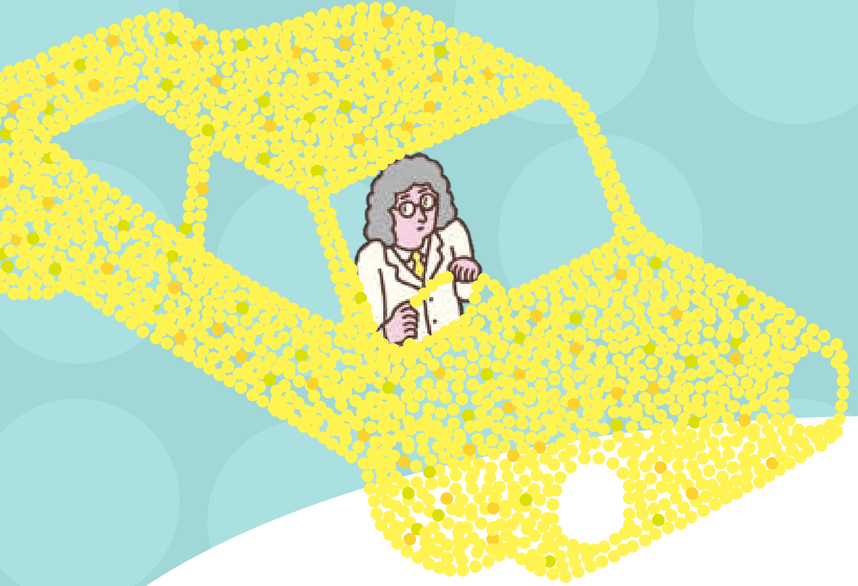
2021

NIMS NOW INTERNATIONAL No. 6

NATIONAL INSTITUTE FOR MATERIALS SCIENCE

EXPLOITING "DEFECTS" FOR MATERIALS SCIENCE



What are "defects" from the perspective of materials science?

How are they formed?

Are they always bad?

"Defect"

The word "defect" generally has negative connotations.
However, for materials researchers, some defects have advantageous traits,
and skillfully exploiting them may open up new horizons.

In fact, some defects are known to be vital in improving the performance of materials.
Finding ways of overcoming or taking advantage
of defects in materials development may lead to new scientific discoveries.

Materials scientists are committed to utilizing defects of various kinds.
Let's take a closer look at defects so that we can see them as these scientists do.

Discussion by
three experts

What are benefits of " defects" in materials ?

The skillful use of "defects" improves the performance of a wide range of materials such as steel, semiconductors and soft polymers. Experts on these materials discussed their approaches to exploiting defects in materials development.

Kaneaki
Tsuzaki
NIMS Fellow

"Defects are crucial components in steel materials. They make steel formable. Understanding their mechanisms will benefit the next generation of manufacturing."

Structural steel material expert

"The history of electronic devices is also the history of compromising defects. Controlling defects in semiconductors is our ultimate challenge. On the other hand, some defects are highly advantageous. We need to deal with defects on a case-by-case basis."

Toyohiro
Chikyow
MaDIS Senior Scientist
with Special Missions
Leader of
the Device Materials
Informatics Group

Semiconductor expert

"Polymers are full of defects. We find ways of effectively using them to improve our products. Skillful defect control may accelerate the development of recyclable polymers in line with the rapidly growing public interest in plastic recycling."

Masanobu
Naito
Leader of the Data-driven Polymer Design Group,
Research and Division of Materials Data and Integrated System(MaDIS)

Polymer expert

The advent of electron microscopes in the 1950s made it possible to observe defects.

Tsuzaki: Defects are crucial components in steel materials. Steel forming has traditionally been done by two types of professionals: foundry specialists and blacksmiths. A foundry specialist forms steel by pouring liquefied steel into a cast, while a blacksmith shapes steel by hammering it. Forming steel using external force (hammering) is impossible without mobile dislocations—a type of crystallographic defect—within a steel material.

If all the crystals were perfect, blacksmiths would have gone out of business long ago. Humans benefitted from steel for many centuries without knowing of the existence of the defects that enabled steel forming.

At some point, scientists began to suspect the existence of defects to explain some metal-related phenomena. The existence of defects was finally confirmed in the 1950s when electron microscopes were developed.

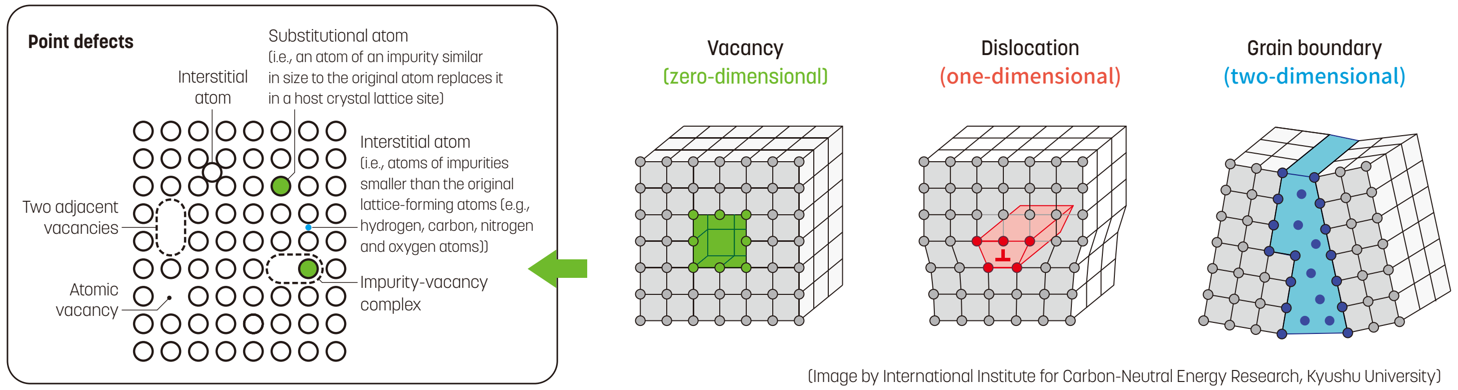
There are several ways of shaping metals, including casting, plastic forming and cutting. All of these methods—except casting—rely on the mechanisms of lattice defects*. Without this knowledge, proper metal forming is impossible. Among the several types of lattice defects known, dislocations play the most important role in metal forming.

