other products. For example, it will be possible to follow locally on the nanoscale what happens inside a battery in operation during the normal charge and discharge processes. We will be able to see how and why it ages and to develop ways of preventing this. The same applies to a whole range of material samples – in the field of aircraft construction or lightweight engineering, for example, where you will be able to follow, at atomic

resolution, exactly what happens when such materials are produced and as they wear.

The insights provided by X-ray nanoanalytics will enable pioneering applications in the fields of energy, communications, security, transport and healthcare.

“Using PETRA IV, we can see on the nanoscale what happens inside a battery in normal operation”

femto: The new free-electron lasers, which include FLASH at DESY and the European XFEL, also promise to follow processes with atomic resolution. Where are the differences?

Schroer: The two kinds of facility complement one another in their potential for research. Free-electron lasers produce extremely short and intense pulses of X-ray laser radiation, which you can use to produce genuine snapshots of

a chemical reaction. When you combine a lot of these snapshots in a sequence, you get essentially a film of a molecular process, just like an animation on a time scale of quadrillionths of a second. However, the sample is destroyed by the highly intense radiation used to produce each snapshot, so the reaction has to be repeated again and again.

For a split second, an X-ray laser is 10 billion times brighter than PETRA IV, but over the space of an entire second, both are equally bright. This means that PETRA IV will produce a more continual illumination, which will make it possible to observe nanoparticles in detail over a longer period – such as the processes in a catalytic convertor or a battery. Depending on what you want to know, you need either an X-ray laser or a synchrotron radiation source.

femto: What's the current state of planning for PETRA IV?

Schroer: We will have to rebuild the accelerator within the existing PETRA ring tunnel. The experimental stations will have to be modified or rebuilt from scratch. First of all, there will be a preparation phase. We will draw up a conceptual design report by mid-2018, which will point out the project's scientific and strategic potential and present a technical solution for the new PETRA IV storage ring. There will then be a period of detailed technical planning until 2020, followed by the production of the new components. Reconstruction could then begin by mid-2024 and be completed by 2026.

Gamma-ray astronomy centre

Scientific centre of CTA observatory comes to DESY

In a major step towards the realisation of the Cherenkov Telescope Array (CTA), a large-scale international project in gamma-ray astronomy, the shareholders' meeting of the company CTAO GmbH has decided to locate the Science Data Management Centre and the seat of the CTA scientific director at the DESY location in Zeuthen. The administrative headquarters of the CTA organisation will be in Bologna,



Picture: Jahn Architekten & Ingenieure

Architectural design draft for the CTA scientific centre on the DESY campus in Zeuthen

Italy. "We are very pleased that we have won the international bid and managed to bring the scientific coordination of CTA to Germany," said Beatrix Vierkorn-Rudolph from the German Federal Ministry of Education and Research and deputy chairperson of the shareholders' meeting of CTAO GmbH.

The Cherenkov Telescope Array is a worldwide unique project aiming to build an observatory for gamma-ray astronomy. This



Picture: DESY, Milde Science Comm.

Visualisation of two particle showers over the array of CTA telescopes

observatory will consist of over 100 individual telescopes located at two sites, one in the southern hemisphere and another in the northern hemisphere. Over 1000 scientists and engineers from more than 30 different countries have joined forces to set up the facility over the next five years and operate it for at least 20 years. Negotiations concerning sites in Chile and on La Palma are under way and scheduled for completion by the end of this year.

Helmholtz Prize for science at FLASH

Five scientists from the Goethe University in Frankfurt am Main have been awarded the Helmholtz Prize in Metrology for their high-precision measurements carried out at DESY's X-ray laser FLASH. The team led by atomic physicist Reinhard Dörner used a special apparatus to study extremely weakly bound helium molecules. In the process, the scientists also discovered a molecule made of three helium atoms, which had been predicted 40 years ago but which scientists had hitherto failed to find. The Helmholtz Prize is awarded for outstanding achievements in metrology, the

science of measurement. It has a value of 20 000 euros and is presented to European researchers every three years by the independent Helmholtz Fund.

As a noble gas, helium does not normally form chemical bonds but rather occurs as solitary atoms. Under special circumstances, however, quantum physics does allow for very weakly bonded helium molecules consisting of two or even three atoms. Using the COLTRIMS (Cold Target Recoil Ion Momentum Spectroscopy) reaction microscope developed at the Goethe University, Dörner and his colleagues Till Jahnke, Maksim Kunitzki, Jörg

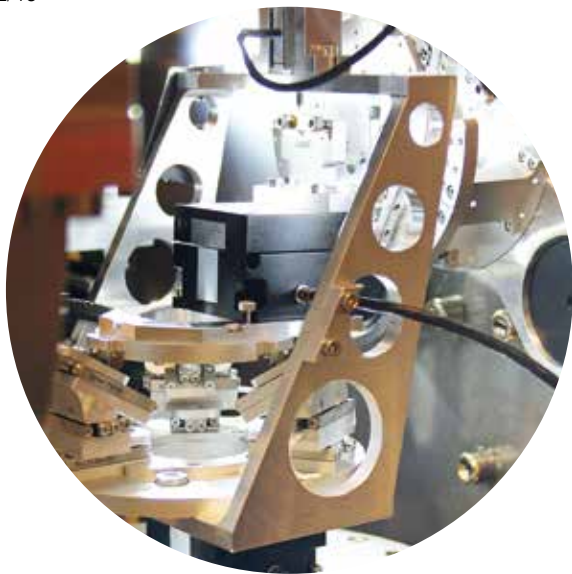
Voigtsberger and Stefan Zeller succeeded in precisely measuring the minute bonding energy of He_2 molecules to within a few nanoelectronvolts (neV).

