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From Gems to New Materials

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Diamonds, sapphires, rubies, crystal quartz . . . The pieces of minerals which are called gemstones have begun to be used as new materials because of their crystal structures and properties. Research on artificial gemstones, that are conceived based on the environments in which they are to be used, is also progressing. This Special Issue introduces gemstones as new materials, and their applications to optical and electronic materials.

Carlo Dolci
The Vergin of the Annuciation c.1653-55

Gemstones have value as ornaments because of their vivid colors and high refractive index. Gems can lose their value as possessions if they broke easily, and they cannot be inherited as family treasures if their shape or color is changed by erosion or discoloration in 10 years or so. These properties of color, hardness, and stability are also the reason why gemstones have an important meaning for industry.

Hardness of gemstones

The relationship between people and stones dates from antiquity. The first tools used by humans were stone tools. In the Stone Age, it is conceivable that the hardness and workability of stones determined their value. For example, in knives and other tools with blades, hardness and the ability to form a sharp edge are two essential requirements.

As a matter of fact, modern human technologies are similar to those used with stone implements. For example, consider gear wheels. In mechanical watches, you may know that the words "17 jewels" indicate the value of the timepiece. This means that sapphires and other hard jewels, which are unbreakable, are used in the shafts of the important gears. As another example, diamonds, which are the hardest material, are used in the edges of drilling tools when extracting oil and natural gas from deep underground.

Vivid colors of gemstones

The stone called lapis lazuli, which originally came from the Silk Road, has a beautiful blue color. Valuing that blue color, the aristocrats of the Renaissance displayed their wealth in paintings that made bold use of a paint called ultramarine, which is produced by powdering this stone. The mantle of the

From treasures to materials: Industrial uses of gemstones.

Division Director,
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Naoki Ohashi

Virgin Mary in the Annunciation by Carlo Dolci (1616-1686) is masterpiece that you must see if you have a chance.

Including this example of lapis lazuli, deep-red rubies, deep-blue sapphires, colorless transparent diamonds and crystal quartz, in all these stones, color is important. Their colors are determined by the interaction between the stone and visible light.

There are three representative interactions with light: diffraction, reflection, and absorption. Diamonds and crystal quartz are transparent because they do not interact with visible light, while rubies and sapphires produce their distinctive colors because their compositions include elements that absorb visible light.

In actuality, both rubies and sapphires are corundum type aluminum oxides (α-alumina) and differ only in the impurities that they contain. Because this α-alumina has an extremely wide bandgap, it is completely transparent to visible light. When α-alumina is used as a substrate for nitride light emitting diodes, or LEDs, the substrate does not absorb the light emitted by the LEDs.

Titanium-doped α-alumina is a laser material which emits light due to the transition of titanium. In this case, α-alumina can be used as the matrix crystal precisely because it is a material that does not absorb the light emitted by the titanium.

Also, there are crystals which change the property of light that passes through them. When garnets contain a magnetic element, a magneto-optical effect can be obtained. With crystal quartz, on the other hand, the wavelength of light can be changed by applying an electro-optical effect. This makes it possible to change infrared light to visible light, and visible light to ultraviolet light.

Gemstone? Ceramics?

In many general ceramics, the interfaces between the particles scatter light. For this reason, gemstones (single crystals) have an important significance in the applications of light wavelength conversion and laser light oscillation.

However, gemstones also have one an weak point. Because a gemstone is a single crystal grain, the atoms are arranged in a well-ordered, regular manner. If a crack is once introduced, it will propagate immediately through the crystal, corresponding to the atomic arrangement, resulting in fracture of the crystal. Recently, therefore, ceramics have come to be used in machine parts as materials which possess the necessary hardness and enable precision machining.

For example, single crystal garnets had been used in garnet lasers, but in recent years, it has become possible to produce transparent garnet ceramics (polycrystalline materials), and ceramics can now be applied to lasers.

Polishing and making gemstones

Cutting and polishing are important to the value of precious stones as gemstones. The sense of value that a gemstone is valuable precisely because it is polished is the same when gemstones are used as industrial materials.

For example, when α-alumina is used in wafers in the manufacture of semiconductor devices, its surface roughness is reduced to the level of a single atom. Technologies for producing this kind of extremely smooth surface have had an extremely important significance in the development of modern science and technology. The principle of polishing objects is the same as in brushing your teeth: Polishing is performed by rubbing fine particles against the surface being polished, but in industrial applications, polishing powders, we say abrasive powders, that utilize the full potential of technology are used. For example, the "abrasive powder" may consist of alumina particles with a size of less than 1 micron, in which the size of those particles is controlled with extreme precision, and this is dispersed in a solution with a precisely controlled pH. Thus, in comparison with polishing for gemstone use (mirror polishing), which is performed by visual inspection, far more advanced technologies may be required in industrial polishing.

Sapphires, garnets, diamonds, opals, and crystal quartz. The industrial value of these respective materials is clear. Today, these materials are not only underground resources, but can also be produced by industrial means. Crystals which are produced industrially by controlling impurities and size may have higher added value than natural crystals which contain unwanted impurities.

The research and developments conducted at NIMS are to find new ways to produce materials that were regarded as treasures in ancient times artificially with high efficiency, and to enhance their added value by controlling their purity and shapes, thereby contributing to a more abundant society.

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Diamond MEMS and NEMS

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Diamond: ideal for MEMS/NEMS

Microelectromechanical systems (MEMS) are typically defined as the devices with a characteristic length of less than 0.1mm but more than 1 µm, which integrates mechanical elements, sensors, actuators, and electronics into a common substrate through microfabrication batch-processing technology. The terminology nanoelectromechanical system (NEMS) is utilized when the feature size is pushed into submicron. The typical examples of MEMS devices include accelerometers for airbag sensors, radio-frequency switch, microphones, projection display chips, blood and tire pressure sensors, optical switches, biosensors and many other products. The current MEMS devices are dominated by silicon due to the well-established microelectronics technology and the easy integration of MEMS with CMOS. However, silicon has intrinsic limitations such as poor mechanical/ tribological properties, poor thermal stability, and a narrow bandgap. Therefore, the present MEMS have the problems of reliability and poor performance, especially under extreme conditions such as high temperatures, environments with corrosive chemicals, high power, and high frequency, etc.