Chikyow: As far as defects in semiconductors are concerned, we're primarily interested in large-scale defects (i.e., dislocations) and small-scale point defects (i.e., atomic vacancies and interstitial atoms).

As you all know, the silicon metal shortage has become a serious problem. Silicon metal is elemental silicon containing impurities which affect its electrical conductivity. The history of semiconductor crystals can be characterized by efforts to increase their purity. Currently, purity is extremely high: "eleven-nine" (99.999999999%) pure. However, high-purity silicon itself is unsuitable for use in semiconductors. The electrical conductivity of semiconductors is controlled by adding trace quantities of impurities and defects to pure silicon.

An atomic vacancy is a defect which occurs when a constituent atom leaves its silicon crystal lattice site. The departed atom moves about within the silicon crystal. When impurities (e.g., phosphorus and boron) are added to silicon, they enter the crystalline lattice with an atomic vacancy, causing it to generate electrons or making "hole" which is positively charged.

Naito: While I was listening to the two of you, I realized that we all look at defects differently. Dr. Chikyow talked mainly about nanoscale point defects while Dr. Tsuzaki talked mostly about microstructures, which are larger in spatial scale than point defects. Defects of various scales directly affect the functions and physical properties of materials. With regard to polymeric



(Image by International Institute for Carbon-Neutral Energy Research, Kyushu University)

***Lattice defects**
"The constituent atoms of crystals in metals and alloys generally have orderly arrangements," Tsuzaki said. "However, when they undergo deformation, they form various types of crystallographic defects, such as point or vacancy defects (i.e., an atom that originally occupied a lattice point is missing), line defects or dislocations (around which the atoms of the crystalline lattice are misaligned) and planar defects (the formation of grain boundaries where the crystallographic direction of the lattice abruptly changes). These defects occur in large numbers during mass processing of metals and alloys." (Tsuzaki)

materials, defects wide-ranging in scale, from the nano to visible sizes, impact their functions. Defects can form in any size of polymer at any processing stage. Polymeric materials are therefore full of defects that we constantly need to deal with. Defects include nanoscale structural defects, which are difficult to control, and large, visible cracks. Polymers can never be 100% crystalline; they are always a mixture of crystalline and amorphous components*. Defects are formed at the boundaries between these two structurally different components. Polymers are mainly composed of spherulites, a type of crystal with a unique structure. Spherulites extend meanderingly and their constituents are held together by amorphous polymers. When these polymers break, the whole material cracks.

Chikyow: The physical properties of Gore-Tex*—a popular outdoor clothing material—were also enhanced by defects, correct?

Naito: That's right. Gore-Tex was created by stretching PTFE (Teflon™), a type of fluorine resin. This process produced a porous ("often thought as defect") material that allows water vapor to pass through while repelling liquid water. This is an example of a successful use of microscale defects.

Tsuzaki: I said earlier that defects in steel enable blacksmiths to form it. In addition to this advantage, defects can also strengthen steel when they are present in large numbers. This is because different defects can immobilize each other, preventing the steel from collapsing.

Strong steel therefore can be created by adding many defects to it. However, very strong steel loses its ability to self-repair when it cracks. This steel snaps when only a weak force is applied to it. In addition, while strong steel retains its strength even when ground into a thinner piece, once it is scratched, it becomes susceptible to snapping. Very hard materials are vulnerable to scratching and embrittlement.

We're eager to develop stronger and lighter products, but they also need to be unbreakable. To satisfy these conditions, we need to control the distribution and density of lattice defects.

The development of formable metals requires optimization of their internal microstructures. We have been working to figure out ways of creating strong, ductile and unbreakable metallic materials. Advanced research has shifted the focus from developing stronger materials to developing materials that break in a desirable manner. This approach to materials research led to the development of hi-ten steel*, for example.

Hydrogen's mixed impact on semiconductors

Chikyow: Semiconductor quality has improved by eliminating a series of defects. Silicon itself is very brittle, but incorporating oxygen makes it stronger. Accordingly, a single crystalline silicon substrate containing 1% oxygen is very strong. This substrate is used to produce large silicon wafers* 300 mm in diameter which are sufficiently strong to be carried around.

On the other hand, some impurities severely harm the performance of semiconductors. These include metallic particles which may contaminate semiconductors during production and airborne impurities, such as sodium and sulfur. Contamination by only tiny amounts of these impurities can considerably change the electrical conductivity of semiconductors.

The gettering process was invented to address this problem. Gettering reduces impurities within the vital components of a silicon wafer by localizing them in predetermined areas containing iron, etc. on the backside of the wafer. Although this technique had been used widely until recently, it is less common today because the purity of silicon has significantly increased. The remaining major source of defects is hydrogen.

Tsuzaki: That's interesting. I also happen to be researching hydrogen's effects on steel materials.

