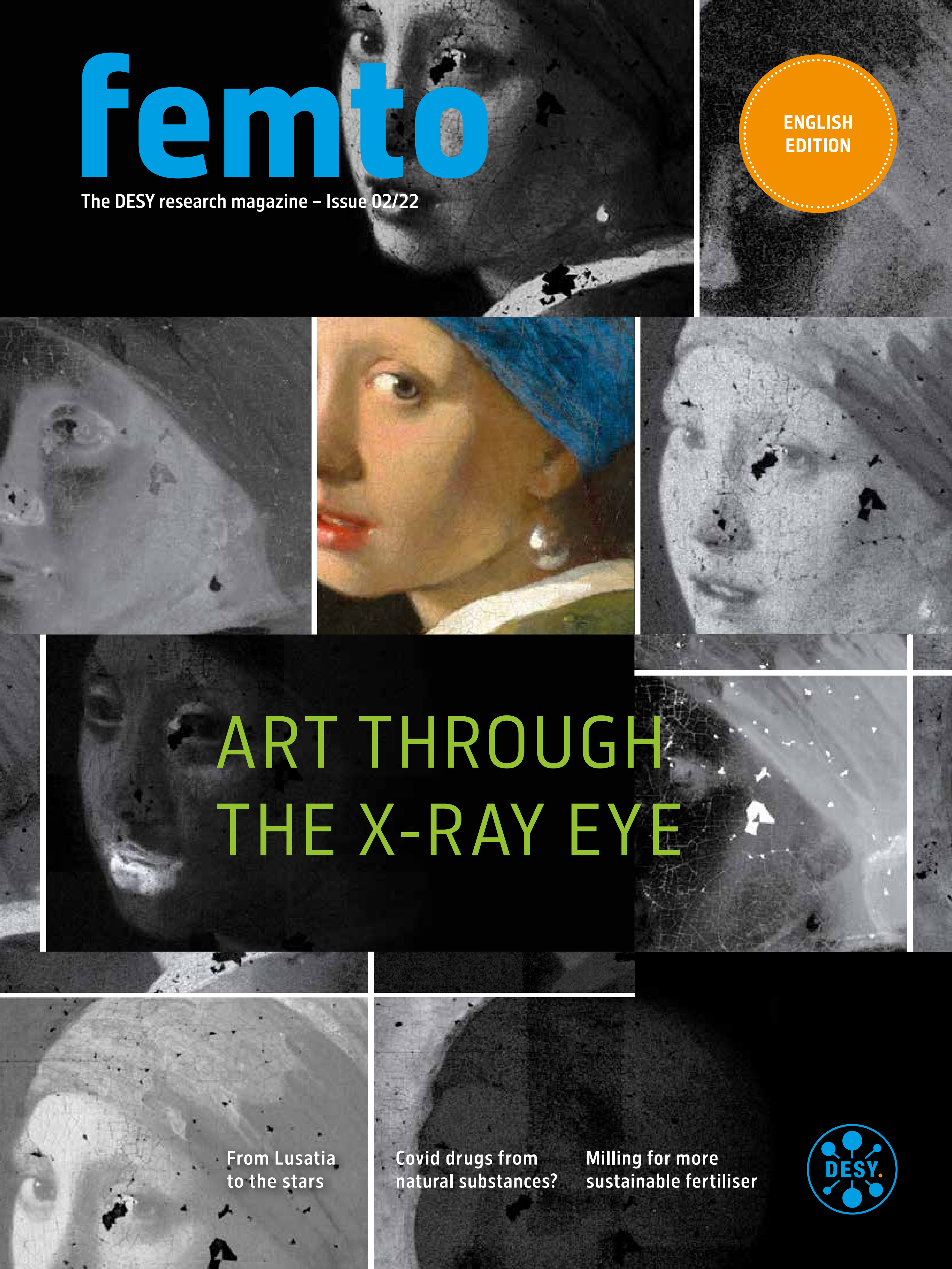


femto

The DESY research magazine – Issue 02/22

ENGLISH EDITION

ART THROUGH THE X-RAY EYE

From Lusatia to the stars

Covid drugs from natural substances?

Milling for more sustainable fertiliser

DESY.

Cosmic particle accelerator at its limit

Using special telescopes, researchers have looked into a cosmic particle accelerator in greater detail than ever before. The observations, made with the H.E.S.S. gamma-ray telescopes in Namibia, show for the first time the course of the acceleration process in a so-called nova, which involves strong eruptions on the surface of a white dwarf star. In this process, a shock wave is created that tears through the surrounding medium, pulling subatomic particles along and accelerating them to extreme energies. Surprisingly, due to ideal conditions, the observed nova RS Ophiuchi seems to accelerate particles to speeds reaching the theoretical limit.

Thermonuclear explosion

White dwarves are burned-out old stars that have collapsed in on themselves to form extremely compact objects. Novae occur, for example, when a white dwarf orbits in a binary system with a large star and picks up material from its more massive companion due to its gravity. Once the gathered material exceeds a critical level, it spurs a thermonuclear explosion on the surface of the white dwarf. The H.E.S.S. telescopes were pointed at the nova as quickly as possible after the event was reported by an amateur astronomer. This allowed the researchers to follow the development of the nova in real time and to observe and study cosmic particle acceleration for the first time as if in a film. H.E.S.S. continued to register high-energy gamma rays for up to a month after the explosion. "This is the first time we have ever been able to carry out observations like this, and it will allow us to gain even more accurate insights in future into how cosmic explosions work," says team member Dmitry Khangulyan, a theoretical astrophysicist at Rikkyo University in Tokyo.

The artistic representation shows the white dwarf and red giant binary system after the nova outburst. Material ejected from the surface of the white dwarf generates shock waves that expand rapidly, forming an hourglass shape. These shock fronts accelerate particles, which collide with the dense wind of the red giant star (sphere in the centre of the picture) to produce very-high-energy gamma-ray photons. The image is taken from an animation of the phenomenon created by DESY and the Science Communication Lab in Kiel.

Science, DOI: 10.1126/science.abn0567

youtu.be/XE3mapcBboc

Picture: DESY/H.E.S.S., Science Communication Lab


femtoscope

Contents

Dear Readers,

Vincent van Gogh's famous "Sunflowers" are wilting. The bright chrome yellow for which the painter is so well known has darkened considerably. By using X-rays to examine tiny paint samples taken from the painting, a research team has managed to establish what happened. It seems that Van Gogh used different chrome yellow pigments, one version of which is light-sensitive. Over time, the chromium in it has been reduced from the highest to a lower oxidation state, causing the pigment to change colour.

X-rays can provide unique insights into cultural artefacts. They can be used to explore the painting techniques of old masters as well as their preferred paints; they can reveal ancient writings and hidden paintings, unravel the techniques used to produce metal objects and peer inside sealed relics without damaging them. Findings like these have some very practical benefits too: They can be used to better protect cultural assets, for example by adapting the lighting in museums to the needs of light-sensitive paints. X-rays can also be used to check the success of protective measures, for example the conservation of crumbling sandstone façades.

The current issue looks at the many uses of X-rays in the examination of cultural artefacts. And we have a new section in this issue: *femtoweb* (p. 41) will introduce you to interesting online offers that bring research to life on the World Wide Web. We hope you enjoy reading this issue and surfing the web and find both enlightening. We welcome your criticism, praise and suggestions at femto@desy.de.

Till Mundzeck
Editor

Pictures: DESY, Staab Architekten; Rijksmuseum Amsterdam; private; DESY, Gesine Born

From Lusatia to the stars

The German Center for Astrophysics is to be built in Saxony

Germany is getting a new large research centre for astrophysics: The "German Center for Astrophysics – Research. Technology. Digitization." (DZA) is to be built in the Saxon region of Lusatia. It is meant to bring together the streams of data from astronomical observatories around the globe, develop new technologies and give German science access to future large-scale international projects, thus also opening up opportunities for industry to bid for contracts.

"Germany lacks a national centre for astrophysics," explains DESY's Director in charge of Astroparticle Physics, Christian Stegmann, one of many renowned scientists who submitted the application to create the DZA. "This will be a great asset for Germany's scientific community, giving it an international appeal. It's wonderful that this is to be built in eastern Germany."

Together with the Center for the Transformation of Chemistry (CTC), the DZA managed to win the competition "Knowledge Creates Perspectives for the Region" organised by the German Federal Ministry of Education and Research (BMBF) and the German federal states of Saxony and Saxony-Anhalt. The CTC is to facilitate a circular economy in the chemical industry and will be located in the Central German mining district in Saxony-Anhalt. The federal government and the two federal states are funding the centres with a total of 2.2 billion euros.

High-tech with innovative power

Günther Hasinger, Scientific Director of the European Space Agency (ESA), was instrumental in the DZA initiative and is its designated founding director. "This competition opened up new perspectives, for the regions in Saxony and for our society – an important sign for the future in difficult times," he says. "Following a demanding one-and-a-half-year application process, during which our concept was thoroughly vetted, we are happy that we can now go ahead with our project. For many reasons, Lusatia in Saxony is the ideal place for this."

Astrophysics was and is a high-tech science with great innovative powers. Progressive lenses, ceramic hobs, key components of mobile phones, navigation systems

Pictures: DESY, Staab Architekten; European Southern Observatory (CC BY 4.0)

An open campus for cutting-edge research is planned in Görlitz.

and high-speed electronic bank transfers via satellite – all these have become possible thanks to astronomical research. Astrophysics is experiencing a real boom at the moment. Half the Nobel Prizes in physics in the past decade were awarded for astronomy, astrophysics and astroparticle physics.

Astronomical measurements today are very different from the astronomical data of the past, though. Modern telescopes are huge facilities, spread across the globe, with international teams collaborating on them. They are situated in the Chilean highlands, in the expanses of Australia and deep in the Antarctic ice. They require extremely precise measurement techniques, and the entire data traffic on the Internet today is just a fraction of what will be collected by future new observatories.

The world's largest civilian data set

In future, this data from all over the world will be collected in Saxony, creating the world's largest civilian data set. The challenges facing the DZA as a result are also relevant to society. Forecasts predict that information technologies will soon consume 20 percent of global electricity production. The DZA intends to meet these challenges, promote green computing and resource-friendly digitalisation and develop new technologies for the society of tomorrow.

"Astronomy is currently opening new windows to our cosmos. These are not only fascinating to science – as drivers of technology and innovation, they also have the potential to change our world," says Michael Kramer, President of the German Astronomical Society and Director of the Max Planck Institute for Radio Astronomy in Bonn, who is also one of the signatories of the DZA application. "In setting up the DZA, we are creating a large research centre with an advanced scientific programme."

"Germany lacks a national centre for astrophysics. This will be a great asset for Germany's scientific community"

Christian Stegmann, DESY

Three pillars

The concept for the DZA rests on three pillars: For one, the centre will conduct cutting-edge astronomical research. This will extend across the entire electromagnetic spectrum and also include gravitational waves. In view of the many existing synergies, the centre will initially focus on radio and gravitational wave astronomy. In the long term, it will devote itself to all astronomical data.

The second pillar will be the data arriving from all over the world, which will be collated and processed in the DZA – including data from future large telescopes. The data streams from these telescopes will amount to several times the data traffic on today's Internet and will require new technologies. The centre is to tame this data tsunami and thereby accelerate digitalisation within Germany.

The third pillar will be a technology centre where, among other things, new semiconductor sensors, silicon-based optical systems and control technologies for observatories will be developed. Building on the experience and modern industrial setting available in Saxony, new companies and additional high-quality jobs will be created via spin-offs.

A subterranean research laboratory is also to be built in the district of Bautzen. Seismic waves that are constantly travelling through the Earth interfere significantly with gravitational wave detectors. Extremely calm geological conditions are also necessary when developing new measuring and production technologies. Lusatia lies on one of the largest known slabs of ››

Picture: DESY, Gesine Born

granite, offering unparalleled vibration-free conditions. The DZA's Low Seismic Lab is therefore going to be embedded in the Lusatian granite in a region between Hoyerswerda, Bautzen and Kamenz, for research and for the development of new equipment. It will also be available for industrial applications, such as developing quantum computers.

Three-year start-up phase

The DZA will be located in the city of Görlitz, because of its proximity to the university cities of Dresden, Wrocław and Prague and because of promising greenfield developments in the innovation and high-tech sector. An open campus for cutting-edge research is to be embedded in the city, including the centres for

"This competition opened up new perspectives, for the regions in Saxony and for our society"

Günther Hasinger, ESA, designated DZA Founding Director

astrophysics and data science, the technology centre and the centre for innovation and transfer. The concepts also includes a visitors' park.

The funding provides for a three-year start-up phase before the centre can be formally established. The Dresden University of Technology will be in charge of project management during this period and will also contribute its technical expertise in the field of data analytics, artificial intelligence and high-performance computing.

www.dza-lausitz.de

femtopolis

RAMMSTEIN ROCKS PARTICLE ACCELERATOR

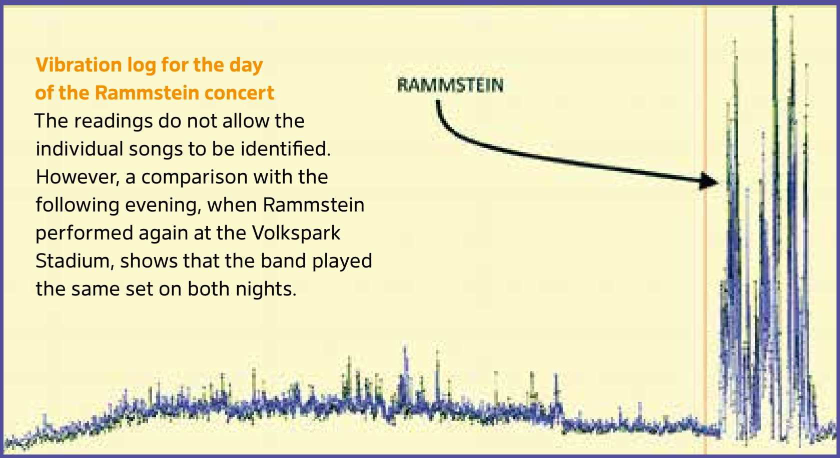
Tuesday, 14 June 2022, was not in itself a remarkable day. While experiments were going on as usual at DESY's X-ray source PETRA III, a not-so-unremarkable band was setting off its famous pyrotechnics in Hamburg's Volkspark Stadium, about two kilometres away: Rammstein, known for controversial lyrics and polarising music videos, was turning up the heat on Hamburg.

Hamburg's ground shook from the live concert of the industrial metal band – and so did the particle accelerator. As the concert began, the vibrations reaching PETRA III through the ground shot up to the highest values of the year. So-called seismometers automatically measure and record the movements of the ground, which have to be corrected for to stabilise PETRA III's sensitive X-ray beam. This can happen when there is an earthquake, for example. "We want to know how strongly external factors affect the system and, above all, how much they impact the beam," explains DESY accelerator physicist Michael Bieler. The automatic system can quickly correct for small deviations.

During the Rammstein concert, the most powerful frequencies were well below the hearing threshold. The expert suspects this can be explained by the synchronous hopping, stomping and jumping by more than 50 000 spectators. **"This kind of thing can happen when tens of thousands of people start moving to the beat,"** says Bieler.

