Steel portfolio: Today, materials are optimized for each individual application. In this context, increasing the lifespan of aircraft turbines poses a major challenge.

Quantum Mechanically **Engineered Steel**

Car bodies, aircraft wings or turbine blades – alloys today are customized for any purpose. Roughly 2,500 different types of steel already exist, and that number continues to grow. **Jörg Neugebauer** and **Dierk Raabe**, Directors at the **Max-Planck-Institut für Eisenforschung** in Düsseldorf, are also developing new varieties, and in their search for innovative materials, they even apply the laws of the quantum world.

TEXT **KARL HÜBNER**

"You could try mixing the titanium with 30 percent niobium or molybdenum." Several years have passed since Jörg Neugebauer gave Dierk Raabe this piece of advice. Back then, Raabe had been searching for a new titanium alloy for hip replacement implants. The material needed to be more elastic under pressure than pure titanium, meaning it had to be about as flexible as human bone. Up until then, titanium prostheses tended to become loose over time due to the fact that they are very rigid and therefore absorb a much greater amount of force than the bone. Since the bone is no longer challenged, it subsequently starts to recede. Jörg Neugebauer and Dierk Raabe developed a material that is more suitable than titanium, and a number of manufacturers have already started using this new alloy.

Raabe is head of the Department of Microstructure Physics and Alloy Design at the Max-Planck-Institut für Eisenforschung in Düsseldorf. Despite the fact that the institute's German name contains the word "iron" (*Eisenforschung* = iron research), the research conducted there also focuses on other metals, and even on biomaterials.

Before Raabe begins examining specific material formulas, he first contacts his colleague, Jörg Neugebauer, head of the Department of Computational Materials Design, just as he had done in the case of the new titanium alloy. At the institute, they can almost wave at each other when standing at the right windows of their two buildings. However, as far as their respective work is concerned, they are orders of magnitude – or as Raabe calls it, many scales – apart. Neugebauer works with material samples that are merely nanometers (millionths of a millimeter) in size. He simulates these extracts using a computer.

QUANTUM MECHANICS REQUIRES POWERFUL COMPUTERS

All Jörg Neugebauer needed to do to later arrive at his precise 30 percent tip, he says, was "to conduct some quantum mechanics" with virtual atoms. As a theoretical physicist, he studies matter on a purely theoretical level, without having to carry out any experiments in a laboratory. He does, however, require powerful computers. It therefore comes as no surprise that the institute's basement houses an infrastructure with computa-

Photo: fotolia

A winning team: Jörg Neugebauer (right) calculates the properties of a material with the help of quantum mechanics. Based on these findings, Dierk Raabe then analyzes how an alloy's microstructure influences the behavior of a large work piece. In this manner, the two Max Planck Directors and their teams jointly develop steels for the future.

tional power that ranked among the top 500 worldwide several times.

The computers Jörg Neugebauer and his team use apply a number of fundamental physical parameters, but most importantly, the calculations are based mainly on sophisticated quantum mechanical equations.

Quantum mechanics becomes relevant when studying particles that are so minute that they can no longer be explained using classical physics, and simply exceed the human power of imagination. After all, who could conceive of an electron as a wave? Or comprehend why its energy doesn't change in a continuous manner, but rather only in discrete quantum portions?

Jörg Neugebauer believes that quantum mechanics starts to get really tricky when it comes to calculating the quantum mechanical behavior of systems consisting of many atoms. The problem is that all of the particles – the atomic nuclei and the electrons – are interrelated, the physicist explains. Calculating a structure made up of many atoms and their numerous electrons is thus such a profoundly complex task that even the most powerful computers reach their limits.

Thankfully, there are a number of simplifications that can be applied. One approach is the density functional theory (DFT), which dates back to the 1960s and for which a Nobel Prize in Chemistry was later awarded in 1998. This theory showed that one doesn't necessarily need to know the exact position of every single electron in a system – only the electron density at a particular location is important. Over the course of the past decades, the mathematical formalism used to determine electron density has been significantly refined. Today it yields results that are also helpful for practical applications. And above all, it reveals the link between this density and the energy contained in a system.