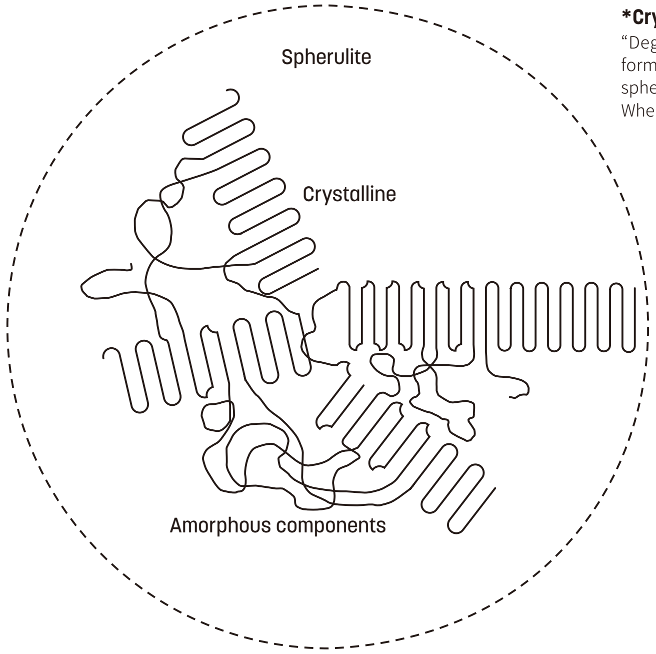
Chikyow: Hydrogen within silicon can be both advantageous and disadvantageous. Even perfect silicon crystals contain holes through which hydrogen can sometimes enter. Hydrogen is advantageous when it binds to a dangling bond (i.e., an unsatisfied valence on an immobilized atom) at the interface between two different materials, thereby maintaining a neutral and stable electrical state. For this reason, semiconductor devices are treated with hydrogen through sintering processes during fabrication to improve their performance though it is not the major process in recent. On the other hand, hydrogen may disrupt the stable performance of semiconductor devices by inducing reduction reactions, leading to the removal of oxygen, which is very detrimental. To prevent this, some device parts are coated with silicon nitride to prevent hydrogen from entering them. Some recent semiconductor devices haven't required silicon nitride coatings because hydrogen contaminants are thoroughly controlled in current semiconductor manufacturing processes.

For semiconductor researchers, controlling virtually invisible, fast-moving hydrogen is the last frontier to be explored.

Tsuzaki: Absorption by hydrogen also makes most metal materials brittle. I said earlier that scratched metals are more breakable. If hydrogen absorbs them, they become even more fragile. Hydrogen weakens bonds between metallic atoms. It is very difficult but critical to prevent hydrogen from entering materials and to neutralize it when it has already done so. I'm surprised that hydrogen also poses serious challenges to silicon material researchers. I just looked up this topic on Google while listening to Dr. Chikyow and surprisingly quite a few search results showed up.

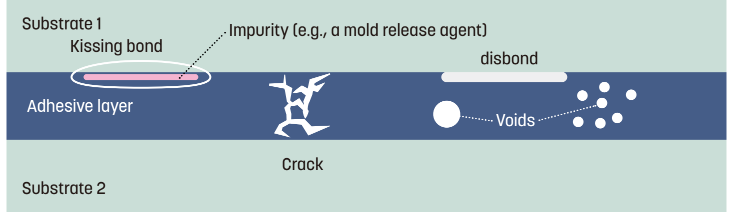
Defects: a persistent issue during polymeric synthesis and processing

Naito: As I said earlier, polymer researchers need to deal with defects every step of the way from polymeric synthesis to processing. In polymer research circles, adhesives have been a hot topic in addition to some other materials.



***Crystalline and amorphous polymers**
"Degradation of a crystalline polymer begins with the disintegration of its spherulites, forming nanovoids (tiny pores) within them. At this early stage of disintegration, adjacent spherulites are barely held together by molecular tie chains—a type of amorphous polymer. When these chains break, nanovoids develop into cracks." (Naito)

***Kissing bonds**
"A kissing bond is an adhesive bonding defect in which voids and other defects are formed at the interfaces between the adhesive and the joined materials (e.g., metals and resins). The adhesive joint appears to be sound, but in reality no chemical interaction has taken place between the bond and the joined materials to achieve adhesion." (Naito)

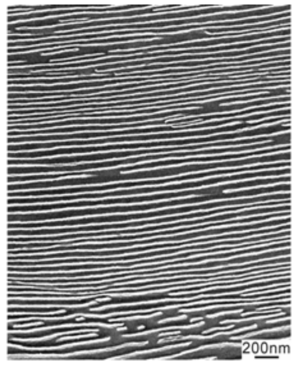


***Crystalline grain boundaries**
"A polycrystal composed of many crystallites of varying orientations has grain boundaries (a type of planar defect) where lattice arrangements abruptly change. The video clip accessible below would be very helpful in understanding grain boundary mechanisms." (Tsuzaki)

A video clip showing an example of effective use of grain boundaries in materials development (in Japanese only) can be accessed here.
Manganese can be added to a magnesium alloy to facilitate grain boundary sliding, thereby preventing the alloy from cracking along the boundaries and enhancing its deformability.

●Magnesium alloy deformable at room temperature: grain boundary sliding is the key

***Piano wire**
What is commonly called "piano wire" today actually refers to industrial wire and differs from the wire currently used in piano strings. Steel piano wire is stronger than ordinary wire. It was originally made for use in piano strings which produce sound when struck by a hammer. Extremely thin, strong piano wire was later developed, enabling pianos to produce higher pitch sound.



SEM image of the internal components of a piano wire. A number of interfaces are stretching in parallel, resembling mille-feuille layers.
(Photo provided by Rintaro Ueji, Principal Researcher, Research Center for Structural Materials, NIMS)

For example, the use of CFRPs (carbon fiber reinforced plastics)—a type of composite—as auto body materials has been increasing in addition to very strong, elastic hi-ten steel. Firmly bonding a metal and a resin using adhesives is difficult because various defects develop at the interface between them. A kissing bond* is one such defect. This is physically attached to the surfaces of both materials, but no chemical interaction has taken place between the bond and their surfaces to achieve adhesion. The bond appears to be sound and defect-free, but in reality it does not adhere to the joined materials and easily peels away. Detecting defects leading to adhesion failure is of critical importance for the industrial sector, and I've participated in research projects related to this issue.

Chikyow: Adhesives have become popular in vehicle manufacturing in recent years. I was very surprised when I heard the news that adhesives were used for the first time to join frame components of the Lotus Elise* in the 1990s. I suppose this practice has been widely adopted since.

Naito: While the use of adhesives to join various structural materials is gradually increasingly, bolting is also used in combination for reasons of safety. I agree with Dr. Tsuzaki that stronger materials also need to be reliable and stable in performance. For example, the adhesives used to join automotive parts are capable of not only ensuring structural stability but also of enhancing ride comfort by reducing vibration.