"This excellent work is an outstanding example of high-precision metrology and demonstrates the enormous potential of DESY's free-electron laser FLASH," says Edgar Weckert, Director in charge of Photon Science at DESY.



Picture: Uwe Dettmar, Goethe University Frankfurt

Reinhard Dörner (left) and Maksim Kunitzki with the reaction microscope



A nano-indenter enables live observation of stress in thin layers of a sample.

Live images of material stress

Researchers at DESY's synchrotron radiation source PETRA III have for the first time succeeded in observing, in situ, stress fields within microscopically thin layers of metal-based ceramics. A new technique enables this unprecedented live view of the effects of pressure at the atomic level.

"We use a tiny diamond tip to apply pressure to the samples, while at the same time illuminating the volume below the tip with X-rays from PETRA III," explains Christina Krywka from Helmholtz-Zentrum Geesthacht, who has set up the experimental station together with colleagues. "Users have wanted to carry out this kind of study for a long time, but the means have not been available before." In addition to an extremely fine X-ray beam with a sufficiently high energy, the scientists also require a special apparatus for mounting the sample during investigation. Special optics were required for the X-ray beam, capable of focusing it to a diameter of just 250 nanometres.

The new technique should help to improve wear-resistant coatings. There is a growing need for materials of exceptional resilience and strength in more and more areas of daily life. The metal-based ceramic investigated here – titanium nitride – can be used as a protective coating only a few micrometres thick, for example to harden tools.

Scientific Reports, 2016; DOI: 10.1038/srep22670

First undulator for the European XFEL

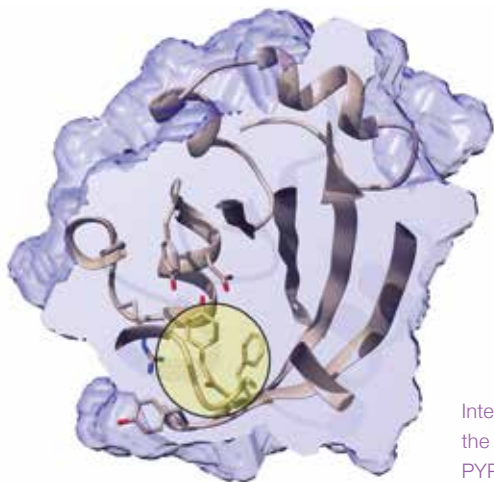
Installation of the 35 undulator segments of the first of three X-ray radiation-generating systems of the European XFEL has been completed. Undulators are the core components of the X-ray laser responsible for producing X-ray flashes a billion times brighter than the radiation produced by conventional X-ray sources. The undulator segments of the European XFEL are installed in underground tunnels. Each one is five metres long, weighs 7.5 tonnes and comprises two opposing girders, each fitted with a long sequence of permanent magnets arranged so that the poles alternate.

When accelerated electrons pass through the field generated by the magnets, ultrashort flashes of X-ray radiation are produced. These X-ray pulses are the basis for a variety of revolutionary scientific experiments that will give scientists new insights into the nanocosmos, with potential applications in many fields, including biochemistry, astrophysics and materials science.

The installation of the undulator segments is a major step towards completion of the European XFEL, a 3.4-kilometre-long X-ray free-electron laser facility currently under construction in the Hamburg region. It is one of Europe's largest research projects, scheduled to open its doors to researchers from around the globe in 2017, when it will be the brightest X-ray radiation source available anywhere in the world.

The first undulator of the European XFEL





Internal structure of the photoactive protein PYP. The light-sensitive chromophore is marked by a highlighted circle.

Atomic motions in biosensor

With the help of a special high-speed X-ray camera, an international team of scientists including researchers from DESY has been able to observe a protein's ultrafast response to light. The study shows light-driven atomic motions lasting just 100 quadrillionths of a second (100 femtoseconds). The technique promises to provide insights into the dynamics of various light-sensitive biomolecules that are involved in key biological processes such as photosynthesis and vision.

Using the bright flashes produced by the LCLS X-ray laser at the SLAC National Accelerator Laboratory in the USA, the researchers investigated the light-sensitive part of photoactive yellow protein (PYP). This protein helps certain bacteria to sense blue light and thereby stay away from light that is too energetic and potentially harmful.

For their investigation, the scientists injected the light-sensitive protein into a reaction chamber, where it was activated by a flash of blue laser light. This was followed almost immediately by an X-ray laser pulse, which enabled the protein's spatial structure to be investigated right down to individual atoms. By systematically varying the time delay between the two laser flashes, the researchers were able to analyse how the activated protein changed its structure over time. "By placing the various obtained molecular structures in order of the time delay between the optical and X-ray flashes, we obtain a molecular movie of the reaction as it evolves from the first step at 100 femtoseconds to several thousand femtoseconds," explains first author Kanupriya Pande, originally from the University of Wisconsin–Milwaukee and now at the Centre for Free-Electron Laser Science (CFEL) at DESY.

