Unusual sounds at the Max Planck Institute for Iron Research: Dierk Raabe tests the acoustics of the staircase. The French horn was his main instrument at the Wuppertal Conservatory. The only thing he didn't like was polishing the corrosion-prone metal.

A Commuter between **Metallic Dimensions**

As a 16 year old, **Dierk Raabe** studied double bass and French horn at the Wuppertal Conservatory. Today he pursues the quantum revolution of materials science as Director at the **Max Planck Institute for Iron Research** in Düsseldorf.

A PORTRAIT BY **ROLAND WENGENMAYR**

Had the career dreams of the young Dierk Raabe come true, he would not now be sitting in the conference room at the Max Planck Institute for Iron Research in Düsseldorf with light streaming through the windows. Fittingly, heavy iron girders reminiscent of the Eiffel Tower provide a solid framework for the Bauhaus architecture, which has been modernized with a great deal of glass. For Raabe, it was love at second sight with metallic materials. His first intense contact was rather unfavorable. This was due to his musical instrument, a French horn. "Those old instruments had to be polished every week with a revolting metal polish," he says: "That was more something for friends of corrosion." The materials scientist clearly falls into the camp of corrosion haters.

At 16, he passed the entrance examination to the Wuppertal Music Conservatory. This was primarily thanks to a committed music teacher. A life as a professional musician between Brahms, Beethoven and Wagner seemed mapped out for him. "In the afternoons after school I went to Wuppertal," explains Raabe. He enjoyed the very personalized lessons at the Conservatory. He diligently practiced the double bass, which had now become his main instrument, and the French horn. But he increasingly lost interest in school: "I no longer wanted to complete my school-leaving examination." But then crisis struck.

FROM BRAHMS AND BEETHOVEN TO METAL PHYSICS

Dierk Raabe tormented himself with thoughts about whether he had made the wrong decision for his life. His early professional training as a musician made it clear to him that the rest of his life would revolve around "two, three instruments." "I have to be careful how I say this, because I don't wish to step on any artist's toes," he says, "but that was a little bit too one-sided for my taste." So he took his school-leaving examination. He had early contact with the topic of steel through his father and his uncle, who worked at Krupp. His family's background was one of the reasons he studied metallurgy and metal physics at RWTH Aachen University. "I was interested in the subject because it is at the interface between the engineering sciences and the natural sciences," explains Raabe, "because the courses included chemistry and physics."

This was obviously the right decision, because his research area is anything but one-sided. It's true that almost everything revolves around metallic materials, but they are everywhere; they shape our environment like hardly any other material. "It is a very old field, dating back to the Bronze Age," he stresses, "and today it is one of the backbones of our industrial society." Accordingly, our conversation develops into a gallop through our technical culture. In the hours that follow, the conversation touches on high-temperature materials for power plant turbines, high-strength steels for car bodies, special alloys for aircraft undercarriages, hip joint implants, gold contacts in electronic chips and corrosion-resistant components for seawater desalination plants. >

Photo: Frank Vinken

top | Complete insight: Dierk Raabe looks into the sample chamber of the new atom probe. This instrument can decipher the structure of the tiny crystals in metallic materials atom by atom.

bottom | The ultra-fine sample tips are kept in the ultra-high vacuum chamber (center of picture). The flange-mounted vacuum tube (foreground, right) contains a pole with which the researchers can move the samples into the large analysis chamber (background), where pulses of laser light or high electric voltages remove the sample tip atom by atom. An electric field accelerates these electrically charged atoms (ions) to a large area detector. The time-of-flight to the detector reveals the type of atom, and the impact location shows its original position in the crystal.

It is quickly becoming apparent that Raabe shares a love of one particular word with Mr. Spock from the science fiction series Star Trek: "Fascinating!" Otherwise, he has little in common with the cool, reserved space traveler with the pointy ears. Words just come gushing out in a slight Rhenish accent. He repeatedly jumps up from the table, rapidly sketches something on the board, then seats himself opposite his guest again. He expects his discussion partners to have the ability to take in a maximum of information in a minimum of time, of course. Boredom does not set in, at any rate.

