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Quantum materials: key to unlocking the cryptic quantum world

Quantum materials: key to unlocking the cryptic quantum world

Quantum technologies are expected to become a reality in the near future, including unbreakable quantum cryptographic communications and quantum computers capable of performing a vast number of calculations instantaneously.

Unlike conventional technologies, these new technologies take advantage of seemingly strange quantum mechanical phenomena and states.

However, these phenomena and states are possible only under perfectly controlled physical conditions and disappear in the blink of an eye unless various disturbances are kept under control.

Advances in quantum materials are critical to making quantum technology a reality. What’s the current status of quantum materials research?

Taichi Terashima
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Xiao Hu
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International Center for Materials
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Researchers' discussion

NIMS' storehouse of expertise gives it the lead in quantum materials development

Interest has been growing in quantum technologies in recent years.
NIMS was assigned to carry out quantum materials R&D in line with the quantum technology innovation strategies laid out by the Japanese government.
More than 40 researchers are engaged in this project. We asked their three leaders about their views on quantum materials and expectations for the project.

Materials vital to the development of quantum technologies

—Why has interest in quantum technologies been growing?

Taniguchi: I think people see quantum technologies (e.g., quantum communications, quantum information processing and quantum sensing) as something that could enrich human life and make society safer. Google announced in 2019 that a quantum processor it developed had surpassed conventional computers in computational power. This news probably convinced the public that quantum computers had become a real possibility. According to other media reports, the use of quantum computers may dramatically expedite the process of identifying promising drug candidates for diseases.

Hu: Performances of many current technologies, including computers, have nearly reached their limit. This is one reason for the growing expectations for quantum technologies. Another reason is that many of the scientific and technical tools needed to develop quantum technologies have become available in recent years. These include new theories on condensed matter physics and rapidly evolving nano-processing, measurement and evaluation techniques.

Terashima: Conventional electronic technologies were developed based on the understanding that electrons are particles with electrical charges or particles capable of generating magnetic fields. However, as Dr. Hu just mentioned, many recent technological demands cannot be satisfied using traditional methods. I believe this issue has motivated some materials scientists to actively exploit the quantum mechanical properties of various systems.

Hu: As a matter of fact, quantum mechanics has already been incorporated into technology used in these days. For example, the band theory based on quantum mechanics has been used to determine energy band structures for electrons in solids and its application has significantly advanced semiconductor technologies. However, the latest quantum technology developments involve not only controlling electron energy but also controlling the wave functions of electrons and light. I agree with Dr. Terashima that the application of quantum mechanics to materials research is accelerating.

—Considering the increasing interest in quantum technologies, what is the essential quality of quantum materials?

Hu: Japan's quantum technology innovation strategies define quantum material as "phenomena and materials with advanced functions derived by precisely controlling the quantum states". I like this definition. Because many such materials have been engineered in a variety of ways and sometimes people combine two or more different materials, quantum material does not necessarily mean a material with single component.

Terashima: For me, topological materials (see the boxed text on p.8) and superconductors typify quantum materials. Electrons within these materials behave completely differently from classical electrons—particles with electrical charges which flow when voltage is applied.

Taniguchi: I view quantum materials as components of a broader system. An actual quantum technology is composed not only of a quantum-state-generating core material but also various other parts, including an underlying substrate layer and peripheral electronic circuits that control quantum states. I think these systems as a whole can be called quantum materials.

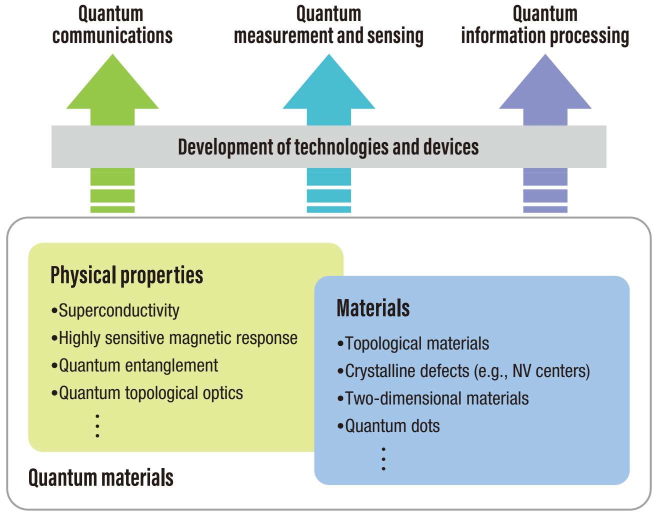
A succession of emergent quantum materials

—Which materials capable of exhibiting quantum states are you most interested in?

Taniguchi: I've been involved synthesis study of diamond with luminscent crystalline defects for the purpose of developing a magnetic sensor (see p.10). This project has made significant progress and this sensor—which uses light to detect distant magnetic field changes at room temperature—may be put into practical use in the near future. The sensor may be used to develop transportable, easy-to-use magnetic resonance imaging (MRI) scanners. I'm also interested in discovering materials other than diamond with luminescent crystalline defects.

In addition, I'm captivated by two-dimensional materials, especially graphene. Research on graphene has progressed rapidly in recent years and three researchers who studied graphene received this year's NIMS Award (see p.7).

Hu: Professor Allan MacDonald, one of the NIMS Award winners this year, theoretically predicted in 2011 that the "twisted bilayer graphene" (two graphenes, the atomic sheets of carbon atoms arranged in honeycomb pattern, stacked with a tiny angle twist) would have very unique wave functions. Professor Pablo Jarillo-Herrero, another NIMS Award winner, then succeeded in realizing the material in 2018 and found that it exhibits superconductivity. This discovery surprised many scientists. Subsequent researches have revealed that twisted bilayer graphene also exhibits magnetic and topological properties. These discoveries were made possible by the high-purity boron nitride substrates developed by Director Taniguchi's team. While to achieve practical application might take time, its unique features, such as simple structure, free of defects, and moreover, being able to tune property merely by changing the twist angle, make the twisted bilayer graphene very important in understanding the controlling quantum states.



Quantum technology innovation and quantum materials
List of quantum properties and materials potentially applicable to the development of quantum technologies described in Japan's quantum technology innovation strategies

What is a quantum?

Although physical quantities (e.g., energy) apparently look continuous, actually there are smallest units for them (thus they can only take discrete values). This smallest unit is called "quantum". The theory that describes physical properties and behaviors of electrons and light based on the concept of quantum is called "quantum mechanics". In quantum mechanics, electrons are considered both particles and waves, and their physical properties and behaviors are explained in terms of their wave functions (mathematical equations describing how such waves travel). Similarly, light can be considered as both particle (photon) and wave of electromagnetic radiation. Quantum technologies are intended to exploit unique phenomena and states of materials that are described by quantum mechanics.

──What are the accomplishments of Professor Tsuneya Ando, another 2021 NIMS Award winner?

Hu: Professor Ando is a prominent theoretician of condensed matter physics, who clarified properties of graphene and carbon nanotubes from quantum mechanics. He theoretically indicated the existence of the quantum Hall effect several years before it was experimentally discovered in 1980. Actually, quantum Hall effect is the phenomenon which led to the development of the concept of topology of matter (see p. 8).

Terashima: Topological materials are very intriguing. There were previously only two types of materials: electrically conductive or not. However, some non-conductive materials (i.e., insulators) were found to be topological while others were not. I found this new theory on topological materials—which was derived from a paradigm shift in solid state physics—to be a very interesting research subject.

