Field: ***Physics/Astrophysics***

Planning Group Members:

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Session Topic:

Atomistic Simulation of Materials

Cutting-edge basic science often leads to new technologies and vice versa. One recent example of such good relation between science and technology is “smart material”. This material has sensor and actuator functions so that they can act by themselves under a change of external fields. Oldest smart material is “piezo ceramic” which can change shape by external voltage. It has been widely used for a long time as high-voltage source, fine positioner and so on. Today, many researchers in material science seek for new smart materials having functions required by technology side. In this session, we will see the wonderful new or future smart materials created by the collaboration between science and technology.

The supplementation of electrical equipments to mechanical systems leads to so called mechatronic systems: Its semantic definition (mechatronics = mechanics + electronics) closely follows the development step from passive to actively controlled systems. In order to improve the functionality of mechanical structures, e.g. of automobiles by active reduction of disturbing vehicle vibrations or noise, three types of electronic aggregates are supplemented to solely passive mechanic structures:

- sensors, that measure forces or kinetic quantities,
- control units, that calculates optimal driving for actuators, and
- actuators, that react against the disturbing forces or reduce the kinetic quantities.

The success of such mechatronic systems can be emerged not only from automobile industries, but also from aerospace industries, robotics, medicine technologies and many other technology areas. In order to reduce the volume, the weight and the energy consumption it is required to follow the way of the new technology of smart materials. Smart or functional materials are structurally integrated into so called adaptronic systems. They serve as sensors and actuators in a multifunctional sense because they still have load carrying capabilities. Recent developments in adaptronics are very promising even the actuator power supplies, the sensor conditioners and the controller units are still external aggregats. The synergetic combination of innovative key technologies leads to the generation of a new class of smart material systems. New fabrication methods based on self-organizing effects are proposed to meet required nanoscaled geometries. Furthermore the session will include the outlook to future nanoscaled sensor-actuator systems as fully adaptive systems for technical applications.

Physics/Astrophysics
Planning Group Members: Jens Günster and Sakura Nishino Takeda

Smart Materials: from Macroscopic to Nano Devices

Speaker:
Naruo Sasaki, Seikei University

Theory of friction in nano-machines: Toward near zero-friction lubricant

1. Introduction

Nano- and micro-machines have been expected to trigger the creation of a new and future prominent industry. However, previous work on nano- and micro-machines has produced poor results, and micro-machines have been considered "machines incapable of movement" because of a marked increase in friction. Thus, the realization of a novel lubricity system and/or a novel lubricant, making it possible for microscopic machines to move easily, are strongly desired. Such a lubricant can also contribute to move variety of macroscopic objects.

Therefore in this talk, we will discuss our recent theoretical works of nano-mechanics on evaluating friction force and interaction force acting between the microscopic objects, and costructing near-zero lubricant system, which is one of goals of our works.

2. Basis of nano-friction

As the size of the machine becomes smaller, effects of friction and adhesion due to physical bonding force (ex. van der Waals interaction) and chemical bonding force (ex. covalent bond), become stronger, which prevents machines from moving smoothly. Therefore it is necessary to evaluate atomic-scale friction force by dragging the nano-size needle on the sample surface.

First we have developed the numerical method of evaluating atomic-scale friction force acting between the needle and the sample surface, and have succeeded in reproducing and interpreting the observed results of two-dimensional friction force map of graphite surface[1)-2)]. The mechanism of imaging the two-dimensional map is clarified by studying the stick-slip motion of the tip.

3. Superlubricity of carbon composite - graphite/C_{60}/graphite, and C_{60} intercalated graphite film

Next we have recently developed graphite/C_{60}/graphite system[3)-4)] [Fig.(a)] and C_{60} intercalated graphite films consist of altenating close-packed C_{60} monolayers and graphite layers[5)] [Fig.(b)].Here Graphite/C_{60}/graphite system, where a C_{60} (soccer-ball-shaped fullerene molecule) monolayer is confined between graphite planes, exhibits nearly zero dynamic friction force.Furthermore, C_{60} intercalated graphite films results in superlubricity where both static and dynamic friction forces are observed to be very small, 0.4 nN or less.