Chikyow: We've been conducting accelerated aging tests—measuring the endurance of semiconductor devices in continuous operation at different extreme temperatures (e.g., 120°C and 150°C). This test expedites the estimation of their endurance at room temperature by exposing them to higher temperatures, thereby speeding up their normal aging processes. The results of these tests are used to ensure the reliability of devices. By the way, I have a question for Dr. Tsuzaki: do high densities of defects tend to develop in materials with unique microstructures, such as piano wire*, over time?

Tsuzaki: I think so. For materials containing planar defects (i.e., grain boundaries), including piano wire, their arrangements and densities are important determinants of the materials' physical properties. While the grain boundaries in most materials are oriented in various directions, those in piano wire are oriented in the same direction. They somewhat resemble the layered structures in croissants and mille-feuille. These dense, parallel grain boundaries are what give piano wire its very high tensile strength.

Chikyow: The invention of piano wire in around 1800 is said to have revolutionized music. The pitch range of musical instruments available during the Mozart era was much narrower than that of modern instruments. The advent of piano wire led to the development of a fortepiano—an early piano—with a wider pitch range. This is why pitch ranges used in symphonies widened significantly from the Beethoven era to the Brahms era and beyond. Successful defect control has transformed music.

Tsuzaki: One could say that materials changed music which then transformed the world. Similarly, the evolution of materials led to the evolution of automobiles, which dramatically changed the world and accelerated economic growth. These chains of events driven by materials inspire me as a materials scientist.

Chikyow: These historical perspectives make me appreciate defects even more.

Growing interest in research contributing to a circular economy

Tsuzaki: Blacksmiths in the distant past used their know-how to create relatively small metallic products. However, the first Industrial Revolution drove the creation of larger structures, such as steam locomotives and iron bridges, and mass production—an abrupt transition from craftsmanship to industrialization. Early industrial manufacturers had to find new ways of creating products. At the time, optical microscopes were a mainstream scientific tool. Subsequent microscopy advancement later enabled materials researchers to observe microstructures within materials in more detail.

Naito: I'm not too concerned about the existence of defects in polymers. Some of them may even be useful. One exciting thing about polymeric materials is their potentially high reusability and recyclability by skillfully exploiting defects within them. For example, biodegradable polymers are drawing growing attention due to increasing public interest in a circular economy. Their biodegradability tends to decrease with increases in the degree of crystallization and an increasing number of branched structures. In other words, highly crystallized polymers are strong but low in biodegradability, while amorphous polymers with many defects are more conducive to biodegradation. It's vital to control polymers' biodegradability by integrating defects into them while giving them desirable functions in a balanced way. It's also important to develop biodegradable polymers with appropriate durability for use in various environments (e.g., soil, aqueous and Arctic environments). Research contributing to a circular economy is expected to become more popular in the future.

Tsuzaki: Only 70 years have passed since 1950, when the existence of lattice defects was presumably confirmed for the first time and when efforts to understand their characteristics began. During this time period, scientists' understanding of defects has greatly advanced. We will need to research defects from new angles.

It's vital to understand the movement of defects under various conditions. I believe this information will benefit the next generation of manufacturing. I'm sure that we will learn new facts about defects as the research environment changes. Research on lattice defects will continue for many years to come.

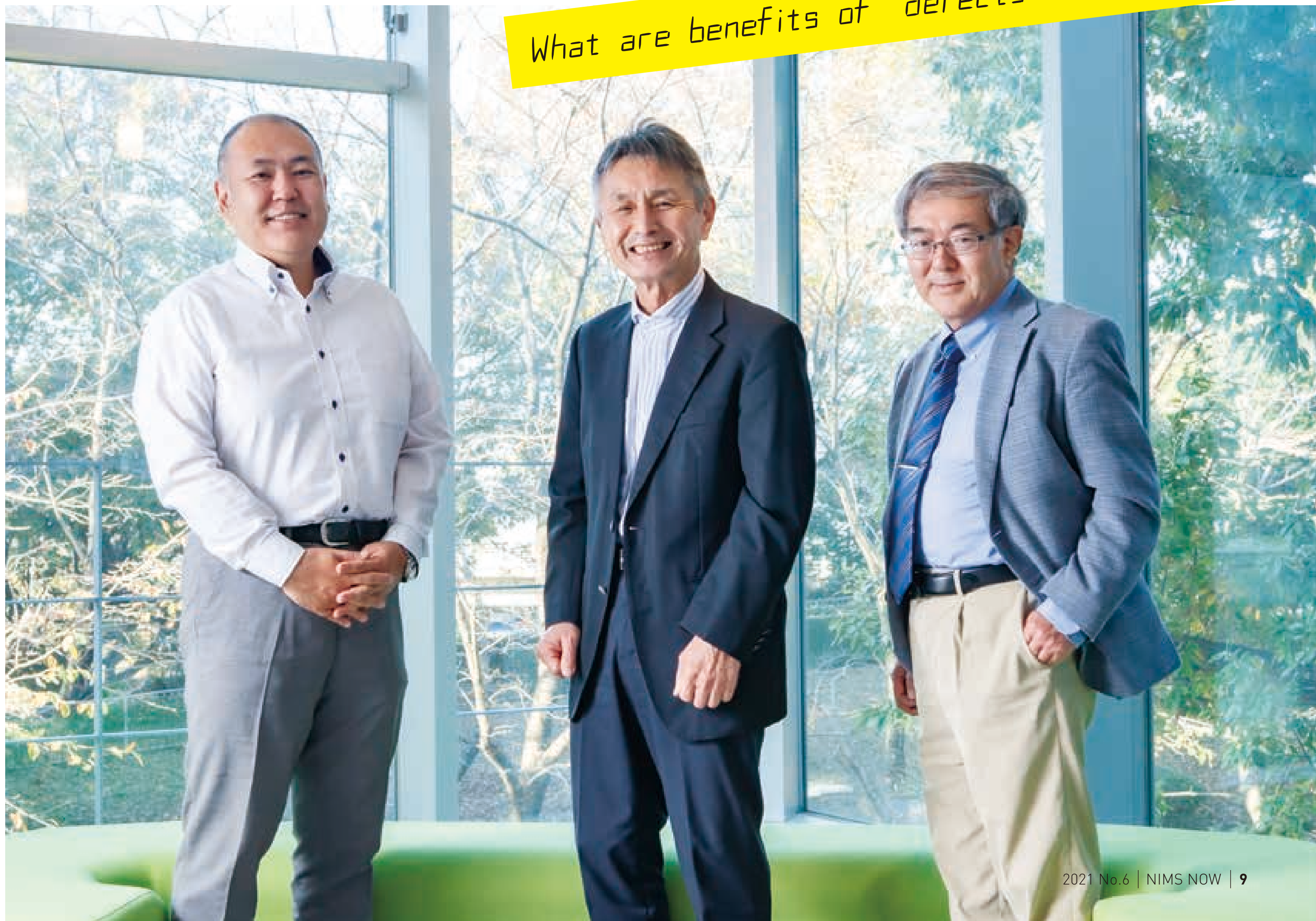
Chikyow: We should change our negative perception of defects and find ways of effectively exploiting them. Our efforts to tackle defect-related issues have no end: solving one problem will lead to the identification of another. Some defects are like troublemakers and others like close friends.