NIMS' three strengths: synthesis, characterization and theorization

──What are the objectives of the NIMS quantum materials project?

Taniguchi: We didn't set simple, short-term goals, such as developing the last piece of elemental technology needed to put a nearly completed quantum technology into practical use. Quantum materials R&D requires serious and persistent effort. Our general goal is to advance basic materials research, thereby promoting the discovery of new materials in the future and improving the performance and quality of selected materials.

As I said earlier, the definition of quantum materials can be broad and diverse. The participants in this project are carrying out research on a variety of topics, including topological materials, quantum communications and extraction of light. In addition to my responsibility to oversee individual research projects, I am researching techniques to synthesize diamonds and boron nitride. Through these activities, I reaffirmed NIMS' many strengths in quantum materials research.

First, NIMS has a long history of developing material synthesis techniques dating back to the time of its two predecessor organizations and is equipped with large synthesis equipment. NIMS also has researchers skilled in evaluating synthesized materials using advanced measurement equipment. Because the performance of quantum materials is influenced even by subtle changes in the amounts of impurities within crystals, it is very convenient that NIMS has all the resources we need: we can synthesize materials here, they can be evaluated immediately after synthesis by experts and we can engage in immediate in-depth discussion on the evaluation results. Moreover, NIMS has theoretical scientists who can advise us about the directions and focuses for our projects, such as a project intended to identify materials with superior performance to diamonds.

Terashima: I also appreciate the resources NIMS can offer. Our team is attempting to detect intangible particles that were theoretically predicted to exist by using a structure composed of a combination of a topological material and a superconductor (see p. 9). We often ask for advice and help from researchers with expertise in sample preparation and various measurement techniques and know-how on a wide range of topics beyond our project.

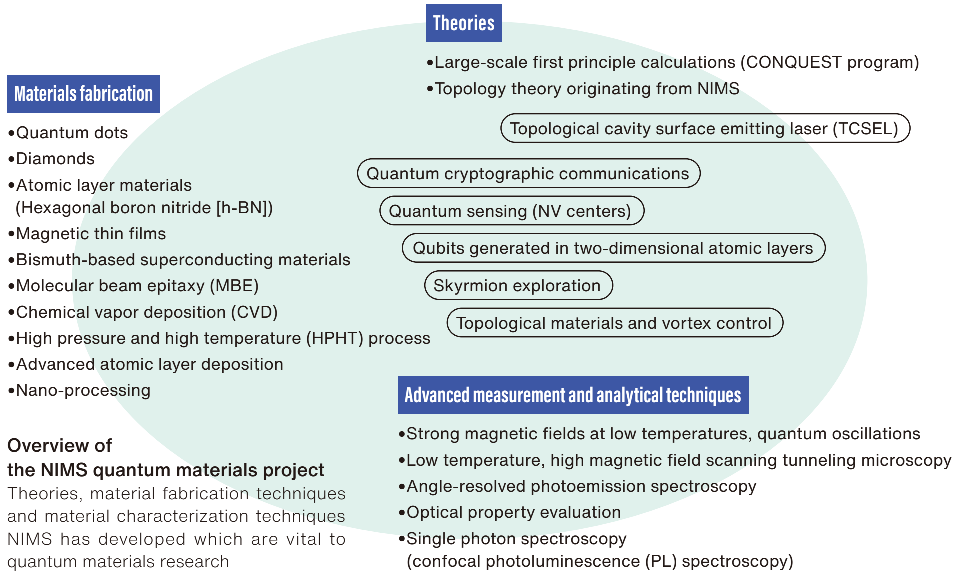
Hu: In this project, our team is exploring the new field of quantum topological optics and developing an advanced laser called topological cavity surface emission laser (TCSEL) (see p. 8). As a theorist, I hope to identify universal principles behind various phenomena and propose principles for materials development.

──Lastly, please share your expectations for this project.

Taniguchi: There is currently a lot of confusion about what quantum technologies really are. I envisage that as the project progresses, individual quantum materials researchers and developers will find their own answers, and the collection of these answers will eventually form the quantum technology concepts. Although our project may only have a small impact on the global quantum physics community, it may potentially have a big impact on materials science if we are able to produce materials for utterly amazing quantum technologies. Achieving this feat and developing it into a scientific concept would be a really joyous experience.

(By Seiko Aoyama)

Types of NIMS' basic materials research potentially leading to quantum technology innovation



Overview of the NIMS quantum materials project
Theories, material fabrication techniques and material characterization techniques NIMS has developed which are vital to quantum materials research

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NIMS AWARD
National Institute for Materials Science

Winners' Comments

NIMS has given the NIMS Award to a distinguished person or a group who had made significant progress in Materials Science. The NIMS Award 2021 was given to three distinguished scientists who have achieved outstanding results in the field of "research on quantum materials."

Prof. Tsuneya Ando
Honorary Professor, Emeritus Professor, Tokyo Institute of Technology/ Emeritus Professor, University of Tokyo

Q.1 What inspired your 2021 NIMS award-winning research on two-dimensional electron systems?

I was inspired to carry out the research by a published article in which the electrical conductivity of silicon surface inversion layers in MOSFETs was measured in strong magnetic fields. To understand the electronic transport in this system, I theoretically calculated the diagonal conductivity and the Hall conductivy of two-dimensional systems subjected to strong magnetic fields. The subsequent experimental discovery of the integer and fractional quantum Hall effects significantly advanced this area of physics. During this research, I noticed that new physical phenomena are realized in semiconductor devices. This experience led me to research various physical properties, including electronic states, transport properties, and optical properties in low-dimensional systems realized in semiconductor devices.

Q.2 What inspired you to research graphene?

In the extreme relativistic limit, electrons travel at the speed of light. The motion of electrons in graphene is formally the same as that of such relativistic particles. Carbon nanotubes can be regarded as cylinders with these electrons confined on their surfaces. I became fascinated by the potentially unique physical properties these systems may have and began researching newly discovered nanotubes, and then graphene, which had yet to come into physical existence at the time. Graphene was later successfully realized experimentally and this success has significantly advanced the graphene research. Although I formally retired from my university position a few years ago, I've continued my theoretical research on graphene and related materials, in particular, on galvanomagnetic effects in these systems.

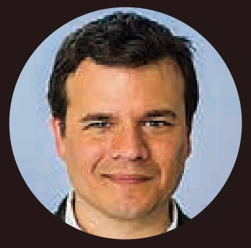
Prof. Allan H. MacDonald
Professor of Physics, University of Texas at Austin

Q.1 What made you work on the research which is awarded the NIMS Award this time?

It was clear from earlier work that electrons in graphene bilayers slowed down when twisted. I understood that the small twist angle limit of this behavior was independent of many microscopic details of the electronic structure, that it was mathematically and numerically complicated, and that it could lead to strong electronic correlations. What happened at small twist angles? - a sharp question with no sharp answer and therefore a warm invitation for theory. With this motivation, my postdoc Rafi Bistritzer and I developed a simple physical picture of the moiré superlattice physics, and used it to discover the magic twist angles. An important secondary goal of this work was to explain why effects related to commensurability between the moiré superlattice and the underlying atomic lattice were unobservable at small twist angles.

Q.2 How would you like to develop the research, which is awarded the NIMS Award, in the future?