IT'S AMAZING THAT WE GET BACK OUT OF IT ALIVE

But Raabe issued a reminder very early on, saying "you have to recognize the central thread." This concern is unwarranted. Each of the many examples makes it clear that the focus is always on the complex inner life of metallic alloys. Science has by no means reached the stage of completely understanding the microscopic behavior of these mixtures of iron, nickel, carbon, cobalt, titanium, chrome, aluminum and other ingredients from the elemental supermarket of the periodic system. This is why industry still has to work painstakingly and empirically to develop structural materials to meet new mechanical requirements or withstand extreme temperatures.

So the search for new materials is still all about intelligent trials based on experience. If there was a sound theory, materials scientists could proceed in a much more focused manner and would be more open to new discoveries at the same time. "There is no such theory for the development of new alloys," says Raabe, thus already introducing the dream goal of his research: "I can only design really new materials for a specific purpose when I, as a scientist, understand precisely what happens there."

These connections and the properties of materials never cease to amaze him. He is already talking about materials that most of us would trust with our lives without giving it a further thought. "Take an airplane," says Raabe enthusiastically: "I'm always amazed to get back out of it alive!" He uses his hands to illustrate how the pressurized cabin made from an aluminum-copper alloy expands its diameter by almost 20 centimeters in the thin air at altitude: "Did you know that?" Then he moves on to the turbine vanes, which are located directly behind the combustion chamber of the aircraft's engines and reach scorching temperatures of up to one thousand degrees Celsius. "We can only go down on bended knee and thank our maker that they don't fly out the back in bits and pieces," says the researcher with a laugh.