Naito: I agree. Precise defect manipulation may become an important focus for materials researchers.

(This discussion took place at NIMS on November 8, 2021)

***Lotus Elise**
"The Lotus Elise is a roadster-type sports car developed in 1995 by the British manufacturer Lotus Cars. The company developed a lightweight car body in an innovative way: adhesives were used to join the different body parts. This was big news at the time." (Chikyow)

What are benefits of "defects" in materials ?



***Gore-Tex :** See p.13
***hi-ten :** See p.12
***Semiconductor silicon wafers :** See p.13

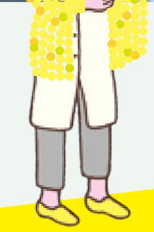
NIMS lab
mini tour

Researchers focusing on materials with "defects"

Some researchers at NIMS are fascinated by materials with intentional defects. Please join us in visiting these passionate people so that we can learn a bit about their ongoing projects.

Morio Kawai
Graduate Student of the University of Tokyo

"Dr. Naito approaches research from a variety of angles and has keen foresight about the practical application of materials being studied. He suggested that I research my current project: recyclable plastics."

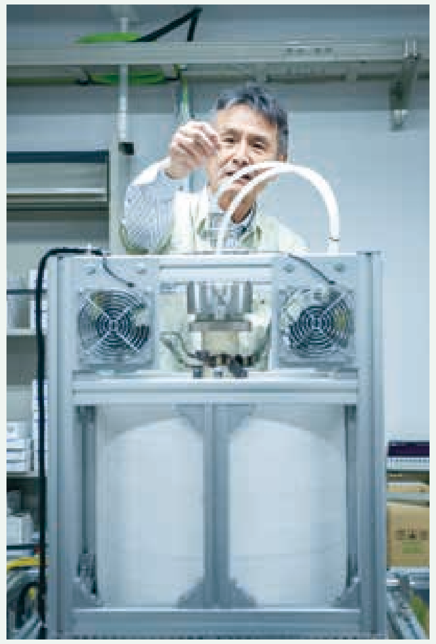


"Recently, our main research focus has been the development of **adhesives as well as materials that can be recycled economically.** We're hoping to create recyclable structural materials that decompose in specific ways. Unfortunately, I can't tell you much about them yet as they're trade secrets." (Naito)

"Our primary research focus has been **martensitic transformation and hydrogen embrittlement** in steel. Very strong martensitic steel can be created by rapidly cooling heated austenitic steel. We've been microscopically observing changes in microstructures and lattice defects in steel that occur during this process. While martensitic transformation is a vital process in strengthening steel, it also makes steel prone to hydrogen entry—a source of embrittlement. We're investigating ways of creating martensitic steel resistant to hydrogen embrittlement." (Tsuzaki)

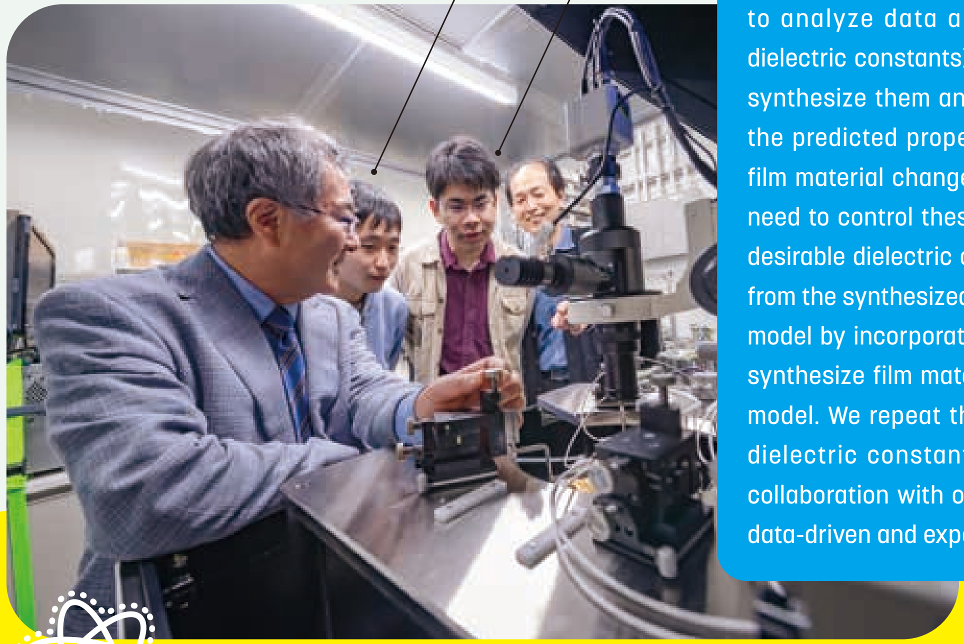
Xiaodong Lan
NIMS Postdoctral Researcher
Steel Research Group,
Research Center for Structural Materials

"I'm originally from China and joined NIMS after graduating from Kyoto University. Dr. Tsuzaki has frequently offered me helpful advice since I became a member of the Steel Research Group led by Dr. Akinobu Shibata."