Diamond, the king of jewels, has demonstrated itself an extreme semiconductor for electronic and photonic devices, thanks to its outstanding properties such as a wide bandgap of 5.5 eV, the high carrier mobility, high electric breakdown field, etc. It also possesses the highest merits for MEMS/NEMS due to the highest mechanical hardness, the highest Young's modulus, extremely low friction coefficient, and high corrosion resistance upon caustic chemicals, etc. Especially, the electrical conductivity of diamond can be tailored from insulator to metallic conductor through impurity engineering. Therefore, it is highly expected that by using diamond, both the reliability and the performance of MEMS/NEMS will be markedly improved.

Diamond MEMS/NEMS devices

We developed a unique process to produce suspended structures of single crystal diamond for MEMS/NEMS with different dimensions (width: 0.1 to 10 µm, length: 1-100 µm, thickness: 0.2-2µm). In this process, a unique device concept of diamond-on-diamond is utilized. A damaged carbon layer (called the "sacrificial layer") was firstly formed locally within a single crystal diamond substrate by high energy ion implantation. This was followed by the growth of a p-type diamond thin film with electrical conductivity by a microwave plasma chemical vapor deposition process. The carbon layer was transformed into graphite under high temperature. The graphite sacrificial layer was then removed by solvent etching to produce a suspended structure. In principle, suspended or free-standing single crystal diamond mechanical resonators with arbitrary geometry could be fabricated in a batch production. As shown in Fig. 1, single crystal diamond cantilevers and bridges were fabricated with different feature dimensions from 0.1 to 10 µm. The formation of a 200 nm air gap can be clearly observed between the substrate and the suspended structure. The resonant frequency of the diamond resonators were measured by piezoelectric actuation and optical detection. A typical frequency response from a cantilever was shown in Fig. 1 (c). The obtained resonant frequency is around1.36 MHz and the quality factor is as high as 4000. The Young's modulus was calculated to be 1100 GPa, suggesting the single crystal diamond nature.

A single crystal diamond NEMS switch was fabricated based on the above procedure by using a lateral device concept. The boron-doped p-type diamond layer was functioned as the conductive source, drain, and gate like a transistor. The on/off operation of the nanoelectromechanical switch can be controlled by the gate voltage. In the off-state (Fig. 2 (a), the cantilever does not contact to the drain. When the gate voltage reaches or is higher than the pull-in voltage (V_P), the electrostatic attraction between the gate and cantilever leads to the deflection of the cantilever contacting to the drain. This is called as on-state (conductive), as illustrated in Fig. 2(b). The pull-in voltage can be varied from 10 to 100 volts by designing the cantilever dimensions. Due to the intrinsic hydrophobic property of diamond, no clear adhesion was observed during the on/off operation. In addition, stable operation at a high temperature environment (525 K) was confirmed, which provides the possibility for the application in aircraft, automobiles, and railway equipments under harsh environments.

In comparison with the current silicon-based MEMS, diamond MEMS exhibit greatly improved performance, including high quality factor, high reliability, long life time, and high speed. The developed diamond MEMS/NEMS may find promising applications in scanning microscopy probe, high-resolution sensor, and harsh-environment MEMS/NEMS devices.

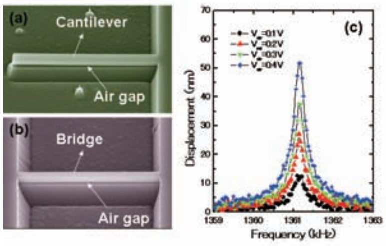

Fig. 1 Suspended structures of single crystal diamond. Scanning electron microscope images of **(a)** cantilever, **(b)** bridge, and **(c)** typical frequency response spectra driven at different voltages applied on a piezoelectric ceramics.

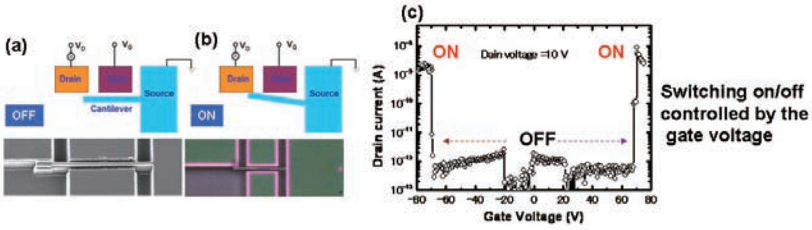

Fig. 2 Schematic diagram showing the operation principle of the single crystal diamond 3-terminal nanoelectromechanical switch in **(a)** OFF state and **(b)** ON state. **(c)** The diamond NEMS switch and its switching behavior.

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Development of Optical Materials from the Viewpoint of Opals

Group Leader, Applied Photonic Materials Group,
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Tsutomu Sawada

Opals and light

Among gemstones, opals are slightly unusual in the unique way they give off light. When a gemstone opal is observed, it has a mysterious way of shining, and change colors depending on the angle of illumination and the angle from which it is viewed.

The composition of natural opals is mainly silica and is a colorless substance. If the microstructure is observed with an electron microscope, you can see that spherical silica particles are arranged regularly in 3 dimensions. Since the period of that arrangement has a length which is almost the same as the wavelength of light, an interference effect occurs due to the phenomenon of light diffraction. This phenomenon is the same as Bragg reflection*, in which ordinary crystalline materials diffract X-rays, and is in fact Bragg reflection of light in the visible range. In other words, although the material of opals is itself colorless, the unique way that opals give off light is due to Bragg reflection of visible light.

Creating artificial opals

From the viewpoint of materials, opals are understood as a material that displays Bragg reflection of light. Materials with this property are generally termed photonic crystals, and it has been clarified theoretically that they are not simply beautiful, giving off rainbow-colored light, but also possess mysterious and useful properties, such as retarding the speed of light, enclosing light, etc.

How can opals be produced artificially? Using silica and organic polymers as the basic materials, it is possible to create fine particles with excellent size uniformity by chemical synthesis. If those particles can be arranged in 3 dimensions, the result will be an artificial opal. So, how can those fine particles be arranged in a regular order? It is a surprising fact, but in a dispersed system of fine particles, in other words, a colloidal system, the particles form an ordered structure by themselves, with virtually no human intervention. This phenomenon is called colloidal crystallization. We simply arrange the macro conditions for that phenomenon and give it a little help.