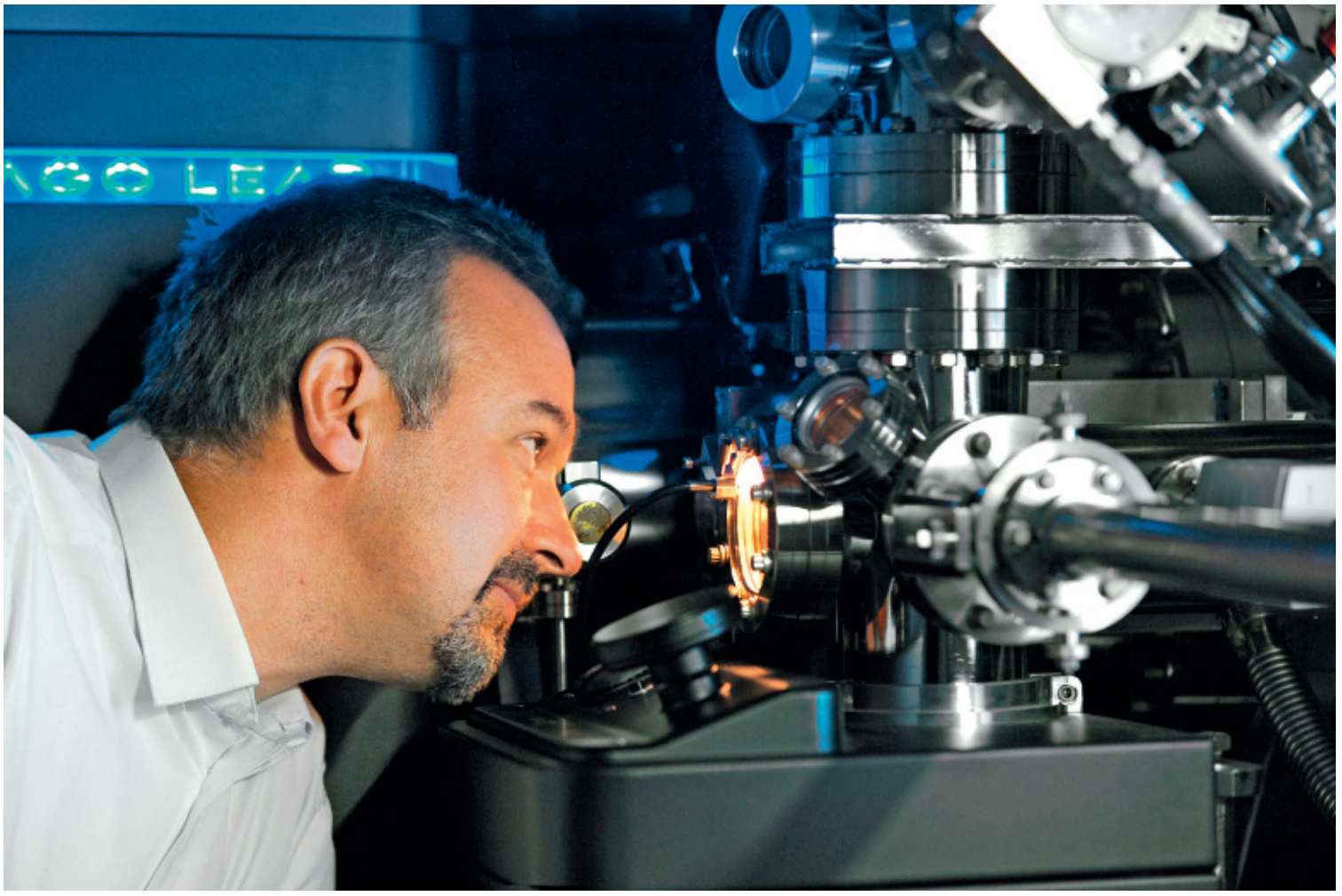
Of course he knows very well why this doesn't happen. But he wants to have an in-depth understanding of the mechanical behavior of such materials. And this is where quantum mechanics comes into play, which describes the behavior of individual atoms and electrons. The engineer-to-be first came into contact with this fundamental but difficult to understand theory as a student via a good physics lecture. It has now become a workhorse for him, thanks to the intense collaboration with his fellow Director Jörg Neugebauer and his theory group. It is unusual to learn about the fundamentals of quantum mechanics when studying materials science because the field is close to mechanical engineering at most universities. And if you want to develop materials for large technical components, you traditionally don't need to worry about individual atoms and electrons.