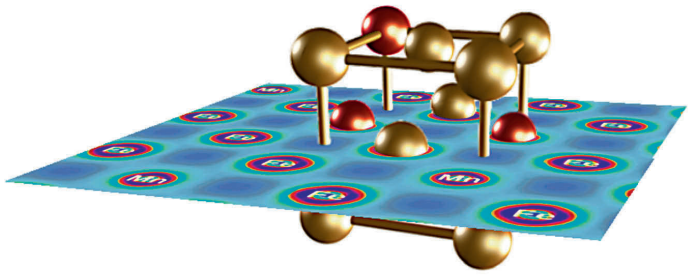
It is precisely these energies that Neugebauer is most interested in when performing his calculations, because they provide information about how stable a given arrangement of atoms is compared with a different structure.

THE DIVERSITY OF METAL LATTICES

In all metal elements, the atoms are arranged according to very specific rules. This arrangement takes the shape of three-dimensional lattices in which the atoms are evenly spaced in all spatial directions. In order to understand how the available space is used in the most efficient manner possible, the lattice can be compared to a pile of oranges. From the third layer onward, there are two different possibilities. Depending on how the depressions are filled, either the third or the fourth layer of oranges will be stacked directly in line with the first layer. The same principle applies to metal atoms. The different crystal lattice types are known as hexagonal close-packed and cubic close-packed (also called face-centered cubic). There is also another important lattice structure that experts call body-centered cubic.

The structure formed by a metal depends on various factors, including the size, nuclear charge and electron configuration of the atoms. Temperature and external pressure also influence the structure. As a result, there are numerous metals that change their preferred lattice structure depending on these conditions. Such phase transitions are of key importance for researchers studying the behavior of metals, and therefore also for materials developers seeking to create metals with specific properties.

Photo: Frank Vinken



Using an electronic map to discover new materials: The distribution of the electron density – depicted here on the horizontal plane using different colors – tells the researchers how much manganese (Mn; red spheres) they must incorporate in an iron (Fe; gold spheres) lattice to make a steel particularly solid.

One of the great achievements of Neugebauer's department is the fact that they adapted the density functional theory so that it can also be applied to such complex systems as structural materials made from metal.

ATOMS DON'T REMAIN FIXED IN ONE POSITION

"We tell our computer program how 100 titanium atoms should be spatially arranged, for example," says Neugebauer. The program knows that a titanium atom has 22 electrons, 4 of which are in the outer shell, where they play a role in binding to other atoms. It can also take into account the fact that atoms don't remain fixed in a position without moving, but that they actually oscillate in relation to one another. The computations can even correctly reflect the magnetic properties of some chemical elements.

The great thing is that, in order to perform his calculations, Neugebauer doesn't even have to know the actual position of the titanium atoms in a real metal lattice. "I can assign the positions at will – and then calculate the energy contained in the system. If I do that often enough using complex optimization algorithms, then the program will automatically come up with the structure that is most favorable in terms of energy at a given temperature," the scientist explains.

This means that he can even specify completely unstable arrangements simply for the purpose of studying their mechanical properties, for example. That is exactly what Neugebauer did in the case of the titanium. "We simply computed a body-centered cubic titanium lattice," he says. In real life, such a lattice would be stable only at a temperature of more than 882 degrees Celsius. But that didn't matter initially. The physicist just wanted to find out how this type of titanium would react to external stress. Once again, he determines these results on a theoretical level. First he calculates the energy states of stretched or compressed atomic arrangements, then he uses this information to deduce the amount of force that would be needed to produce such deformations. "We can use these results to show that body-centered cubic titanium can, in fact, be more easily distorted in certain spatial directions – meaning it is also less rigid," explains Neugebauer. A first step in the right direction.

The next task was to find a way to stabilize the body-centered cubic titanium (see box on p. 60) at room temperature. Other metals automatically form such a lattice, including molybdenum, vanadium, tantalum, niobium and tungsten. It therefore seemed an obvious choice to mix these atoms into the titanium. Once again, Neugebauer and his team first simulated this scenario on the computer, trying out different mixing ratios each time. "In the end it turned out that, if the amount of niobium or molybdenum exceeded 30 percent, then in terms of energy, a body-centered cubical arrangement would be more favorable than the compact hexagonal lattice of pure titanium," says Neugebauer. His part of the work was thus complete, and the ball now in Raabe's court.