Our early work on twisted bilayer graphene made it clear that artificial crystals are associated with moiré patterns formed between any two-dimensional host crystals that are semiconductors or semi-metals, and that each system would be its own artificial universe – a distinct type of moiré material. I would like to help expand the types of artificial crystals that can be engineered using this approach. The physics of magic angle graphene bilayers, for example its superconductivity and its quantum anomalous Hall effect, is unlike that of any bulk crystals because of the prominence of topological effects of crossing bands. On the other hand, as we proposed a few years later, transition metal dichalcogenide moiré materials are quite similar to common strongly correlated atomic materials that are approximated by Hubbard models. These are the two examples that are developed at present. I believe that we are still at the beginning of discovering what types of electronic and optical properties can be created by forming moiré materials.



Prof. Pablo Jarillo-Herrero
Cecil and Ida Green Professor of Physics, Massachusetts Institute of Technology

Q.1 What made you work on the research which is awarded the NIMS Award this time?

The motivation to work on twisted bilayer graphene was that the angle between two crystalline lattices was a new "knob" in physics and materials science, something that could not be changed before in the history of materials science. Therefore, I was convinced that playing with this new knob would bring interesting surprises and discoveries. Quantum materials are sufficiently complex that when one takes risks and explores unchartered territory… new things are bound to happen.

Q.2 How would you like to develop the research, which is awarded the NIMS Award, in the future?

I would like to continue exploring more exotic systems based on moiré heterostructures. I believe these systems bring together two of the most intriguing themes of modern physics: strong correlations among electrons and the topology of electronic bands. I hope that we will be able to ascertain what are the key essential ingredients for the emergence of complex quantum behavior. With a bit of luck, this fundamental knowledge will also be translated later on by my engineering colleagues into new quantum technologies.

Research 1

Exploiting photonic topology to develop a laser beam that exerts torque

Xiao Hu

Most quantum technologies derived from the topology of matter exploit electron quantum states. However, Xiao Hu found optics to be more interesting, since currently electron quantum states require ultralow temperatures or strong magnetic fields, whereas optics make it possible to create devices that function at room temperature without a magnetic field. As an example, Hu is working to develop a high-performance laser as part of the NIMS quantum materials project.

Electrons travel freely around the perimeter of a sample of a two-dimensional topological insulator (see the boxed text below), while the interior of the sample continues to act as an insulator. Hu was interested in reproducing this electronic phenomenon with light. However, electron spin plays an important role in topological insulators, and light does not exhibit spin. To address this issue, Hu studied ways of inducing an analog to electron spin in photons. In 2015, he found that an assembly of dielectric cylinders arranged in a honeycomb pattern can be used to achieve this goal.

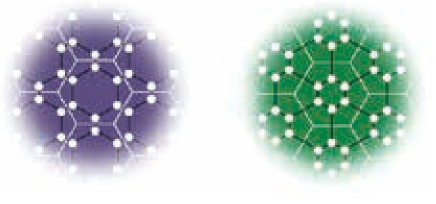
The effect that Hu was focusing on happens at shorter wavelengths when the composite structures are smaller in size. Achieving this with visible light requires a precise array of dielectric cylinders several tens of nanometers in diameter and several micrometers in height. However, fabricating such structures is extremely difficult. Hu therefore decided to first verify his theory using a much larger structure composed of dielectric cylinders several millimeters in diameter and microwaves, which have much longer wavelengths than visible light. Experiments demonstrated that microwaves traveled around the perimeter of the sample, as predicted by Hu's theory. This success set the stage for him to conduct similar experiments with light of shorter wavelengths by fabricating smaller structures on thin semiconductor film. He named this structure a topological photonic crystal.

Hu then tried to develop a high-performance laser using the topological photonic crystals. First, he carried out theoretical calculations and found that a slight modification to the honeycomb pattern would suppress the topological property. He then clarified that wrapping the topological photonic crystal in the modified crystal would induce laser radiation. These photonic crystals were successfully fabricated by overseas collaborators using nano fabrication technology, and the emission of laser radiation was successfully confirmed in 2019.

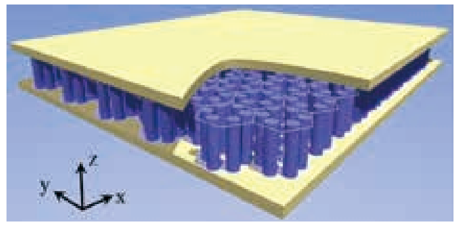
This laser radiation had a wavelength of 1.55 micrometers (near-infrared band). In the quantum materials project, Hu's group is aiming to develop a laser that emits visible light (e.g., green and blue light) at shorter wavelengths. "Laser light emitted from topological photonic crystals exerts torque, which is useful for manipulating very small objects, such as DNA," Hu said. "It is vital to make the wavelength shorter for this purpose."

Making a shorter wavelength laser will require further refinement of the structures of the semiconductor photonic crystals. In addition, a technique needs to be developed to selectively induce laser radiation that can exert clockwise or counter-clockwise torque. Hu is tackling these challenges in collaboration with experimental specialists on his team.

(By Seiko Aoyama)



Schematic cross-sections of the two types of crystals used to generate laser radiation
Topological photonic crystal (left) and matching non-topological photonic crystal (right). Wrapping the crystal on the left with the crystal on the right forms an optical resonator required for a laser.



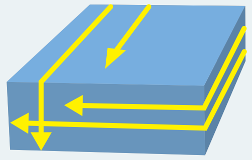
Schematic of the topological photonic crystal
Dielectric cylinders are arranged in a honeycomb pattern. Light rotates around the outer perimeter of the two-dimensional crystal.

What are topological materials?

Topology is a branch of mathematics that classifies objects based on properties invariant upon continuous deformation of their shapes. For example, a donut and a coffee cup, both of which have a single hole, would fall into the same category, whereas a ball would be classified differently because it has no hole.

Since the 1980s, topology has been used to categorize materials' electronic states in terms of the shapes of the wave functions they exhibit, and it has been found both theoretically and experimentally that materials can be classified in ways different from previous ones. As a result, the concept of the topological insulator was proposed in 2005. Conventional insulators and topological insulators are classified differently. When the surface of a topological insulator is brought into contact with a conventional insulator, it becomes electrically conductive with quantum features. Subsequent experiments conducted in both air and a vacuum—both conventional insulators—confirmed the existence of materials in which quantized electrical current can flow only on their surfaces, supporting the concept.

Like topological insulators, the existence of topological superconductors has been predicted theoretically, driving active research to develop them for use in quantum computing. Materials like topological insulators and topological superconductors that exhibit unique properties due to their unconventional topology are called topological materials.



Topological insulator
Conventional insulators do not conduct electricity internally and on their surfaces, while metals (i.e., electrical conductors) do. By contrast, topological insulators allow electricity to flow on their surfaces but not internally.

Research 2

Detecting intangible Majorana particles: a potential major player in quantum technologies

Taichi Terashima

A Majorana fermion is a peculiar elemental particle which is both a particle and its own antiparticle. This particle, which was first predicted to exist in 1937, is believed to exist based on circumstantial evidence. Because Majorana particles are thought to emerge in topological superconductors and to be a potentially promising quantum computer component, global competition is underway to discover them. Taichi Terashima and his colleagues—members of the NIMS quantum materials project—are contenders in this race.

Among the various Majorana particle detection methods that have been proposed, Terashima's group uses a two-layered structure in which a thin topological insulator film is placed on the surface of a superconductor. This structure can be used to induce superconductivity on the surface of the insulator. The subsequent application of a magnetic field to the superconductive surface generates superconducting vortices. Theories predict that Majorana particles appear within these vortices.