The mechanism of the above low friction has been tried to be explained by reducing the problem to the C_{60} motion in graphite/C_{60}/graphite system, proposing a concept of single molecular bearing [Fig.(c)]. Furthermore the role of dynamics of C_{60} molecule in ultra low friction is investigated by using atomistic simulation [Fig.(d)].

4.Conclusion

We have developed a simulation method of atomic-scale friction and recently studied superlubricity of carbon composite - graphite/C_{60}/graphite system and C_{60} intercalated graphite films, developed by our group, which are expected to provide an exciting breakthrough in industrial development.

References

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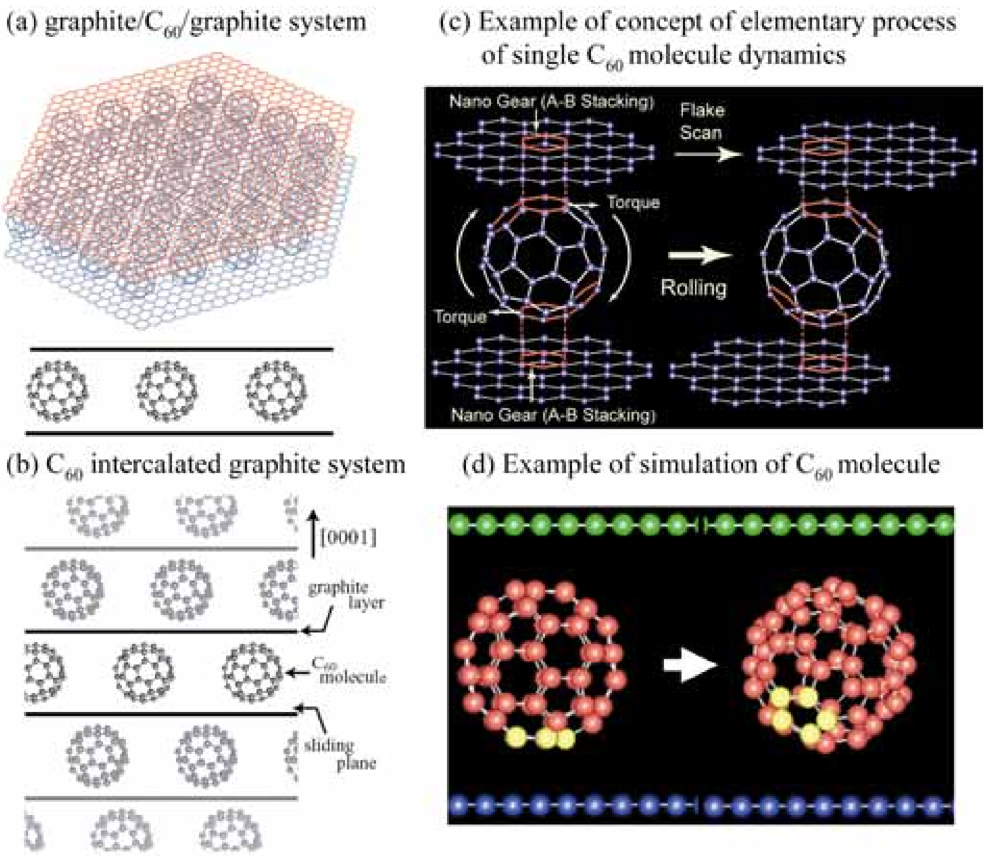
Figures



Physics/Astrophysics
Planning Group Members: Jens Günster and Sakura Nishino Takeda

Smart Materials: from Macroscopic to Nano Devices

Speaker:
Kazuya Terabe, National Institute for Materials

1. Introduction

Many electric devices created by exploiting semi-conducting properties are used in information communication equipment. Advancement in this equipment is greatly dependent on the performance of semiconductor devices. Current advances in micro-structuring and integration technology enable further development of these semiconductor devices. However, their development will be restricted in the near future owing to limitation on their down sizing. Therefore, nanoelectronic devices based on new principles are being investigated in recent years. We have developed a new type of nanodevice, an atomic switch, that could overcome the limitations of current semiconductor devices(1). Atomic switching is accomplished by local control of solid-state electrochemical reaction with a mixed ionic and electronic conductor. Here, we introduce the operation principle, development process, and unique functionality of an atomic switching device.

