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FEATURE

Reaping the Benefits of Collaboration and Integration

An interview with four scientists involved with MANA's programs to encourage interdisciplinary collaboration

RESEARCH HIGHLIGHTS

Vol. 13

Reaping the Benefits of Collaboration and Integration

An interview with four scientists involved with MANA's programs to encourage interdisciplinary collaboration

MANA established in 2016 several special research programs, in the belief that "science can make strong advances through the integration of research".

Four of the key researchers in these programs — Dr. Waka Nakanishi and Dr. Ayako Nakata in the Theory-Experiment Pairing Program (TEPP), and Dr. Toshikaze Kariyado and Dr. Takuya Iwasaki in the Challenging Research Program (CRP) — sat down with MANA e-Bulletin to discuss their work and their experience with these programs.

Forming collaborations

– Let's start with a description of your research.

Nakanishi: In organic chemistry, we create organic molecules in the desired form by connecting carbon atoms. Since their structure is directly related to their functions, I focus on realizing functions through designing molecules.

Nakata: I do theoretical research using first-principles calculations. Ideally, we can know the electronic state of a material from calculations. However, it's difficult to simulate systems with many atoms, because it requires vast computational resources. Therefore, we developed a program called CONQUEST to determine the state of systems and molecules containing many atoms. We are now applying it to various real-life material systems.

Kariyado: My research is on clarifying the properties of materials using theory. There are many meanings to the term "properties of materials," but I focus on how to control the electronic state in matter.

Iwasaki: I am interested in electron transport, which is the source of electric current, and my research aims to clarify the properties of materials. I am particularly interested in two-dimensional materials, mainly graphene. Ideally, graphene is flat, but if the substrate is uneven, it loses its exceptional properties. To solve this problem, we are developing a technique to superimpose graphene on a very flat 2D material.

– **How did you start your collaboration?**


The Interview was conducted online to comply with countermeasures policy for COVID-19.

Nakanishi: In organic chemistry, we often look at the function of a molecule as an "overall average" under easy-to-measure conditions, such as a large amount in a solution or organic solvent. Experiments that look at the shape and function of single molecules are still in their infancy.

In 2017 I participated in the Nanocar Race, an international competition to manipulate single molecules (nanocars) around a track. We were looking a theorist to investigate the function of our molecules, and Dr. Christian Joachim, a MANA satellite principal investigator and director of the Nanocar Race, introduced me to Dr. Nakata.

Nakata: Actually, the project here had three parts. The first was to calculate the behavior of a single molecule that was first designed. It didn't move as expected, so we designed a new one. That in turn had some unexpected functions, so we applied to study them, and summarized our research in a paper.

Kariyado: In our case, we had originally been connected with separate research groups, but decided to deepen our collaboration.

In graphene research, there is a lot of interest in the effective mass, a measure of the mobility of electrons. The lower the effective mass, the easier electrons move, but graphene has zero effective mass, so it moves a little too much! We want to manipulate it and control it in a usable way, and we focus on stacking two sheets of graphene slightly out of alignment, which increases the effective mass.

Iwasaki: Creating new functions with graphene layers is now a worldwide trend. That wasn't the aim of the experiment — it just happened by accident. Even before we started the project, we were wondering what the mechanism behind the emergent functions produced by superposition.

– **What did you learn about communication between theorists and experimentalists?**

Kariyado: In our case, our goals and backgrounds were similar, so the only difference between us was method — calculation or experiment. In graphene research, theory and experiment have always been close, and there is no difference in terminology or research direction.

Nakata: I mainly work on developing computational methods, and I haven't done much applied calculation. Perhaps because of this, when I talked with Dr. Nakanishi, who is an experimentalist, at times I could not fully explain the calculations, or conversely, could not properly understand the experimental results. So it was difficult at first. But eventually, we were able to communicate smoothly.

Nakanishi: I respected and trusted Dr. Nakata as an expert, but as we were in different fields, I couldn't fully understand, so I listened to every detail. We had many hours of intense discussions.

– **How did MANA's environment help you in proposing research to TEPP and CRP?**

Nakanishi: We rented a conference room and had a half day of discussions. MANA has a "melting pot" environment, and it's easy to move around.