Participants in
the NIMS Joint Graduate School Program:
(From Graduate School of Meiji University)
Masaya Morita

Participants in
the NIMS Joint Graduate School Program:
(From Graduate School of Meiji University)
Yuki Daimon



"We've been working on **high-throughput materials synthesis techniques combined with data-driven materials science.** For example, when we develop dielectric films, we use a model to analyze data and predict the physical properties (e.g., dielectric constants) of film materials to be synthesized, actually synthesize them and verify their physical properties relative to the predicted properties. Because the dielectric constant of a film material changes in relation to the defects present in it, we need to control these defects during film synthesis to achieve a desirable dielectric constant. To this end, we take measurements from the synthesized films, improve the accuracy of the prediction model by incorporating the collected data into it and once again synthesize film materials using the parameters predicted by the model. We repeat these processes until we achieve a targeted dielectric constant. We've been carrying out this project in collaboration with other teams with different expertise, such as data-driven and experimental research." (Chikyow)

Principal Researcher,
Device Materials Informatics Group, MaDIS
Yukinori Koyama

Hiori Kino
Senior Researcher,
Device Materials Informatics Group,
MaDIS

Takahiro Nagata
Leader of
the Nano Electronics Device Materials Group,
Research Center for Functional Materials

Who would have thought?

Products whose performance is enhanced by “defects”

Exploiting them

Controlling them

Japanese swords

“The strength of a Japanese sword can be increased by introducing various lattice defects into it through a heating and quenching treatment. The blade of the sword is composed of martensite, a very hard crystalline steel structure. Traditionally, the temperature to which swords were heated and of the cooling water needed to create high-quality swords were kept secret, and only experienced swordsmiths were able to masterfully craft swords. It would be very difficult to conduct a scientific investigation into the mysteries of precious, centuries-old Japanese swords because taking samples from them is severely restricted.”

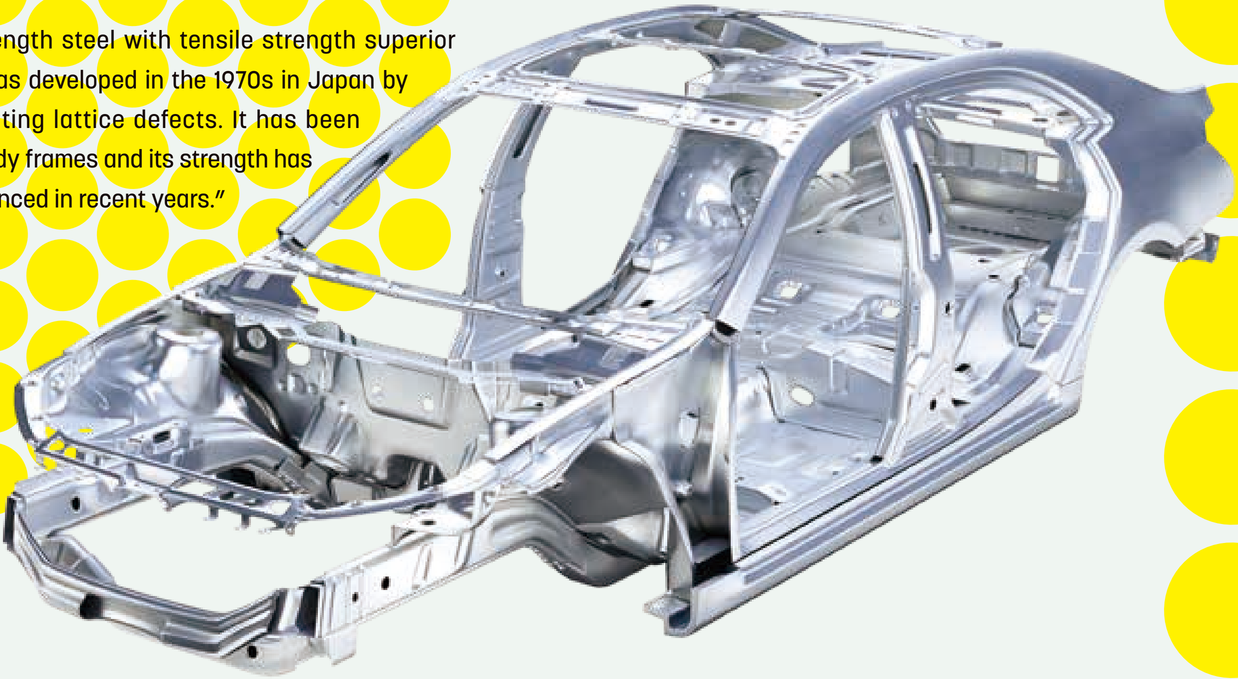
Backscattered electron SEM image of a cross-section of a Japanese sword. Martensite can be seen at the tip of the blade material.
(Photos provided by Mr. Kazunori Tsukamoto and Dr. Takashi Kimura, JEOL Ltd.)

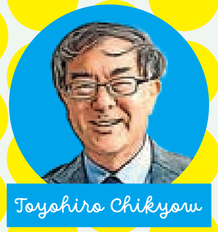
Duralumin

“Duralumin is a very strong aluminum alloy invented in Germany in 1906. According to a famous story, the metallurgist who later invented duralumin began measuring the hardness of a heat-treated alloy on a Saturday but didn’t complete it that day. When he resumed the hardness measurement early the following week, he found that the alloy was much harder than usual. This led him to discover the phenomenon called age hardening: when alloys are allowed to harden slowly after they are heated and quenched, their hardness increases. Age hardened alloys form many nanocrystals with different structures within them, immobilizing crystallographic dislocations.”

High tensile strength (hi-ten) steel

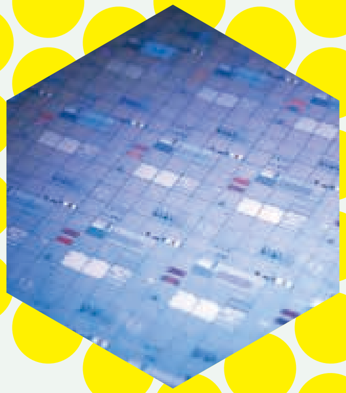
“High tensile strength steel with tensile strength superior to normal steel was developed in the 1970s in Japan by effectively exploiting lattice defects. It has been used in vehicle body frames and its strength has been further enhanced in recent years.”