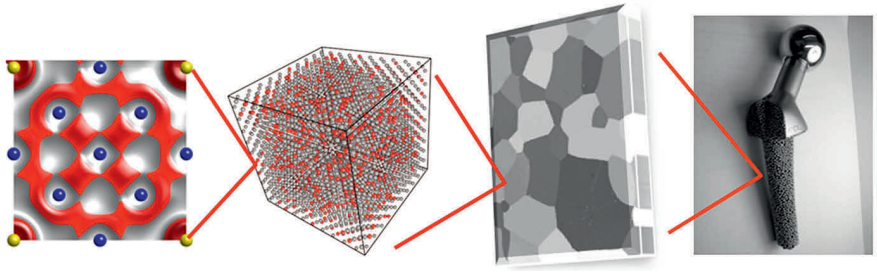
Raabe was able to confirm the lattice structure predicted by the theory. "It turns out that the body-centered cubic structure is, in fact, stabilized when niobium or molybdenum is added," says Raabe. Yet before the exact material mix was finalized, the results were analyzed by the computers in Raabe's department, as well.

"You have to remember that quantum mechanics studies only a miniscule section of a given crystal," the scientist explains. Metals, however, don't usually exist as a single crystal in which all atoms are evenly arranged. What actually happens is that, when molten metal solidifies, countless tiny monocrystals known as grains are formed, and these grains border on each other.

THE ROLE OF GRAIN BOUNDARIES AND CRYSTAL DISTRIBUTION

"My team studies how these grain boundaries and the distribution of crystals influence the macroscopically measurable mechanical properties," explains Raabe. In the case of the titanium alloy, this task was still relatively simple. "In

From an electron to a hip replacement implant: The electronic structure can be used to deduce the atomic structure. This, in turn, produces the microstructure, which largely determines the properties of a macrostructure. By following this path, the researchers in Düsseldorf developed a titanium alloy for hip replacement implants that are more similar to human bone than pure titanium. As a result, the bone surrounding the implant doesn't recede.



Graphics: MPI für Eisenforschung

that case, the individual crystals are arranged in virtually no particular order, meaning there is no preference for any specific spatial direction," says Raabe. Thus, with the help of simple statistics, it was possible to use the data that Neugebauer fed into the computer, and extrapolate it to a larger component, such as a hip replacement implant.