Nakata: When Dr. Joachim came to MANA, we often talked with him as well. Since the relationship between young and experienced researchers is not that of master and disciple, which is unique to Japan, the environment is very easy to talk to.

Kariyado: MANA's system makes it easy to take on new challenges. In my proposal I talked about building on my existing work — this is normal. But I also added brand-new things, and made clear that although there was no guarantee of success, I wanted to try anyway.

Nakanishi: In a “Grant-in-Aid for Scientific Research” application, the standard way is to propose to do something as a next step, based on what you’ve already done. But in a MANA application, I feel like I’m being asked to draw up a dream of the future. This is rare in Japan. Writing about the future is American style, and it’s appreciated in MANA’s international environment.

Interdisciplinary Support

– **What are your thoughts on MANA's support for interdisciplinary research?**

Iwasaki: My research with Dr. Kariyado is progressing steadily, so I hope we can continue in the same way. I have no complaints about the research or the budget.
Nakanishi: I worked at MANA until 2018, then was transferred to another NIMS center. I joined this project because even after leaving MANA, I can still collaborate with people here. Many research funding systems approve research that is useful and contributes to society. But if you want to try something new or a fusion of things. I think MANA is a good place for that.
Iwasaki: This year, MANA added another research program, the Synthesis-Characterization Pairing Program. I’d like to see all kinds of collaborations. The program was set up based on MANA Director Taniguchi's own experience of collaborations, and I expect to see some very interesting research projects.
Nakata: Collaboration is important in research, and it’s important to think about who you can work with. Some of us at MANA have never met, and it would be nice to have more opportunities to get to know each other.

– **What do you want to do in the future?**

Nakanishi: Before working with Dr. Nakata, I didn't know about single-molecule design, but through TEPP, I was introduced to this field. I’ll continue my research with the single molecule perspective in mind.
Nakata: Working with experimentalists, I have found several gaps in my understanding and points for improvement, and I want to clear them up in my future research.
Kariyado: Theoretical research is all about explaining and predicting. I found interesting things in Dr. Iwasaki's experimental results from a theorist's point of view, and asked him to try the experiments. I was able to provide both explanations and predictions, which is a theorist’s job. I will continue to make it my goal to prove that theorists are still necessary!
Iwasaki: In the past, I often chose experimental 2D materials quite vaguely, using materials that happened to be on hand in the laboratory. In this project, Dr. Kariyado suggested materials that might be interesting. I hope we can continue this relationship and deepen our research together.

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RESEARCH HIGHLIGHTS

[Vol. 68]

New GaN MEMS Resonator Is Temperature-Stable up to 600 K

A team at MANA has demonstrated a highly temperature-stable GaN resonator that boasts high-frequency stability, high Q factor and the potential for large-scale integration with silicon technology.

The finding could result in faster 5G electronics devices thanks to better integration of GaN-based micro-electromechanical and nano-electromechanical systems (MEMS/NEMS) with the current semiconductor technology.

The GaN resonator was fabricated on a silicon substrate, and had a low temperature coefficient of frequency (TCF) of several ppm/K (parts per million per degree Kelvin) and high quality (Q) factors without degradation up to 600 K.

The millimeter-wave 5G system that is driving the much-anticipated “internet of things” requires increasing modulation complexity to improve data bandwidth. But conventional quartz oscillators are limited by their inability to integrate well with semiconductor electronics. Using MEMS/NEMS for reference oscillators is one way to achieve high resonance frequencies with less phase noise and high temperature stability.

Silicon-based MEMS resonators usually have a large negative TCF of around -30 ppm/K. Temperature compensation techniques, including geometry modification, impurity doping and multilayer structures, have been proposed to improve the TCF, but these degraded the system's Q factors.

The MANA team used elastic strain engineering, a technique to modulate the strain at the heterojunction of the resonator structure, which helped to store energy and thereby increase Q factors.

In contrast to conventional flexural modes, the internal thermal stress at high temperatures improved the TCF of the GaN MEMS resonator by over 10 times, without losing the high Q factor.