While this method has been widely adopted, there are many possible combinations of topological insulators and superconductors: more than 10 different types of topological insulators have been discovered and many different superconductors exist. Terashima's group uses not only the well-recognized Bi2Se3 topological insulators but also other less common insulators, including lead (Pb) compounds. The group also uses several different types of iron-based superconductors. In principle, they synthesize all of their two-layered structural samples themselves.

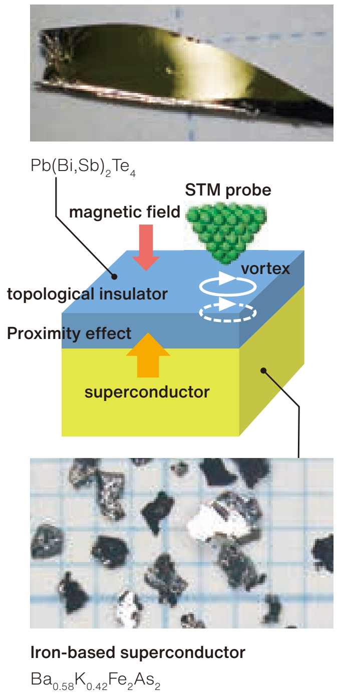
What is NIMS' competitive advantage in the global race to detect Majorana particles? "We have a group of experts capable of performing various types of electronic state measurements," Terashima said. "That's our biggest strength."

A fundamental requirement for making Majorana particles appear is ensuring that topological insulators fully exhibit their unique physical properties. "Slight compositional deviations sometimes cause there to be too few or too many electrons within a topological insulator," Terashima said. "To prevent this, we need to carefully synthesize them and inspect their electronic states before using them."

The electronic state measurement techniques Terashima's group uses are not only useful for inspecting the quality of topological insulators; they are also potentially effective in detecting Majorana particles. These techniques include the use of a scanning tunneling microscope (STM), a powerful tool potentially capable of directly detecting Majorana particles from vortices. In addition, Terashima uses quantum oscillation measurements—his specialty—to determine the precise range of energy levels electrons may occupy within a material. The group is also skillful in determining the relationship between electronic energy and momentum using an angle-resolved photoemission spectroscope (ARPES).

Terashima's group is currently working to identify optimum insulator-superconductor structures for detecting Majorana particles. The group hopes to observe these particles in the near future using a combination of the three measurement techniques.

(By Seiko Aoyama)



Majorana particle detection method
This two-layered structure (middle) in which a topological insulator is placed on the surface of a superconductor can be used to induce superconductivity on the surface of the insulator. The subsequent application of a magnetic field to the superconductive surface generates vortices. Theories predict that Majorana particles exist within these vortices. Terashima's group hopes to detect Majorana particles by optimizing this structure. Examples of insulating and superconducting materials tested are shown on the top and bottom photos.

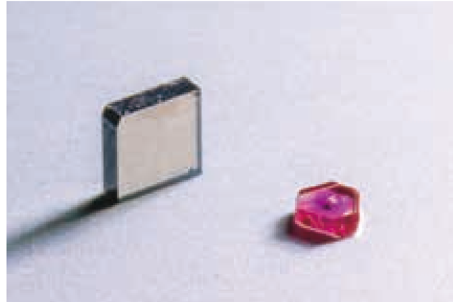
High-performance diamonds for quantum sensors by unique growth technology

Diamond jewelry has long fascinated people the world over. Known as the hardest material on Earth, diamond has also been widely used for industrial purposes and has been researched and developed as a novel semiconductor material. Recently, diamond was found to be a potentially promising quantum material for high-performance sensors. To be effective as a sensor material, diamond needs to meet a number of performance criteria. Tokuyuki Teraji and his team have been working to grow precisely designed diamonds for this purpose through the NIMS quantum materials project.

Quantum material usable at room temperature

According to high school chemistry textbooks, diamonds are crystals solely composed of carbon atoms. However, in reality, diamonds often incorporate a small amount of nitrogen atoms from the surrounding air which replace carbon atoms in the crystalline lattice. In addition, some carbon atoms are missing from lattice sites, forming vacancy defects. When a substitutional nitrogen atom is adjacent to a vacancy defect, a nitrogen-vacancy (NV) center may form.

Basic research on NV centers, which began around 2000, has revealed that NV centers have electron spin that can store quantum states. Their quantum spins are highly sensitive and responsive to slight changes in environmental conditions, such as magnetic fields, temperature and pressure. Changes in NV centers' quantum states have been found to correlate with changes in the intensity of the red fluorescence they emit when irradiated with green laser light (see the front cover). These findings indicate that NV centers with quantum properties can be used as highly sensitive environmental change sensors. In addition, the quantum states of NV centers can be preserved at ambient temperatures and do not require the very low temperatures many other quantum materials need because the quantum states are protected by a strong diamond crystal.



Two diamond crystals containing NV centers

The crystal on the left was grown using the CVD process, while the one on the right was grown using the HPHT process and then irradiated with electron beams.

Further research has revealed that the quantum states of NV centers can be well controlled. This discovery triggered rapid intensification of research around 2010 with the goal of artificially creating NV centers for use in various types of sensors. The use of NV centers as magnetic sensors is especially appealing. They may be used to develop nuclear magnetic resonance (NMR) systems with ultrahigh spatial resolution capable of analyzing individual molecules and compact magnetocardiography and magnetoencephalography devices capable of taking various magnetic measurements, including magnetic field direction. Teraji's team aims to develop diamonds for these purposes.

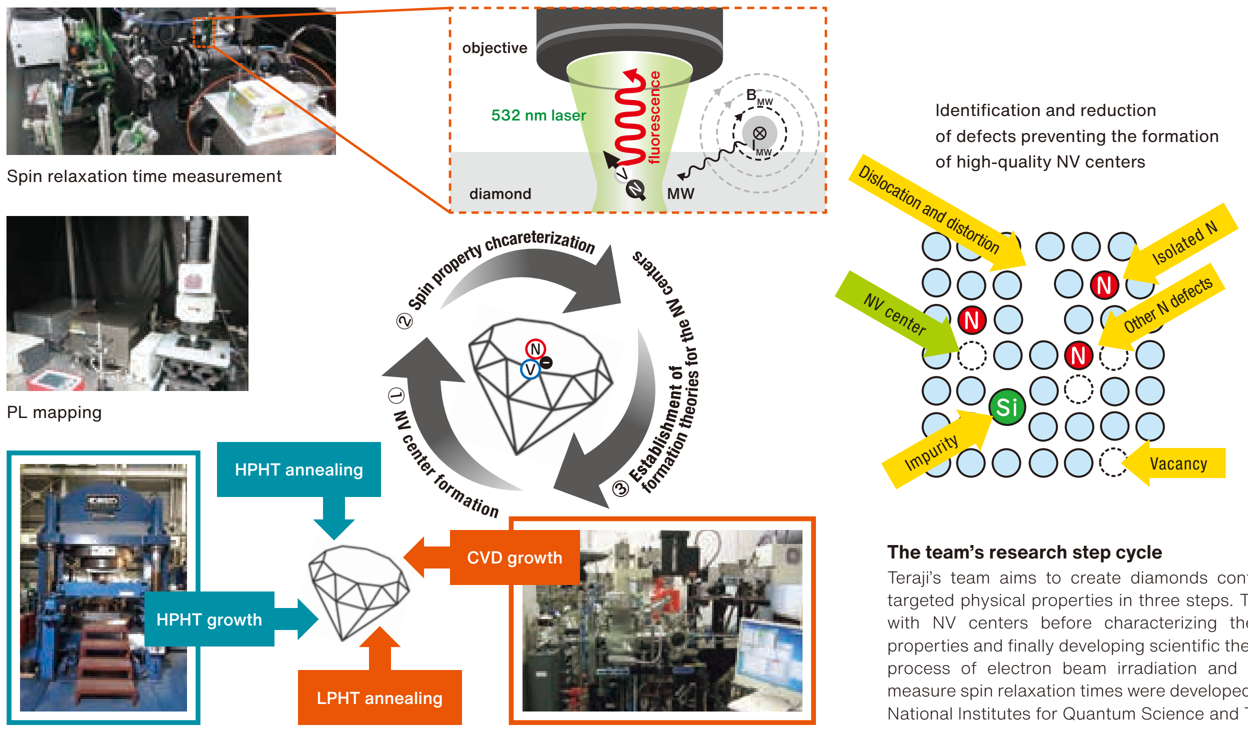
Repeated diamond growth and crystal characterization for feedback