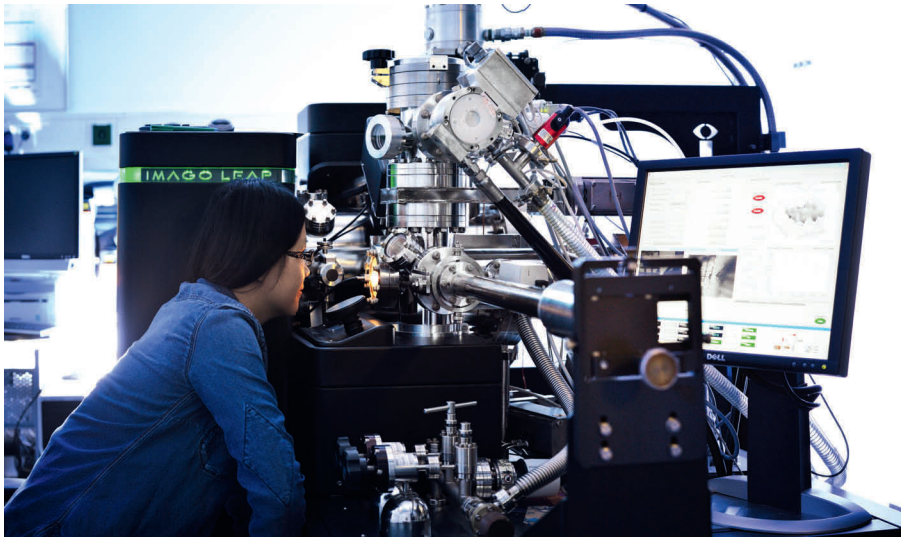
PRECISELY PREDICTING THE DESIRED BEHAVIOR

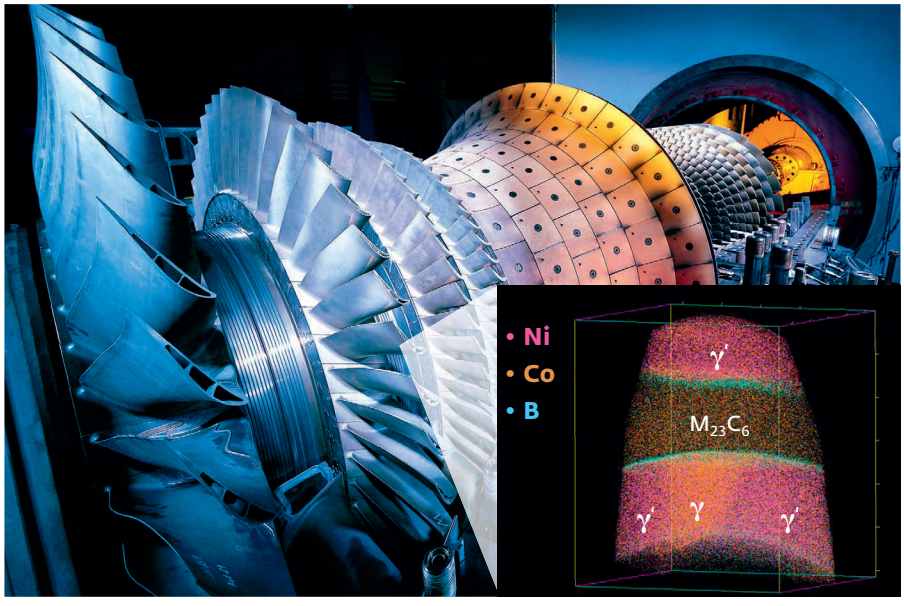
After completing all of their observations and experiments, the scientists had now defined a specific alloy that contained not only titanium and niobium, but also some zirconium and tantalum. Experiments showed that this material was only twice as rigid as human bone. Pure titanium, by comparison, is more than five times as rigid. Even after all this time, Raabe is still impressed by the quality of the predictions computed with the help of quantum mechanics.

Raabe and Neugebauer have been working together like a well-oiled machine on a regular basis ever since. And they certainly have their work cut out for them. New metal materials are needed for all sorts of applications. The more lightweight types of steel are preferred in automobile manufacturing to reduce fuel consumption. Improved metals could also increase the average lifespan of power plant and airplane turbines. And the ideal variants of steel for durable wind turbine transmissions have yet to be discovered.

These types of requirements are usually much more complex than in the case of the titanium alloy, due to the fact that some of these properties are often even required to change within the lifespan of a material. "A piece of sheet steel should initially be easily malleable so that it can be formed into a radiator hood, for example, without requiring a lot of energy," says Raabe. As part of the car, however, the radiator hood must then be stable and robust so that it doesn't instantly become deformed when subjected to external pressure. Yet it shouldn't be rigid and brittle, either. "Otherwise it would shatter when you hit a tree with your car," explains Raabe. "In the event of a collision, though, it should become deformed and, in the process, should absorb as much energy as possible."

Adapting materials as precisely as possible so that they exhibit the desired behavior is one of the central aspects of the work carried out by the materials researchers in Düsseldorf. And just like in the case of the implant, they begin by observing the positions of the atoms in a metal lattice. "The deformability of metals is based largely on the crystallographic defects present in the crystal lattice," explains Raabe.