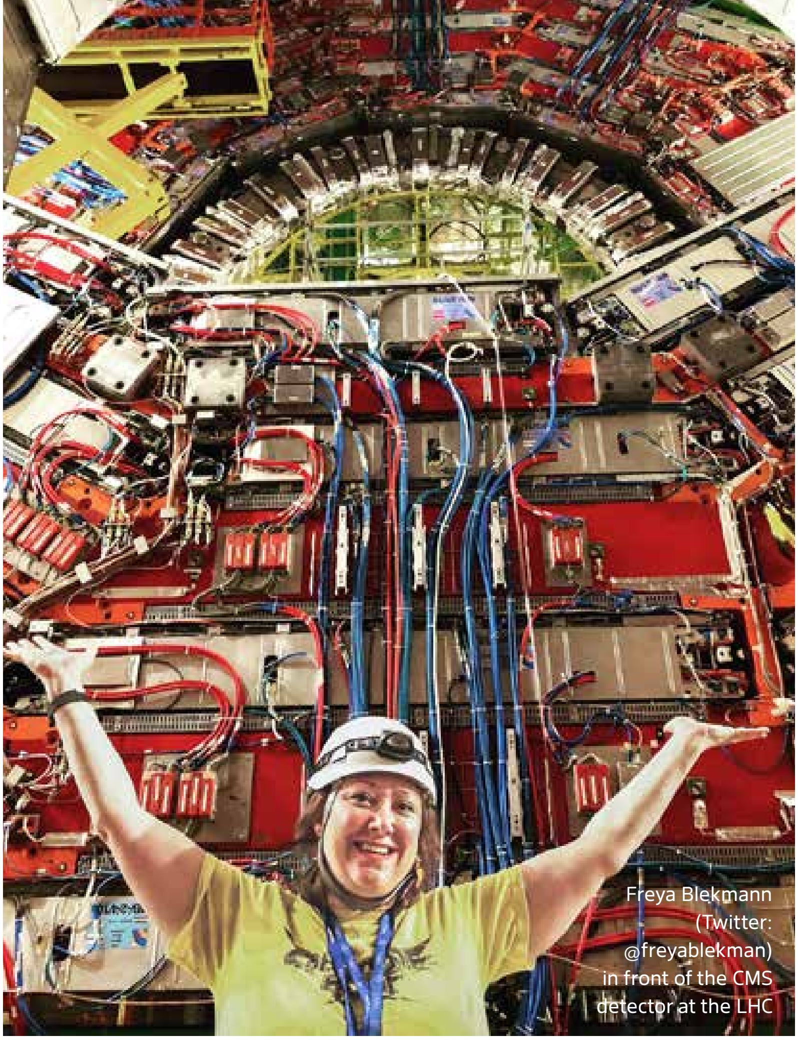
The sensitive seismometers record even distant earthquakes, in Chile or Japan. "The seismic waves propagate through the Earth, and eventually we see what is left of them," the accelerator physicist reports. He notes that the measurements are so precise as to clearly show a difference between week days with rush hour traffic and the quieter weekends. Concerts stand out even more.

Fortunately, PETRA III was unperturbed by the Rammstein fans hopping up and down. The systems routinely corrected for movements of the ground within fractions of a second. Just as well, really, because just two weeks later, on 26 June 2022, the accelerator faced an even bigger test: The vibrations of the ground that evening were in fact three times as strong as those caused by the rock musicians. This time, pop icon Harry Styles was playing at the Volkspark Stadium – while star violinist André Rieu was performing at the Barclay Arena next door.



Vibration log for the day of the Rammstein concert
The readings do not allow the individual songs to be identified. However, a comparison with the following evening, when Rammstein performed again at the Volkspark Stadium, shows that the band played the same set on both nights.

Picture: DESY



Freya Blekmann (Twitter: @freyablekman) in front of the CMS detector at the LHC

"We are looking for a crack in the Standard Model"

Ten years after the discovery of the Higgs boson, particle physics is exploring new horizons

Freya Blekman, who hails from the Netherlands, has been a lead scientist at DESY since October 2021. For many years, she has been involved in the CMS experiment at the LHC particle accelerator at the European particle physics centre CERN, outside Geneva. On Twitter, she is one of the female physicists with the largest following, making particle physics research accessible to a wider audience. With a circumference of 27 kilometres, CERN's Large Hadron Collider (LHC) is the biggest and most powerful accelerator in the world. It accelerates protons (hydrogen nuclei) and allows them to collide head-on. Huge detectors, such as CMS and ATLAS, observe these collisions and analyse whether any rare, exotic elementary particles are created in the process. That is how the Higgs boson was discovered ten years ago – the last missing building block in the structure of the Standard Model of particle physics.

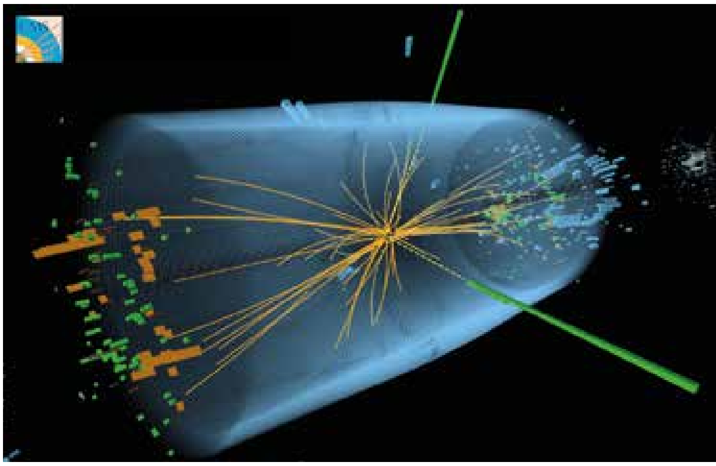
femto: In 2012, CERN in Geneva announced a significant discovery: The long-awaited Higgs boson had been detected at the LHC. What did this discovery mean for physics?

Freya Blekman: It is an extremely important particle. It was predicted way back in the 1960s, in particular by the theoretical physicist Peter Higgs. The reason the Higgs boson is so important is that it helps explain why other elementary particles, such as quarks, have mass in the first place. For decades, various accelerators had been searching for the Higgs, but only the LHC was powerful enough to create this particle, and in the course of an elaborate search we managed to identify it with the help of the two detectors CMS and ATLAS. This discovery marked a final milestone for our current theoretical framework, the Standard Model. The Higgs was the final missing piece of the puzzle in the Standard Model.

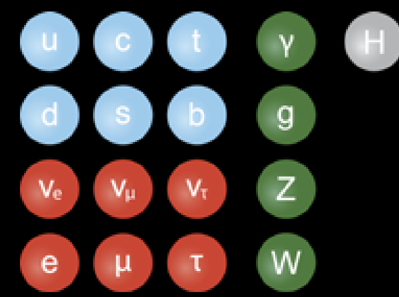
femto: Since the Higgs boson was first discovered in 2012, CMS and ATLAS have taken a very detailed look at it. What has come out of this? What have the experts learned about the Higgs since then?

Freya Blekman: We have measured the mass of the Higgs boson with great precision, as well as its spin and whether it is its own antiparticle. And we have measured how the Higgs interacts with other particles. In all of these measurements, I was surprised at how well the LHC and the detectors worked and that by using intelligent analyses we were able to extract more information from the data than expected. All this has allowed us to thoroughly test the predictions of the Standard Model. So far, our measurements have been consistent with this theory. But ultimately, we are hoping to discover deviations from theory in our experiments – and thus a crack in the Standard Model. Because we know that the ››

Picture: private



Left: Typical signature of the Higgs boson in the CMS detector at the LHC



The Standard Model of particle physics comprises quarks (blue), leptons (red), force particles (green) and the Higgs boson (grey).

Standard Model is not the final truth. It does not explain the mysterious dark matter that must exist in the universe, nor the puzzling fact that there is much more matter than antimatter in the cosmos. This is why we want to study the Higgs boson even more closely at the LHC, to find a crack in the Standard Model that will give us clues about a new, more comprehensive theory.

femto: Over the past three years, both the LHC and the detectors have been upgraded and made even more powerful. The particle collider started up again in the summer of 2022. What has improved?

Freya Blekman: The accelerator now produces more particle collisions and thus more Higgs bosons, some 50 percent more than before. At the same time, we have modified our detectors to handle this larger number of particle collisions and measure them more precisely. In a few years, there will be another, even bigger upgrade. Right now, we are building some components for it at DESY, both for ATLAS and CMS – really cool stuff. After this major upgrade, the LHC should be able to generate up to ten times as many Higgs bosons. That will allow us to study the particle with much greater precision than before.

femto: What are you hoping for in terms of the future measurements? What could they lead to?

Freya Blekman: The hope is still to identify anomalies in the behaviour of the Higgs boson and thus to detect a crack in the Standard Model. But we will also be looking out for signs of entirely new particles in the measurement data, particles that are beyond the Standard Model. We will be assisted by artificial intelligence algorithms, among other things. Some of them work along similar lines to the algorithms used for image recognition. They can help us to detect hidden patterns in the data that would otherwise go unnoticed.

femto: One of the most fundamental questions in physics is: What's behind the dark matter that appears to hold galaxies together like an invisible glue? Could there be a connection between the Higgs boson and this dark matter, and could it be detected as a result?

Freya Blekman: If dark matter has mass, it should interact with the Higgs boson. The question is: Can this be observed? In principle, that should be possible: The Higgs boson is not stable; it decays into other particles immediately after being created. It might well decay into dark matter particles in the process. Our detectors will not be able to observe this directly, but by using certain tricks it should be possible to detect such invisible Higgs decays. It's difficult, but it doesn't seem impossible. However, we will have to make very precise measurements to see if such phenomena exist.

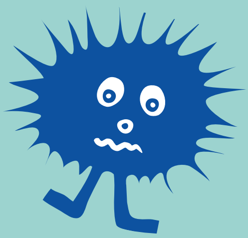
femto: So the LHC will be studying the Higgs boson much more closely in the future. Will it be able to answer all the questions about the particle that still remain open, or will other, new accelerators be needed?

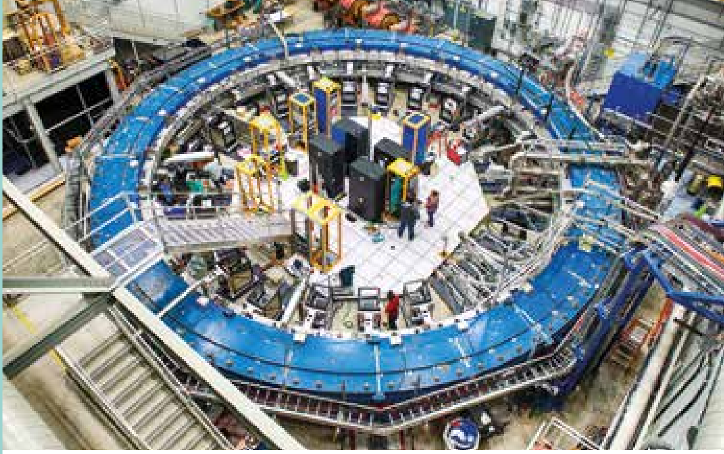
Freya Blekman: The LHC fires protons at each other, but even more precise measurements would be possible if electrons were allowed to collide with their antiparticles, that is, positrons. The plans for such an accelerator already exist, and DESY in particular has a lot of know-how on the subject, both with regard to the accelerator and the detectors and to the data analysis and the theory. In principle, the Higgs boson could also be studied extremely precisely using a facility that allows muons to collide, heavy but very short-lived relatives of the electron. A muon collider like this is a very beautiful, ambitious dream. But making it a reality would require a great deal of research and development.

Pictures: CERN, DESY

Mathematical magic to track down the **magnetic moment** of the muon

International team of theoretical physicists cracks new level of precision





The centrepiece of the Muon g-2 experiment, which attracted a lot of attention in 2021: The magnetic ring, some 17 metres in diameter, generates a strong, uniform magnetic field in which researchers measure the magnetic properties of the muon and compare them with theoretical predictions.

Every particle has specific properties. These include, for example, its charge, its spin, or how it reacts to other particles. Some of these properties have the potential to shake our world view – if the experimentally determined values for these properties do not match the values predicted by theory. A team of theoretical physicists, including Karl Jansen, an expert in lattice quantum field theory at DESY, has now managed to make high-precision calculations for a subrange of such a value that was previously considered extremely difficult to calculate. These calculations can now be compared with the data from an experiment that has held the world record for precision since 2021.

Hoping for a deviation

The hope is always to find a deviation, a small discrepancy somewhere deep in the decimal places, which would point to a revolutionary new phenomenon. Dark matter or dark energy could be responsible for such deviations; other candidates are extensions to the Standard Model of particle physics discussed in the literature. “We are not there yet, however,” explains Karl Jansen. “As yet, no real deviation is apparent.” Nonetheless, these calculations are important for all future theoretical and experimental results. “Above all, our result shows one thing: that we are actually able to perform such complicated calculations! Because in the past, there were considerable doubts about this.”

The research group in which Jansen is working has set its sights on a specific aspect of the muon’s magnetic moment. The magnetic moment is one of the particle properties mentioned above; in this case, for example, it describes how a muon reacts to a magnetic field. The magnetic moment of the muon is one of the best known and most accurately calculated quantities in physics. This is why it is often used in comparisons with “real”, i.e. experimental data – such as that from the Muon g-2 experiment in the USA, which made the headlines in 2021 when it recorded a deviation from the theoretical predictions, even though this was not significant enough to be considered a discovery.

When making theoretical predictions, the magnetic moment is considered in relation to other physical quantities – such as the forces acting between particles. In the case of the electromagnetic force and the weak force, perturbation theory is used. This describes a complicated quantum system (interactions between particles) in terms of a simpler system, using a series of approximations, called perturbations; and the predictions for the magnetic moment are very precise. However, perturbation theory cannot be applied to the strong force acting between quarks and gluons. So predictions in this area have been fairly inaccurate – until now.

Four-dimensional space-time lattice

Jansen’s research group has been using an approach that relies on the computational method of lattice quantum chromodynamics, which allowed them to reduce the error, especially the systematic error. “We have taken the equations from the Standard Model of particle physics and expressed them mathematically on a four-dimensional space-time lattice. That way, we can solve the equations numerically and transfer the results to the magnetic moment. However, this requires the best supercomputers available.” After a worldwide campaign that lasted ten years, the researchers have now achieved a level of precision in their calculations that comes very close to that of the experimental data.

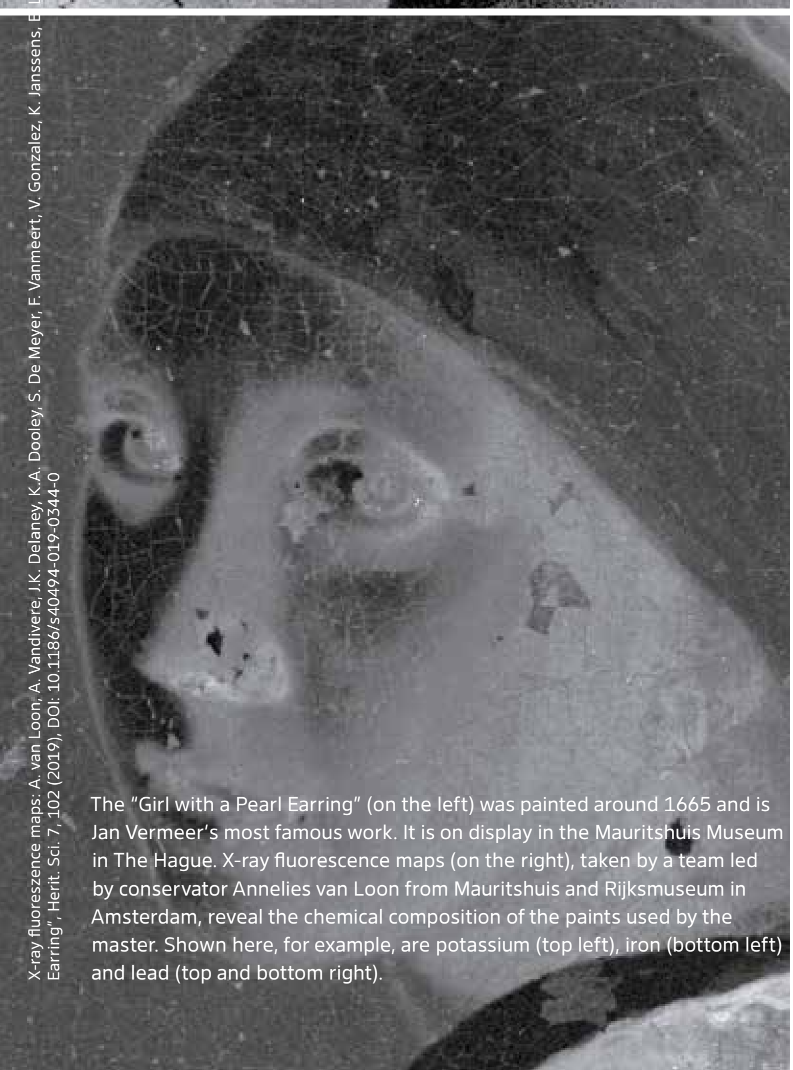
Picture: Fermilab, Reidar Hahn

ZOOM

Picture: Mauritshuis, The Hague

ART THROUGH THE X-RAY EYE

What technique did Jan Vermeer use to paint his pictures? Why is the sky in Giotto’s frescoes developing green blotches? And what did Sumerians write to each other in their clay correspondence 5000 years ago? X-rays provide unique insights into cultural artefacts that would otherwise be inaccessible. The analyses not only reveal new facts about valuable works of art, but also improve the methods used to preserve them.