Science, 2016; DOI: 10.1126/science.aad5081

Helmholtz Innovation Lab

Green light for industrial alliance MicroTCA.4 TechLab

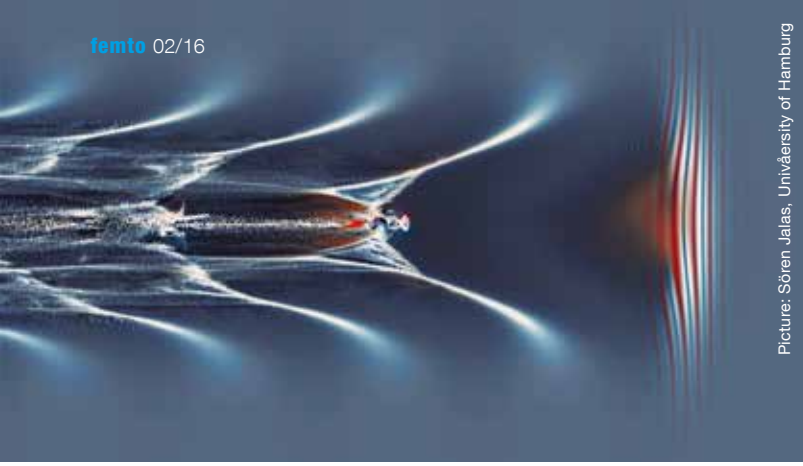
DESY is setting up the MicroTCA.4 Technology Lab in cooperation with partners from industry. The collaborative venture will push ahead with the development of the MicroTCA.4 electronics standard and establish it for a large market. Over the next three years, the project will be funded as a Helmholtz Innovation Lab, with the Helmholtz Association providing almost 2.5 million euros. Additional funds from DESY and industry will raise the total budget of the Innovation Lab to 5.07 million euros. "DESY is fundamentally restructuring the way in which innovation is promoted on the campus. The MicroTCA.4 Technology Lab is an important building block in the research centre's innovation strategy," says DESY Director Helmut Dosch. "It will open up a new dimension of cooperation between DESY and private enterprises."

The MicroTCA.4 (Micro Telecommunications Computing Architecture) electronics standard combines ultrafast digital electronics with the optional integration of analogue components in a very compact format. Its tremendous reliability and scalability make it ideal for controlling particle accelerators. However, there are many potential fields of application in industry as well, including telecommunications, online inspection, aviation, medical engineering and precision metrology.

MicroTCA.4 printed circuit boards have a universal range of application.



Picture: DESY, Heiner Müller-Eisner



Plasma wakefield acceleration involves generating a wave of electrically charged gas – a so-called plasma – inside a narrow capillary tube. There are various ways of doing this, which are being tested in different projects on the DESY campus in Hamburg. LUX uses the 200 terawatt ANGUS laser, which fires ultrashort pulses of laser light into hydrogen gas. These laser pulses strip the hydrogen molecules of their electrons, which are swept to the side as if by a snowplough. The electrons collect in the wake of the light pulse and are accelerated by the positively charged plasma wave in front of them – just like a wakeboarder riding the stern wave of a boat.

Plasma accelerator produces first electron beam

A pioneering accelerator project at DESY has generated its first electron beam. Known as LUX, this experimental facility is a collaborative project with the University of Hamburg. It is based on the highly promising technology of plasma wakefield acceleration, which, it is hoped, will one day enable the construction of smaller and more powerful particle accelerators. Using a plasma cell of only a few millimetres in length, LUX was able to accelerate electrons to around 400 megaelectronvolts in an initial test run. This is very close to the energy produced by DESY's 70-metre-long linear pre-accelerator, LINAC II.

“The result is a first important milestone on the path to developing compact laser/plasma-based accelerators in Hamburg,” explains Reinhard Brinkmann, Director of the Accelerator Division at DESY. The LUX facility was designed and built by the junior research group headed by Andreas R. Maier, which is part of the accelerator physics unit of the University of Hamburg led by physics professor Florian Grüner at the Centre for Free-Electron Laser Science (CFEL). Before viable application, however, the new technology must still overcome a number of hurdles. LUX is operated as part of the LAOLA cooperation between the University of Hamburg and DESY, in which various groups from these two institutions work closely together to study pioneering new accelerator designs.

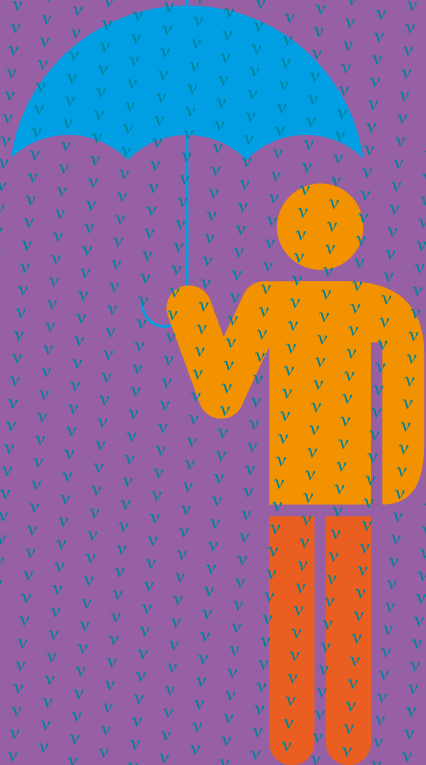
femtomenal

Ghostly!