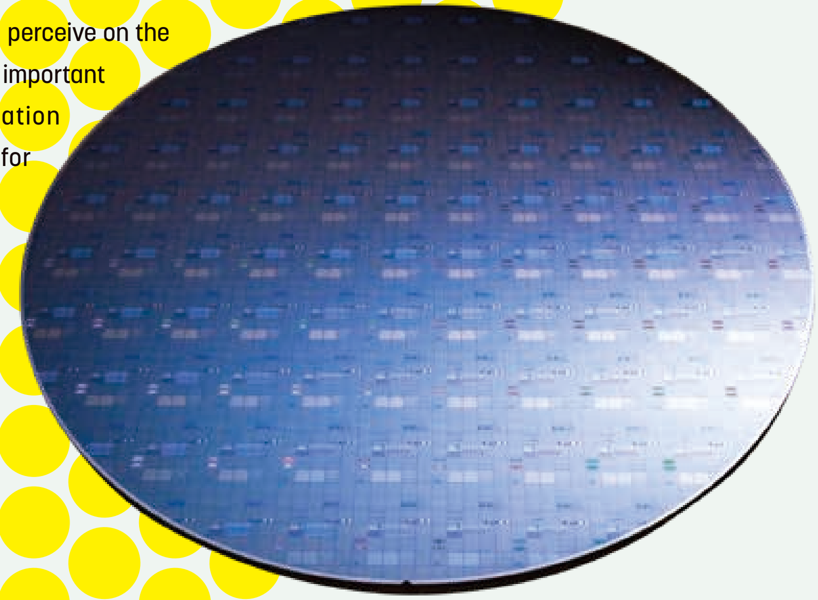


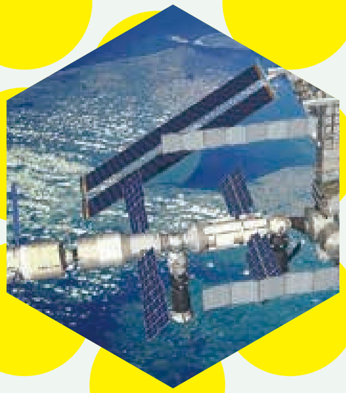


Semiconductor silicon wafers

“This is an example of an integrated circuit (IC) fabricated on the surface of a wafer substate 300 mm in diameter. The ICs widely used today have circuit traces 30 nanometers in width and it becomes less than 7 nm in high performance devices. These traces are narrower than the colorful, fine, glowing patterns the naked eye can perceive on the wafer surfaces. Controlling defects becomes increasingly important with increasing IC sophistication. The final IC fabrication process sometimes involves heat treatment at 450°C for approximately 10 minutes to terminate defect formation.”



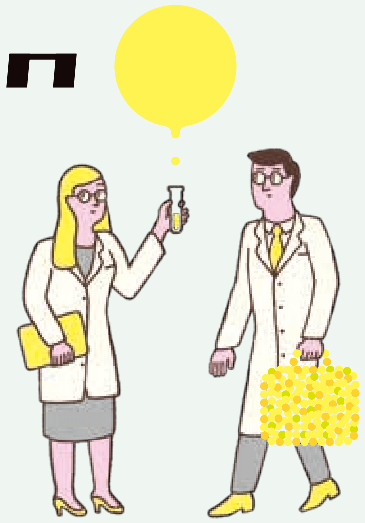




“ePTFE” polymer known as Gore-Tex

“Gore-Tex—which allows water vapor to pass through while repelling liquid water—is composed of stretched PTFE (Teflon™), a type of fluorine resin. Early efforts to slowly stretch PTFE rods without breaking them had been unsuccessful until, by accident, they were stretched to 10 times their original length by applying a sudden, accelerated yank. Gore-Tex materials with numerous pores (“often thought as defect”) have been an indispensable component in a variety of products, including clothing, medical equipment and electronic cables.”

A new generation explores "defects"



Younger researchers at NIMS have been investigating the mechanisms of defects in materials they have been studying in an effort to put them into practical use.

Unique mechanisms in necklace-like structures potentially applicable to the development of strong materials

A polymer is composed of long, entangled, noodle-like chains of repeated molecular units. When an external force is applied to it, voids—nanosized defects—form within it. For example, when a soft plastic material, such as a clear file folder, is bent sharply, the bent portion turns white. This is because bending it creates numerous voids that scatter light. Applying a force to harder plastic materials often causes them to crack as soon as voids are formed.

Preventing void formation within polymeric materials is very difficult. However, identifying void formation mechanisms, including void-inducing structural defects, may facilitate the development of stronger materials.

I have been researching polyrotaxane glass, a material resistant to void-induced cracking despite its high hardness. I'm investigating this material's potentially unique ability to strengthen itself locally in response to void formation, preventing voids from developing into cracks. Although other strong polymeric materials exist, their structures are difficult to analyze in detail even with the aid of x-rays and electron microscopes. By contrast, a polyrotaxane molecule is easier to analyze because of its relatively simple necklace-like structure consisting of ring components through which a string component extends. The mechanisms by which polyrotaxane glass fortifies itself locally in response to void formation may be used to reinforce many other polymeric materials.

Kazuaki Kato

Invited Researcher,
Data-driven Polymer Design Group, MaDIS
(Lecturer, Department
of Advanced Materials Science
Graduate School of Frontier Sciences,
The University of Tokyo)

Development of electrically conductive organic materials with "defects" created by extracting protons

Yuka Kobayashi

Principal Researcher,
Molecular Design and Function Group
Research Center
for Functional Materials

In general, organic materials are electrical insulators. Their use as practical electrical conductors had not been widely pursued until the discovery of conducting organic polymers by Professor Hideki Shirakawa et al. (Nobel Prize, 2000). These polymers, however, are somewhat unstable chemically due to a doping strategy for obtaining conductive properties; inherently stable molecules are doped with other molecules, making them less stable. This chemical instability makes long-lasting conductivity difficult depending environmental conditions, such as heat. A new idea had come to me; we might develop chemically stable conducting molecules by removing something from insulating molecules, rather than adding anything. Based on this concept, I have designed new electrically conductive organic materials with protonic defects, which are stabilized by using hydrogen-bonding networks. These defects are intended to effectively balance the charge of the materials.