The "Girl with a Pearl Earring" (on the left) was painted around 1665 and is Jan Vermeer's most famous work. It is on display in the Mauritshuis Museum in The Hague. X-ray fluorescence maps (on the right), taken by a team led by conservator Annelies van Loon from Mauritshuis and Rijksmuseum in Amsterdam, reveal the chemical composition of the paints used by the master. Shown here, for example, are potassium (top left), iron (bottom left) and lead (top and bottom right).

X-ray fluoreszence maps: A. van Loon, A. Vandivere, J.K. Delaney, K.A. Dooley, S. De Meyer, F. Vanmeert, V. Gonzalez, K. Janssens, E. Leonhardt, R. Haswell, S. de Groot, P. D'Imporzano, G. Davies: "Beauty is skin deep: the skin tones of Vermeer's Girl with a Pearl Earring", Herit. Sci. 7, 102 (2019), DOI: 10.1186/s40494-019-0344-0

FINE ART AND FAST BEAMS

How particle accelerators are helping to analyse the paintings of famous masters

Paintings were created for eternity – but even famous masterpieces are vulnerable to the ravages of time. Some pigments fade over the years, or they may change colour like a chameleon. Bright yellow can become sombre brown, bright white can mutate into dull black. The details of what causes the colours to degenerate like this can be determined using high-intensity X-rays from particle accelerators. Facilities like DESY's storage ring PETRA III offer exciting insights into legendary masterpieces by Rembrandt, Munch and van Gogh. The results can be used to help preserve the paintings more effectively in the future.

Taking X-rays of paintings has long belonged to the repertoire of art experts. With a bit of luck, it is possible to vaguely see any changes made during the painting process or even whether another picture was painted over. But what if you use the most powerful X-ray sources on Earth for your analyses – huge particle accelerators like those operated at DESY? "In 2007, we started bringing entire paintings to Hamburg and scanning them using synchrotron radiation, which at that time still came from the storage ring DORIS," says Koen Janssens, a chemist at the University of Antwerp in Belgium.

Among other things, the experts discovered that Vincent van Gogh had painted his "Grasgrond" on top of one of his older works – the portrait of a woman. Instead of using a simple X-ray image, the experts analysed the so-called X-ray fluorescence for this study. This allows conclusions to be drawn about the combination of elements present; as a result, the work that has been painted over can be seen much more clearly than on a conventional X-ray image.

Pictures: Rijksmuseum Amsterdam (left), DESY (top right), private (portrait)

In the elaborate research and restoration project "Operation Night Watch", which was carried out by the Rijksmuseum in Amsterdam, the entire painting by Rembrandt van Rijn, dating from 1642, was analysed with the help of a mobile X-ray scanner.

X-ray analyses at DESY revealed the portrait of a woman underneath Vincent van Gogh's "Grasgrond" (1887)

Detective work on paint fragments

However, transporting valuable works of art to the accelerator for analysis proved to be difficult. So experts designed specialised compact mobile X-ray devices for scanning paintings. These can be used in the museums themselves, which greatly simplifies the procedure. "Since then, we've been concentrating on the accelerator's true strengths – analysing tiny paint fragments using extremely narrow but high-intensity X-rays," explains Janssens, one of the pioneers in the field.

Examining these specks of paint, which are carefully removed from the masterpieces by practised hands, can reveal surprising details about the artworks. "Among other things, we gain information about the pigments originally used by the masters," says Janssens. "And we can find out whether and how these pigments have altered over time."

At DESY, such measurements are being done at the beamline P06, one of 25 beamlines along the PETRA III accelerator. Electrons moving close to the speed of light orbit the 2.3-kilometre storage ring. As they travel around their circular path, they pass through special magnetic chicanes, which force them to emit an extremely powerful and narrowly focused X-ray beam. "The distinctive feature of this particular beamline is that we can focus the X-ray beam coming from the accelerator to make it particularly narrow," says Gerald Falkenberg, the DESY physicist who is in charge of the beamline. "Our X-ray optical systems focus the beam on a spot that is only 200 to 300 nanometres across, a fraction of a micrometre." A micrometre, in turn, is one thousandth of a millimetre. This allows even the smallest samples of a material to be scanned and analysed with extreme precision – for example, the tiniest specks of pigment taken from a historical painting.

"Among other things, we gain information about the pigments originally used by the masters"

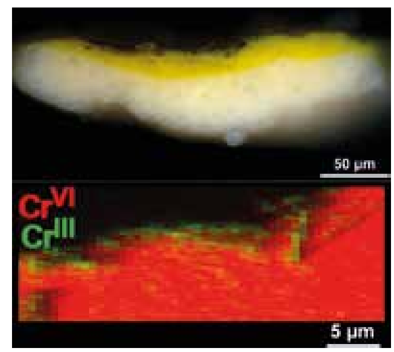
Koen Janssens, University of Antwerp

Grey instead of white

To take the measurements, several different analytical methods are combined: X-ray fluorescence can reveal the composition of the elements that are present – for example, whether the samples contain substances such as lead or chromium, as used in white or yellow pigments, and in what quantities. However, some of these elements have reacted chemically over time – and have lost their luminosity or characteristic colour as a result. An originally white lead carbonate can mutate into a dark oxide: As a result, regions of a painting that once shone brightly now take on a drab grey appearance. "Chemical changes like this can be detected using other techniques, such as X-ray diffraction," says Falkenberg. "It allows us to determine in which crystal forms and chemical compounds elements such as chromium, arsenic, lead or iron are present."

Falkenberg enters the so-called experimental hutch of the beamline. Its solid metal walls shield anyone outside against the X-rays, making it safe to be outside the hutch while an experiment is in progress. Inside the hutch, we are greeted by a jumble of tubes, cables and vacuum chambers mounted on massive granite tables. "The X-ray beam from the storage ring comes out of this tube," explains Falkenberg, ››

Van Gogh's famous "Sunflowers" (left) have changed colour over time. An X-ray analysis has revealed that this is due to the mixture of pigments. On the surface of the chromium yellow used, chromium III compounds (green) have replaced the orange-yellow chromium VI compounds (red) (below).



pointing to a stainless steel tube, as thick as an arm, sticking out of the end wall of the hutch. From here, the beam travels through a metal box where a special X-ray optical system focuses it on a tiny spot.

The sample, such as a fragment of a painting, is placed on a rotating holder at the focal point of the optical system. "During the experiment, the sample is slowly rotated in the X-ray beam and scanned point by point," explains Falkenberg. "The sample scatters and absorbs the X-rays, and we capture the corresponding signals using a range of different detectors." These "X-ray cameras" produce a veritable flood of data – some individual images consist of millions and millions of pixels, with megabytes of data for every pixel. "A series of measurements can quickly add up to many terabytes," says Falkenberg. During the subsequent data analysis, elaborate computer programs determine the composition of elements and the crystal structure of the pigment sample under investigation.

More chemically active than assumed

Painters such as Vincent van Gogh and Edvard Munch are particularly interesting for the analyses. "A revolution took place in chemistry during their time; new pigments such as chromium yellow and cadmium yellow were developed," Koen Janssens reports. "But some of these materials turned out to be more chemically active than was realised at the time." In consequence, quite a number of paintings have darkened over time, including van Gogh's famous sunflower paintings. Experiments at DESY have helped to identify the cause: Over the decades, sunlight turned the bright chromium yellow used by the master ››

Ancient eye colours in X-ray light

The Battle of the Teutoburg Forest was a famous event in Roman antiquity. In AD 9, a Germanic army led by the legendary Arminius destroyed several Roman legions, halting the Roman advance into what was then Germania. Archaeological excavations at Kalkriese bear witness to this battle against the troops of Publius Quinctilius Varus and have unearthed, among other things, bones, Roman militaria and coins as well as, most recently, an almost completely preserved set of a legionary's armour. The remarkable items found on the battlefield also include six small glass eyes, each barely larger than a fingertip, some of them blue, others black, the function of which is not yet fully understood. These were examined at DESY using high-intensity X-rays from PETRA III to find out exactly what materials the Romans mixed into the glass to achieve the colours. The measurements show that black seems to have been produced by using a higher iron content, while white glass contains large amounts of lead, suggesting that lead white was used. Blue regions, finally, are conspicuous for their high copper content.

Pictures: Van Gogh Museum Amsterdam; Letizia Monico et al., Angewandte Chemie, DOI: 10.1002/ange.201505840; DESY, Katrin Zerbe

Proton accelerator analyses frescoes

Portable accelerator looks inside valuable art treasures

MACHINA uses accelerator components from CERN.

The European particle physics centre CERN specialises in building accelerators for protons (hydrogen nuclei) – such as the LHC. With a circumference of 27 kilometres, this giant ring is currently the largest accelerator in the world and is being used to unravel the mysteries of the building blocks that make up our universe. At the same time, CERN also wants to exploit its technologies for practical purposes. For example, it has modified a type of accelerator based on a radio frequency quadrupole (RFQ) so that it can be used for medical applications, such as tumour therapy.

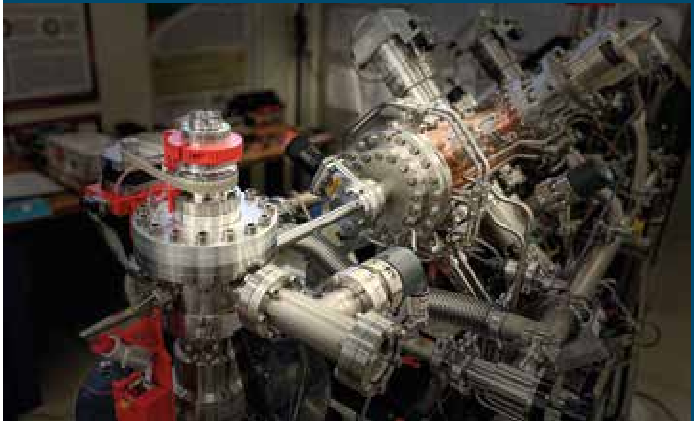
In collaboration with Italy's National Institute for Nuclear Physics (INFN), a transportable proton accelerator called MACHINA has been designed, which can be used to examine ancient art treasures. INFN has a great deal of experience in controlling accelerators as well as in analysing materials, in particular historical cultural artefacts. The partners wanted to refine the RFQ technology in order to analyse valuable cultural assets. MACHINA (Movable Accelerator for Cultural Heritage In-situ Non-destructive Analysis) was to be compact, portable and energy-efficient enough to be brought to artworks that are too difficult, too expensive or simply impossible to transport to a laboratory. Furthermore, the device was to be inexpensive and emit as little radiation as possible.

Different layers

The idea emerged at a meeting in 2016. "An expert from CERN presented the different applications of RFQ accelerator technology, while I reported on our projects for studying cultural assets," INFN physicist Francesco Taccetti recalls. "Afterwards, we decided to launch the joint project." The idea was to build a compact device that would accelerate protons and bunch them into short pulses – 200 per second. When these proton pulses strike a material, they generate X-ray pulses, which can be recorded by detectors and analysed. The key point is that different elements produce different types of X-ray pulses, meaning that the chemical composition of a sample can be determined with great accuracy. In works of art, this makes it possible to determine which pigments were used for a painting or whether there is another painting underneath the visible one.

Such analyses can also be done using X-ray machines. However, for certain applications, proton accelerators offer definite advantages. "Using MACHINA, we can roughly vary the energy of the protons," says Taccetti's colleague Lorenzo Giuntini. "Among other things, the protons penetrate a painting to varying depths, revealing different layers of the painting."

It was decided to base MACHINA at Opificio delle Pietre Dure in Florence, one of the world's most renowned institutes for the restoration of ancient works of art, which was founded in 1588 by Grand Duke Ferdinando I de' Medici. "Among other things, MACHINA will be able to detect images that have been painted over," explains Taccetti. "The different proton energies mean that several different image planes can be viewed." Another area of focus might be the analysis of frescoes: Since paintings on walls cannot be transported to a laboratory, the analytical equipment has to come to the work of art. "Exactly that is possible with MACHINA," Giuntini emphasises. "Its size of around two metres means that it fits easily into a van."



Among other things, the portable proton accelerator can detect images that have been painted over.

Pictures: MACHINA Collaboration, CERN

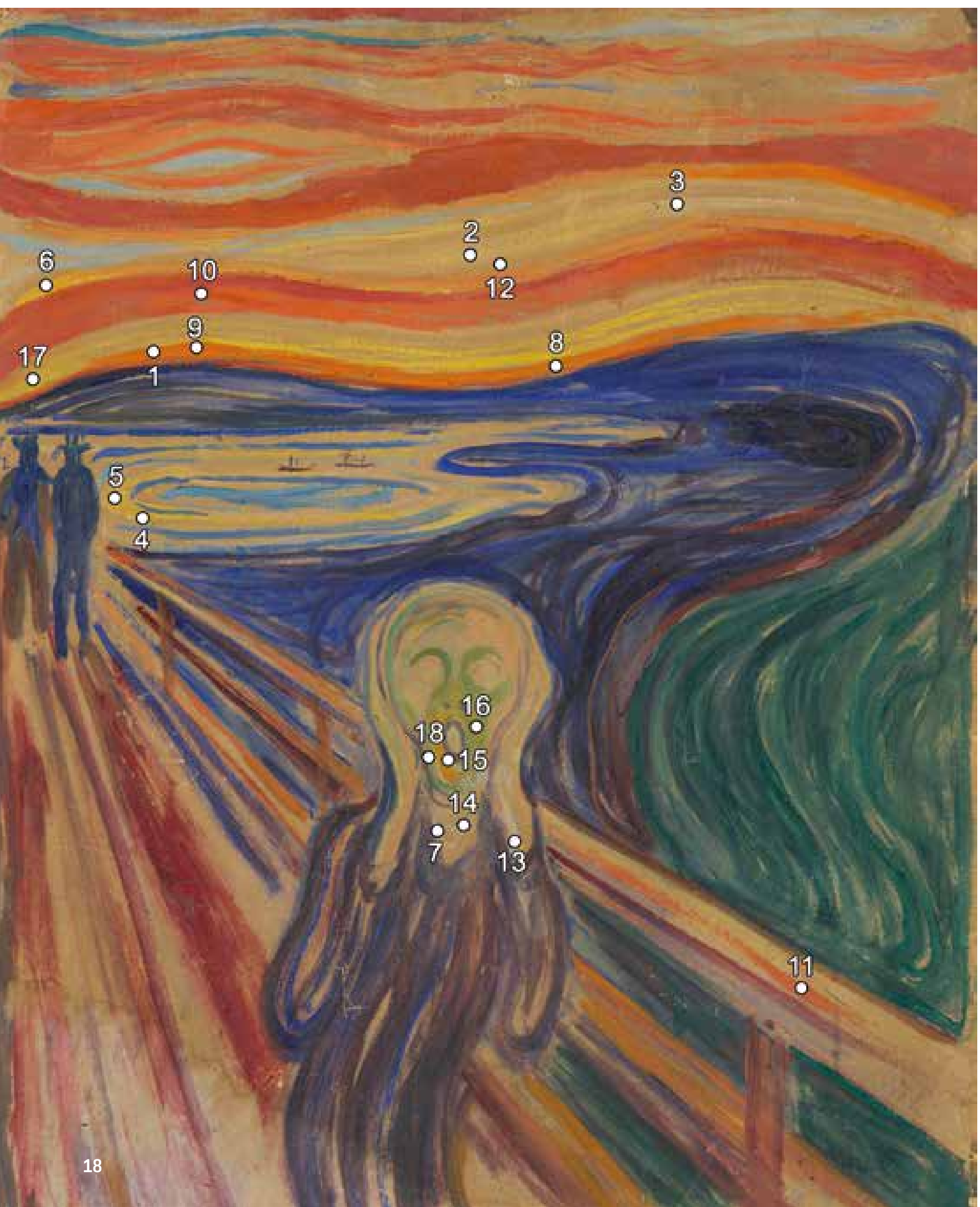
into drab brown pigments – in chemical terms, chromium VI was reduced to chromium III. In addition, van Gogh sometimes deliberately used pale yellow paint, which may have accelerated the dulling of the luminous yellow.