Every second of the day, some 60 billion neutrinos hurtle through each square centimetre of our skin. Not that this should cause us to worry, for over the course of our entire life only one or two, on average, will remain in our body. Almost all of these neutrinos originate in the sun.

An exploding star spews around 18 000 000 000 000 000 000 000 000 000 000 000 000 000 000 000 000 000 000 000 (18 octodecillion) neutrinos into space during the first 10 seconds of a supernova. Around 99 percent of the energy of a supernova explosion is emitted in the form of neutrinos.

IceCube, the world's largest particle detector, is on the lookout for highly energetic neutrinos from the far-flung reaches of the cosmos. The detector comprises a cubic kilometre of Antarctic ice packed with highly sensitive sensors. Detection of the ultralight elementary particles poses a real challenge – so much so that they're sometimes called “ghost particles” because they hardly interact with anything.



A sign of a new particle?

Great suspense in the world of particle physics: Data collected in 2015 at the world's largest particle accelerator, the Large Hadron Collider (LHC) at the Geneva research centre CERN, show a conspicuous deviation from the expected results. This bump in the mass spectrum at 750 gigaelectronvolts (GeV) could possibly indicate an unknown particle. On the other hand, as Eckhard Elsen explains, it may well just be a statistical fluctuation. At the beginning of the year, Elsen moved from DESY to Geneva to become the new Director for Research and Computing at CERN.

Editorial note

The original version of this article, now abridged, appeared in July in the German issue of femto, before the particle physics summer conference ICHEP 2016 in Chicago. At ICHEP 2016, the ATLAS and CMS collaborations reported on first analyses of a five times larger data sample collected so far in 2016. The new data sample gave no indication of an enhancement at the same mass so that both collaborations independently declared the previous bump a statistical fluctuation.

Physicists think in curves and graphs.

They have a very precise theoretical model, which they use to draw up their calculations and predictions based on simulations. These are then compared with data from real collisions. The predictions and the real data are plotted as curves on a graph. During analysis of the collision data collected at the LHC last year, scientists spotted a bump in one of the curves – an outlier that projects outside of the corridor of expected results. Might this indicate a new particle?

- Observed
- - Predicted
- One standard deviation
- Two standard deviations

femto: Mr Elsen, there's a flood of scientific papers right now, all trying to explain the observed deviation. You've been research director at CERN since January. What do you think is causing the deviation?

Elsen: Well, let us not forget it may just be a statistical fluctuation. Just imagine, you're a fashion scout on the lookout for the latest trends. You see two people on the street, both wearing a blue-and-red checked jacket. Is that a new fashion or just a coincidence? Before investing in the same jacket yourself, what you do is keep your eyes open and look for more information.

It's exactly the same situation at the LHC. At 750 GeV, we're seeing more events than expected. It's a bump, but it's not yet statistically significant. It's certainly encouraging that the two large detectors ATLAS and CMS, each of which uses different detection technologies, are both picking up this deviation. But it's also true that these two bumps, while close together, are perhaps not in exactly the same place. We simply need more information.

On the other hand, we can certainly exclude the possibility of a measurement error, since the measurement itself is very clear. The detectors registered events involving two high-energy photons, i.e. quanta of light. It's unlikely that they would falsely interpret this signature, since these two photons are pretty prominent among the other signals registered by the detectors. More data will show us whether the bump increases or flattens out.

femto: How long will that take?

Elsen: The teams from the two detectors are currently publishing their observations from last year. The LHC started up again early this year, following a winter break. And it's been in top form to date. Physicists are now busy comparing

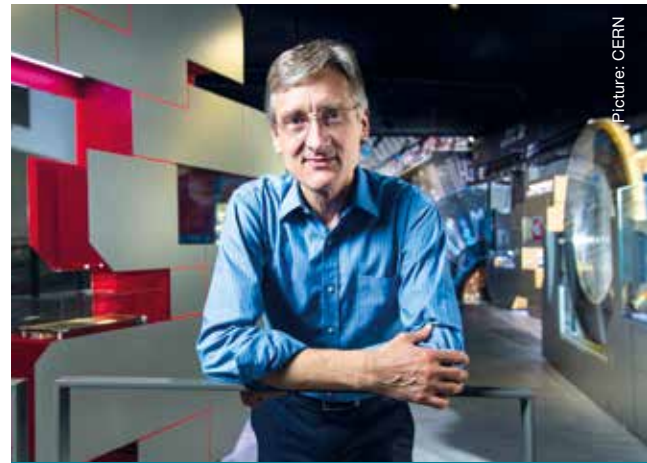
the results coming in with those from last year. With a bit of luck, we'll be able to tell in summer whether we're about to make a big breakthrough, or whether the statistics has played a trick on us. All the people involved are very well prepared and, of course, extremely excited!

femto: Apart from this noteworthy deviation, what else is on the research list before the LHC shuts down again for a longer break in 2018?

Elsen: The more collisions we can observe at the LHC's design energy of 13 teraelectronvolts, the higher the quality of the statistical analyses, and the more clearly effects become visible. Moreover, the more data we have, the better we can observe particles with a greater mass. The sensitivity of our measurements for greater masses increases. This, in turn, enhances our chances of finding either evidence of supersymmetrical particles or further exclusion limits for them.