Because of the general preconception that defects are always undesirable in organic materials, the electrically conductive organic materials I developed were largely dismissed initially. However, it was gradually accepted when it was found to be stable for use even under extreme conditions, such as light irradiation in solar cells. The technique used to develop the electrically conductive organic materials could be applicable to a wide variety of semiconductors and metals. In addition, it may be used to develop inexpensive electrodes potentially capable of replacing rare-metal-containing ITO (indium tin oxide) electrodes. Moreover, because this technique is compatible with drop casting, a method of depositing electrode materials, it may be used to develop organic electrodes for industrial use where inorganic electrodes are unsuitable. I am going to continue fundamental researches aiming for future practical applications.

Ascertaining defect mechanisms using atomistic simulations

Dislocations are a type of lattice defect. When present in a metallic material, dislocations with high mobility often reduce its strength. However, other lattice defects can be used to reduce dislocation mobility, making a material stronger and more resistant to deformation. I have been researching interactions between lattice defects by running atomistic simulations on a computer.

One current major focus in structural materials is developing materials with high strength and high toughness. Although various strong structural materials have already been used, we still lack enough knowledge about atomic-scale mechanisms—including the role of defects—that make materials stronger. Atomistic simulations are a powerful tool that can be used to investigate these mechanisms. I believe that understanding fundamental lattice defect mechanisms will facilitate the efficient development of materials with outstanding properties.

The importance of computational simulation has increased in recent years because of the improved accuracy of the computational evaluation by the more powerful computers available today. Combining the strengths of experimental and computational research makes an in-depth understanding of physical phenomena possible. Research on the behavior of lattice defects at extremely small spatial scales is very challenging and continually fascinating to me.

Masato Wakeda

Senior Researcher,
High Strength Materials Group
Research Center
for Structural Materials

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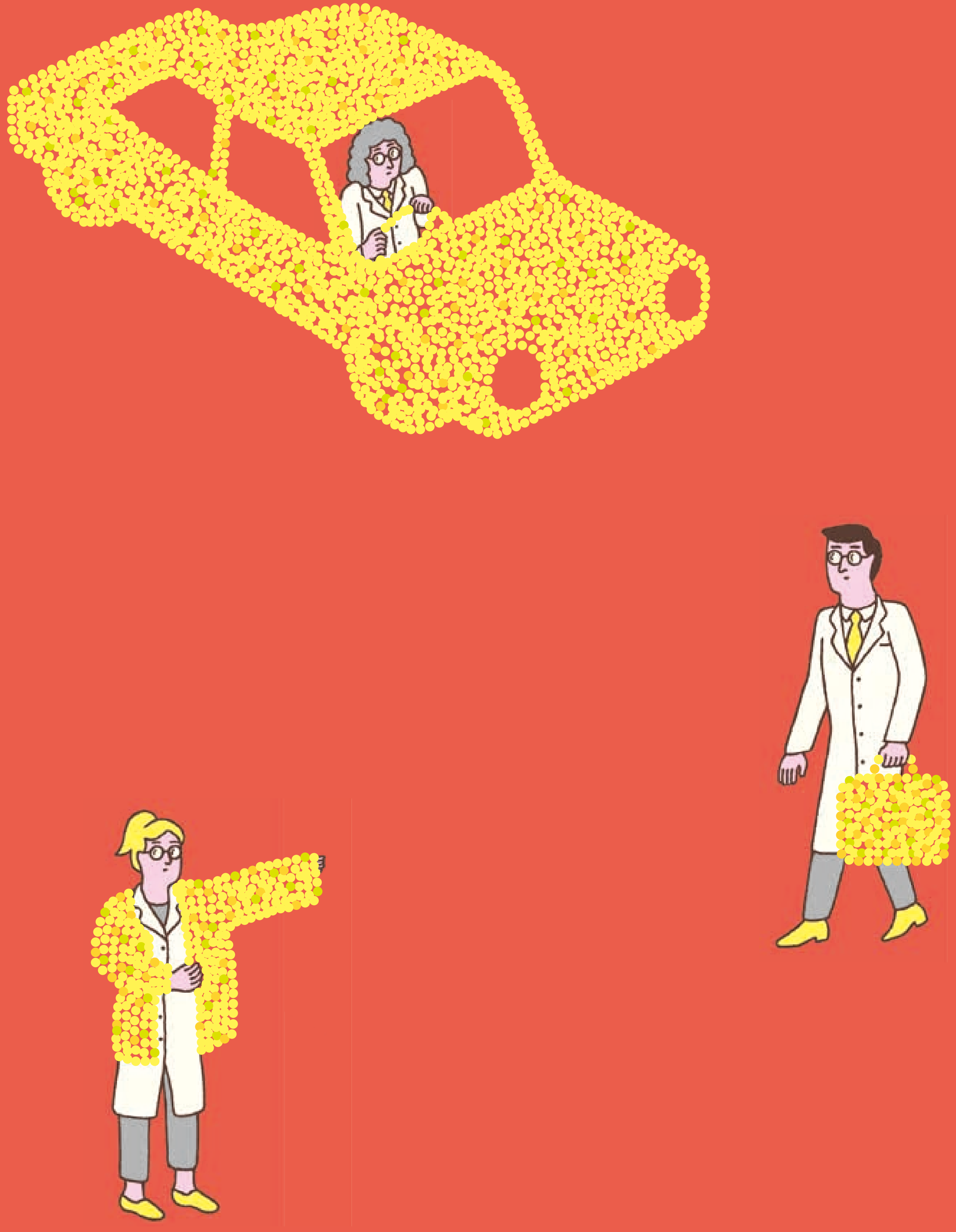
Exploiting “defects” for materials science



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