"In order to make a good sensor using the NV center, their concentration and distribution within a diamond need to be optimized for each specific sensing target and they need to have long spin relaxation times (i.e., the time periods during which a quantum state can be preserved)," Teraji said. "Meeting these criteria will require the growth of high-purity, high-quality diamond crystals and doping techniques capable of precisely controlling the nitrogen content of diamonds."

There are two representative ways to grow diamond crystals: one is the HPHT (high pressure and high temperature) process, in which carbon is melted in a metallic solvent and allowed to precipitate and crystallize under HPHT conditions, and the other is the chemical vapor deposition (CVD) process, in which diamond crystals are grown layer by layer on a substrate within a chamber containing methane gas which decomposes and undergoes chemical reactions. At NIMS, Takashi Taniguchi (see p.4) is highly skilled with the HPHT process, while Teraji succeeded in growing a diamond of the highest purity in the world in 2015 using the CVD process.

Teraji's team adds nitrogen when growing diamond crystals using either method to create nitrogen defects and then irradiates fully grown diamonds with electron beams to create vacancy defects, resulting in the formation of NV centers. "Diamonds grown using the HPHT and CVD processes differ not only in shape and size but also in their nitrogen defect configuration in each crystal," Teraji said. "Our strength is the ability to create NV centers with several different feature by purposely combining the different characteristics of these two methods."

After synthesizing diamonds with NV centers, the next step is to assess their physical properties. The team measures the concentration and distribution of NV centers using photoluminescence (PL) mapping and measures their spin relaxation times by applying microwave radiation to diamond specimens while they are fluorescing. Based on the results of these assessments, the team readjusts the diamond growth conditions, including the amount of nitrogen added and the intensity of the electron beams applied, in an effort to bring the physical properties of the NV center closer to the target value.



The team's research step cycle

Teraji's team aims to create diamonds containing NV centers with targeted physical properties in three steps. They first grow diamonds with NV centers before characterizing the NV centers' physical properties and finally developing scientific theories and principles. The process of electron beam irradiation and the equipment used to measure spin relaxation times were developed in collaboration with the National Institutes for Quantum Science and Technology.

The challenge of optimizing performance

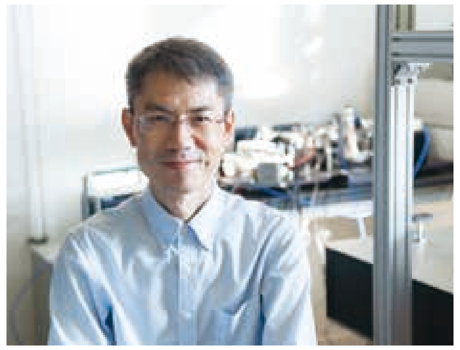
The development of highly sensitive, high-performance magnetic sensors poses many challenges. Increasing the sensitivity of a magnetic sensor will require increasing the number of NV centers. However, the processes used to create NV centers will also create various forms of nitrogen defects (e.g., various combinations of N and V, such as NVN and VNNN) which do not contribute to increasing diamonds' sensitivity to magnetic fields. Methods of creating NV centers selectively and densely have yet to be developed. In addition, while a larger number of NV centers can be created by increasing the nitrogen concentration, this approach will undesirably shorten the NV centers' spin relaxation times. The creation of NV centers with long spin relaxation times is critical for the development not only of magnetic sensors but also many other quantum devices.

Moreover, magnetic sensors used for different purposes require NV centers with different characteristics. For example, magnetocardiography and magnetoencephalography devices need to be able to sense changes in the intensities of subtle, distant magnetic fields and therefore require diamonds with high concentrations of uniformly distributed NV centers with spin relaxation times of at least 10 microseconds. By contrast, ultrahigh spatial resolution NMRs require diamonds with low concentrations of NV centers located near their outer crystalline surfaces (within a depth of approximately 100 nanometers) with spin relaxation times of approximately 100 microseconds. However, NV centers near the crystalline surfaces generally have shorter spin relaxation times, making it difficult to satisfy both conditions. The team needs to find ways to increase the spin relaxation times of NV centers near the surface.

"The level of specifications required for quantum diamonds is even higher than that for semiconductor diamonds," Teraji said. His team includes theoretical and computational researchers working to establish theoretically grounded diamond growth and crystal engineering methods and examining measurements taken from the grown diamonds.

"By sharing our researcher's talents and working together closely, we should be able to create diamond NV centers capable of satisfying the requirements for magnetic sensors and other quantum devices," Teraji said. We may even discover next-generation NV centers superior in performance to diamond NV centers." Teraji's team continues to challenge in quantum material research, including the search for new color centers beyond the NV center in diamonds.

(By Kaori Oishi)



Tokuyuki Teraji
Chief Researcher,
Wide Bandgap Semiconductors Group
Research Center for Functional Materials

Research 4

Developing next-generation tap-proof quantum communications using NIMS’ original quantum dots

Quantum communications technologies may potentially enable tap-proof communications for use in networking quantum computers in the future. NIMS has been researching and developing original quantum dot photon sources vital to quantum communications. This R&D is accelerating under the framework of the NIMS quantum materials project.

Quantum dots as single photon sources for quantum communications

Quantum communications R&D is underway globally to develop safe, secure, anti-eavesdropping communications technologies. Quantum communications, a type of optical communications technology, exploit photons in quantum states as information carriers. While current optical and quantum communications both employ optical fibers, they differ significantly in the number of photons involved. Existing optical communications, in which pulsed lasers are used to transmit information, require as many as 100,000 to 1 million photons to transmit one bit of information. Due to the huge number of photons involved, photon eavesdropping is difficult to detect. By contrast, quantum communications use only a single photon to convey one bit of information. This characteristic enables prompt detection of photon eavesdropping, making the communications highly secure.

Putting quantum communications into practice will require overcoming some major hurdles. First, a photon source capable of emitting individual photons on demand needs to be developed. Quantum communications experiments currently use pseudo single photon sources: lasers that emit pulsed light passed through an attenuation filter to greatly reduce the number of photons in each pulse. A research team led by Takashi Kuroda has been researching and developing a true single photon source using quantum dots and also quantum entangled photon sources.

Entangled photon emitting quantum dots: a key technology to developing long-distance quantum communications

A quantum dot is a minute crystalline structure of semiconductor materials with sides approximately 10 nanometers in length. A quantum dot containing one electron-hole pair can generate one photon. This structure may potentially be used as a single photon source.