We want to stake out the ground and see if there's anything new to be found within it. We plan to collect more than 100 inverse femtobarns of data up until the next big shutdown in 2018. That would be 20 times as much data as has been collected at this energy so far, and it would also be several times the amount of data collected during the LHC's first running period.

With more statistics, the physicists will also be able to focus on rarer processes such as unusual decays of heavy quarks. And, of course, we will also be taking a closer look at the properties of the Higgs particle, which was discovered in 2012. Two things will help us here: the higher collision rate of the LHC at high energies and the higher production rate of Higgs particles. The decay rates are like a fingerprint of the particle type. They can tell us whether it exists as a single scalar particle or whether there are



CERN Research Director Eckhard Elsen was leading scientist at DESY for some 25 years and, among other achievements, coordinated the activities for the proposed International Linear Collider.

Picture: CERN

brother or sister particles, which would then indicate a more complex theory involving, for example, a supersymmetrical Higgs particle.

femto: Assuming that the observed bump is not a statistical fluctuation and you discover a new particle: it would be a scientific sensation. Which of the many proposed theories is your favourite?

Elsen: I've not yet seen a theory that can describe these measurements with full plausibility. As a rule, there's a hitch somewhere in the explanation and further assumptions have to be made. The particle – if that's what it is – decays into two photons. But nothing else? That alone would be spectacular enough. But first, the experiments have the floor.

Mathematics reveals molecules in motion

New algorithm improves time resolution at X-ray lasers by a factor of 300

Thanks to an ingenious computational algorithm, researchers are now able to follow the ultrafast movements of molecules and other dynamic processes in the nanocosmos with a time resolution of a quadrillionth of a second. In developing this method, an international team has made a crucial advance in the analysis of dynamic processes. Their work provides a comparatively simple way of determining the sequence of events during elementary reactions with a very high time resolution. The research team led by

Abbas Ourmazd, a professor at the University of Wisconsin–Milwaukee, has developed a special mathematical technique to extract new information from experimental data recorded at free-electron lasers such as DESY's FLASH. The results have been confirmed by quantum-mechanical simulations carried out by DESY scientist Robin Santra and colleagues from the Hamburg Centre for Free-Electron Laser Science (CFEL), a cooperative venture between DESY, the University of Hamburg and the Max Planck Society.

“This method has unbelievable potential,” explains Santra, who is also a professor at the University of Hamburg. It provides completely new insights into the events taking place during numerous ultrafast chemical and biochemical reactions, including electrochemical applications and industrial processes. These are all areas in which scientists have hitherto been restricted to speculating about the sequence of events occurring at the microscopic level. “Dynamic time measurements using FELs are subject to extreme uncertainty,” explains Santra. “This new method of data analysis can increase their accuracy by a factor of 300 – which is astonishing!”

“This new method of data analysis can increase their accuracy by a factor of 300 – which is astonishing!”

Robin Santra, DESY

Snapshots out of sequence

Chemical reactions and the movements of biomolecules are incredibly fast and are therefore not normally observable. They occur within a matter of femtoseconds, i.e. quadrillionths of a second. Until now, no effective method has been available for observing such molecular processes in detail. While today’s X-ray free-electron lasers do enable exposure times in the femtosecond range, the result is merely a series of snapshots taken at different times during the process under investigation. These images cannot be turned directly into a film of dynamic processes, because it is not possible to determine the exact time at which they were recorded.

In order to study a particular reaction, scientists first trigger the process by means of a pulse of optical laser light and then take a snapshot of it directly afterwards, this time using an X-ray laser pulse. This process destroys the sample, however, so that the same reaction has to be repeated with a new, practically identical sample. This time, the X-ray laser pulse takes the snapshot at a slightly later stage of the reaction – and so on. The result is a series of countless snapshots, which scientists must then string together, like a flipbook, to form an animated film. But the exact temporal sequence of the snapshots is corrupted by timing uncertainty, a fluctuation that experts refer to as jitter. This

Robin Santra is leading scientist at DESY and professor at the University of Hamburg. He is head of the theory group at the Centre for Free-Electron Laser Science (CFEL).



can lead to the individual snapshots being arranged in the wrong order.

Twelve million dimensions

“This temporal uncertainty is a curse in many areas of science,” says Ourmazd. “You have lots of data, but no accurate time stamps.” For snapshots to be able to document the sequence of events during a reaction with femtosecond accuracy, the optical and X-ray lasers must be very precisely synchronised. “None of the experimental solutions known to us so far has been able to achieve a temporal resolution better than around 14 femtoseconds, and most measurements are limited to 60 femtoseconds or longer,” says Santra.

“This temporal uncertainty is a curse in many areas of science. You have lots of data, but no accurate time stamps.”

Abbas Ourmazd, University of Wisconsin–Milwaukee (USA)

Ourmazd and his team therefore opted for a different approach: They developed a mathematical algorithm that would enable them to extract information from the available data with a temporal accuracy of one femtosecond. For this purpose, the individual snapshots with the fuzzy time stamps are represented as individual points in a highly multidimensional space. In the paper now published, this space has around twelve million dimensions. Using a mathematical pattern recognition procedure, the scientists then reduce the number of dimensions by looking for curved, multidimensional surfaces upon which the points lie. The aim is >>

to eventually find a single, one-dimensional curve upon which all the points are located. For if the individual points only differ in terms of a change in a single parameter – in this case, time – they must necessarily form a curved line in the space under consideration. If this curve can be found, the points on it will all be ordered in the correct temporal sequence.