In work until now, we have developed a method of artificially producing opals with a large surface area by applying an independently-developed technique to the phenomenon of colloidal crystallization.

Opals as a new photonic material

A stable material is formed by embedding resin or polymer in the matrix between fine particles arranged in 3 dimensions, and fixing the resulting material so that its ordered structure is not destroyed. A hard opal is formed when the matrix is hard, and a soft opal which is easily deformed is obtained when the material is soft.

In previous work, we succeeded in creating a laser oscillation device by utilizing the features that the speed of light is greatly retarded and light can be enclosed in opals. When a fluorescent dye is added to this opal and excited with external light, laser light of a wavelength corresponding to the Bragg wavelength is emitted from the opal. If a soft opal is used, the laser emission wavelength can be varied freely. In addition to this, because soft opals are a material that changes color when stretched or compressed, sensor applications in which deformation is visualized by color and application as decorative materials can also be expected.

* Bragg reflection: A phenomenon in which a group of designated lattice planes in a crystal reflect only light of a designated wavelength like a mirror when light is irradiated on a 3-dimensional periodic structure. This reflection is not reflection by a single lattice plane, but rather, is the total effect of the sum of the reflection by a group of layered lattice planes.

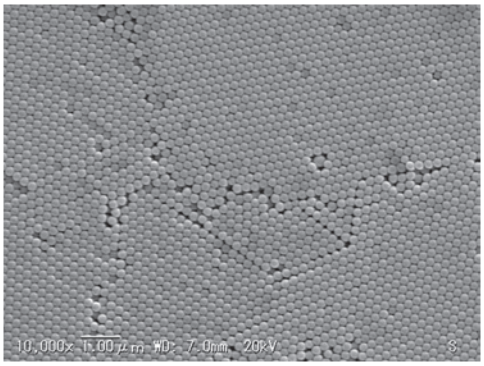

Fig. 1 Regular ordered structure formed naturally by fine particles. The figure shows a scanning electron microscope image of polystyrene particles.

Fig. 2 Artificial opal film fixed by a polymer gel matrix (colloidal crystal gel). The rainbow coloration is caused by Bragg reflection of light.

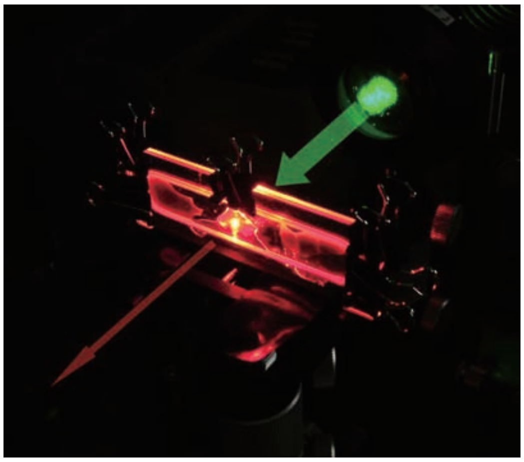

Fig. 3 Laser oscillation by a fluorescent dye-added artificial opal film fixed by a polymer gel. Laser oscillation of the color red, corresponding to Bragg reflection, occurs as a result of irradiation with green excitation light. (Courtesy of Dr. Seiichi Furumi of the Applied Photonic Materials Group.)

Tsutomu Sawada Ph.D. (Physics) NIMS Chief Researcher. His fields of specialization are crystal growth science and colloid science. Following previous research on the fundamentals of crystal growth, pressure-controlled crystal growth, and crystal growth experiments under microgravity conditions, he has been engaged in development of colloidal single crystal materials since 2000. He is currently the Group Leader of the Applied Photonic Materials Group.

Garnets: From gemstones to industrial applications

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García Víllora

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Garnet crystals received their name from the iron silicate minerals that exhibit a shape and color similar to the pomegranate fruit. Depending on their composition they present beautiful colors and therefore have been used since the ancient times as gemstones. Garnets are cubic crystals with a complicated structure of three differentiated cationic sites (Fig.1). Nowadays, they are industrially used as laser crystals (Nd:YAG), for optical communications (YIG), high-power laser machinery (TGG), etc. Taking into account the flexibility of the garnet structure for cationic substitution, we design and grow garnet crystals for the following applications.

Rare earth doped YAG single crystal phosphors for white LEDs

Cerium-doped YAG exhibits an intense and broad band luminescence in the visible region (yellow) when excited with blue light. Ce:YAG powders embedded in the resins covering blue light emitting diodes (LEDs) are commercially used for the fabrication of white LEDs. The phosphor resins, as they suffer from photodegradation, are critical for the fabrication of demanded high-brightness (HB) white LEDs. As alternative we have developed rare earth-doped YAG single crystal phosphors (Fig.1). These, placed over the blue LEDs, avoid overheating, and have higher quantum efficiencies than defect-rich powder phosphors. We have demonstrated the growth, excitation-photoluminescence and quantum efficiency of these phosphors, as well as the adequate color rendering and exceptional temperature stability of the resin-free white HB-LEDs fabricated with them.

$Tb_3(Sc,Lu)_2Al_3O_{12}$ (TSLAG) garnet Faraday rotators for high power laser machinery

Materials processing by laser machinery has evolved from the traditional Nd:YAG and CO_2 lasers to high-power fiber-amplified laser diodes (LDs). The power of current lasers is increasing rapidly and the protection of semiconductor LDs from back-reflections is a crucial issue. This is achieved with Faraday rotators, which can rotate the polarization plane of light under an applied magnetic field (Fig.3). At present, terbium gallium garnet, TGG, is the only material in use in spite of several material deficiencies. In order to substitute TGG, we have designed TSLAG and have demonstrated its remarkable advantages such as easier growth from congruent melt composition, higher homogeneity and stability, higher rotation so that smaller magnetic fields can be used, and higher damage threshold. This crystal and related optical isolators are under industrialization by Fujikura Corp. This work has been awarded the President's Prize inside company.