Even Edvard Munch's legendary painting "The Scream", of which various versions exist, has undergone some unsightly changes. Some of the yellow paint, containing cadmium, has faded and is crumbling away, for example in the region of the sunset. Some time ago, an international team examined tiny fragments of paint that had become detached from the painting, using high-intensity X-rays produced by an accelerator, and compared them with artificially aged paint samples made from original pigments. They found that bright yellow cadmium sulphide had oxidised to become colourless cadmium sulphate. The experts identified excessive humidity as being a major contributor to this process.

In the case of the Old Masters, on the other hand, the art world long believed that the pigments used in those days were for the most part stable. "But in recent years, it has turned out that these materials are not as stable as expected," says Janssens. "The paintings of the Old Masters are up to 700 years old, and slow chemical processes can certainly take place over that time."

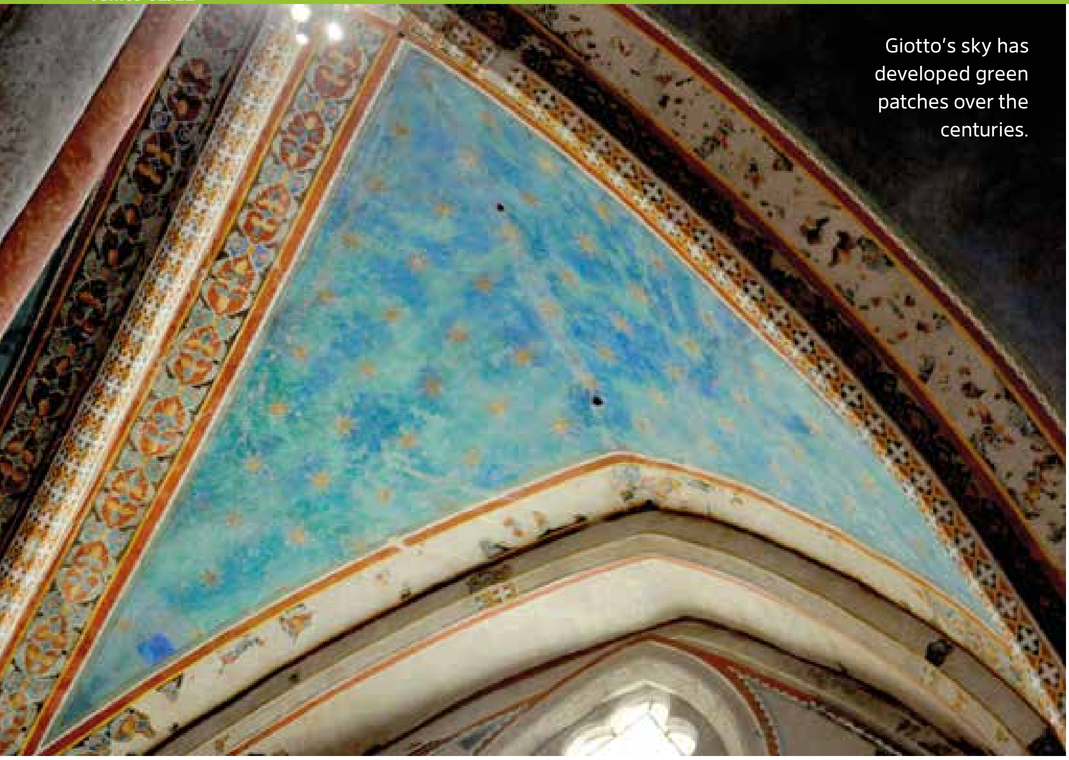
Mercury droplets

For example, Ermanno Avranovich, a member of Janssens's team, recently inspected the murals in the Basilica of Saint Francis of Assisi in Italy, whose walls and ceiling were painted in the



Edvard Munch's painting "The Scream" (1910) was analysed in 18 places using X-ray reflection and fluorescence spectroscopy.

Picture: Munch Museum, Oslo



Giotto's sky has developed green patches over the centuries.

"Some of the pigments used by Giotto have undergone substantial changes in colour"

Ermanno Avranovich, University of Antwerp

14th century by famous Italian artists, including Giotto. In 1997, a powerful earthquake caused parts of the building to collapse, badly damaging some of the wall and ceiling paintings. Many have since been restored, but Janssens and his team have been able to analyse some of the paint remnants using sophisticated X-ray techniques.

According to Avranovich, "some of the pigments used by Giotto have undergone substantial changes in colour. Most of the vermilion used on the ceiling has turned black because the mercury compound in it, a mercury sulphide, has reacted with chlorine." Tiny, finely dispersed mercury droplets formed, which appear black. Another finding concerns a famous ceiling fresco by Giotto, depicting what should be a blue sky with stars. In the meantime, however, numerous green blotches have appeared in the blue areas.

The analyses carried out at the accelerator have revealed the cause. The blue pigment azurite, a copper carbonate, appears to have reacted with chlorine and turned into an exotic mineral, a carbonate chloride – which is green instead of blue. "Presumably, strong chlorine chemicals were used in the cleaning of the basilica over several centuries," Janssens believes. "Our research shows that even the pigments used in paintings that are normally considered stable may interact with the environment. More attention therefore needs to be paid to the chemical surroundings of artworks." For some old art treasures, it may be important in the long term to afford them even better protection against external factors – in the form of glass panels, climate chambers or special ventilation systems, for example.

Operation Night Watch

Even the lighting in the museum can play a role. Some time ago, Janssen's team discovered that the comparatively strong green and blue components in the spectrum of LED lamps can damage some of the pigments used by van Gogh. Other works of art, on the other hand, are far less sensitive to green or blue light. In such cases, there is nothing to stop energy-saving LEDs from being used in museums.

Samples from another famous painting were also analysed at DESY – tiny pieces of Rembrandt's "Night Watch". Some of the results were surprising: "Before we started, the art world believed that Rembrandt was very parsimonious and reluctant to spend money on his painting utensils," says Koen Janssens. For white, for example, he was said to have always used the cheapest lead pigment available at the time – ››

Example of millimetre-sized fragments of paint from Giotto's works that were made available for the scientific study

Pictures: University of Antwerp, Ermanno Avranovich; istockphoto/Gito Trevisan

"A series of measurements can quickly add up to many terabytes"

Gerald Falkenberg, DESY

or so it was believed. "But we found out that this was not the case," says Janssens. "Rembrandt did in fact use different types of lead white, some of which were probably significantly more expensive than others." This would put a dent in the myth of "Rembrandt the Miser".

The "Night Watch" was also recently the subject of an elaborate international project: "Operation Night Watch". "In this project, we wanted to understand how Rembrandt painted his pictures, what condition the painting is in, and how we can preserve it for future generations," says Katrien Keune, chief scientist at Rijksmuseum Amsterdam, where the large painting is on display. To do this, the experts use a wide variety of methods, from X-ray images and microscopy techniques through chemical analyses and computer simulations to photographic digitisation of the image with an enormous image resolution.

Unexpected pigment

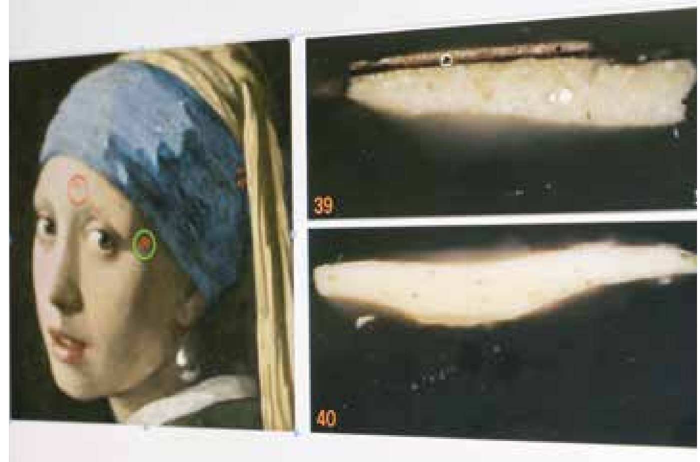
Here too, measurements carried out at DESY have contributed to a better understanding. The team came across a paint that art experts did not expect Rembrandt to have used – a yellow-orange pigment containing arsenic, which the master used to paint the gold embroideries in the picture. "We were very surprised to find it in one of the main characters of the 'Night Watch',

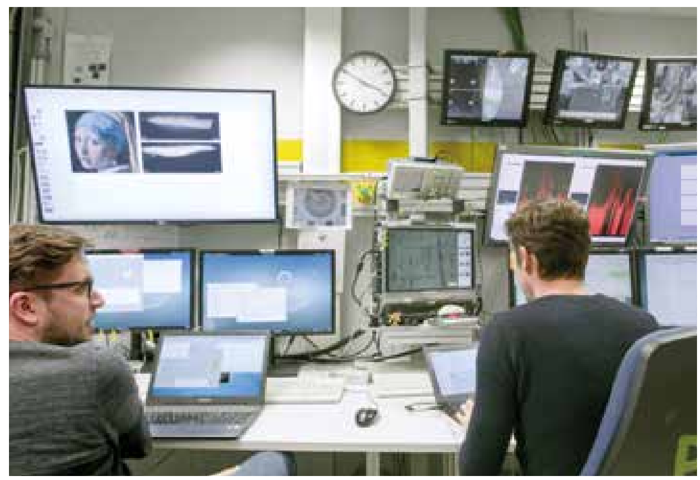
Medieval metal art
Casting or embossing – how was this medieval chalice made more than 1200 years ago? A team from Germanisches Nationalmuseum in Nuremberg, the Curt-Engelhorn-Centre of Archaeometry and DESY is trying to answer this question. The scientists have been using the high-intensity X-ray beam from PETRA III to explore the internal structure of the silver cup, which can provide information about how it was manufactured. It is not only paintings that can be analysed using X-rays.

Pictures: DESY, Marta Mayer

"We wanted to understand how Rembrandt painted his pictures"

Katrien Keune, Rijksmuseum Amsterdam





X-ray analysis of microscopic paint samples taken from the forehead and temple of the "Girl with a Pearl Earring" reveals how Vermeer went about painting the masterpiece.

on his jacket," Keune recalls. The experts also took a closer look at the primer used on the canvas. Completed in 1642, the painting had been restored several times over the centuries. Among other things, a second canvas had been glued to the back of it using a wax–resin mixture in order to stabilise it. "We are still trying to determine to what extent this mixture contributed to the darkening of the painting," says Keune. "Our measurements have certainly provided new insights concerning the sizing. We now suspect that Rembrandt applied a layer of sizing containing lead and that this lead was then able to migrate into the primer due to the subsequent treatment with the wax–resin mixture."

Unravelling Old Masters' techniques

X-ray analysis of the "Girl with a Pearl Earring" also reveals the technique used by Jan Vermeer, who created the famous painting around 1665. On Falkenberg's beamline at DESY's X-ray source PETRA III, a team led by Annelies van Loon from Mauritshuis Museum in The Hague and Rijksmuseum in Amsterdam was able to X-ray tiny paint samples from the "Girl's" forehead and temple. The analysis revealed three layers on the temple: The uppermost is just a hundredth of a millimetre thick and contains plenty of lead white as well as traces of vermilion. Underneath lies a layer of the whitish sulphate mineral palmierite, probably produced during the decomposition of lead white. The lowest layer is comparatively thick – a tenth of a millimetre – and consists of a mixture of calcite and lead white. The "Girl's" forehead is also made up of three layers, but here the upper and middle layers are somewhat thicker. Comparing the two paint samples also reveals that Vermeer used different types of lead white for the forehead and for the temple. Thus the techniques of the Old Masters can still be unravelled centuries later.

And the future? Many more insights could be in store for the art world, because in a few years' time, DESY intends to replace the current X-ray source PETRA III with a more powerful facility. The X-rays produced by PETRA IV will be much narrower, more tightly focused and more intense than now. This would allow researchers to observe in detail how pigment nanoparticles in a chemical reactor change when they are being subjected to heat, moisture or reactive gases – corresponding to a speeded-up ageing process. "After all, you can't very well do an experiment that lasts 400 years," Koen Janssens explains. "But we hope that the planned time-lapse experiments will allow us to observe how and why pigments change under certain external conditions."

On the one hand, the results should help the art world to better understand the properties of its masterpieces. On the other hand, the findings could give conservators new hints as to how to treat and restore the paintings in the future so as to preserve this human cultural heritage for the sake of posterity.

Pictures: Perspektive Media

Ancient hill settlement with brick buildings on Elephantine Island on the Nile

JOURNEY INTO THE PAST

X-ray exploration of ancient cultures

The Middle East is considered to be the cradle of civilisation. The first advanced cultures arose in Mesopotamia and Egypt; pyramids and temple complexes still bear witness to a complex society in ancient Egypt. To explore these long-gone cultures in greater depth, experts are examining the relics they left behind, analysing stone ruins, ancient writings and faded wall paintings. Particle accelerators and X-ray equipment can help reveal important details. They allow us to read hidden texts and help analyse and conserve ancient frescoes.

A thousand kilometres south of Cairo lies an archaeological site with an abundance of ancient writings. Elephantine is a small island in the middle of the Nile, not far from the border with ancient Nubia, now Sudan. For many millennia, it was an important military border fortress, but also a vibrant trading post. “It was very international, a multicultural place,” says Verena Lepper, an Egyptologist at Staatliche Museen zu Berlin. This is because Elephantine was home to a wide variety of cultures, each with a different language and writing system – including hieroglyphics, Greek and Arabic, but also Coptic, Syriac and Aramaic.

“Elephantine is the only place in the world where we can access 4000 years of cultural history through written documents”

Verena Lepper, Staatliche Museen zu Berlin

Picture: istockphoto/nexusimage

In addition, each culture left behind traces in the form of papyrus documents – covering an astonishingly long period of time. “Elephantine is the only place in the world where we can access 4000 years of cultural history through written documents,” say Lepper with enthusiasm. “There are religious, medical and literary texts, but also contracts and administrative documents. They reflect the entire range of life on the island over a span of 4000 years.”

Rolled up, folded and sealed

Today, these manuscripts are distributed all over the world; important examples are found in the Louvre in Paris and Ägyptisches Museum in Berlin, among other places. Until recently, however, only a fraction of these mauscripts had been analysed. In order to decipher further documents, in 2014, Lepper successfully applied for a project called ELEPHANTINE funded by the European Research Council (ERC). “Our Berlin collection included metal boxes from excavations conducted 100 years ago,” explains Verena Lepper. “But we have only now opened them and sorted through their contents.” However, not all the documents could be deciphered. This is because they had been carefully rolled up, folded and sealed. Trying to open them could cause them to crumble or disintegrate into countless fragments; the texts threatened to be irrevocably lost.

To solve this problem, Lepper teamed up with a physicist: Heinz-Eberhard Mahnke, now an honorary professor at Freie Universität Berlin and physicist at Ägyptisches Museum, who used to work at Helmholtz-Zentrum Berlin. Its accelerator BESSY II is one of the most powerful X-ray sources in Germany. “Initially, there was some doubt whether such hidden texts could be revealed with the help of a special X-ray technique known as tomography,” Mahnke recalls. “But it turned out that it can in fact be done!”

In tomography, a 3D image of the object is created using X-rays, resulting in a spatial representation. “Special mathematical algorithms can use the data collected to unroll or unfold the document in virtual reality,” Mahnke explains. “That way, we can reconstruct the writing in the document.” However, the prerequisite is being able to distinguish the ink from the papyrus to which it was once applied. “This is difficult with inks based on carbon black because, like papyrus, they consist essentially of carbon,” Mahnke continues. “It is more favourable if the documents were written in iron gall ink, because the image contrast is significantly higher.”

“Special mathematical algorithms can use the data collected to unroll or unfold the document in virtual reality”

Heinz-Eberhard Mahnke, Fellow at the Einstein Center Chronoi

Spectacular insights

The team first tested the new technique on “papyrus mock-ups”, which they wrote themselves and then folded up. This allowed them to test whether the method was in principle suitable for deciphering hidden texts. Once this had been successful, Lepper and her team turned to the originals, in other words actual documents from Elephantine. Some of these originals were scanned at BESSY II, others using smaller X-ray machines.

Physicist and Egyptologist: Heinz-Eberhard Mahnke (l.) and Verena Lepper (r.) examined the written documents from Elephantine together (bottom).