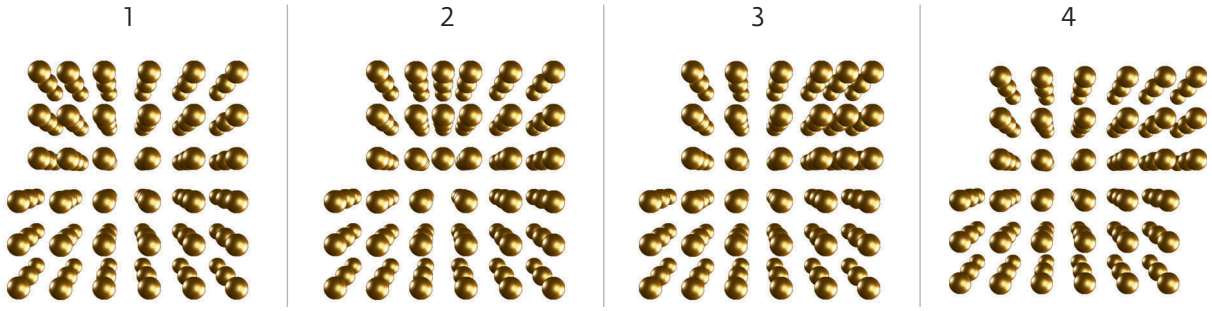


DISLOCATIONS FACILITATE DEFORMABILITY

The arrangement of atoms in a lattice is never quite perfect. Individual atoms or even whole rows of atoms are missing at statistically distributed sites within the lattice. It is these line defects (also known as edge dislocations) in particular that facilitate the deformability of metals. "When you bend a piece of cop-

Where are the atoms located? Mengji Yao operates the atom probe (top), which shows precisely how the elements are distributed in a sample. By applying this method, the Düsseldorf-based researchers discovered that, in the case of a particular alloy that contains nickel (Ni), cobalt (Co) and boron (B) and is used for power plant turbines, the boron is located along the crystallite boundaries in different compositions and structures (γ; γ' or $M_{23}C_6$); here, the boron serves as a type of "cement," strengthening the bonds between the crystal grains (bottom).

Photos: Frank Vinken (top), Siemens (bottom, large image), MPI für Eisenforschung (small image)



A migrating fault: An edge dislocation – in which a layer of atoms in the crystal lattice is incomplete – migrates through a crystal when a material is deformed. Figure 4 in this schematic sequence illustrates how such a dislocation leads to plastic deformation.

per wire, these line defects are each passed on to the next row, thus initiating one step in the atomic deformation process. This effect can propagate itself throughout an entire crystal so that, in the end, an entire layer of metal will have slightly shifted," says Raabe. This scenario is comparable to a rug with an upward fold that travels forward as you push it along with your foot. By the time the fold reaches the end of the rug, the entire rug will have slightly shifted its position. And pushing it along in this way requires much less effort than if you had tried to move the whole rug at once.

Today, the Düsseldorf-based scientists are skilled at using the atomic structure to deduce the force needed to deform metals. Neugebauer begins by observing a finite framework composed of roughly 100 atoms and determining the amount of external force needed to cause some of the missing atoms to dislocate by exactly one row. These findings then flow into Dierk Raabe's observations of larger sections of the respective material.

However, Raabe also has to take into account a series of other effects, such as the fact that dislocations can also encounter obstacles and subsequently split up into numerous new dislocations, for example. That is why the number of dislocations keeps growing as the deformation progresses. "In the case of a larger work piece with a size of about one cubic meter, the total length of such defects triggering the deformation can add up to one light-year," says Raabe. That's almost ten trillion kilometers.

If the external force persists, the dislocations eventually become so numerous that they start obstructing each other. "The deformability then starts to decrease," says Raabe. This effect can be easily explained using a paperclip as an example. The pre-bent parts of the wire are especially hard to deform. Occasionally, they even snap.

The researchers in Düsseldorf specialize in modeling the behavior of dislocations. This field of research is known as crystal lattice defect dynamics. "We examine how fast the dislocations propagate within a crystal when subjected to force, where they fan out, where they become obstructed, and how they interact with each other," says Raabe. This is an incredibly complex endeavor in light of the fact that a single miniscule crystal can easily contain one million of these line defects. And they even influence each other over a certain distance. "Imagine a bus jam-packed with passengers," says Raabe. "If one more passenger boards at the front, the effect will be noticeable all the way in the back of the bus, because every single passenger has to scoot back a little bit – those in the front more so, and those in the back gradually less so."

FROM AN INDIVIDUAL LATTICE DEFECT TO AN ENTIRE CRYSTAL

In the end, Raabe and his team are faced with a series of complicated equations that need solving. This is where the findings derived from Jörg Neugebauer's quantum mechanical calculations come in handy again. "Here at the institute, we invented the method of deducing the mechanical behavior of an entire crystal based on the quantum mechanical description of a single lattice defect," says Raabe.