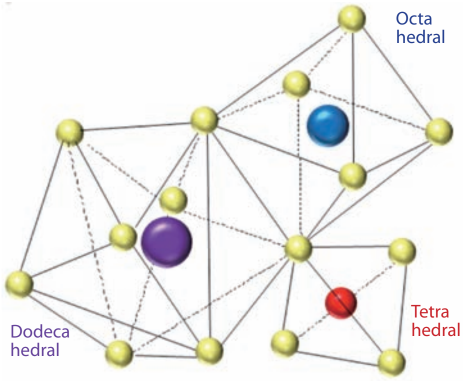

Fig. 1 The garnet structure is very complicated (contains 8 formula units $C_3A_2D_3O_{12}$ in one unit cell) in spite of belonging to the highly symmetric cubic system. Simplifying, it has three distinguishable cationic sites with dodecahedral, octahedral and tetrahedral coordination, respectively. These sites give a high flexibility for the design of new crystal materials by cationic substitution.

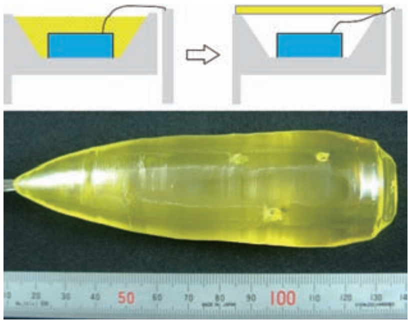

Fig. 2 (Up) White LED structures: (left) resin with embedded yellow phosphor, (right) resin-free single crystal garnet phosphor. (Down) Ce:YAG phosphor single crystal.

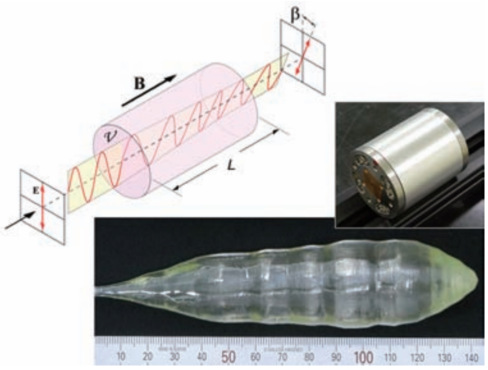

Fig. 3 (Up) Rotation of the light polarization plane by a garnet in a magnetic field. The inset shows a TSLAG-based Faraday isolator of 70 mm in length. (Down) TSLAG single crystal.

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Development of Optical Devices from the Viewpoint of Crystal Quartz

Optical Crystal Group,
Optical and Electronic Materials Unit,
Sunao Kurimura

From fortune-telling and clocks to advanced lasers

Rose quartz, which is sometimes called the love stone, is said to have a healing effect and give women a sparkling aura. Amethyst, with its noble color, brings inner stability and a favorable turn to human relations. The unique colors of these crystals are caused by impurities such as iron and manganese. Colorless crystals have long been used in fortune-telling, in the eyes of the Buddha statues, and in lenses of eyeglasses, and crystals of quartz are frequently included in mineralogy specimens (Fig. 1). Although people with worries in love and human relations desire these crystals as power stones, here, we will discuss the applications of quartz, which is a transparent single crystal, to ultraviolet (UV) lasers.

Application of artificial crystal quartz to new UV laser light sources as an optical material

SiO_2, which is the basic component of quartz, is also the main component of sand that is found in abundance at beaches. Its reserves are virtually inexhaustible, and it is environment-friendly. Crystal quartz is widely used in every-day lives, as it is extremely hard, with a Mohs hardness of 7, and has excellent chemical and heat resistance. Common applications include not only quartz clocks, but also crystal oscillators producing the timing signal for data processing in cell phones and televisions, and low-pass filters that eliminate noise in camera images. Development is continuing in the material itself, where the properties of filters are improved by reducing the moisture content in the crystal, and, light absorption are suppressed by reducing the contents of impurities such as Al, Na, and Li. A mass-production technology for crystal quartz by hydrothermal synthesis has already been established, and NIMS is engaged in research to extend applications of this material (Fig. 2) to new UV lasers as a wide bandgap optical material.

Realizing wavelength conversion of laser light to vacuum-ultraviolet light by ultra-fine structure

Because quartz crystals have a nonlinear optical property, they have the function of converting the wavelength of laser light. Although the nonlinear optical property itself was reported in crystal quartz for the first time in 1961, quartz crystals were not applied to wavelength conversion thereafter due to their extremely low efficiency. There was an anecdote in the paper published in 1961 on the effect, where the light at the converted wavelength was so weak that the publisher erased the light spot by mistake. With other nonlinear optical materials, research has demonstrated that wavelength conversion efficiency can be dramatically enhanced by creating a structure in which spontaneous polarization is periodically reversed.[1] Therefore, NIMS focused on "polarity reversal by application of stress," which had been studied in connection with earthquake prediction, as a method of introducing a polarity-reversed structure. This is a phenomenon in which electro-magnetic waves are generated by polarity reversal underground when stress is applied to crystal quartz deep in the ground before an earthquake. By combining this phenomenon and state-of-the-art semiconductor processing technology, we fabricated a structure with narrow steps and applied stress at high temperature. As a result, we realized a periodic polarity-reversed structure with alternating plus-minus polarity for the first time in the world (Fig. 3).[2] Considering that the thickness of typical Japanese hair is 70-90 µm, perhaps the reader can understand just how small the period of 11.9µm is. At present, we are the only group in the world that possesses this technology. By realizing wavelength conversion of laser light to vacuum-ultraviolet light (wavelength: 193nm) using this ultra-fine structure, we demonstrated a completely new application of crystal quartz. Because this laser wavelength of 193nm is widely used in microprocessing of semiconductors and in ophthalmological treatments such as LASIK, a miniature light source is highly expected for use in the semiconductor industry and medical fields.[3] We have already begun material development matched to applications in new fields, namely, reduction of UV light absorption for a stable light source.

1) Miyazawa and Kurimura, eds., "Fundamentals and Applications of Polarity-Reversed Devices" (Optronics, 2006). (in Japanese)
2) S. Kurimura, M. Harada, K. Muramatsu, M. Ueda, M. Adachi, T. Yamada, T. Ueno, Optical Materials Express 1, (2011) pp.1367-1375 (Invited).
3) Nikkei Sangyo Shimbun, Jan. 24, 2011, p. 11. (in Japanese)

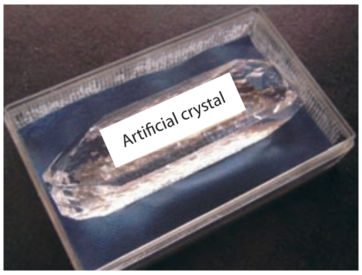

Fig. 2 Artificial crystal quartz grown by hydrothermal synthesis process.