πχοε[ις]

The reconstructed hidden Coptic manuscript “Oh Lord” after being unfolded (Louvre L/EI227b/1-pC)

The results were spectacular: Analysing a folded amulet from the fourth century AD from the Louvre collection, the experts were able to decipher a phrase written in the Coptic alphabet – Oh Lord Jesus Christ. “That was a real sensation,” says Verena Lepper. “The phrase is an expression of personal piety, and for scholars it was impressive evidence of early Christianity on Elephantine Island.”

This success is to some degree a result of the cooperation between two completely different research disciplines: Egyptology and physics. “The papyrus collection in my museum includes ten different languages and writing ››

Pictures: Anke Weber, Felix Herter, Zuse Institute Berlin systems," Lepper recalls. "Working with Heinz-Eberhard Mahnke meant learning yet another language, namely that of physics. But it was worth it; the cooperation worked wonderfully!" Another discipline also played a key role. Without the work of Daniel Baum's group in the field of computer science at the Zuse Institute Berlin, neither the imaging nor the virtual unfolding and unrolling would have been possible.

Promising pilot tests

This work is to continue, and the X-ray methods will be refined. "In the future, we would also like to decipher documents written in carbon black ink," explains Mahnke. "We have already carried out some promising initial pilot tests at DESY's PETRA III." The approach is based on the observation that, in certain X-ray techniques, carbon black ink absorbs or scatters the radiation slightly differently from the papyrus on which it was used. The result would be a weak but discernible image contrast, which might well allow the writing to be deciphered.

A special accelerator is also expected to play an important role: the X-ray source SESAME in Jordan. This went into operation in 2017 and involves several countries from the Middle East, including Egypt, Bahrain and Turkey, but also Palestine, Israel and Iran. SESAME not only aims to boost science in the region, but also to bring together hostile nations that have little contact with each other at the political level. "It is an advantage that Egypt is participating in SESAME," points out Verena Lepper. "I expect that, in the future, cultural treasures from the region will also be brought to Jordan to be X-rayed at SESAME." New experimental stations at SESAME funded by the Helmholtz Association will contribute significantly to these studies.

The Al-Khasneh treasury is probably Petra's most famous building.

Ruins of the rock city

SESAME's possibilities are also benefiting the project of Maram Naes, a researcher at Technische Universität Berlin. She is studying relics from the famous ancient city of Petra in what is now Jordan. 2000 years ago, several nomadic tribes in the Middle East joined forces to create the Kingdom of Nabataea, and Petra was its capital. Its remains are among the most impressive city ruins in the world, serving, among other things, as the backdrop to the famous "Indiana Jones" adventure film franchise. "I first visited the rock city when I was a schoolgirl," says Naes. "To get there, I first had to pass through the Siq, a sandstone gorge over a kilometre long and in places only two metres wide. Once I was standing at the end of the gorge in front of Al-Khasneh, the 39-metre-high Nabataean treasury, it took my breath away."

It was this fascination that later moved the Jordanian-born scientist to take a closer look at Petra and to subject the ruins to painstaking scientific scrutiny. Her interest lay especially with the murals that once adorned the ancient city. "Today, you can no longer see that the walls of Petra were almost completely covered in paint; everything used to be full of colours and pictures," says Naes. "The Nabataeans did this not only to beautify the city, but apparently also to protect the delicate sandstone against weathering." Most of the images were decorative; in some cases, geometric shapes are recognisable. "To my mind, this suggests that the Nabataeans were fond of mathematics," says Naes.

Picture: istockphoto/cinoby

The inside of buildings in Petra are richly decorated with murals (left). Using a mobile X-ray scanner, Maram Naes led the first non-destructive and non-invasive on-site investigation of Nabataean wall paintings (right).

Examining the remains in more detail, the researcher discovered that some of the relics were once gilded, but have since darkened. “I wanted to understand the composition of these materials,” she says. “And I asked myself how we could best conserve them, so as to preserve this valuable cultural heritage for posterity.” In search of answers, Maram Naes used a variety of experimental techniques to study the objects. Among other things, she collected tiny fragments of material to analyse them under the narrowly focused X-ray beam of a particle accelerator. The experiments were conducted at the storage ring BESSY II in Berlin, but also at SESAME in Jordan.

“Today, you can no longer see that the walls of Petra were almost completely covered in paint; everything used to be full of colours and pictures”

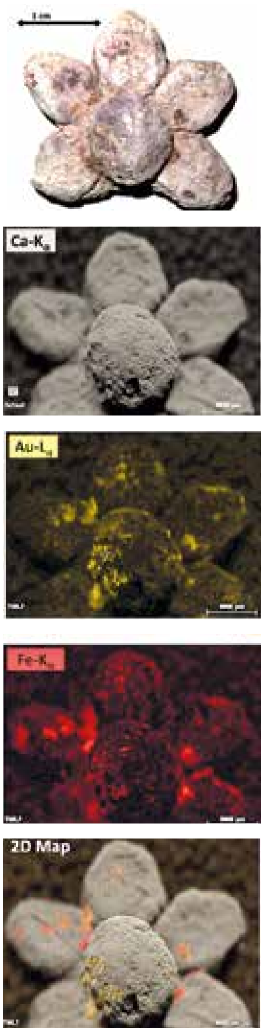
Maram Naes, Technische Universität Berlin

New conservation method

As a result, the experts were able to determine what materials are located above and below the layer of gold. They also determined the impact of restoration work carried out in the 1990s. “The preservative that was used at the time permeated the entire structure, from the top of the gilded layer all the way to the foundation,” Naes reports. “In some cases, layers of oxalate have formed on the surface, causing the gold to darken.” However, the paintings are in a stable condition, so these dark layers do not necessarily need to be removed.

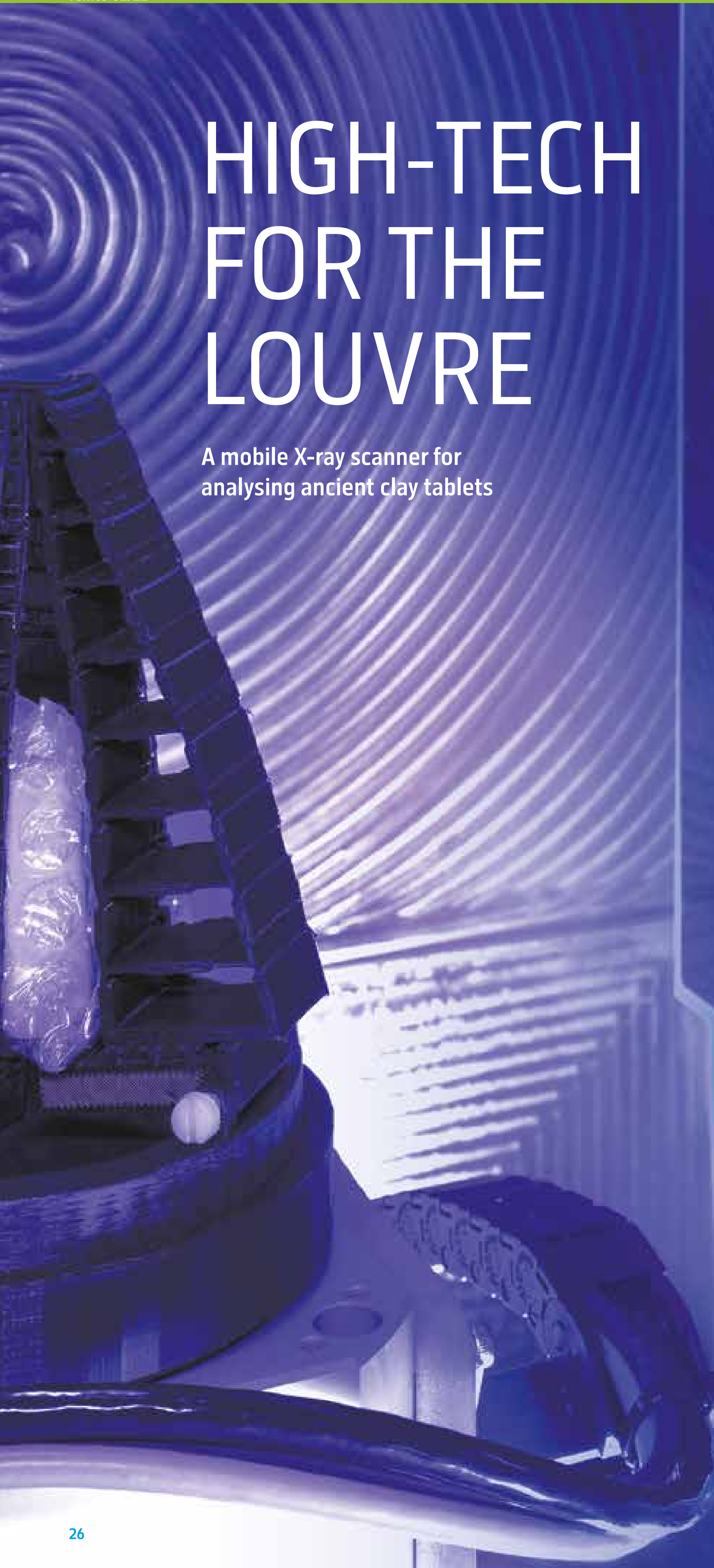
On the other hand, action is necessary in those areas where the gold coating threatens to flake off. “This is why I developed a new preservative, which is supposed to reattach the gold to the underlying surface,” explains Naes. “It is based on a mixture of a polymer and gold nanoparticles and can be injected underneath the gold layer of the affected murals using fine needles.”

Using a new experimental station by the name of HESEB, the researcher now wants to find out how this agent works on a molecular level. This Helmholtz–SESAME Beamline is the result of a DESY initiative and was recently set up at the Jordanian storage ring. “The soft X-rays from SESAME will allow us to observe in detail how well the gold reattaches to the underlying surface with the help of the new preservative,” says Maram Naes. “HESEB provides perfect conditions for those analyses.” If the experiment is a success, the new conservation method could soon be put into practice and help to preserve the art treasures of the Nabataeans for future generations.



X-ray examination of once-gilded stucco (top) reveals calcium (Ca), residual gold (Au) and iron (Fe) in a combined fluorescence map (bottom).

Pictures: Maram Naes



HIGH-TECH FOR THE LOUVRE

A mobile X-ray scanner for analysing ancient clay tablets

The first ancient civilisations wrote on clay tablets. But by no means all these tablets can be read – they are encased in thick envelopes, also made of clay. As part of a Cluster of Excellence at Universität Hamburg, DESY experts have constructed a special X-ray tomograph that should finally reveal the contents of these hidden documents. This could lead to completely new insights into the customs of antiquity.

It may be the oldest writing system in the world: Starting around 3300 BC, the Sumerians in Mesopotamia immortalised themselves using a script called cuneiform, by pressing a stylus into soft clay. This technique was later adopted by other cultures, such as the Babylonians, Assyrians and Persians – until it was finally supplanted by more modern forms of writing about 2000 years ago.

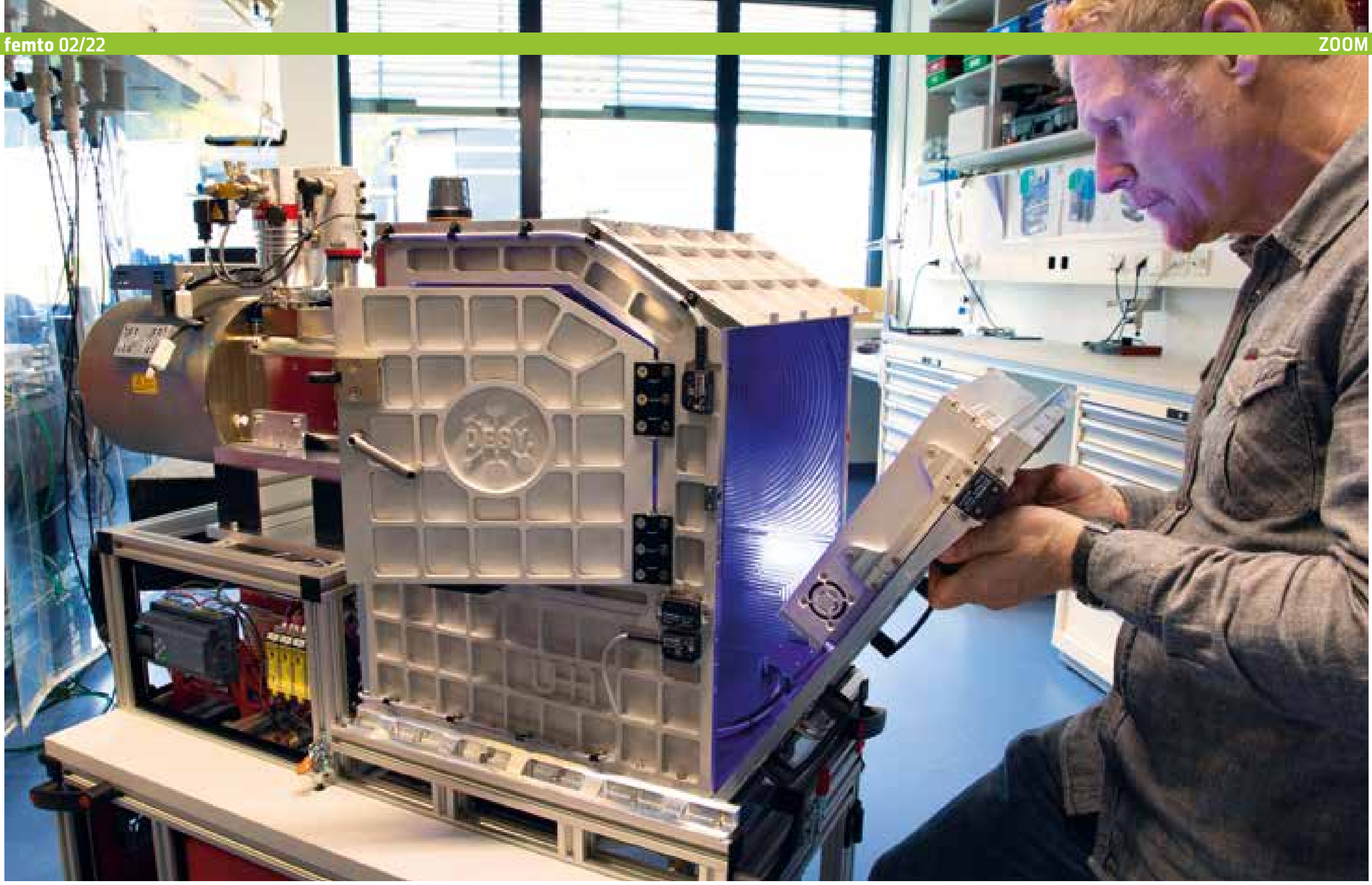
The fascinating thing is that, even back then, correspondence appears to have been confidential. Many of the inscribed clay tablets were sent in addressed envelopes, themselves also made of clay. “These were private letters, but also contracts and official documents,” says DESY physicist Christian Schroer. “Studying these tablets teaches us a huge amount about what life was like thousands of years ago. How did people communicate, how was their society organised, and which paths did their trade routes follow?” Once the letter reached the right address, the clay envelope was broken, revealing the tablet and its cuneiform message.

Forever unopened

However, not every document reached its destination – and some remained unopened forever. Today, archives and museums hold thousands of such sealed letters. As interested as the experts are in studying their contents, they do not want to open the old treasures – after all, this would mean destroying them. Yet the X-ray machines that museums have been using up to now cannot penetrate the clay envelopes in order to read the contents of the tablets inside. This is because such machines produce comparatively low-energy radiation. While these X-rays are adequate for analysing paintings and have the big advantage that proper radiation protection is comparatively easy to implement, the low-energy radiation is simply not strong enough to penetrate the thick clay envelopes. That requires a higher-energy X-rays with noticeably more “penetrating power”.

Christian Schroer’s group is now making a fresh, more technically sophisticated attempt. It

Picture: DESY, Marta Mayer,



has constructed a mobile X-ray device that uses high-energy radiation to look inside the clay letters and reveal their contents. This work is being conducted within the Cluster of Excellence "Understanding Written Artefacts" at Universität Hamburg, comprising experts from various northern German research institutions who are taking a closer look at the evolution and function of written documents from all over the world. Schroer's team has been working particularly closely with the Hamburg Assyriologist Cécile Michel.

"The Sumerians are now thought to have first dried the actual clay tablets," says Schroer. "Then they wrapped the envelopes around the tablets fairly loosely, leaving a narrow air gap between the two." The idea is that this air gap will provide the necessary contrast in the X-ray image, allowing the tablet to be distinguished from the envelope and its contents to be deciphered.