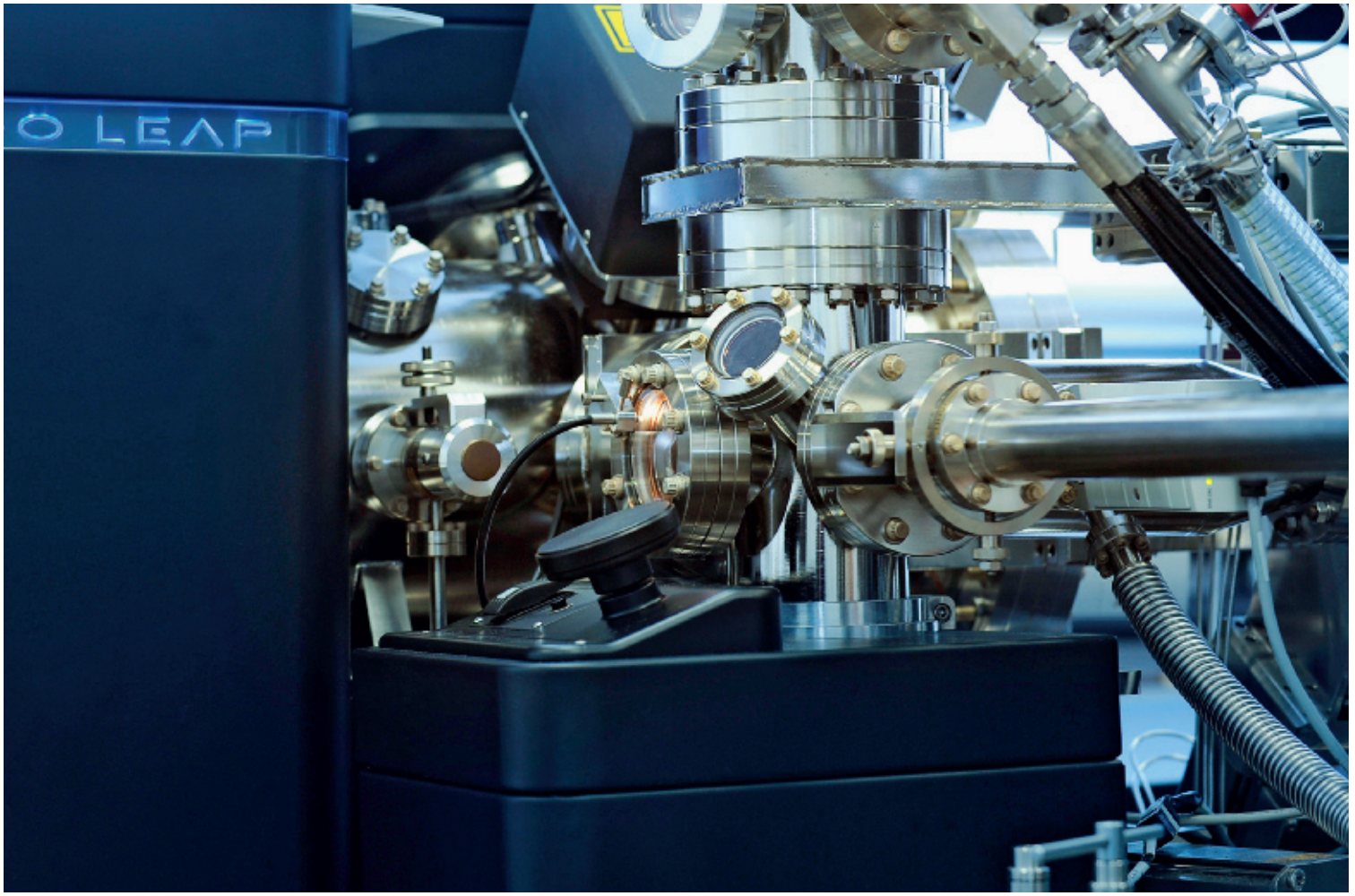
QUANTUM THEORY BECOMES A WORKHORSE

But Dierk Raabe and his colleagues at the institute want to radically change this attitude. If Raabe's dream comes true, the same will happen to mechanical engineers as happened some time ago to electrical engineers: they had to get used to quantum mechanical design tools about sixty years ago after the invention of the transistor. "We want our long-term research work to contribute to materials being developed completely on the basis of quantum mechanics within 15 years or so," says Raabe: "I absolutely believe in this vision!"

Very early on in his scientific career, Raabe was already developing computer simulations that could be used to theoretically predict the properties of materials. This has been his main field of research since obtaining his doctorate in Aachen in 1992. At that time, he was heading a group at the Institute for Metallurgy and Metal Physics. The German Research Foundation rewarded his excellent findings

Photo: Frank Vinken (2)




LEAP

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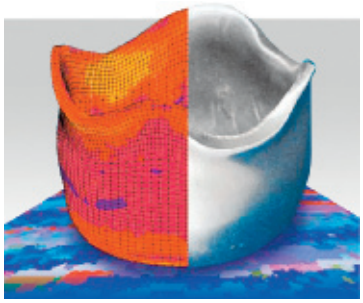


The metal does not flow uniformly everywhere in the press like viscous honey, but moves in preferred directions. This critical "earing" can be realistically simulated by the software developed by Raabe's team (left).

with a prestigious Heisenberg fellowship. In 1997, after gaining his postdoctoral lecturing qualification, he used the fellowship to go to the US. He carried out research at Carnegie Mellon University in Pittsburgh and at the High Magnetic Field Laboratory in Tallahassee, Florida. The Max Planck Society was so impressed by Raabe's innovative methods that, in 1999, at just 34 years of age, he was appointed to the Max Planck Institute for Iron Research as one of the youngest Max Planck Directors.