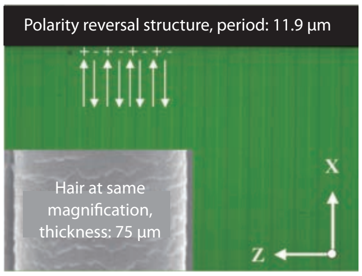

Fig. 3 Crystal quartz with periodical polarity-reversed structure by applied stress.

Fig. 1 Crystal quartz family: From the left, the rose quartz, amethyst, and crystal quartz.

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Optical Material Development from the Viewpoint of Sapphire

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Kiyoshi Shimamura

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Sapphire single crystals

Single crystals are widely used, not only as gemstones but also as components in many devices of daily life. One representative example is the sapphire single crystal, Al_2O_3. Cr and Fe/Ti doped aluminum oxides are two of the most common gemstones. These, known as ruby and sapphire, exhibit beautiful red and blue colors, respectively.

Colorless transparent sapphire is widely used in the industry. This material possesses outstanding properties such as high hardness, high mechanical/chemical stability, high heat resistance, and high transparency. Besides its wide use as watch window and as a mechanical element in semiconductor production, recently it is widely applied for projector windows and especially as substrate for blue/white LEDs (Light Emitting Diodes).

Development of gallium oxide (β-Ga_2O_3) single crystal substrates for high brightness LEDs

With the development of white LEDs, the potential to substitute currently used lightning stuffs for general illumination by low energy-consumption LEDs has become a reality. In order to achieve this, it has become an urgent issue to increase the current flow of LEDs, leading to so called HB (High Brightness) LEDs. The substitution of the insulating sapphire by a conductive substrate is of fundamental importance, so that the horizontally-structured LED can be replaced by the efficient vertically-structured one.

For this purpose, we have developed a new transparent conductive oxide, namely gallium oxide, β-Ga_2O_3. This material exhibits a large band gap (4.8 eV), an excellent chemical stability and a high electrical conductivity (resistivity ~ 0.005 Ωcm). The weak point of this material is its cleavage* nature, which was considered to impede any cutting and polishing procedures. We could overcome these difficulties by the growth of large bulky single crystals of high crystalline quality (Fig. 1), which can be processed as substrate for epitaxial growth. Additionally, we have found that Si is an efficient n-type dopant, so that the carrier concentration of β-Ga_2O_3 can be controlled by several orders of magnitude.

β-Ga_2O_3 wafers have been used to fabricate vertically-structured blue LEDs based on the InGaN-system. Multi-quantum-well layers were deposited on β-Ga_2O_3 by the MOCVD (metalorganic chemical vapor deposition) as shown in Fig. 2. At an operating voltage as low as 3.3 V at 200 mA current flow was obtained through the 300 μm square LED prototype (Fig. 3). This result contrasts with the 4.7 V of commercial LED with horizontal structures of the same size and current. The light output of this LED prototype at 1200 mA was as large as 170 mW, i.e. more than 5 times higher than horizontal LEDs (Fig. 3). The present estimations indicate that the light output of these HB-LEDs may be still enhanced by a factor of two.

The potential of β-Ga_2O_3 for LED at shorter wavelengths is also feasible. We have demonstrated the homoepitaxial growth of high quality β-Ga_2O_3 using oxygen plasma as well as ozone gas as oxygen sources. The free carrier concentration of these films can be controlled by Sn doping, while high insulating films can be obtained by Mg doping. Band gap engineering by solid solution with Al has been also demonstrated. P-type layer was demonstrated, however, there are issues to be improved and optimized.

Present and future perspectives of β-Ga_2O_3 development

We started the development of β-Ga_2O_3 in 2002 in the frame of a NEDO joint project between the Waseda University (under Prof. Ichinose, today Emeritus) and Koha Co., Ltd. From 2007 we put emphasis on the prototype development with Koha Co., Ltd., and Tamura Corporation. What HB-LEDs concerns, commercialization is planned to start at the beginning of 2013. Other promising applications are also under consideration such as different types of sensors (solar-blind, gases) and power devices. The good performance of β-Ga_2O_3-based Schottky-barrier diodes has been already demonstrated. It is estimated that β-Ga_2O_3 Baliga's figure of merit is 10 and 4 times higher than those of SiC and GaN, respectively.

One of the most important features of β-Ga_2O_3 is perhaps the fact that high quality large-scale bulk single crystals can be grown from the melt. On the contrary, due to their high vapor pressures GaN and SiC cannot be grown from the melt, and other techniques to grow these crystals in large scale with sufficient high quality encounter numerous difficulties and are very expensive. More than 10 years have passed since we started the development of β-Ga_2O_3. We expect further rapid progress in the future.

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* Cleavage: Splitting of crystals in a preferred plane or direction.

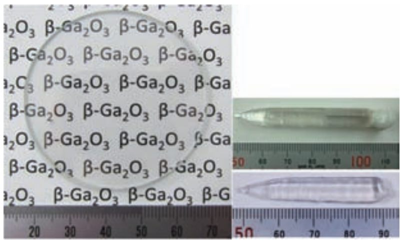

Fig. 1 (left) 2-inch β-Ga_2O_3 single crystal substrate that was processed to a round shape (presented by Koha Co., Ltd.; grown by EFG technique), (upper right) β-Ga_{2}-xAlxO_3 single crystal with further increased bandgap (grown by FZ technique), and (lower right) highly insulating Mg:β-Ga_2O_3 single crystal (also grown by FZ technique).

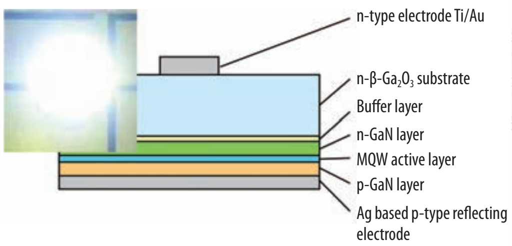

Fig. 2 Schematic of a GaN-based LED on an n-type β-Ga_2O_3 substrate. The upper left photograph shows a white light emitting diode (presented by Koha Co., Ltd.).