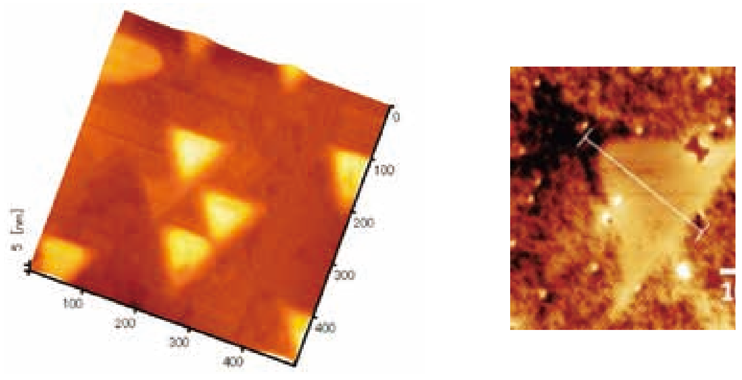
In addition to this amazing property, quantum dots may also be used as quantum entangled photon sources. The transmission distance of photons through optical fibers is currently limited to dozens of kilometers due to their fragile quantum states. A way to extend transmission distance has been devised which involves the use of entangled photon pairs as information carriers and relays capable of restoring collapsed quantum states. Developing an entangled photon source is the key to bringing this concept into reality.

How can quantum dots generate entangled photon pairs? “A quantum dot containing two electron-hole pairs can generate two photons almost simultaneously,” Kuroda said. “Theoretical studies have revealed that when a quantum dot is sufficiently symmetrical, the pair of photons it generates is entangled.” Researchers in different countries have been attempting to synthesize highly symmetrical quantum dots without success.

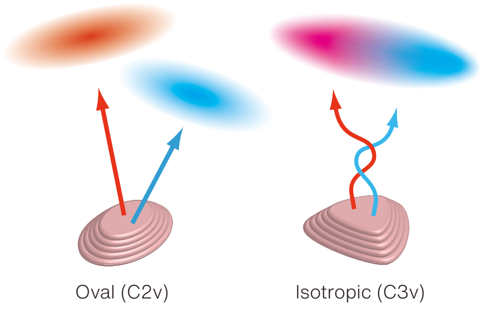
In 2013, Takaaki Mano (NIMS Epitaxial Nanostructures Group) succeeded in synthesizing highly symmetrical quantum dots using a droplet epitaxy technique NIMS developed. These quantum dots were able to generate entangled photon pairs of the world’s highest quality, attracting a great deal of attention.

Kuroda’s team has since been researching and developing ways to optimize quantum dots for use in quantum communications. The team’s main focus has been extending the wavelengths of photons emitted by quantum dots from the original 0.7 micrometers (in the visible spectrum) to 1.55 micrometers (in the infrared spectrum). The reason for this is that photons at a wavelength of 1.55 micrometers have the highest transmission efficiency through optical fibers for long-distance communications.

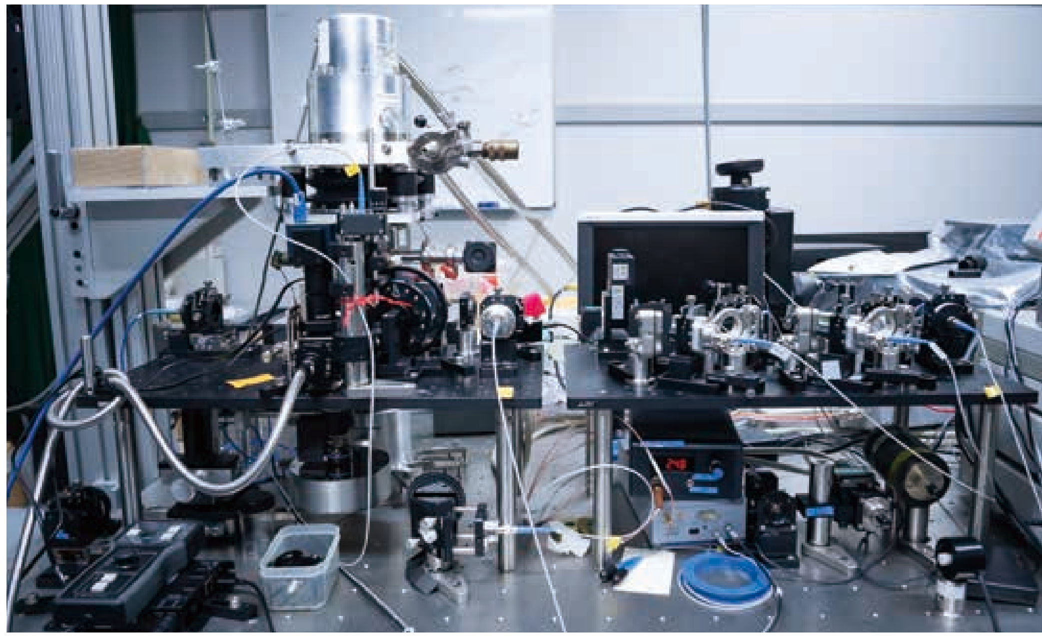
“To extend wavelengths, we switched quantum dot materials from gallium arsenide (GaAs) to indium arsenide (InAs),” Kudoda said. “In fact, we’ve already succeeded in fabricating InAs quantum dots capable of generating single photons at 1.55 micrometers. However, these quantum dots had a lower degree of symmetry than GaAs quantum dots, requiring us to improve their symmetry by optimizing crystal growth conditions. We are currently working on this through trial and error. Concurrent with this project, we are developing a system used to measure the degree of quantum entanglement in the infrared wavelength region.”



GaAs quantum dots (left) and a cross-section of one of them (right)
These GaAs quantum dots were synthesized using a droplet epitaxy technique. Nanometer-sized hemispherical Ga droplets were first formed on the surface of a GaAs substrate, which were then crystalized by adding As. This technique can be used to synthesize high-performance quantum dots made of a variety of semiconductor materials. A large-scale project to synthesize quantum dots using this technique is ongoing in the European Union.



Schematic showing classical (left) and quantum entangled (right) photon pairs
A more highly symmetrical quantum dot can generate a more thoroughly entangled photon pair. The triangular quantum dot (right) has a higher degree of symmetry than the oval quantum dot (left), causing the former to induce a more thorough quantum entanglement. When a pair of photons is entangled, the quantum state of one photon (measured by the orientation of polarized light) determines the quantum state of the other. This relationship may be leveraged to develop long-distance quantum communications with relays capable of restoring the collapsed quantum states of photons.



System used to measure infrared quantum entangled photon pairs.
This system measures the quantum properties of quantum-dot-emitted photons traveling through optical fibers.

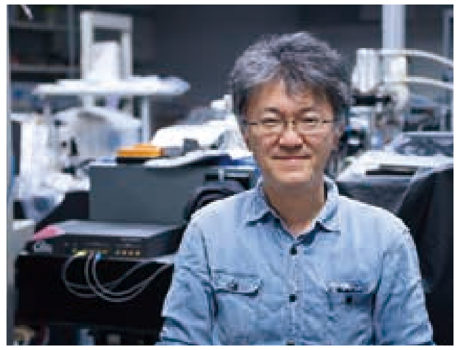
Improving energy efficiency and portability by achieving higher operational temperatures

Kuroda’s team is also working to increase operational temperature for quantum dots. This is challenging because higher temperatures cause the electrons confined within a quantum dot to escape from it. An extremely low temperature of around 10 Kelvin (-263.15°C) is currently needed to keep the electrons confined. Creating this cryogenic condition requires the use of a large liquid helium cooling system, which has significant negative environmental impacts. Kuroda’s team is developing quantum dots capable of confining electrons at 80 Kelvin (-193.15°C). This temperature can be achieved using a liquid nitrogen cooling system. Unlike a helium cooling system, a nitrogen cooling system can be miniaturized to a transferable size and may therefore be applicable to the development of highly secure mobile communications via quantum Wi-Fi instead of optical cables.