In the study now published, the scientists used their algorithm on data that had been collected by a research group led by the Stanford scientist Philip Bucksbaum. Back in 2010, the group had studied the dynamics of doubly charged ions of nitrogen, using the X-ray free-electron laser LCLS (Linac Coherent Light Source) at the SLAC National Accelerator Laboratory in California. The scientists created these unusual nitrogen ions by firing X-rays at the molecules. Such ions are also formed in the Earth's atmosphere as a result of the constant bombardment by high-energy cosmic radiation from outer space.

The experiment resulted in a large number of snapshots of different vibrational modes that occur in intact and split nitrogen molecules. The correct sequence of those snapshots could not be clearly ascertained, however. With the help of their algorithm, Ourmazd and his colleagues were able to determine the vibrations of the molecules to an accuracy of one femtosecond. This allowed them to reconstruct the dynamic behaviour of the nitrogen molecules with a precision enhanced by a factor of 300.

Revolutionary analysis technique

Santra and his team at CFEL then carried out a quantum-mechanical calculation of the processes involved, which confirmed the accuracy of one femtosecond. "We concluded this from the fact that the extracted periods of the oscillation correspond to our quantum-mechanical calculations with exactly this level of precision," says Santra. And not just that: It was only through the simulation calculations carried out by Santra's team that the scientists were able to explain what was causing the vibrations observed in the experiment, what these vibrations mean, and when and why doubly charged nitrogen molecules break apart.

In addition to making the analysis of future experiments more precise, this new method can also be used to re-examine existing data. The only requirement is the availability of sufficient data. As the researchers explain, this can be a problem particularly when it comes to investigating three-dimensional structures. In crystallography, for example, where it takes a tremendous number of

X-ray exposures to produce even a single snapshot, it can be difficult to obtain a statistically significant set of data. "But perhaps this problem will also be solved by the European XFEL," says Santra. The 3.4-kilometre-long X-ray free-electron laser, which is currently under construction in the west of Hamburg, will produce 100 times more pulses per unit of time than existing FELs.

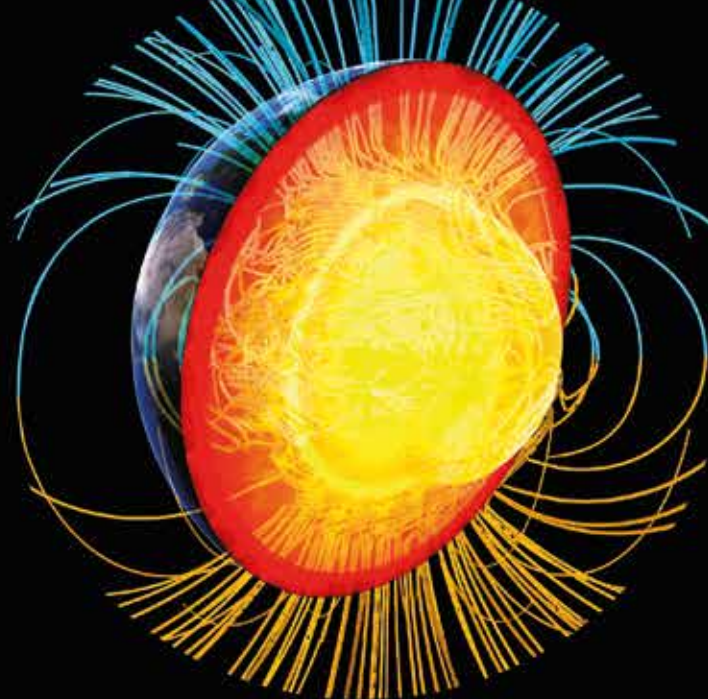
"This method has what it takes to revolutionise the research conducted at FEL facilities"

Robin Santra, DESY

"This method has what it takes to revolutionise the research conducted at FEL facilities," says Santra. And it has a huge advantage too: Instead of resorting to complex technical solutions, it makes ingenious use of mathematical operations. "This approach is not only simpler, but also more successful, because the results are much more exact," says Santra. He envisages numerous possible applications: "This method can be used as a far more precise tool in all areas in which we would like to know what matter is doing – viewed dynamically on short time scales." This includes enzyme reactions in biology and chemistry, for example, as well as the investigation of unusual states of matter, such as those occurring inside planets and stars. Abbas Ourmazd, the project leader, goes even further and is hoping to use his algorithm to more accurately calculate the sequence of an even wider range of processes, such as past climatic events.

Nature, 2016; DOI: 10.1038/nature17627

What drives the dynamo in the Earth's core?



The Earth's magnetic field has existed for at least 3.4 billion years – thanks also to the low thermal conductivity of iron in our planet's core. This is the result of the first direct measurement of the thermal conductivity of iron at pressures and temperatures corresponding to the conditions in the Earth's core.

The geodynamo that generates the Earth's magnetic field is powered by convection in the outer core of our planet. This convection stirs up the molten, electrically conductive, iron-rich material like boiling water in a pot. In combination with the rotation of the Earth, this gives rise to a dynamo effect, which in turn produces the Earth's magnetic field. "The magnetic field shields us from harmful high-energy particles from space, the so-called cosmic radiation, and its existence is one of the things that make our planet habitable," explains DESY researcher Zuzana Konôpková. "We measured the thermal conductivity of iron because we wanted to know what the energy budget of the core is to driving the dynamo. Generation and maintenance of our planet's magnetic field strongly depend on the thermal dynamics of the core."