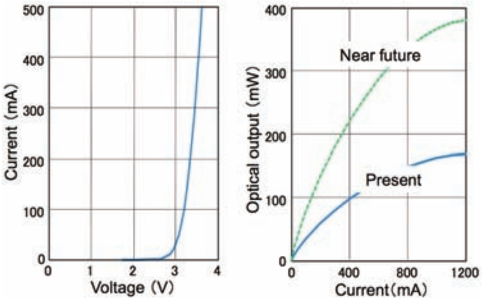

Fig. 3 Prototype of a GaN-based LED on β-Ga_2O_3 single crystal substrate, showing a low operating voltage (left) and a high light output (right) (presented by Koha Co., Ltd.).

Kiyoshi Shimamura See Profile on page 6. / **García Víllora** See Profile on page 6.

Interview

Clarifying Unsolved Problems by Searching for Overlooked Parameters

Naoki Ohashi, **Division Director, Environment and Energy Materials Division**

**Dr. Naoki Ohashi is not only the Unit Director of the Optical and Electronic Materials Unit,
but also Division Director of the Environment and Energy Materials Division. With this wide range of responsibilities,
he always asks himself where and how he can find new materials that are truly useful,
from optical applications to the field of materials as a whole.**

── Your research on crystals is research on optical and electronic materials?

Ohashi(O): As also described in this Special Issue, single crystals are certainly important if we consider the light transmission. Also, glass is extremely important in optical applications, although we haven't mentioned in this Issue.

I was involved in research on high Tc superconductors when I was a student, and then I did work at the intersection between ceramics and electronics. As it happened, I began using optical properties in characterization of materials, and before I knew it, I was in charge of optical and electronic materials at NIMS. During that whole time, I was involved in research related to crystals.

The fact that the paper on high Tc superconductivity by Bednorz and Mueller appeared during the year that I began research for graduation thesis at university, and the blue LED which was developed in Japan during the year (1993) when I became an assistant professor had a great influence on my career. The discovery of high temperature superconductivity, and the realization of blue LEDs: everybody is searching for new discoveries with the potential to be that kind of social phenomena, but finding things of the similar impact is always very difficult.

── You are also the head of the Environment and Energy Materials Division?

O: Energy and the environment issue isn't just difficult, it's also extremely complex. We can't say that expensive products are acceptable simply because some new technologies to produce renewable or clean energy is installed in those products. If I said that these will be valuable technologies when the price of crude oil rises by a factor of 10, people would laugh. It's such an important and also difficult problem that energy-related research and development has become an issue in this year's Presidential election in the United States. In any case, we can only do our best to obtain renewable energy and highly efficient systems that's inexpensive, safe, and secure.

── What do you consider important in the quest for new optical and electronic materials?

O: I'd like to solve the fundamental, unsolved problems that have been left behind until now. In the world of materials, and particularly in the development of ceramics, there had been a strong aspect of proceeding by trial and error. In other words, repeating a process of looking for good results, and then trying to improve on them. Although technology advanced as a result of those efforts, there are many cases where there's no answer to the question of what will produce good results. For this reason, I think the first priority is to look at those questions from a slightly different direction from that in the past, clarify those unsolved problems logically, and then see if this will produce some kind of new results.

── What is the origin of material properties, and from there, questioning the existing common sense?

O: Perhaps there are parameters that everybody has overlooked until now. For example, if everybody believes that impurities control the properties of a certain crystal, everybody will earnestly analyze impurities. However, it is also possible that impurities are unrelated to those properties, and those properties are determined by something else. We have to look at things that we haven't seen before.

── In other words, a different perspective from research to date?

O: Considering the fact that there are so many chemists and so many physicists, and still only one hundred elements that are on the Periodic Table, a lot of people may presume that there are no more substances that none has seen. What's more, much research has already been done on general combinations. Nevertheless, new materials may appear, and that is why we continue to investigate the true essence of things and look at phenomena from every angle. What is the origin of this property? Can this property possibly used in a different situation? From that kind of study, we can find hints which, while uncertain, may lead to new materials. If the result of repeating that process is a new material that can actually be used, there's nothing better!

Naoki Ohashi Ph.D. (Engineering) Before joining NIMS, he was engaged in research and development of ceramics at Tokyo Institute of Technology and Massachusetts Institute of Technology (MIT). Involved in research and development on wide gap semiconductors at NIMS since 2000. Currently Division Director of the NIMS Environment and Energy Materials Division and Unit Director of the Optical and Electronic Materials Unit of the same Division.

NIMS AWARD 2012

Prof. Harry K.D.H. Bhadeshia
Tata Steel Professor of Metallurgy,
University of Cambridge

——Could you describe the work for which you received your NIMS Award?

For a long time, we have been trying to establish principles to allow us to calculate the structure of steel. So that instead of doing experiments first, we aim to make predictions of properties and structures. We're not going to be able to do that for 100% of the problem which is very complex, but we calculate first, then design an experiment. Then we archive all the material for everyone to use, the algorithms, and hopefully in that way, we can generate progress in the field. We've created a huge algorithm library, accessible throughout the world, free of charge.

In that way, we have had several commercial successes, some of which I talked about today in my lecture, "The First Bulk Nanostructured Metal."

——How did you originally get into this field?

When I was 16, I took a job as a technician in British Oxygen Co.'s metallurgy lab, and I got hooked on the subject. The company sponsored me for further education, and I did a degree at the City of London Polytechnic, then went to Cambridge for my Ph.D. I still work with that company – they still support my research.

——You started working at a young age – does that have a good impact?

I think so. You're not frightened of industry, because you've worked there, and that's a very useful perspective to have. And you realize how difficult it is to create a product, compared to just writing a paper. Of course, if you go on that career path you have to be lucky for a company to sponsor you. The normal path is probably the right way to go.

——You've had a long relationship with NIMS.

Yes, since 1987, when it was NRIM. Dr. Hiroshi Harada introduced me to NRIM and I first visited in 1989. Then between 1990-1995 there was a huge project between NRIM and Cambridge, with hundreds of man-hours of Japanese scientists working at Cambridge on atomic arrangements and control.

Ever since then, there has been a systematic stream between Cambridge, NIMS and Japan of Ph.D. students and professors on sabbaticals. Also, NIMS supported a new office at Cambridge. We now have seamless interaction with NIMS.