Group III nitrides have been excellent wide bandgap semiconductors for high-frequency electronics in the 5G era. The integration of such MEMS with electronics is therefore promising for IoT sensors and communications devices.

This research was carried out by Liwen Sang (MANA Independent Scientist, WPI- MANA) and her collaborators.

Reference

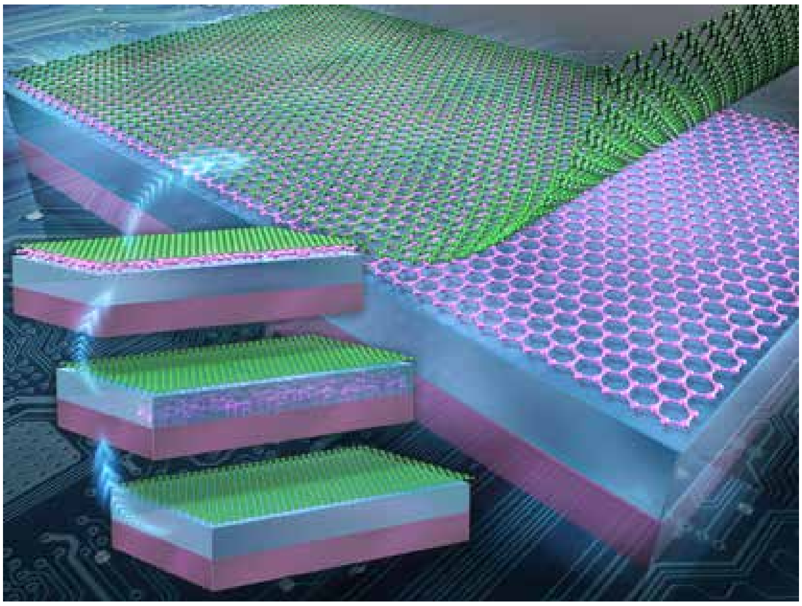
“Self-Temperature-Compensated GaN MEMS Resonators through Strain Engineering up to 600 K”
Liwen Sang *et al.*,
2020 IEEE International Electron Devices Meeting (IEDM) (2020)
DOI : 10.1109/IEDM13553.2020.9372065

[Vol. 69]

Direct Growth of Germanene Marks a Major Step for Electronic Device Fabrication

A team at MANA has succeeded in the direct growth of h-BN-capped germanene on the surface of silver Ag(111). They believe this could be a promising technique for the fabrication of germanene-based electronic devices in the future.

The MANA group grew the germanene at interfaces of graphene/Ag(111) and hexagonal boron nitride (h-BN)/Ag(111) by segregating germanium atoms. A simple annealing process in nitrogen (N_2) or hydrogen/argon (H/Ar) at ambient pressure led to the formation of germanene, which indicated that ultrahigh-vacuum conditions are not necessary in this process. The resulting germanene was stable in air and uniform over the entire area covered with a van der Waals (vdW) material.



Germanene is one of a group of elements with two-dimensional honeycomb lattices, such as silicene, stanene and plumbene, which are collectively known as Xenes. These substances have electronic properties similar to those of graphene, including extremely high carrier mobility. In contrast to graphene, however, the honeycomb-lattice crystal structure of Xenes is not flat, but buckled, which results in their bandgaps being controllable by applying an electric field. Such bandgap controllability would provide a way to overcome the problem of gapless graphene for future electronic device applications. Thus, the utilization of Xenes in electronics is highly desirable.

In another important finding, the group discovered it was necessary to use a vdW material as a cap layer for their germanene growth method, since the use of an Al_2O_3 cap layer resulted in no germanene formation.

The results also prove that Raman spectroscopy in air is a powerful tool for characterizing germanene at an interface.

This research was carried out by Seiya Suzuki (ICYS Research Fellow, International Center for Young Scientists, ICYS-NAMIKI), Tomonobu Nakayama (MANA Principal Investigator, WPI-MANA) and their collaborators.