3D images

In the laboratory at the Centre for X-ray and Nano Science (CXNS), Schroer's colleague Ralph Döhrmann points to the device. Its design is modular, consisting of several segments that can be assembled to form a complete unit. "All the individual parts are portable," explains the engineer. "That way, the device can be transported up stairs and down narrow corridors in a museum." Once assembled, the unit is about the size of an overflowing shopping trolley – and, like a shopping trolley, it can be pushed around on wheels. All the individual parts were manufactured and tested in DESY's workshops, and the programs that control it were developed and written by Schroer's team.

The heart of the device is a special X-ray tube that focuses the radiation onto a spot that is only 20 to 40 micrometres across. A micrometre is one thousandth of a millimetre. The X-rays illuminate a sample holder on which the clay tablet is mounted. "This holder consists of finger-like grippers, which can be used to gently clamp the tablet," explains Döhrmann. "It can be rotated and moved in all directions." As a result, the tablet can be scanned from every angle – the device is a tomograph, which produces three- ››

"Studying these tablets teaches us a huge amount about what life was like thousands of years ago"

Christian Schroer, DESY

Reading aid: The mobile X-ray scanner is to be used to decipher cuneiform tablets inside their clay envelopes.

Pictures: DESY, Marta Mayer; DESY, Gesine Born

"Everything humans have ever written on"

A Cluster of Excellence at Universität Hamburg is investigating the evolution and influence of manuscripts

At Universität Hamburg, the Islamic scholar Konrad Hirschler is coordinating the Cluster of Excellence "Understanding Written Artefacts". DESY is one of the cluster's partners. A first joint project could now turn into steady cooperation.

femto: Since 2019, the Cluster of Excellence "Understanding Written Artefacts" has been looking at the development and role of manuscripts in our world. What exactly is this about?

Konrad Hirschler: We are examining how and when different cultures used and practised writing. How do we explain the numerous differences, in form and function? And how have these practices influenced societies, how have they changed the political, social and economic conditions? We are not only interested in written artefacts made of paper, but also in eggshells, palm leaves, wooden boards or metal rods bearing characters – in other words, everything that humans have ever written on.

Some projects are looking at the oldest written documents in the world, 5000-year-old clay tablets from Mesopotamia. Others are analysing graffiti on the walls of houses in modern-day Hamburg. The humanities are particularly closely involved, including Japanese studies, Arabic studies and Assyriology. But the cluster also has a natural sciences section. This examines how to analyse the materials on which the writing was recorded as accurately as possible. Which region does an Indian palm leaf that was once written on come from, for example, and how old is it? In recent years, we have been cooperating more and more closely with DESY on these issues.

femto: The first joint project with DESY was to develop a mobile computer tomograph for the analysis of Mesopotamian clay tablets. What value will this device have for research?

Konrad Hirschler: It will allow us to decipher the cuneiform writing on clay tablets that has been illegible until now because they are enclosed in envelopes. We don't want to, and we cannot, destroy these envelopes, which are also made of clay, so we need special CT methods that are able to penetrate the envelopes. In principle, we could do this on site at DESY, because Hamburg is home to some of the most powerful X-ray sources in the world. However, cultural institutions are usually not willing to relinquish their valuable treasures.

So we have developed a mobile device with which we can visit the institutions and examine the clay tablets on site. This will enable us to provide scientists with completely new texts in the future; but we will also be able to draw conclusions about how the clay tablets were manufactured. We also want to try out other applications for the new device, such as analysing centuries-old book covers. These were often made by gluing together sheets of old manuscripts. If we could make the writing on these sheets legible with the help of X-rays, this could lead to ground-breaking new insights for our research.

femto: Do you have any additional plans?

Konrad Hirschler: The cooperation has been excellent, and based on this there is a mutual interest in turning it into a permanent collaboration. The problem with collaborations between the humanities and the natural sciences is that they often take the form of research projects with a limited duration of just a few years. Once the project is finished, the know-how associated with it often gets lost. We are hoping for a long-term collaboration with DESY, one that can have a much deeper impact on our respective fields. For example, we are working together to develop new methods of analysing the mineral composition of historical clay tablets. This would help us to determine where these tablets were once made.

We are also hoping to implement new methods of analysing paper. Paper is incredibly difficult to analyse because the organic raw materials have undergone so many processes during its production. That makes DNA analyses virtually impossible, which is why we want to work with DESY to find ways of determining, at the molecular level, how and where a paper document was originally produced.

Pictures: istockphoto/nathan4847; private (portrait) dimensional images. An X-ray detector records the radiation passing through the sample, and the data ends up on an onboard server and hard drive. Depending on the dimensions of the tablet – the largest are the size of a brick – screening can take two to three hours, in extreme cases even a day.

The biggest challenge in designing the tomograph is that it should deliver as much power as possible in the smallest possible space, and yet remain absolutely safe. “Due to the high energy of the X-ray tube, it is not at all easy to screen the outside from the radiation, ensuring radiation protection and keeping the operators safe,” explains Döhrmann. The problem is that,

“The device can be transported up stairs and down narrow corridors in a museum”

Ralph Döhrmann, DESY

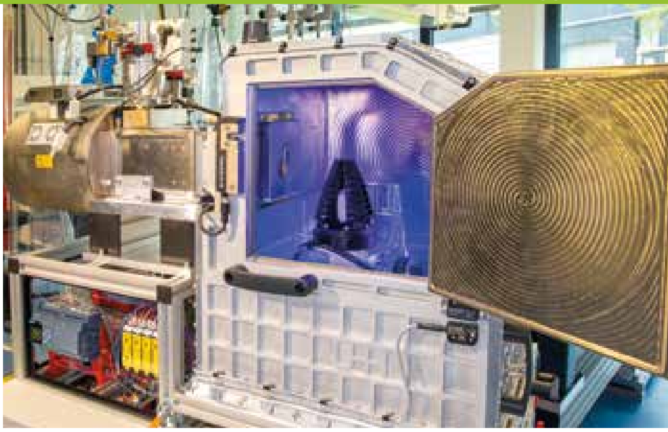
on the one hand, the tungsten–aluminium plates used as shielding need to be thick enough to reliably contain the radiation. On the other hand, they must not be too thick, otherwise the unit would become too heavy for mobile use – it should not weigh much more than 300 kilograms in total.

Laboratory testing

Using a large laboratory tomograph, the experts were able to demonstrate some time ago that the method does work in principle. The object used at the time was a “replica” clay envelope with clay contents. “We were able to separate the inner part from the outer part,” says Ralph Döhrmann. “Afterwards, we managed to print a 3D model of these test clay tablets using the tomography data.” Similar tests are to begin soon with the new, compact model.

The first place to use the mobile tomograph will probably be the world’s most famous museum: the Louvre in Paris. Some 50 sealed clay letters are waiting there to be deciphered. “I could imagine that the experts at the Louvre will be very reluctant to relinquish the device,” says Schroer. “Because it can be used to study many other works of art and cultural treasures.” Ideas for this already exist, including analysing the spines of historical books. These often used to be made from waste paper. If X-ray scanners could reveal what was written on these documents, which were considered superfluous at the time, some surprising insights might emerge. “We have already carried out some initial tests at DESY and found that documents written with ferrous inks can indeed be identified,” Schroer says.

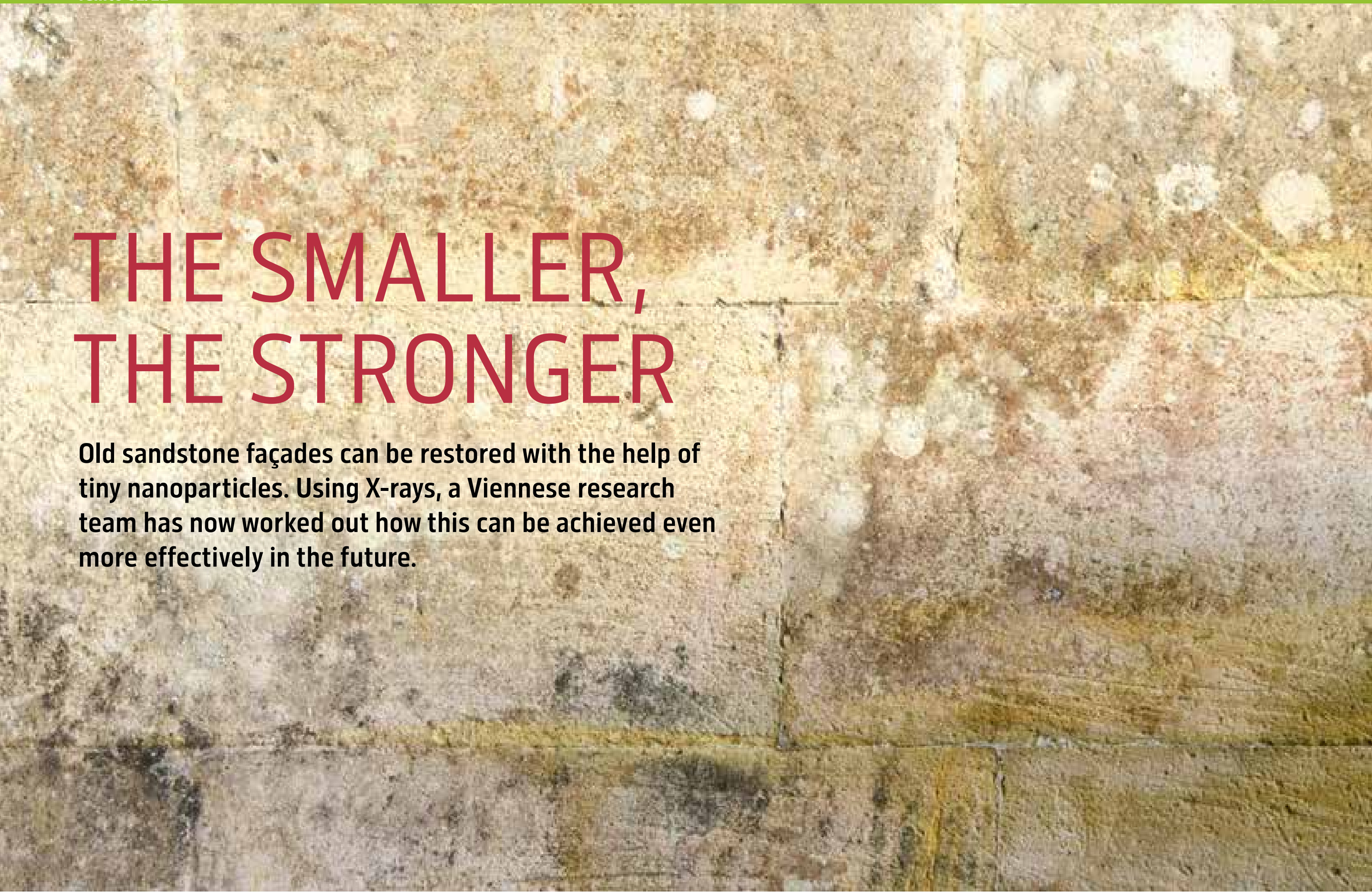
Anyway, the new mobile X-ray tomograph does not have to remain the only one of its kind. Admittedly, its development was complicated and took over two and a half years. But the hardware costs are manageable, so it should be perfectly possible for a company to manufacture a small-batch series of the devices. “Once people see that the tomographs work,” says Christian Schroer, “I think there will be a strong demand for them.”



The clay tablets are clamped in a holder with finger-like grippers.

Clay tablets served as documents thousands of years ago. This specimen from today’s Central Anatolia records a loan contract that is about 4000 years old.

Pictures: DESY, Marta Mayer; Universität Hamburg, Cécile Michel



THE SMALLER, THE STRONGER

Old sandstone façades can be restored with the help of tiny nanoparticles. Using X-rays, a Viennese research team has now worked out how this can be achieved even more effectively in the future.

Numerous historical buildings are made of sandstone – St. Stephen's Cathedral in Vienna, for example, the Berlin Cathedral or parts of Dresden's Zwinger. Although the material is easy to work with, it is also prone to severe weathering. The reason for this is that "sandstone is made up of small loose grains, which are not very strongly bonded to each other," says Markus Valtiner, a physicist at Vienna University of Technology. "This makes the material porous and liable to break, and when it is exposed to changing temperatures, weathering and sulphur dioxide, it eventually crumbles away." As a result, elaborate restoration work is often necessary in order to preserve famous sandstone façades.

For some time now, a comparatively new method has been used for such restoration measures – treating the sandstone with silicate nanoparticles. In this process, the sandstone affected is sprayed with a suspension of silicate nanoparticles that penetrates one or two centimetres into the porous material. Here, the silicate particles act as a kind of glue; as the suspension dries, the particles bond with the sandstone grains, forming reinforcing bridges between them. "However, until now it has been unclear what size of particles has the greatest effect," says Valtiner. "So we have been looking at how these adhesive forces vary for different particle sizes."

"The smaller the nanoparticles, the stronger the adhesive forces"

Markus Valtiner, Vienna University of Technology

Suspension of nanoparticles

The experts resorted to a combination of two experimental techniques. The equipment used by Valtiner's team can precisely measure the forces with which the tiniest particles adhere to each other. His colleague Markus Mezger, a physicist at the University of Vienna, knows all about X-ray methods for determining the structure of nanoparticles in great detail. The experts combined these two techniques,

Picture: istockphoto/Mac99

designing the experiment that measures the forces in such a way that it can be carried out while simultaneously studying the sample with the high-intensity, narrowly focused X-rays from PETRA III, one of the world's most powerful X-ray sources, at DESY's Hamburg site.

"We injected a suspension of silicate nanoparticles into our apparatus and left it to dry," explains Mezger. "While it was drying, we were able to measure an increase in the adhesive forces and, at the same time, use the X-rays to determine how the structure of the particles was changing." The group took several series of measurements, each with particles of different sizes. The smallest were 11 nanometres across, the largest 27. A nanometre is a millionth of a millimetre.

Working on St. Stephen's Cathedral in Vienna

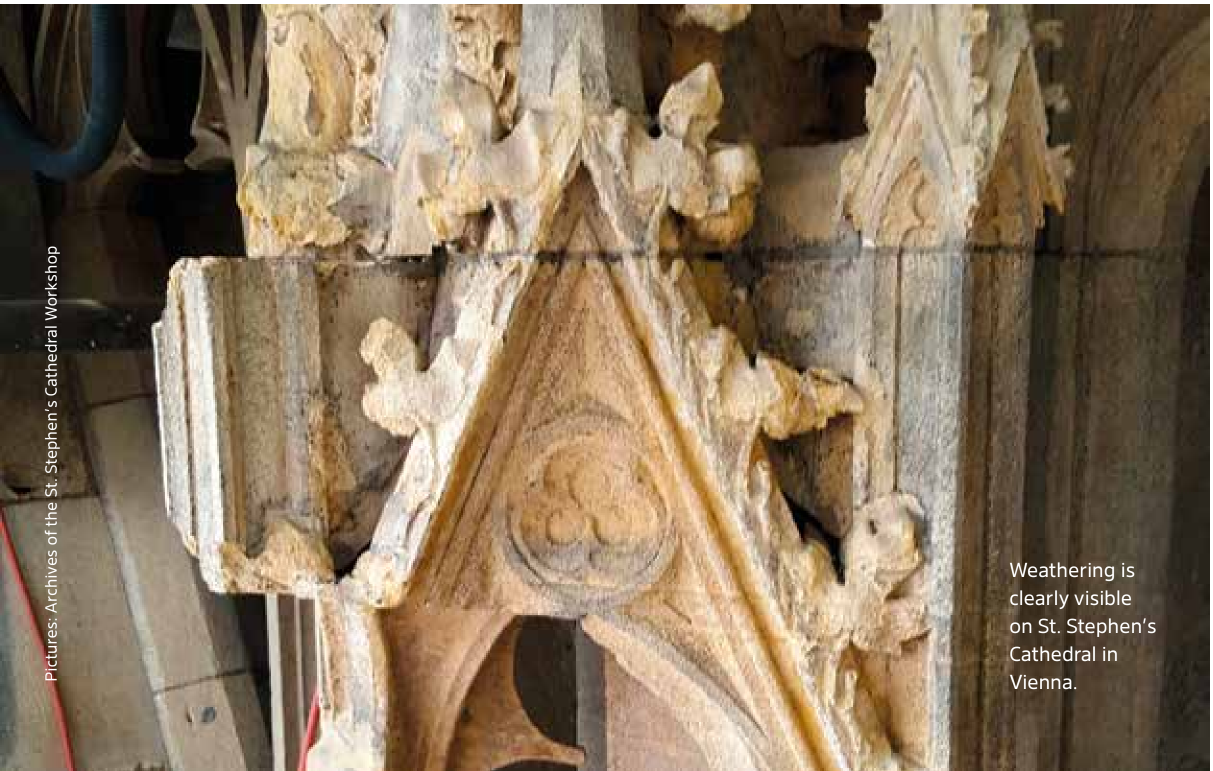
"On drying, crystallisation into a glass-like state set in"

Markus Mezger, University of Vienna

Significantly more contact sites

And the result? "The smaller the nanoparticles, the stronger the adhesive forces," Valtiner replies. The X-ray measurements revealed the reason. Smaller particles formed significantly more contact sites than larger particles. "Initially, we saw the individual nanoparticles with water in between them," Mezger explains. "On drying, crystallisation into a glass-like state set in, and we started to observe more and more interactions between the particles and, at the same time, an increase in the adhesive forces."