——Has the research environment at NIMS changed since you first came here?

Things have changed quite a bit. In those days, national labs were not allowed to cooperate with universities, and couldn't have students. Then the government changed the regulations, and now NIMS is a fantastic place. It always had excellent equipment, but not enough people, because they couldn't take students. Now they have 1,500 people here. Over this weekend I saw presentations by really young students who gave superb technical explanations of their work.

—— Is the research environment here different from at Cambridge?

It's necessarily different, because it's a national laboratory. You don't have teaching at NIMS, though of course, adjunct professors teach at universities. In research you need various structures; you can't get creativity with one standard kind of laboratory. You have outstanding equipment here, very well maintained, and also a strong interaction with industry.

——Any advice for young researchers?

As long as you're interested in your work, and have the drive in your heart to create something new, you will succeed. But in this field you must be driven by your own interest in the work, not by finding a job or making lots of money.

Harry K.D.H. Bhadeshia Professor of metallurgy at the University of Cambridge. Fellow of the Royal Society. Graduated the City of London Polytechnic (now London Metropolitan University) in 1976. Obtained PhD from the University of Cambridge in 1979. He worked with British Steel (now part of Tata Steel Europe) to develop a carbide-free, silicon-rich bainitic steel that was used for rails in the Channel Tunnel. He was awarded the Bessemer Gold Medal by the Institute of Materials, Minerals and Mining for "outstanding service to the Steel Industry" in 2006, and NIMS Award in 2012 for "Understanding phase transformation and precipitation behavior in steel materials at the basic level and the development of new steel materials based on this insight."

Prof. John William Morris, Jr.
Department of Materials Science and
Engineering, University of California, Berkeley

—— First, please tell us about your talk today at the conference, "Theoretically understanding the mechanisms behind strength."

Well, the high-strength steels that really push the properties of steel are called martensitic steels, made by quenching, which changes the physical structure of the metal. It produces a very complicated microstructure that people been trying to sort out for 150 years or so. And we are finally figuring out what the microstructure is all about. It looks very complicated, but if you understand what's going on it really isn't. It is understandable, and that makes it much easier to interpret and control the properties of steel. When you begin with the premise that it's complicated and hard to understand, it's hard to make progress. But when you discover that it's much simpler than you thought, it's easier to manipulate in an intelligent way.

—— How did you originally get into this field?

A couple of things happened at the same time – I was headed to MIT from central Florida where I went to school, and originally wanted to study math. That summer two things happened – I had a summer job working in construction plumbing, hammering metal all summer, and I discovered I kind of liked it – in contrast to math, you actually got to feel something. Also, I happened to read Ayn Rand's "Atlas Shrugged," where the hero was a metallurgist. So I decided to go into metallurgy. It was a good move – it's a fascinating field, and I've never had any regrets.

Thing that got us all really excited in this area back then, was the need to develop good materials for cryogenic applications. That was a hot field in the 1970s to early to mid-80s,

At the NIMS Conference 2012, held this year at Tsukuba, three distinguished materials scientists received NIMS Awards, in recognition of their contribution to research and development in the field of structural materials as well as their contribution to NIMS and its reseach objectives.
The three were: Prof. H.K.D.H. Badeshia (University of Cambridge), Prof. John William Morris, Jr. (University of California, Berkeley), Prof. Subra Suresh, (Director of U.S. National Science Foundation).
During the conference, they kindly took some time to discuss their work with us.

because of LNG storage, particularly in Japan. Also, there was an international effort to make large superconducting magnets for Tokamak fusion reactors, and these require good cryogenic structural steels

In recent years the LNG issue has become even more important. I'm involved in funded research in the U.S. and collaborating with steel companies around the world.

—— You've had a long relationship with NIMS, haven't you?

I first came into contact with NIMS in the late 1970s, when it had just been built. I was in Tokyo, and Prof. Kyoji Tachikawa, who built the first really big high-field superconducting magnet, invited me to come out to Tsukuba to see it. Over the years we've had an ongoing collaboration with NIMS, and we've had a number of NIMS people working at our lab.

It's a very good environment here at NIMS. It's always been a very well-supported organization, especially the steel research group. In the U.S., steel research went out of vogue for a while. So for most of my career, most of my technical contacts have been in Asia, especially Japan and Korea.

—— What advice would you give young researchers thinking of entering this field?

If you go into research to have fun, to enjoy yourself, for the excitement of discovering things, it can be an absolutely delightful career. It certainly was for me. I've had fun every day of my life, and I still am. So my advice is, find a way to do what you want to do, to research things that interest you, because if you take advantage of opportunities to do fascinating things, you can have a career that's both useful and a lot of fun.

I know lots of people in research who are my age, pushing 70, and still excited, still having fun.

John William Morris Jr. Professor of Metallurgy, Materials Science and Mineral Engineering at the University of California, Berkeley, and in the Structural Materials Program at the Center for Advanced Materials in the Materials Sciences Division at Lawrence Berkeley National Laboratory. Received his BS in Metallurgical Engineering in 1964 and ScD in Materials Science in 1969, both from MIT. After working with Bell Aerospace Company in Buffalo, New York, from 1968 to 1971, he joined the UC Berkeley, and the Lawrence Berkeley National Laboratory in 1971. He was awarded NIMS Award for "Theoretically understanding the mechanisms behind strength" in 2012.

Prof. Subra Suresh
Director, National Science Foundation (NSF)

—— How did you get into this research field?

It started when I got my Ph.D. in the late '70s. I was trained as a mechanical engineer, and I was interested in the mechanical properties of materials, especially fracturing. This was a rapidly emerging area where people from theoretical mechanics and materials science were starting to work together. When I became a faculty member at Brown University, it was one of the major focal points of research.

This is not how I planned it, but the way it happened was that I work in a field for 10 years, write a book and then go into some other field. In the 1980s, most of my work was in structural materials, the mechanical properties of large structures – nuclear reactor pressure vessels, airplanes, pipelines, etc. – and I wrote a book on fatigue, which came out in 1991. In 1993 I moved to MIT to work on semiconductor materials, and I started getting interested in nanoscale properties of living materials. I've been working on that for the last 10 years.

—— How do you apply mechanical engineering to human diseases?