"My advantage was maybe that I sit between engineering sciences and natural sciences and have done a lot of simulations," he continues. But one should not think that these complex simulation programs merely ask for a couple of desired material properties to be entered into a template and the computer then spits out the recipe for a new alloy. The simulation programs in materials design are very complex. Many simulations do simplify the metals in one crucial aspect, though: they ignore the complicated microstructure – just as ship designers do not care about individual water molecules. "This is called homogenization," explains Raabe.

Such simplifications are justified in many applications. In reality, however, metals and metallic alloys are grainy in a complicated way. They consist of many small crystals of between a few micrometers (thousandths of a millimeter) and several millimeters in size, depending on the material. The atoms in these small crystals have a very regular arrangement, like that of diamonds or quartz. The situation for alloys is even more complicated, because the atomic composition can vary from crystal to crystal.

However, the interaction of these crystal grains determines important material properties. So what can sometimes happen is that sheet metal acquires unsightly lugs after being cold formed into a fender, for example. The metal does not flow uniformly everywhere in the press like viscous honey, but prefers certain directions. This is due to the small crystals. Their stacked atomic layers mean that they give in a preferred direction – like sandwiches, whose slices of bread prefer to slide parallel to each other on the slippery filling.

AUDI AND MERCEDES USE THE SIMULATION PROGRAM

This is a growing problem for the automotive industry with its tendency to use folded car body parts with ever more complicated designs. So some years ago, Raabe and his team developed a simulation program that is now used by vehicle manufacturers like Audi and Mercedes. They use it to predict the behavior of different steel grades in the presses. This saves on expensive tests and high scrap rates when starting up production lines for a new model.

The researchers in Düsseldorf have found a clever way of translating the behavior of the small crystals into the forming behavior of complete workpieces in their simulation program. If the computer had to simulate the interaction of many millions of virtual crystals, grain by grain, it would