“Developing high-temperature quantum dots will require widening the energy barrier—known as the bandgap—between the quantum dot and the substrate,” Kuroda said. “A wider bandgap will prevent electrons from crossing it, making it more difficult for them to escape from the quantum dot. However, a wider bandgap will also increase the difference in the lattice constant between the quantum dot and the substrate, which makes the synthesis of a highly symmetrical quantum dot difficult, creating a dilemma. We are currently investigating the optimum conditions for the synthesis of highly symmetrical quantum dots with high operational temperatures using InAs. Once the optimum conditions are identified, we may be able to simultaneously elongate the wavelengths of photons emitted from a quantum dot and increase its operational temperature.”

Quantum communications are expected to be indispensable for networking quantum computers. Kuroda and his colleagues intend to further intensify their R&D efforts to optimize NIMS’ original quantum dots for use in quantum communications.

(By Kumi Yamada)



Takashi Kuroda
Leader of the Nanophotonics Group
Research Center for Functional Materials

Exploring the quantum properties of hexagonal boron nitride, a little-known two-dimensional material

Quantum technologies can be roughly divided into those driven by electrons and those driven by photons. Development of photon-driven technologies, such as quantum communications, requires a photon source capable of efficiently emitting individual photons (see p. 12). Hexagonal boron nitride (*h*-BN) is a potentially promising single photon source material. Kenji Watanabe is an *h*-BN expert who has many years of experience studying *h*-BN crystals. We asked him about the appeal of this material and the future direction of his research, which is part of the NIMS quantum materials project.

h-BN in everyday life

h-BN is made up of a stack of honeycomb layers composed of boron (B) and nitrogen (N). "Most people probably haven't heard of *h*-BN, but it is used widely in our daily lives," Watanabe said. For example, *h*-BN powder is the main ingredient in lock lubrication sprays and is used in cosmetic foundations to help them spread more smoothly and evenly over the skin. In addition, because *h*-BN is thermally and chemically stable, it is used in laboratory containers designed to withstand high-temperature chemical reactions.

Watanabe grows *h*-BN crystals using chemical vapor deposition (CVD) processes, while Takashi Taniguchi—a long-time colleague of Watanabe at NIMS—grows it using HPHT (high pressure and high temperature) processes. *h*-BN crystals synthesized via either method have higher purity and surface quality than those used in the *h*-BN-containing commercial products mentioned above. HPHT crystals have been used as graphene substrates in many quantum materials research projects worldwide. Watanabe discovered in 2004 that *h*-BN itself may exhibit quantum properties.

Boron nitride is a group III-V semiconductor composed of the group III element boron and the group V element nitrogen. Many of the group III-V semiconductors, including gallium nitride (GaN)—a blue LED material—are known to emit intense light. On the other hand, zinc-blende structure boron nitride—aka cubic boron nitride (*c*-BN)—has attracted the interest of many scientists not because of its light-emitting properties but due to its similarity to diamond as a potentially promising high-performance semiconductor. Pure *c*-BN is difficult to synthesize, however, because it is prone to incorporate impurities during crystal growth.

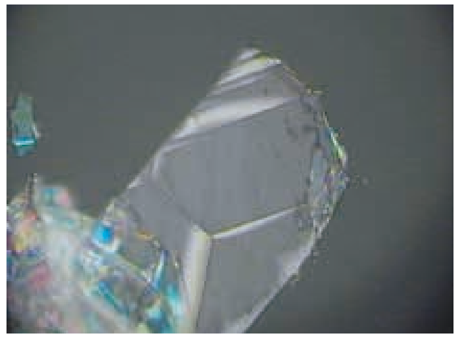
"We needed to create highly pure *c*-BN before we could study its physical properties," Watanabe said. "So we worked to increase its purity. One day we noticed that *h*-BN—a byproduct of *c*-BN synthesis with a different crystalline structure—was highly transparent. We irradiated it with electron beams and found that it was able to emit intense far-ultraviolet radiation at 215 nm." This discovery led to the development of a germicidal UV emission device powered by batteries. Another significant implication of this discovery was that high-purity h-BN crystals may be used as a light-emitting quantum material.

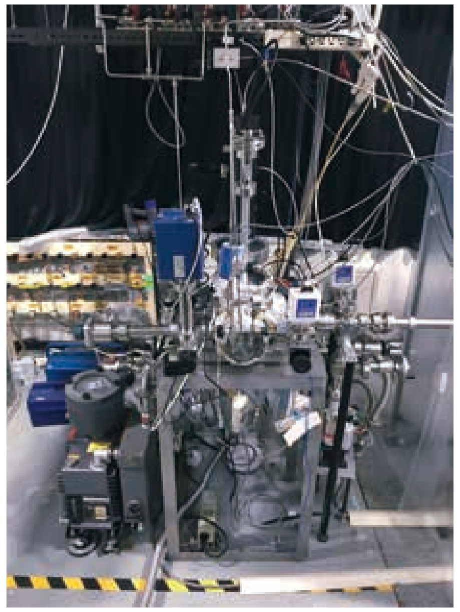
Investigating efficient light emission mechanisms

Development of quantum photonic technologies for communications will require the use of single photon sources. Extensive research efforts are underway to identify effective single photon source materials and single photon emission methods (see also p. 12).