The strength of the convection in the outer core depends on two things: the heat transfer from the core to the Earth's lower mantle and the thermal conductivity of the iron in the outer core. Until now, however, it has proved difficult to measure thermal conductivity under conditions similar to those in the core. Recent theoretical calculations postulated a comparatively high thermal conductivity of up to

150 watts per metre per kelvin (150 W/m/K) for the iron in the Earth's core.

Such a high thermal conductivity would make it improbable that the dynamo effect had begun at an early date. According to numerical models, it would mean that the geodynamo could only have arisen relatively recently in the Earth's history, around one billion years ago. Yet old rocks enable the existence of the Earth's magnetic field to be traced back at least 3.4 billion years. "There's been a fierce debate among geophysicists, because with such a large thermal conductivity it becomes hard to explain the history of the geomagnetic field, which is recorded in ancient rocks," says Konôpková.

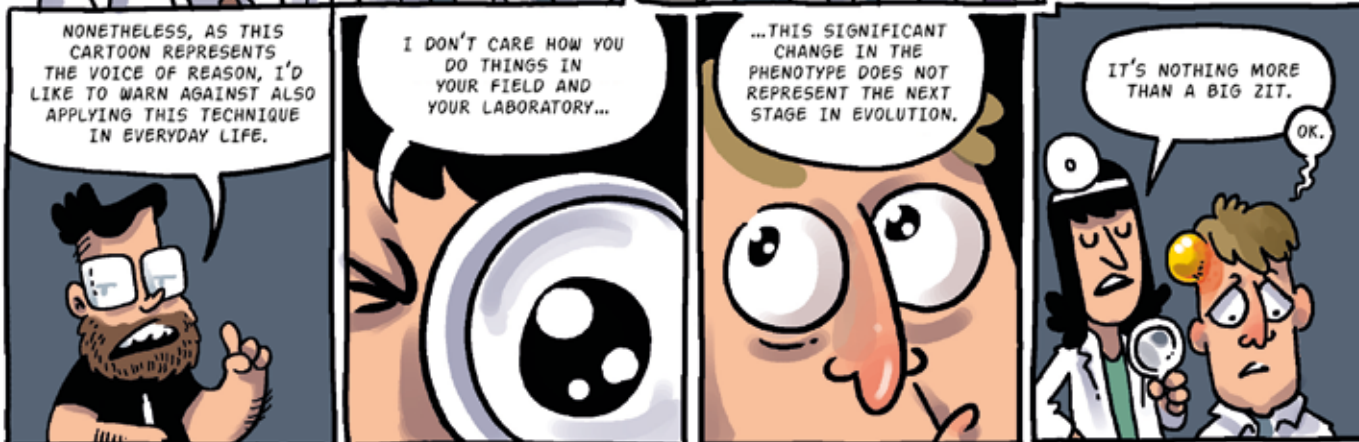
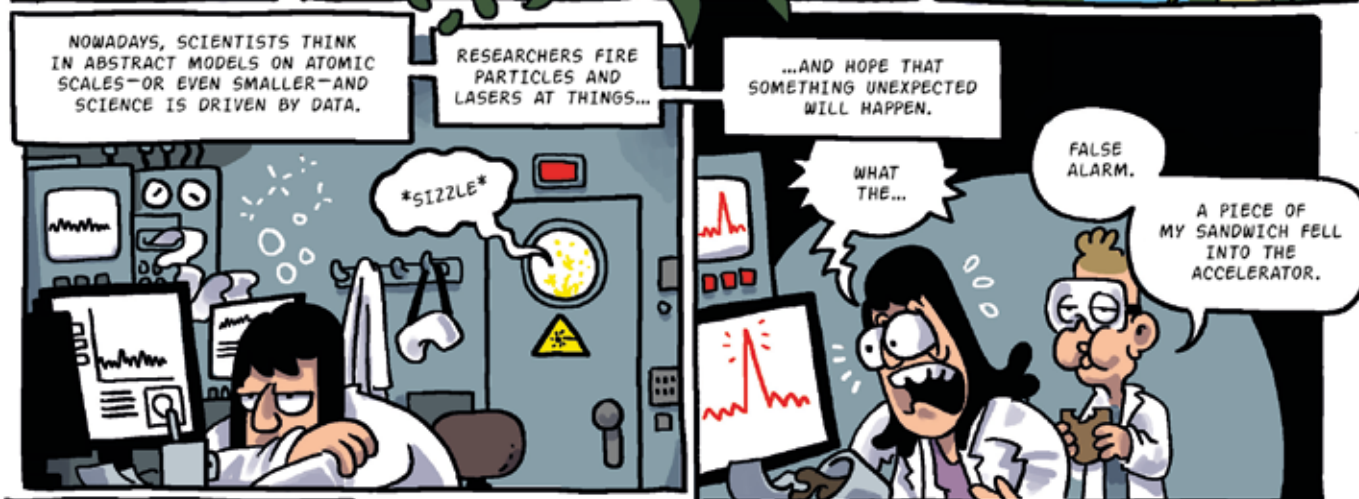
Together with her colleagues Stewart McWilliams and Natalia Gómez-Pérez from the University of Edinburgh and Alexander Goncharov from the Carnegie Institution in Washington DC, Konôpková used a specially designed pressure cell in order to directly measure the thermal conductivity of iron at high temperatures and pressures. "We compressed a thin foil of iron in the diamond anvil cell to up to 130 gigapascals, which is more than a million times the atmospheric pressure and corresponds to approximately the pressure at the Earth's core-mantle boundary,"