If these results are confirmed by future, more practically oriented experiments, this could lead to a noticeable improvement in how old sandstone buildings are preserved. Up to now, the silicate particles used for restoring them have been much larger, measuring 70 to 100 nanometres. "In principle, it should be more favourable to use smaller particles," suspects Markus Valtiner. "They should generate stronger adhesive forces, and I could imagine that, in addition, they will penetrate deeper into the stone." Both effects taken together should significantly increase the strength of the stone, making the restoration measures much more effective. As a result, historic sandstone façades – some of which include ornate embellishments – would be even better protected against decay.

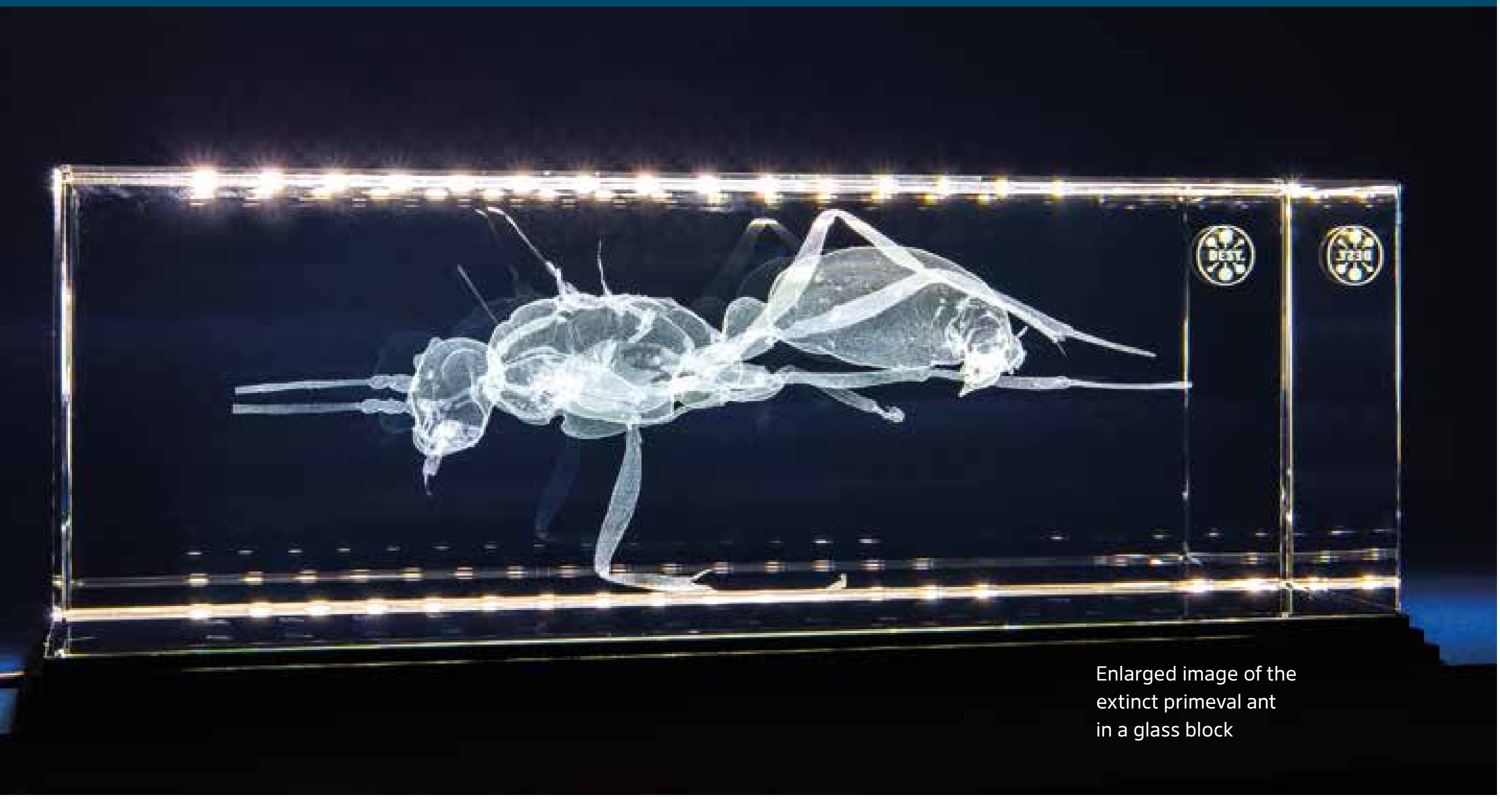


Weathering is clearly visible on St. Stephen's Cathedral in Vienna.

Pictures: Archives of the St. Stephen's Cathedral Workshop

SPECTRUM

News from research



Enlarged image of the extinct primeval ant in a glass block

New ant genus named after DESY

An international team of scientists led by Friedrich Schiller University Jena has identified a previously unknown extinct ant in a unique piece of African amber about 20 million years old. The team used DESY's X-ray source PETRA III to examine the critical fossil remains from 13 individual animals at a specialised measuring station operated by Helmholtz-Zentrum Hereon, and realised that these could not be attributed to any known species. The new species even establishes a completely new genus of primordial ants, as the scientists report. The new genus was named after DESY, the new species after Hereon: With the scientific name †*Desyopone hereon* gen. et sp. nov., the discoverers honour the two research institutions, which contributed significantly to this discovery with modern imaging methods.

The ants studied are only 3 to 3.5 millimetres long. The team therefore used the technique of micro-computed tomography with the brilliant X-rays from PETRA III at the Hereon measuring station to obtain high-resolution 3D X-ray images of the individual ants. The images show details as fine as a thousandth of a millimetre.

According to current knowledge, ants have been around for about 140 million years. To date, about 14 000 living and 763 extinct ant species have been described. They belong to about 350 living and 167 extinct genera. *Desyopone hereon* is the 764^{th} extinct species and the only species of the new (168^{th}) extinct genus so far. However, it would be plausible that some still existing species of the new genus *Desyopone* could one day be discovered somewhere in Africa, the researchers write. There is a corresponding example from a South American ant genus that was believed to be extinct, but was later discovered alive. "*Desyopone* may still be out there," says main author Brendon Boudinot, who is currently working at the University of Jena on a Humboldt Research Fellowship.

Insects, DOI: 10.3390/insects13090796

Picture: DESY, Marta Mayer

Materials researcher Nicola Spaldin wins Hamburg Prize for Theoretical Physics

British scientist Nicola Spaldin has won the 2022 Hamburg Prize for Theoretical Physics. Currently serving as professor of materials theory at ETH Zurich in Switzerland, Spaldin is a trailblazer in the development of a new class of materials known as multiferroics. Theses are materials that can be both permanently magnetised and electrically polarised. These physical properties almost never coexist in nature. Spaldin's theoretical analyses have paved the way for the production of tailor-made ferromagnetic and ferroelectric crystals. This unusual combination could allow for the building of ultrafast data repositories and supersensitive sensors.

The Hamburg Prize for Theoretical Physics, which is presented jointly by the Joachim Herz Foundation, the Wolfgang Pauli Centre at DESY and the Clusters of Excellence "CUI: Advanced Imaging of Matter" and "Quantum Universe" at Universität Hamburg, has been honouring the work of internationally renowned researchers since 2010. Nicola Spaldin is the first woman to win the accolade since its inception. The prize is one of the highest-endowed scientific awards for physics in Germany. The prize money, financed by the Joachim Herz Foundation, is 137 036 euros – an allusion to Sommerfeld's fine structure constant, which plays an important role in theoretical physics.

Picture: Daniel Rihs

Rare insights into growing nanoparticles

How exactly do nanoparticles form in solution? For the first time, researchers from Universität Hamburg and DESY have been able to observe this process in real time using DESY's X-ray source PETRA III.

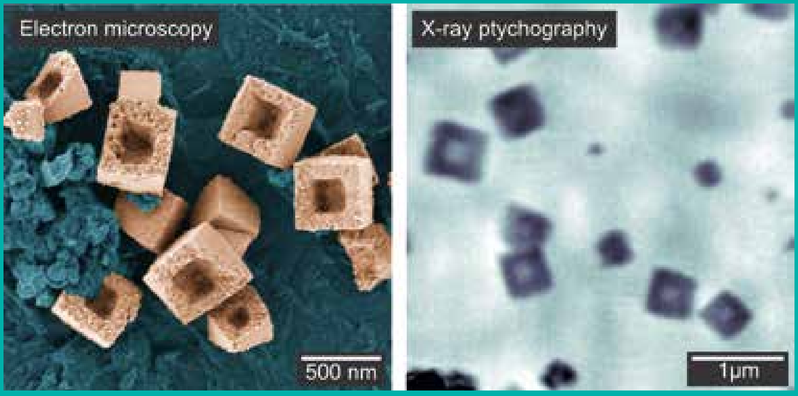
Many pathways exist that lead to such complex materials. Hence, understanding and controlling the course of the nanoparticles' growth remains a major challenge. Hard X-ray microscopy can image growing nanoparticles in chemical reactors with a spatial resolution of up to ten nanometres. A nanometre is a millionth of a millimetre.

The observations showed that particles growing on the walls of the chemical reactor developed a flatter shape, while particles in the middle of the solution took on a regular cubic shape. The nanocubes were eventually reduced to metallic copper in a solid-state reaction. In the process, voids formed in the centre of the particles and expanded towards the surface, resulting in hollow nanocubes.

Hollow nanoparticles with sizes in the range of several hundred nanometres have widespread application potential, for instance in lithium ion batteries, as sensors and for (photo-)catalytic energy production. "To reach the desired functionality and high performance, it is decisive that we achieve precise control over the structure and shape of the nanoparticles during their growth", explains first author Lukas Grote from Universität Hamburg and the Cluster of Excellence "CUI: Advanced Imaging of Matter".

Nature Communications,
DOI: 10.1038/s41467-022-32373-2

Scanning electron microscopy image (left) of the final hollow copper nanocubes outside the chemical reactor. X-ray ptychography (right) does not achieve the same resolution, but it can be used to follow the growth of the nanoparticles live in the reactor.



Picture: Grote et al., Nature Communications, CC BY 4.0

"Dust echo" reveals cosmic catastrophe

In a distant galaxy in the constellation Hercules, a gigantic black hole has torn apart a giant star. The cosmic catastrophe revealed itself through a glistening "dust echo" in the infrared range, as reported by an international team led by DESY.

The giant star had come so close to the black hole that the black hole's gravity tugged much harder on the front side of the star than on its back. This tidal force eventually destroyed the star. The intense radiation produced in this so-called tidal disruption event burned a cavity in the huge dust cloud surrounding the black hole in the faraway galaxy. Within a range of about half a light year, the dust evaporated immediately. Beyond that point, the radiation heated the dust so intensely that it began to glow brightly in the infrared range. Due to the geometry of the light path, this dust echo reached its maximum only about a year after the demise of the giant star. "The dust echo in the infrared range is a key signature of the tidal disruption event," reports first author Simeon Reusch from DESY. "This gave away the nature of this transient object."

The intense radiation from the debris disk around the black hole (centre) heats the dust until it begins to radiate brightly in the infrared. The time delay creates a "dust echo".

Picture: Science Communication Lab for DESY

Physical Review Letters,
DOI: 10.1103/PhysRevLett.128.221101

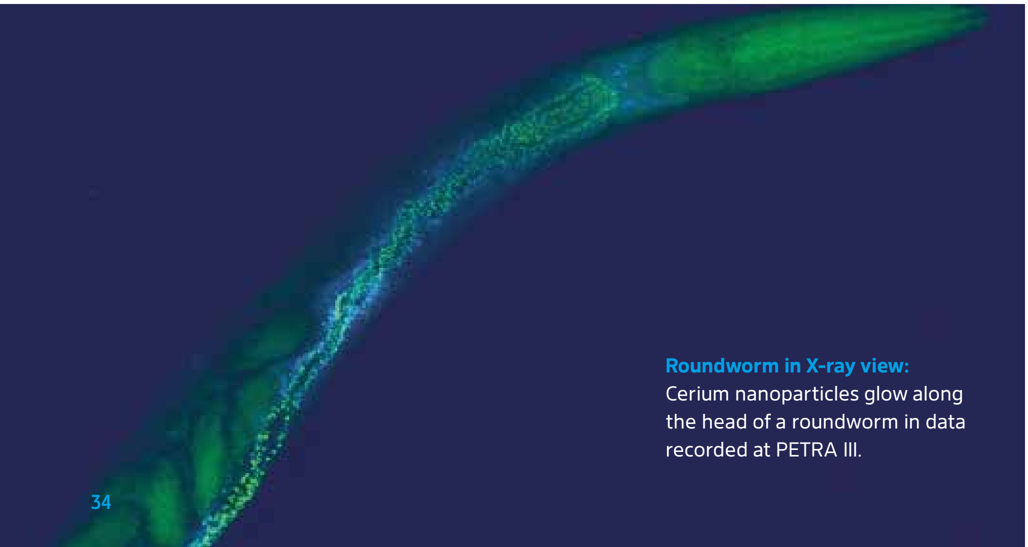
High-resolution X-ray images show nanoparticles in roundworms

An international team of scientists working at DESY's X-ray source PETRA III has generated whole-body images of an organism at such a high resolution that contaminants could be detected in individual cells. The researchers were able to identify nanoparticles of the rare earth metal cerium in the digestive system of the roundworm *Caenorhabditis elegans*, while also determining that the nanoparticles showed relatively low toxicity. The innovative imaging method could prove valuable also for assessing other environmental pollutants, as the team from the Norwegian University of Life Sciences (NMBU), the University of Antwerp in Belgium and DESY reports.

The cerium nanoparticles studied are among the most commonly manufactured nanomaterials due to their unique properties and applications in automobile catalytic converters, fuel cells and materials that block ultraviolet light. The scientists exposed the worms to a high concentration of the nanoparticles, much higher than those found in the environment. "Using X-ray fluorescence spectroscopy with a very fine X-ray beam, we managed to piece together an extremely high-resolution picture of the roundworms and the nanoparticles within them," says co-author Gerald Falkenberg from DESY.

The data were so detailed that the scientists were able to view the entire organism while also zooming in on individual parts of cells in order to localise clusters of nanoparticles within them. "The ability to map the uptake of contaminants at 300 nanometre resolution for full-body X-ray imaging of an intact, non-dehydrated organism enables us to address the consequences of pollutants in a totally new way," explains research leader Ole Christian Lind from NMBU. "This is next-level toxicology, where we can show in detail that the presence of a contaminant in a tissue or a cell is directly related to the effect it causes."

Environmental Science and Technology,
DOI: 10.1021/acs.est.1c08509



Roundworm in X-ray view: Cerium nanoparticles glow along the head of a roundworm in data recorded at PETRA III.

Picture: NMBU

Molecular motor deciphered

A team from the Centre for Structural Systems Biology (CSSB) at DESY has elucidated the architecture, complete functional cycle and mechanism of a molecular motor that is responsible for recombining and repairing DNA in cells. According to the study, "the sequential mechanism, coordination and force generation manner" of the so-called RuvAB branch migration complex "share conceptual similarities with combustion engines," as first author Jiri Wald from the University Medical Center Hamburg-Eppendorf (UKE) explains.