Blood cells, for example, have a certain shape, and to deliver oxygen to different parts of the body, they have to move through very small blood vessels, and have to mechanically deform to do it. If they lose their ability to stretch, you get a disease. A mechanical engineer can bring the tools of mechanical engineering and materials science – spectroscopy, characterization tools, nanotech, atomic force microscopy – to study this deformation.

—— When did you begin your relationship with NIMS?

I've had a lot of interactions with NIMS scientists for many years, and we've had many collaborations. I've had people from NIMS visit my lab at MIT, and about three years ago I joined the NIMS international advisory board. The nice thing about NIMS is that it focuses on broad areas like materials science in a very coherent way.

Of course, the cultures are different. But Japan has always had strength in materials science, especially in areas like electron microscopy, which is essential to the field.

—— Is it important to keep changing your field of research?

You want to change fields, but not too quickly – you need to be in the field long enough to make a substantial contribution; for me that's about 10 years. The exciting thing about switching fields is that you bring a very different viewpoint with you. But it's very challenging, because you don't know the field; the culture, even the language is different, with new technical terms to learn.

One example is when I started working on malaria, I had all these tools for studying blood cells that microbiologists didn't have access to. But I didn't know the biology, so I had to spend a couple of years educating myself. So I had to read a lot, and I immersed myself in a biology group in Paris at the Pasteur Institute for six months. Among all those medical doctors, biologists, chemists and geneticists, it was very exciting, but also intimidating.

—— Do you still do research?

Oh yes, I have a group, and we Skype, mostly on weekends – that's the only time I have. It's a very precious time for me, and these are very good post-docs, so they don't mind if I call them on Sunday mornings. We have two projects, one in nanomaterials, and the other on the mechanical properties of cells related to malaria, cancers, different blood diseases and, recently, diabetes.

Subra Suresh Director of the National Science Foundation (NSF). After graduated Indian Institute of Technology Madras in 1977, obtained his MS from Iowa State University in 1979, and ScD from MIT in 1981. Completed postdoctoral work from 1981 to 1983 at UC Berkeley and the Lawrence Berkeley National Laboratory. Joined Brown University as Assistant Professor in 1982 and became Professor in 1989. Nominated by US President Barak Obama to be the Director of the NSF in June 2010. He was awarded NIMS award for "Establishment of multiscale materials science across disciplines at the macro and nano scale for the study of structural materials and biomaterials" in 2012.

NIMS NEWS

1 NIMS Receives the Commendation in Informatization Promotion Category

(Oct. 1, 2012) NIMS was selected to receive the Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology (MEXT) in the Informatization Promotion Category as part of Japan's 41st Informatization Month.

Informatization Month is an activity for popularization and education in connection with various types of informatization in society, and is conducted in October of each year by 6 related government ministries and agencies, beginning with MEXT and the Ministry of Economy, Trade and Industry (METI). Information-related efforts and achievements are selected by the ministers of the related ministries, who present commendations to the companies and individuals concerned.

This year, NIMS received the Commendation by MEXT in recognition of the results of the NIMS Materials Database system "MatNavi."

MatNavi is a diverse group of databases related to materials, which was created to enable selection and use of the optimum materials for applications, and can be accessed free-of-charge at the NIMS website. It was constructed and is operated as one of the world's largest groups of materials databases by concentrating and applying integrated management to various types of databases. MatNavi presently comprises 12 individual databases (Polymer Database, Inorganic Material Database, Metallic Material Database, Diffusion Database, Superconducting Material Database, etc.), 4 types of applications, such as the Composite Design and Property Prediction System, online editions of NIMS Structural Materials Data Sheets, and a horizontal search system. It was renovated in 2010 and has won high marks as an easy-to-use database system. MatNavi now has approximately 70,000 registered users.


President Ushioda of NIMS receiving the MEXT Minister's Commendation.

2 MANA 5th Anniversary Memorial Symposium

(Oct. 3, 2012) MANA 5th Anniversary Memorial Symposium was held with a total of 257 attendees to commemorate the five years since MANA's inception.

The International Center of Material Nanoarchitectonics (MANA) was launched in October 2007 as one of the research centers of the World Premier International Research Center Initiative (WPI) by the Ministry of Education, Culture, Sports, Science and Technology (MEXT).

The Symposium started with a welcome address by NIMS President Dr. Sukekatsu Ushioda, continued with congratulatory speeches by Director and Officer of WPI Program and Prof. Sir Mark Welland (MANA Satellite Principal Investigator at University of Cambridge).

Subsequently, MANA Director-General Dr. Masakazu Aono spoke about "Five-year journey and future challenges of MANA" and Prof. Yoshinori Tokura from the University of Tokyo gave a special lecture entitled "Emergent electromagnetic phenomena in solids".

The latter part of the program was entitled "Our Future Challenge in MANA" and consisted of eight oral presentations by the MANA researchers.


The participants in the Auditorium of the WPI-MANA building.


Prof. Sir Mark Welland.

Hello *from* NIMS

Dear NIMS NOW readers,

In December 2009 we were offered to come to Japan for a postdoctoral position. To be honest, we were afraid to travel to a non-frequent destiny for Argentinean people but we decided to challenge our opportunity and we arrived to Tsukuba in March 12th, 2010.


With the family in front of the renewed Tokyo Station.

After almost three years living in Tsukuba we found out that there are no ninjas, samurais and geishas everywhere as we use to imagine when we were kids and people talked about Japan. Instead, we discovered a great country full of friendly and respectful people always ready to help whenever you need it. Therefore with not so good Japanese language skills we were able to experience Fuji-san's country. We visited the modern and the ancient capital cities and enjoyed their great history; we were delighted by different types of ramen (noodle) and tempura, and experienced fantastic Matsuris (festivals), wonderful Hanabis (fireworks) and lovely Hanamis (cherry blossoms viewing); and on the top of that, we could learn about this millenary and very rich culture.

The decision we took by 2010 provided us not only with a great personal/professional experience but also with the huge happiness last May when our first son, Matías, was born at Tsukuba University Hospital.

After all we can say (with no doubts) that is always worthy to challenge our fears.


Matías wearing his first Yukata.

Alejandro FRACAROLI (Argentina)
from March 2010 - present
Post Doctoral Researcher
Reticular Materials Unit, MANA

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