Graphic: MPI for Iron Research

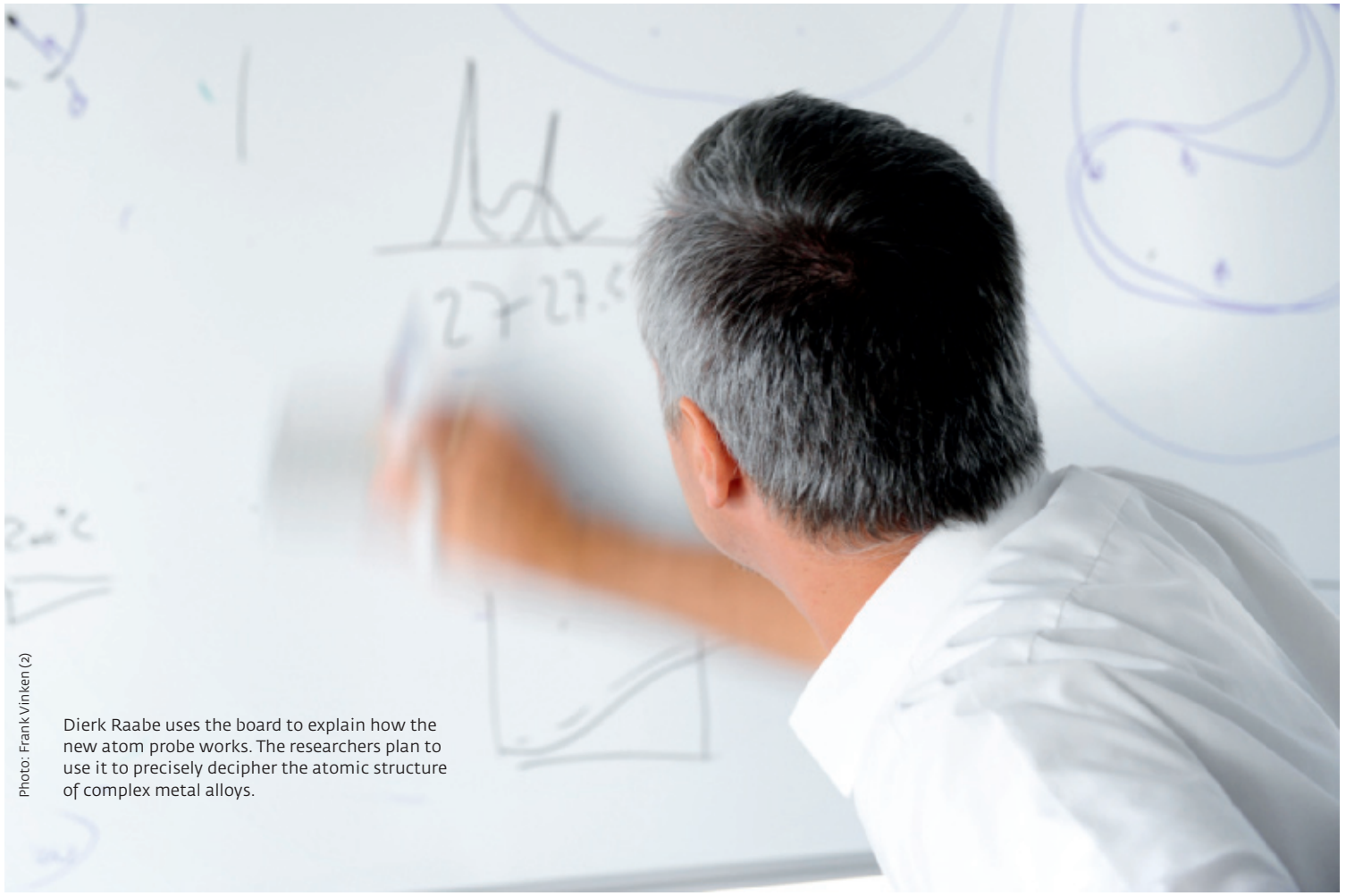
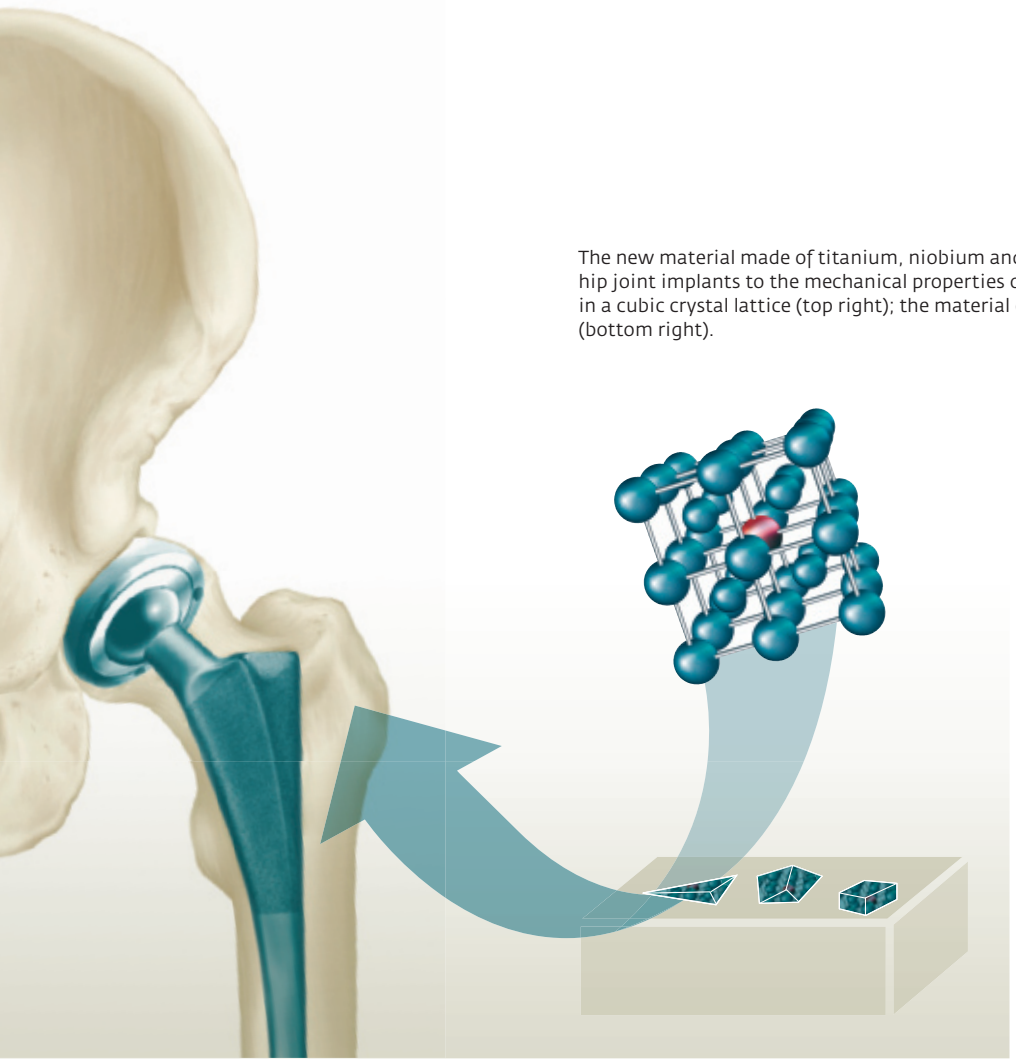