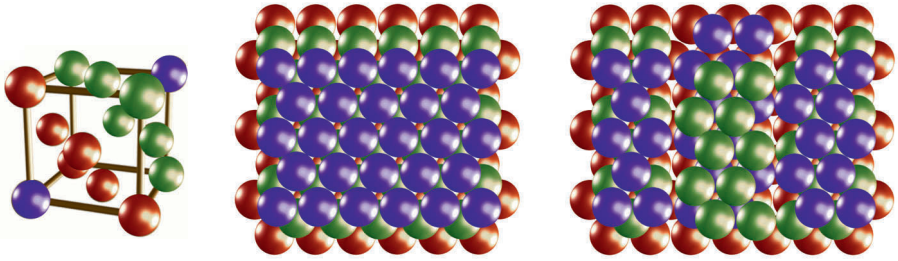
The team also has to take something else into account, a factor that already

GPS FOR ATOMS

Quantum mechanical computations for small sections of material are only partially suitable for deducing the manner in which the atoms of different elements are actually distributed in a larger extract. That is why it is important to observe the conditions in the real materials once they have been created. Atom-probe tomography serves as a sort of GPS for the individual particles. High-voltage pulses knock out single atoms from the ultra-thin material sample one atom at a time, and an electrical field then steers them toward a detector. The time it takes them to travel this distance indicates their mass and charge, thus revealing the element to which they belong. In turn, the location at which they reach the detector allows researchers to draw conclusions about the position of the atoms in the sampled material. This method generates a three-dimensional image of the sample with a high enough resolution to even show individual atoms.

Especially when analyzing complex alloys, this type of imaging grants scientists interesting insights into the actual distribution of elements in a material. That was the case during the development of a new generation of materials for future power plant turbines: a nickel alloy that also contains boron. Not until the sample was subjected to atom-probe tomography did it become apparent that the boron atoms aren't simply distributed in the nickel lattice. Instead, they prefer to settle by the grain boundaries between the individual crystals. There they evidently serve as a type of "cement," strengthening the bond between the grains.

Graphics: MPI für Eisenforschung – Tilmann Hickel



Wrongly stacked: The colors of the individual atom layers represent the positions of the atoms in relation to the next two atom layers underneath. The normal arrangement for a face-centered cubic crystal (the unit cell of which is depicted on the left) is shown in the center using a layered sequence of red–green–purple. When a stacking fault occurs, the positions in one particular area are shifted (right), altering the sequence to red–purple–green. Stacking faults make a material more rigid; they can be incorporated on purpose to make a steel more solid.

played a role in the titanium project: the fact that some metals can form different types of crystal lattices, each featuring different mechanical properties.

Sometimes an external force can cause certain points of a crystal structure to become altered. "Then a layer of atoms in one location is shifted into a less stable position, for example, triggering what is known as a stacking fault," says Raabe. "This fault can cause a nanoscopically small zone of a face-centered cubic lattice to turn into a hexagonal lattice."

STACKING FAULTS INFLUENCE DEFORMABILITY

And that has an impact on the material's mechanical properties due to the fact that the boundary layer between two such types of crystal lattices serves as a stop sign for dislocations. Consequently, the deformability decreases at this site, and this part of the material becomes brittle – and can ultimately even break. Dierk Raabe and his team seek to prevent such premature fatigue. In order to do so, they increase the amount of energy required to cause a stacking fault and thus alter part of the structure. By now, Raabe is able to give his colleague Neugebauer a pretty precise description of what he is searching for. "For example, I ask him what an alloy would have to look like if I wanted the crystal structure to alter only after reaching a tensile stress of 0.8 gigapascals."

Neugebauer and his team would then simulate the atomic shift that leads to a stacking fault and thus alters one part of the lattice structure. "We determine the exact energy threshold that needs to be overcome in order for this to occur," says Neugebauer. This stacking fault energy is in defined proportion to the tensile stress. When performing his complex calculations, Neugebauer would then simulate random combinations of iron atoms and other types of atoms until one particular alloy exhibits the threshold value specified by Raabe.

In this very manner, the researchers in Düsseldorf created a new type of steel – a variant that sets the benchmark in more ways than one. "For the first time ever, we were able to incorporate so much aluminum into manganiferous steel that the resulting material is roughly 10 percent lighter than normal steel," says Raabe. At 10 percent, the total weight of a car could easily be reduced by 100 kilograms. But that wasn't the only highlight. "Until now, steel variants containing a noteworthy amount of aluminum were brittle, thus rendering them unusable," explains Raabe. This new type of steel, on the other hand, is extremely deformable and would absorb a large amount of energy in the event of a collision. This behavior was further improved by the individual aluminum atoms in the crystal lattice.