Reference

"Direct Growth of Germanene at Interfaces between Van der Waals Materials and Ag(111)"
Seiya Suzuki *et al.*,
Advanced Functional Materials 31 [5], 2007038 (12 November 2020)
DOI : 10.1002/adfm.202007038

[Vol. 70]

Flexible Patterning on Liquid Marble Droplets

A team at MANA has created flexible patterning of functional particles on liquid marble droplet surfaces in a patchwork design. Their results show that these droplets can switch their macroscopic behavior between a stable and an active state on super-repellent surfaces in situ by jamming and unjamming the surface particles.

Solid particles in the nanometer to micrometer size range irreversibly attach to liquid surfaces, which has led to new products and concepts, such as powder foam, dry water and liquid marble (LM).

LMs consist of droplets wrapped by hydrophobic solid particles, which behave as a non-wetting soft solid. Thanks to this property, LMs have applications in fluidics and soft devices, and a wide variety of functional particles have been synthesized to form functional LMs. However, it is difficult to form multifunctional LMs by integrating several types of functional particles.

Active LMs hydrostatically coalesce to form a self-sorted particle pattern on the droplet surface. With the support of LM handling robotics, on-demand cyclic activation-manipulation-coalescence-stabilization protocols by LMs with different sizes and particle types result in the reliable design of multi-faced LMs. Based on this concept, the MANA team designed a single bi-functional LM from two mono-functional LMs as an advanced droplet carrier.

The team showed that they can switch LMs' macroscopic behavior between solid and liquid in situ by changing the packing density, whereas most materials require thermal energy and/or pressure to enable switching.

While jamming particles to prepare droplets with solid-like behavior has been studied in the past, the concept of a reversible interfacial jamming transition at the fluid-fluid interface to activate/stabilize LMs offers a new platform for the development of colloidal and soft matter science.
The team believes this property may be of great interest to materials science researchers.

This research was carried out by Mizuki Tenjimbayashi (MANA Independent Scientist, WPI-MANA) and his collaborators.

Reference

"Liquid Marble Patchwork on Super-Repellent Surface"
Mizuki Tenjimbayashi *et al.*,
Advanced Functional Materials 31 [21], 2010957 (19 February 2021)
DOI: 10.1002/adfm.20201095

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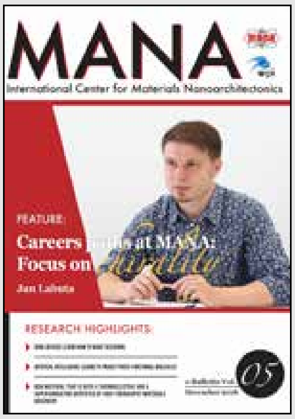

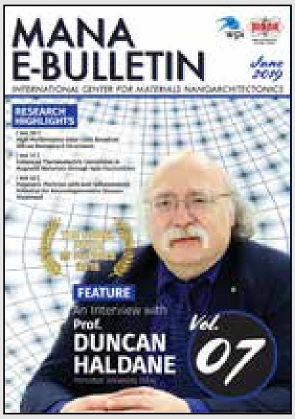

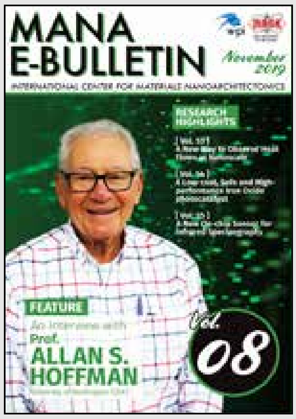

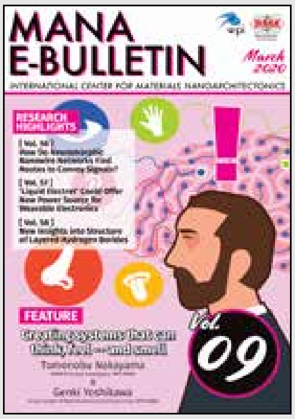

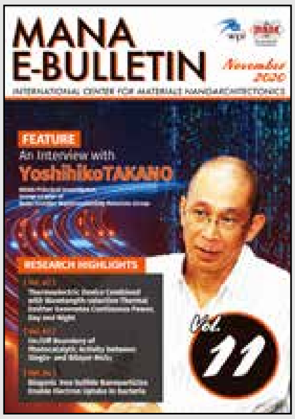

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