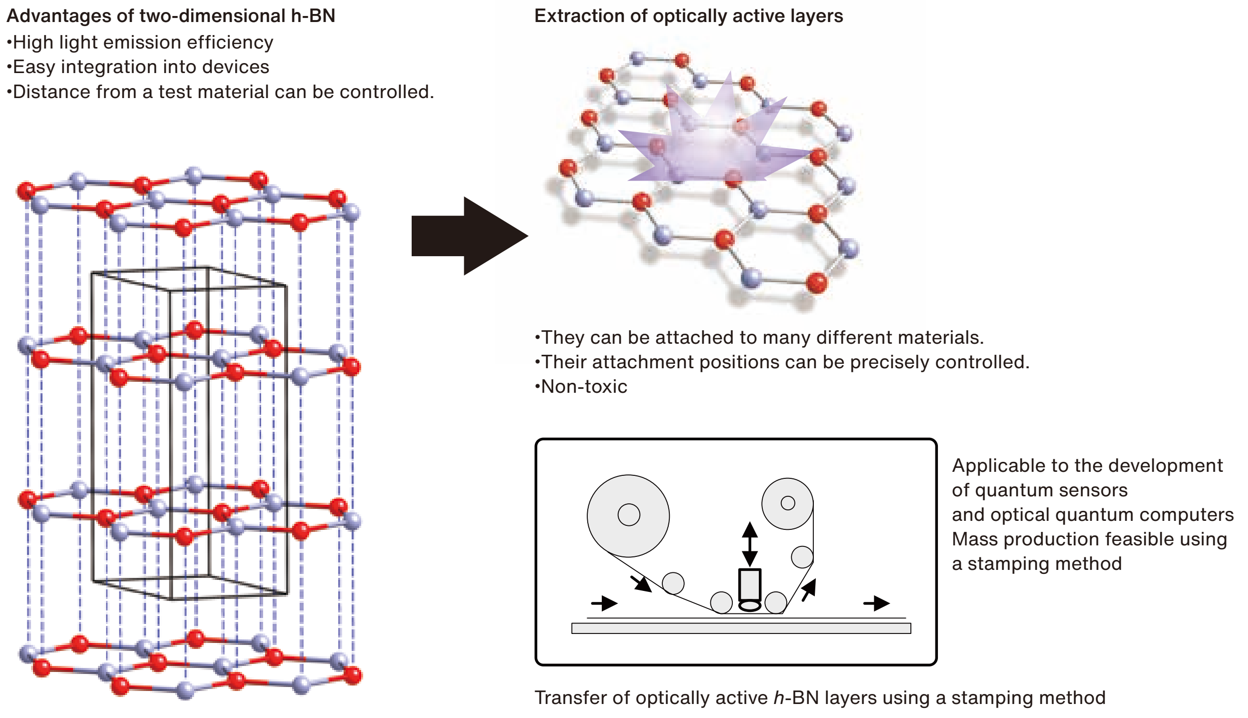
"*h*-BN may be used to develop efficient single photon sources. However, my first and foremost goal is to understand the far-UV emission mechanisms of *h*-BN," Watanabe said. Semiconductors emit light when unpaired excited electrons and vacant holes reunite. This reunion occurs in two ways: direct and indirect transition. Indirect transition recombination involves lattice vibration while direct transition recombination does not, usually causing the former to be less light emission efficient than the latter. Although theories predict—and experiments have demonstrated—that *h*-BN undergoes indirect transition recombination, its light emission efficiency is mysteriously very high.

"Several factors are conceivably contributing to the high electron-hole recombination efficiency in *h*-BN," Watanabe said. "They include the electron confinement effect within two-dimensional B-N layers, the exciton effect by which an excited electron and a hole are attracted to each other by the electrostatic Coulomb force and the fact that easily deformable *h*-BN crystals are prone to be influenced by excited electrons."





(Top) Crystalline thin film of hexagonal boron nitride (*h*-BN).
(Bottom) Chemical vapor deposition (CVD) equipment used to grow the crystal.



Advantages of using *h*-BN as a quantum material
h-BN is made up of stacked layers (left) and they can be peeled off a few layers at a time. *h*-BN-based quantum devices may be mass-produced by extracting layers with light-emitting crystalline defects (i.e., optically active layers) and transferring them onto the surfaces of other materials.

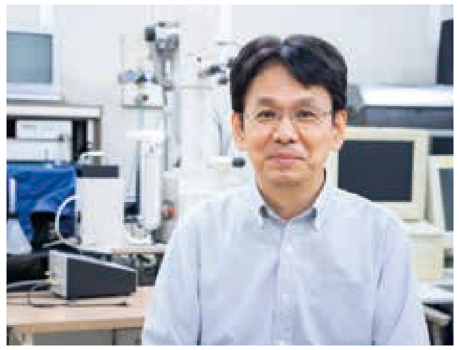
Searching for ways to create light-emitting defects through experiments and by reviewing past data

Although h-BN can emit intense far-UV, this physical property cannot be directly translated into use as a single photon source. Rather, creating light-emitting defects within *h*-BN crystals is a more viable approach. "Defects can be created within *h*-BN crystals by irradiating them with electron beams or adding impurities while growing them," Watanabe said. "Because *h*-BN intrinsically has high luminescence efficiency, its crystalline defects are also likely to emit light efficiently. My plan is to develop single photon sources using these light-emitting defects." Single photon emissions need to be stably repeatable and controllable by such means as magnetic and electrical fields and pressure. In addition, the ideal emission wavelength is approximately 1.55 micrometers because this wavelength is most resistant to absorption by optical fibers. Through experiments, Watanabe plans to determine various requirements for creating desirable light-emitting defects, including the optimum electron beam intensity to apply and the types and amounts of impurities to introduce. Understanding *h*-BN's intrinsic light emission mechanisms first is expected to greatly facilitate efforts to create controllable crystalline defects.

Research on light-emitting defects is more actively carried out in diamonds and other materials. What is the significance of researching them in *h*-BN? "The layers of *h*-BN can be peeled off into two-dimensional materials which then can be easily attached to the surfaces of other materials," Watanabe said. "In addition, *h*-BN-based devices may be mass-produced by extracting layers in which defects were successfully created and attaching them to the surfaces of other materials in a manner similar to stamping documents."

"We're still in an early stage of ascertaining the luminescence properties of crystalline defects," Watanabe said. "However, we have accumulated a large amount of *h*-BN research data over the years since the time of NIMS' predecessor, the National Institute for Research in Inorganic Materials. We will extract defect-related data from the accumulated data and work with theoretical research groups to assess the quantum properties of *h*-BN." Supported by its long tradition of *h*-BN research, NIMS is expected to lead the world in this field of research.

(By Akiko Ikeda)



Kenji Watanabe
Chief Researcher, Electroceramics Group
Research Center for Functional Materials

NIMS NEWS

Special Open Call for Leaders Promoting World-Top-Class Research in Material Science

NIMS announced an international open call for the recruitment of extremely talented researchers who can promote top world-class research in Materials Science. The successful candidate will be required to lead a new independent research group. In addition, several incentives will be made available, including the special allocation of a generous start-up fund of up to 100 million yen within the first year, to enable the candidate to start research at NIMS. All research fields related to Materials Science, regardless of whether they are basic or applied, are eligible for application.

More detail

Impact factor of STAM reaches a record high of 8.090

The impact factor of the journal Science and Technology of Advanced Materials (STAM) has risen to 8.090 according to the 2021 Journal Citation Reports announced by Clarivate Analytics on 30 June 2021. STAM is one of the world's leading materials science journals that is published with support from NIMS and the Swiss Federal Laboratories for Materials Science and Technology. The impact factor is an increase of 38% from last year—when it was 5.866—putting STAM into the 56th position among 335 journals in the field of materials and multidisciplinary science.

As of June 2021, STAM is published by an international team of more than 70 experts from 14 countries including the Editor-in-Chief, Kazuhiko Hashimoto, who is also the president of NIMS. STAM is a Gold Open Access Journal and is internationally recognized as an open-science platform that provides the latest findings on world-class research for materials scientists worldwide.

STAM Impact Factor Trends (Clarivate Analytics, 2021)

Hi! My name is Pelin and I am from Turkey. I joined ICYS in October 2019. My research activities focus mainly on the area of finding novel permanent magnets for energy-efficient devices. I investigate experimentally the magnetic, crystallographic, and microstructure properties of bulk and thin-film materials, in order to discover new compounds for high-performance permanent magnets. NIMS is a top-class worldwide research center for permanent magnets, with the world's most advanced research equipment and a pioneer in the material industry. For that reason, I came to NIMS to continue my research in magnetic materials. There are also many international researchers in NIMS with different expertise, where interacting with them through the seminars, coffee breaks and festivals (before COVID19) give a good opportunity to learn about cutting edge research and extent my interests. Above all, it is nice to live in Tsukuba Science City and explore Japan.

At Ueno park

Pelin Tozman Karanikolas
(Turkey)
ICYS Research Fellow

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