Photo: Frank Vinken (2)

Dierk Raabe uses the board to explain how the new atom probe works. The researchers plan to use it to precisely decipher the atomic structure of complex metal alloys.



The new material made of titanium, niobium and zirconium is better at matching hip joint implants to the mechanical properties of bone. The atoms are arranged in a cubic crystal lattice (top right); the material consists of many such small crystals (bottom right).

take too long. Raabe's team thus had the idea of mathematically grouping all crystals that have the same orientation, because they exhibit the same flow behavior. This shortened the computing time by a factor of one hundred.

THE MULTI-SCALE PROBLEM

It's not just the different orders of magnitude – from the atom to micrometer-sized crystals to meter-sized workpieces – that result in a complicated "multi-scale problem," as Raabe calls it. Even more extreme is the spread of the time scales in which a workpiece corrodes or succumbs to permanent stress as a result of creeping: they range from electron movements within femtoseconds (trillionths of a second) up to years.

"These scales cannot be bridged with computer simulations, not even in 30 years," says Raabe: "So we have to bridge them theoretically." A discovery comes to their aid: the exact quantum mechanical description of what happens on the microscopic scale between a few atoms in the small crystals can already provide good answers. One example is provided by the mechanical properties of the material. "The first work in this field carried out in collaboration with colleagues from the theory side resulted in a precision in predicting certain phenomena that really surprised me," says Raabe. His fellow Director Jörg Neugebauer's team studies the very demanding application of quantum theory. The collaboration works very well: "We are dreaming pretty much the same scientific dreams," comments Raabe.

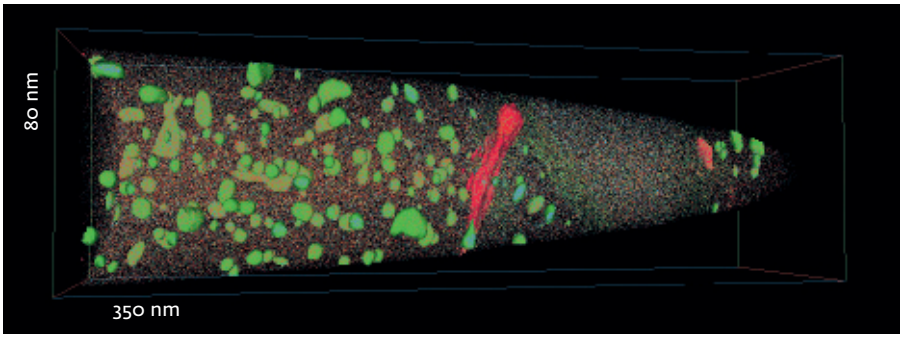
In quantum mechanical materials design, the focus is on the electrons. They form the adhesive that glues the atoms together. Quantum mechanics can describe these adhesive forces very precisely on the atomic scale. The equations can be used to directly derive how the crystal is going to behave mechanically, for example. Although a large, "macroscopic" workpiece consists of many crystals, it is these that determine the limits of the material properties – just as a chain can only be as strong as its individual links.