A cross-section of the Earth together with the field lines of the geomagnetic field (as simulated with the Glatzmaier-Roberts geodynamo model)

Konôpková explains. "Simultaneously, we heated up the foil to up to 2700 Celsius with two continuous infrared laser beams shining through the diamonds. Finally, we used a third laser to send a low-power pulse to one side of the foil to create a thermal perturbation, and measured the temperature evolution from both sides of the foil with an optical streak camera." In this way, the scientists were able to observe the heat pulse travelling through the iron.

These measurements were conducted at different pressures and temperatures. "Our results strongly contradict the theoretical calculations," reports Konôpková. "We found very low values of thermal conductivity, about 18 to 44 watts per metre per kelvin, which can resolve the paradox and make the geodynamo operable since the early ages of the Earth."

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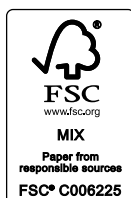
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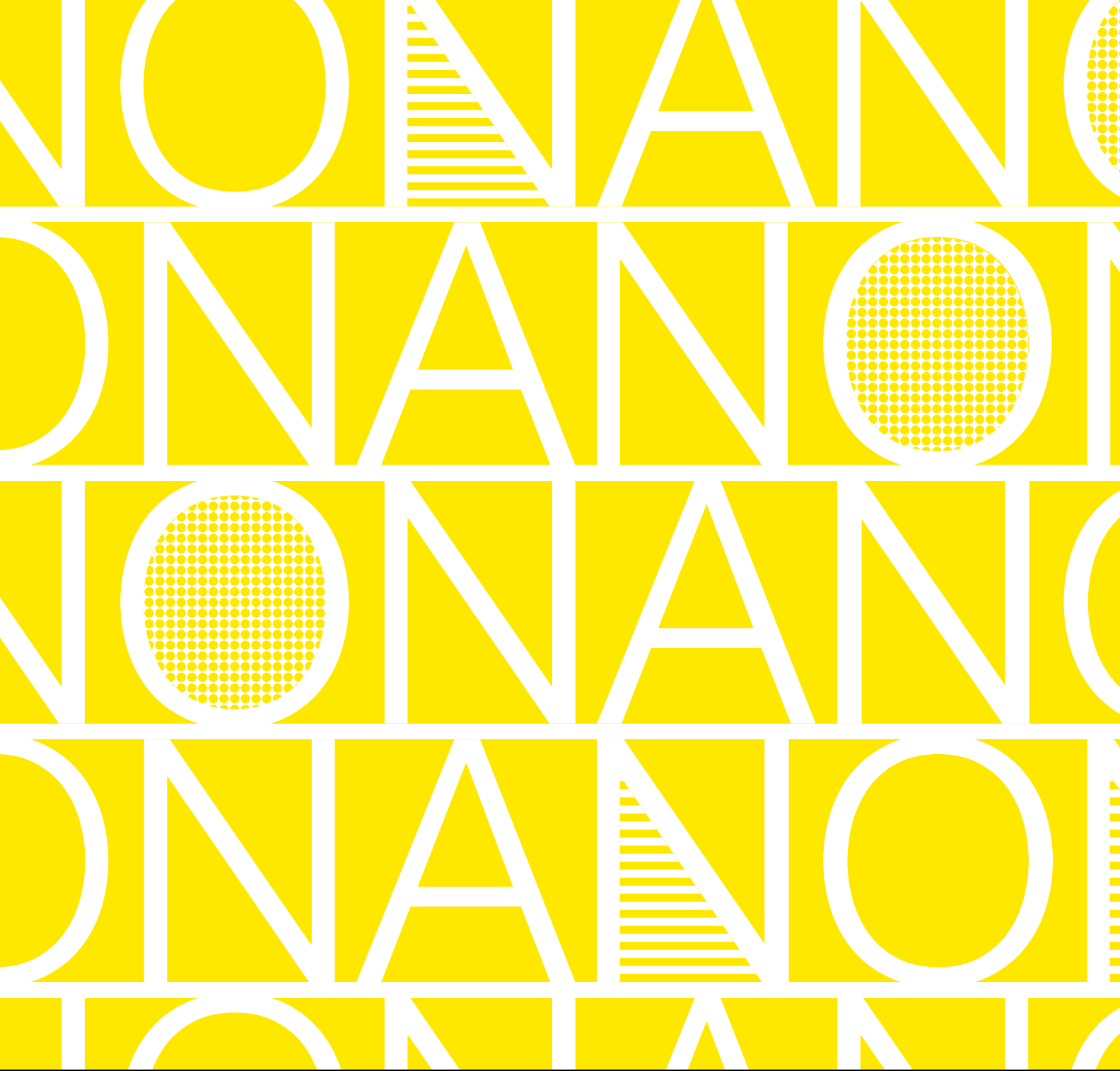
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The DESY research centre

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.