DNA recombination is one of the most fundamental biological processes in living organisms. In the process, four DNA arms separate from their double-helix formations and join together at an intersection known as a Holliday junction. The energy needed for this branch migration to occur comes from a molecular machinery that scientists have tagged as the RuvAB branch migration complex. This complex assembles around the Holliday junction (artist's impression).

The branch migrations energised by the molecular motor are very fast and highly dynamic. To determine the individual steps of this process, the scientists used time-resolved cryo electron microscopy to observe the motor's machinery in slow motion. "We basically provided the molecular motor with a slower-burning fuel, which allowed us to capture the biochemical reactions as they occur," explains research leader Thomas Marlovits from DESY and UKE.

The scientists captured over ten million images of the motor's interactions. Using the high-performance computing facility at DESY, they were then able to put all the puzzle pieces together to generate a high-resolution movie detailing how the RuvAB complex functions on the molecular scale.

Nature, DOI: 10.1038/s41586-022-05121-1

Picture: CSSB, Nicola Graf

femtomenal

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is the upper limit for the weight of the neutrino. This is the result of a precision measurement of the Karlsruhe Tritium Neutrino Experiment (KATRIN) at the Karlsruhe Institute of Technology (KIT). The exact mass of the neutrino is still unknown and very difficult to measure. KATRIN is the world's most sensitive neutrino scale. Researchers have now used it to determine the new upper limit for the neutrino mass. According to the measurements, the ghostly particle weighs a maximum of 1.4 decillionths of a gram or, in the units of particle physics, a maximum of 0.8 electronvolts.


Henna tree


Marigold

Covid drugs from natural substances?

X-ray screening identifies compounds blocking a major coronavirus enzyme

Three natural compounds present in foods like green tea, olive oil and red wine are promising candidates for the development of drugs against the SARS-CoV-2 coronavirus. In a comprehensive screening of a large library of natural substances at DESY's X-ray source PETRA III, the compounds bound to a central enzyme of the virus and can thus inhibit its replication. All three compounds are already used as active substances in existing drugs, as the team headed by Christian Betzel from Universität Hamburg and Alke Meents from DESY reports. However, if and when a Covid-19 drug can be developed on the basis of these compounds remains to be investigated.

"We tested 500 substances from the Karachi Library of Natural Compounds to see if they bind to the papain-like protease of the novel coronavirus, which is one of the main targets for an anti-viral drug," explains the study's main author Vasundara Srinivasan from Universität Hamburg. "A compound that binds to the enzyme at the right place can stop it from working."

Molecular scissors

The papain-like protease (PLpro) is a vital enzyme for virus replication: When a cell is hijacked by the coronavirus, it is forced to produce building blocks for new virus particles. These proteins are manufactured as a long string. PLpro then acts like a molecular pair of scissors, cutting the proteins from the string. If this process is

Pictures: istockphoto/peterschreiber.media

Copperleaf

“By inhibiting PLpro, we can also enhance the cell’s immune response“

Vasundara Srinivasan, Universität Hamburg

blocked, no new virus particles can form. “However, PLpro has another vital function for the virus,” says Srinivasan. “It blocks a protein of the immune system, called ISG15, and that severely weakens the cell’s self-defence. By inhibiting PLpro, we can also enhance the cell’s immune response.”

For the experiments, PLpro was mixed with each of the 500 natural substances in a solution, giving them the chance to bind to the enzyme. With a conventional light microscope, however, it is not possible to see whether a substance binds to the enzyme. Instead, tiny crystals were grown from the mixtures. When illuminated with the bright X-rays from PETRA III, the crystals produced a characteristic diffraction pattern from which the structure of the enzyme could be reconstructed down to the level of individual atoms. “From this information, we can produce three-dimensional models of the enzyme with atomic resolution and see if and where a substance binds to it,” explains Meents.

Copperleaf and marigold

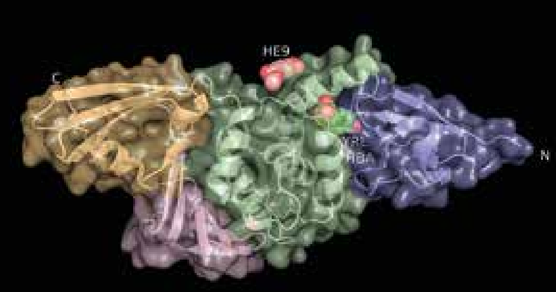
The screening showed that three phenols bind to the enzyme: Hydroxyethylphenol (YRL), isolated for the experiments from the henna tree *Lawsonia alba*, is a compound present in many foods, such as red wine and virgin olive oil, and used as anti-arrhythmia agent. Hydroxybenzaldehyde (HBA) is a known anti-tumor agent and accelerates wound healing. It was isolated from the copperleaf *Acalypha torta*. Methyldihydroxybenzoate (HE9), isolated from the French marigold *Tagetes patula*, is an anti-oxidant with anti-inflammatory effect and is found in green tea.

In subsequent lab tests, established and performed by Hévila Brognaro in Betzel’s group, the three phenols reduced PLpro’s activity in living cells by 50 to 70 percent. “The advantage of these substances is their proven safety,” says Betzel, who is also a member of the Cluster of Excellence “CUI: Advanced Imaging of Matter”. “These compounds occur naturally in many foods. However, drinking green tea will not cure your Covid infection! Just as it would not heal your wounds or cure your cancer. If and how a Covid drug can be developed from these phenols is subject to further studies.”

In a different screening, a team consisting largely of the same scientists had already screened thousands of existing drugs at PETRA III as possible inhibitors of the coronavirus’ main protease (Mpro), which is also a molecular pair of scissors and a major potential drug target. The screening identified several Covid drug candidates, and the most promising have entered preclinical testing. “The corona initiative of DESY and Universität Hamburg is one of the very few worldwide that investigated both of Covid-19’s main targets,” emphasises Betzel.

Communications Biology,
DOI: 10.1038/s42003-022-03737-7

Key protein:
Structure of the enzyme papain-like protease with the binding sites of the identified natural substances



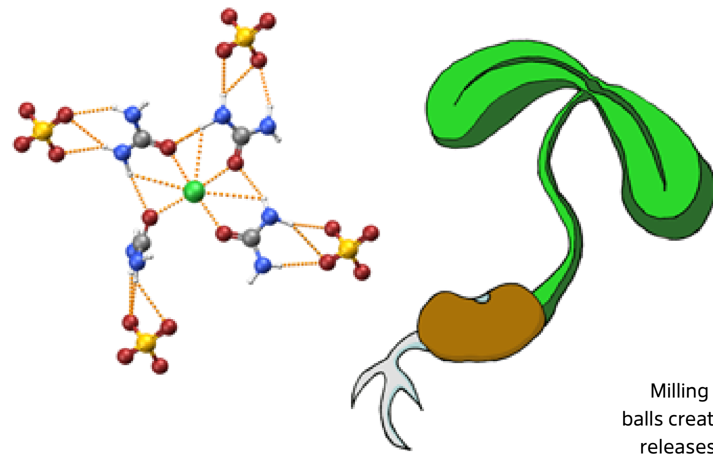
Picture: Universität Hamburg, Vasundara Srinivasan

Chemical mill produces more sustainable **fertiliser**

X-ray study enables optimisation of the production process

The milled fertiliser is intended to protect water systems and the climate.

Picture: DESY, Gesine Born



Milling gypsum and urea with steel balls creates a so-called cocrystal that releases nitrogen (blue) only slowly.

Plant fertilisers are often an environmental problem. Among other things, almost half of the nitrogen they contain seeps into the soil and pollutes water systems. As a method optimised at DESY's X-ray source PETRA III shows, a purely mechanical process can be used to produce a novel, more sustainable fertiliser in a less polluting way. In the process, urea and gypsum are milled until a new solid compound of the two substances is formed. The compound then slowly and gradually releases two chemical elements critical to soil fertilisation, nitrogen and calcium. The fertiliser product can thus help reduce the pollution of water bodies and protect the climate.

The milling process is fast, efficient and clean, as the international research team reports. The method is also scalable and thus has the potential for industrial use. The new fertiliser still needs to be tested in the field, however.

The researchers from the Ruđer Bošković Institute (IRB) in Croatia, Lehigh University in the USA and DESY used PETRA III to follow the production of the fertiliser live in the mill and optimise the manufacturing process. Teams from DESY and IRB have been collaborating for several years to explore the fundamentals of mechanical methods for initiating chemical reactions as an alternative to wet chemistry. Mechanochemistry, as the technique is called, uses various mechanical processes, such as compression, vibration or, in this case, milling, to achieve a chemical transformation.

Thousands of years old technique

"Mechanochemistry is quite an old technique," explains DESY scientist Martin Etter, head of the beamline at which the experiments were performed. "For thousands of years, we've been milling things, for example, grain for bread. It's only now that we're starting to look at these mechanochemical processes more intensively using X-rays and seeing how we can use those processes to initiate chemical reactions."

Etter's beamline is one of the few in the world where mechanochemistry can be routinely performed and the processes analysed using X-rays from a synchrotron. To study fertiliser production, the researchers teamed up with the group of Jonas Baltrusaitis at Lehigh University. The starting materials were fed as powders into a milling container with two steel balls. The powders were then milled by shaking until they combined chemically.

> *"For thousands of years, we've been milling things, for example, grain for bread. It's only now that we're starting to look at these mechanochemical processes more intensively using X-rays"*
>
> ***Martin Etter, DESY***

The setup allowed for direct insight into the evolution of the reaction mixture by illuminating the milling vessel with synchrotron radiation without having to stop the procedure. The researchers could thus determine the exact reaction pathways and analysed the output and purity of the product, which helped them refine the mechanical procedure on the fly. The optimised procedure enabled 100 percent conversion of the starting materials into the target fertiliser.

More robust bonds

That end product is known as a "cocrystal", a solid with a crystal structure comprising two different chemicals that is stabilised by weaker intermolecular interactions in repeated patterns. "Cocrystals can be seen like LEGO structures," says Etter. "You have sets of two kinds of bricks, and with these two bricks you make a repeating pattern." In this case, the "bricks" are calcium sulphate, derived from gypsum, and urea. Through the milling process, the urea and the calcium sulphate become bonded to one another. ››

Picture: Ruđer Bošković Institute, Krunoslav Užarević

"On its own, urea makes for a very weakly bound crystal that falls apart easily and releases its nitrogen too readily," explains Baltrusaitis. "But with the calcium sulphate through this mechanochemical process, you get a much more robust cocrystal with a slow release." The advantage of this cocrystal is that its chemical bonds are weak enough to release nitrogen and calcium, but strong enough to keep the two elements from being unleashed all at once.

"We are optimistic that there's a strong application potential for the procedure around the world"

Krunoslav Užarević, Ruđer Bošković Institute

That method of release is the great advantage of the fertiliser. It alleviates one of the major drawbacks of the nitrogen fertilisers used since the 1960s. "The status quo in fertilisers, for food security reasons, is to dump as much nitrogen and phosphorus on crops as possible," says Baltrusaitis. With conventional fertilisers, only about 47 percent of the nitrogen is actually absorbed by the soil; the rest is washed away and can lead to massive disruptions in water systems. In the North Sea and the Gulf of Mexico, massive "dead zones" are growing, in which algal blooms fed by excess fertiliser absorb all the available oxygen in the water, killing off marine life.

Fast and efficient

In addition, production of common fertilisers through the so-called Haber–Bosch process, which traps atmospheric nitrogen into urea crystals, is energy-intensive, consuming four percent of the world's natural gas supply every year. The new method provides an opportunity to significantly reduce this consumption. "If you increase the efficiency of those urea materials by 50 percent, you need to make less urea via the Haber–Bosch process and you thus reduce all the related problems, such as the need for natural gas," says Baltrusaitis.

The milling procedure is fast and very efficient, resulting in a pure fertiliser without any waste byproducts except water. "Not only are we proposing a better functioning fertiliser," explains Baltrusaitis, "we are also demonstrating a green method of synthesis."

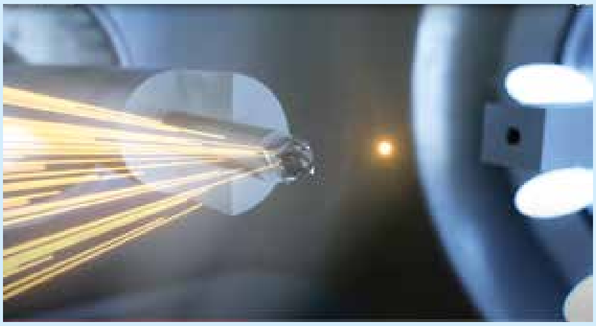
While the analysis for the study involved less than one gram of fertiliser, the research team led by Baltrusaitis and Krunoslav Užarević from IRB in Zagreb has managed to scale up the procedure using the data taken at PETRA III. Thus far, the researchers can produce hundreds of grams of fertiliser, using the same procedure and with the same efficiency. As a next step, the team plans to continue scaling up in order to make an actual proof-of-principle industrial version of the process. Baltrusaitis is already working on such a scale-up and testing cocrystal fertiliser for application in real-world conditions.

"Beyond the product, the mechanochemical process generates virtually no unwanted byproducts or waste", says Užarević from IRB. "We are optimistic that there's a strong application potential for the procedure around the world."

Sustainable Chemistry & Engineering, DOI: 10.1021/acssuschemeng.2c00914

The fertiliser is produced as a powder by purely mechanical means; solvents or other wet chemistry are not necessary.

Picture: Lehigh University, Jonas Baltrusaitis



Drug search in protein crystals

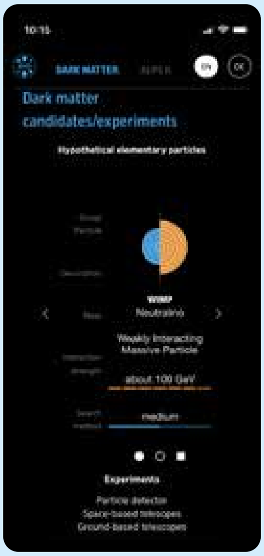
Using protein crystallography, researchers can peer deep into the workings of proteins that are vital for life. To this end, the proteins are formed into tiny crystals, which are then illuminated with intense X-rays. This produces a characteristic diffraction pattern, from which the structure of the proteins can be deduced. Research teams at DESY's X-ray source PETRA III are using this technique, for example, to search for – literally – fitting drugs against the coronavirus. A new animation by the award-winning Science Communication Lab shows the various steps required to achieve this:

youtu.be/Upb-nETh584

femtoweb

Interactive dark matter

Most of the matter in the universe is dark. The mysterious dark matter is more than five times as common as the matter we are familiar with. However, it is not called dark because it merely does not glow, but because it must be an unknown form of matter that hardly interacts with light at all. The ALPS II experiment at DESY, among others, is searching for the as yet hypothetical particles of this mysterious substance. A new interactive digital poster explains the rationale behind the experiment:



darkmatter-alps.desy.de/dark-matter.html

Particle accelerator in compact format

Up to the speed of light at the click of a mouse: A new interactive website illustrates the principle of laser plasma acceleration as explored by the KALDERA project at DESY. The technology should enable the realisation of particle accelerators that are significantly more compact and less expensive than today's facilities. In this approach, an extremely powerful laser flash is used to generate a plasma in a tiny tube. The laser flash sweeps through the gas in the tube like a snowplough, stripping the electrons from the gas molecules. The electrons gather behind this plasma wave, on which they can surf like a wakeboarder on the wake of a ship. How this works can now be explored interactively on any desktop PC:

kaldera.desy.de

X-ray microscope of the future

The world's best 3D X-ray microscope is to be built in Hamburg. The facility, called PETRA IV, will provide 3D images from the nanocosmos and enable insights with unprecedented precision into materials and biological structures – from the makeup of pathogens through catalysts to innovative microchips and quantum materials. A new website presents the project to the public, with pictures, videos and articles. The expansion of DESY's X-ray source PETRA III to PETRA IV is also a cornerstone of the planned Science City Hamburg Bahrenfeld.

petra4.desy.de/index_eng.html

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Cartoon: Nicolas Mahler

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The DESY research centre

DESY is one of the world's leading particle accelerator centres and investigates the structure and function of matter – from the interaction of tiny elementary particles and the behaviour of novel nanomaterials and vital biomolecules to the great mysteries of the universe. The particle accelerators and detectors that DESY develops and builds at its locations in Hamburg and Zeuthen are unique research tools. They generate the most intense X-ray radiation in the world, accelerate particles to record energies and open up new windows onto the universe.

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