There are currently around 2,500 different types of steel – more than twice as many as at the turn of the century. And the demand for further optimizing materials continues to rise. Today it is possible to predict a material's properties solely on the basis of its chemical composition, and thus to design metals that fulfill the desired specifications. A mere ten years ago, that would have been virtually inconceivable. ◀

TO THE POINT

- **Two of the characteristics that the researchers try to customize for each field of application are how rigid a type of steel or other alloy is, and how easily the material can be deformed.**
- **Max Planck researchers compute the material's properties, starting with the quantum mechanical interactions between a finite number of particles. They made it possible to calculate the quantum mechanical behavior of complex materials such as alloys with multiple components.**
- **The mechanical properties strongly depend on the material's microscopic structure. Defects in the crystal lattice play an important role in this regard. The Düsseldorf-based researchers study what happens to such defects when the material is deformed, for example. This gives them clues about how a given material can be optimized for a particular application.**

GLOSSARY

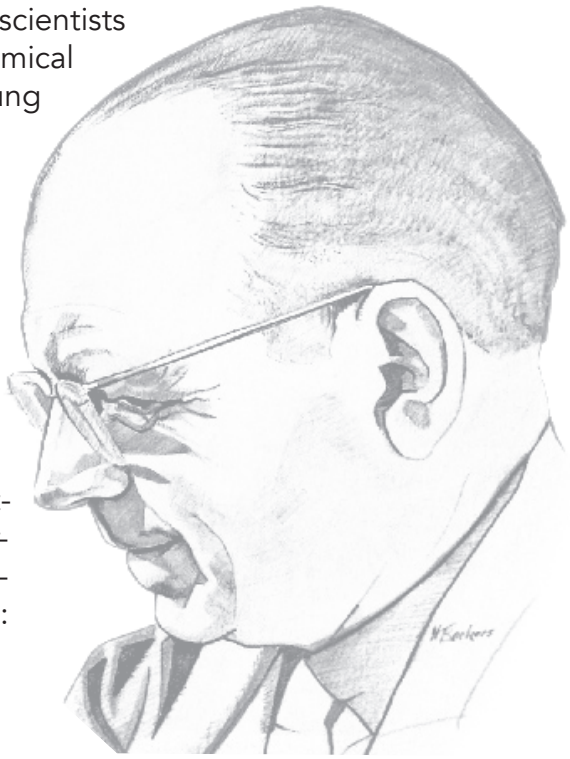
Density functional theory: In order to calculate the properties of a crystal or other system composed of many atoms, this method determines the electron density at each point within the crystal lattice. As a result, it is no longer necessary for researchers to observe the interaction of all the electrons within the entire lattice, thus drastically reducing the time needed to compute these results.

Stacking faults: If you imagine atoms as being spheres that are stacked on top of each other inside a crystal, the third layer of atoms can take on one of two different arrangements: either directly in line with the first layer, or offset to the first layer. This arrangement is predetermined for a given crystal structure, and deviations from this pattern are known as stacking faults.

Edge dislocation: If this fault (also called a line defect) is present in a crystal lattice, a row of atoms abruptly ends, so that the neighboring rows must be dislocated in order to fill the void.

Graphics: MPI für Eisenforschung – Tilmann Hickel

Since 2006 the Ernst Haage-Prize awards young scientists for outstanding achievements on the field of chemical energy conversion and promotes particularly young academics. The award is given in honour of the entrepreneur Ernst Haage who lived in Mülheim and died in 1968. The Ernst Haage-foundation awards the prize which is supported with a prize money of € 7.500,-. Nominees shall be scientists with a doctor's degree of a German research institution/university, who are in general younger than 40 years and have no permanent contract of employment.



Nominations can be submitted instantly until September 30th 2014 to the curatorship of the foundation. The following documents should be part of the proposals:

- Two pages of laudation
- Curriculum vitae in table form
- Complete publication list
- Up to three reprints of works of the nominated person.

Personal applications cannot be considered.

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