"My dream is to achieve the electronic design of materials," adds Raabe. Compared to empirical development methods, this elementary theoretical approach has one great strength: it makes it possible to develop completely new materials. Empiricism, on the other hand, can only vary things that are already known.

BRAND NEW TITANIUM ALLOY FOR HIP IMPLANTS

Dierk Raabe wants to convince mechanical engineers and traditionally minded materials scientists of the possibilities of the quantum mechanical approach. He hopes that some impressive demonstration projects will help. One is a brand new titanium alloy for hip implants. "About a million people worldwide receive this type of artificial hip annually," explains Raabe. Unfortunately, these new joints loosen after a few years and have to be replaced. The problem is the bone, which recedes. Titanium is more than five times as rigid as bone, so the metal joint takes much more strain. Just like a muscle that is no longer trained, a bone that has too few demands put on it grows weaker as a result.

Illustration: dpa Picture-Alliance (left); Christoph Schneider (right)



Dierk Raabe in front of the powerful computer system that evaluates the data from the atom probe. From the measurement data, it must calculate the types and the crystal positions of between 10 and 100 million atoms per analysis. The graphs generated show the greatly enlarged internal atomic structure of a superfine sample as thin as the tip of a needle in an atom probe, for example. This instrument can detect the positions of the different atoms (different colors) of an alloy in the atomic crystal lattice.

The Düsseldorf-based researchers have succeeded in developing a much softer titanium alloy. Mechanically, it adjusts much better to the bone because it has a different crystal structure than titanium. The development of this brand new material, consisting of biocompatible titanium, niobium and zirconium, would not have been possible without quantum mechanics. The group is already negotiating with manufacturers of such prostheses.

The social relevance of his research is very important to Raabe. But the researchers also hit upon titanium alloys because they are still relatively simple to describe on an atomic level. "So, in many ways, it was a strategic decision," says Raabe. He is already dreaming of making high-temperature materials with a much more complex structure even more heat resistant. These are mixtures of more than a dozen different chemical elements. The huge turbines in modern coal-fired power stations give him a reason: if they could increase their operating temperature "from about 580 to 720 degrees Celsius," explains Raabe, they would convert coal into energy much more efficiently and emit considerably less carbon dioxide into the air. "For one kilowatt-hour of electric power, I would then no longer need to shovel in half a kilogram of coal," says Raabe: "It could be less than a third of a kilogram!"

Four years ago, the German Research Foundation awarded Raabe the Gottfried Wilhelm Leibniz Prize. This carries the highest prize money of all German science prizes and increased his research budget by 1.55 million euros. He has now used this money to buy an instrument called an atom probe. It uses a thin sample of material to detect precisely where in the crystal structure the different atoms are located. Raabe hopes to use this data to make even high-temperature steels accessible for quantum mechanical calculations.

When Raabe talks about his many projects, partnerships and contacts with other researchers, the passionate communicator and networker shows through. Did he learn this during his time as an orchestra musician? After a brief pause, he confirms that there was a link with science: artists are also pronounced individualists, but they still have to come together to form a common harmony.

The creativity that studying music imparts is also important to him – but he hardly ever gets to play music now. "The atmosphere at our institute is so good," he laughs "that I prefer to keep myself busy at home with a scientific subject rather than play music." ◂

Photos: Frank Vinken (top); MPI for Iron Research (bottom)