2. Operation principle of atomic switch

Figure 1 shows solid-state electrochemical property of an ionic and electronic mixed conductor, a silver sulphide (Ag_2S) crystal, in which positive silver (Ag) ions and electrons can migrate in the crystal. As is already known, applying appropriate bias voltage to Ag electrodes of positive polarity at both ends of the Ag_2S crystal reduces the mobile silver ions in the Ag_2S crystal to neutral Ag atoms by precipitating electrons and Ag metal . On an opposite Ag electrode of negative polarity, Ag atoms of the metal electrode are oxidized to Ag ions and are dissolved in the Ag_2S crystal. Because the solid-state electrochemical reaction, $Ag_{(metal)} \rightleftarrows Ag^{+}_{(Ag2S)} + e^{-}$, is reversible, the precipitating and the dissolving of Ag metal can be controlled by switching the polarity of bias voltage.

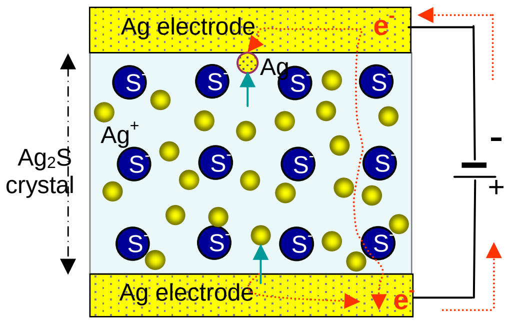


Fig. 1 Solid-state electrochemical property of ionic and electronic conductor (Ag_2S crystal).

The atomic switch that we have developed was achieved by controlling the solid-state chemical reaction on the atomic scale by using tunneling electrons. Figure 2 is a schema of the atomic switch. As shown in the figure, Ag_2S film is stacked on a silver metal electrode. The Ag_2S film faces another platinum (Pt) electrode with a ~ 1-nm gap; this is the key structure of this device. Electrons can tunnel through the gap between the Ag_2S films and the Pt electrode. When an appropriate negative bias voltage is applied to the Pt electrode, tunneling electrons from it reduce the Ag ions in the Ag_2S film to Ag atoms and Ag atoms precipitate on the Ag_2S film, forming an Ag bridge through the gap. The conductance between two electrodes become very high, and in this state the device is switched on. Then, the polarity of bias voltage changes to positive, the silver atoms of the

bridge are oxidized to Ag ions and are dissolved
in the Ag_2S film, thus the bridge shrinks and breaks, so that the device is switched off. Namely, the atomic switch operates by forming and dissolving a silver atom bridge on the atomic scale level, and this can be achieved by local control of a solid-state electrochemical reaction by using tunneling electrons.

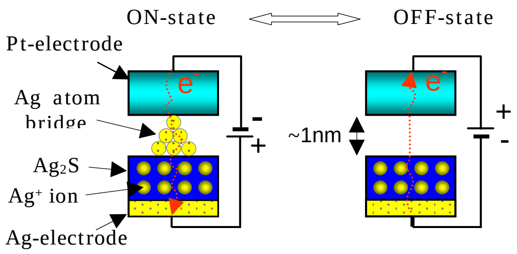


Fig.2 Schema of atomic switch. Switching is accomplished by formation and dissolution of Ag atomic bridge.

3. Development of atomic switch

In initial stage of the atomic switch development, we examined its characteristics with a scanning tunneling microscope (STM) combined with a scanning electron microscope. We used Ag_2S needle-like crystal on Ag wire as an STM tip. The tip was made to approach a Pt substrate until tunneling current could flow between the tip and the substrate; specifically, we obtained a 1-nm gap. We thus confirmed that forming and breaking a silver atom bridge between the tip and the substate could be achieved with local control of the solid-state electrochemical reaction by using tunneling electrons, and further, that switching operations could be achieved. We found that the rate of the formation and dissolution, in other words the switching rate, exponentially increased as the applied bias voltage increased.

Our experiments to date have confirmed a switching rate of 1 MHz. Furthermore, controlling contact point of the Ag atom bridge with the Pt substrate on atomic scale generated quantized conductance. We found that applying a pulsed bias voltage could control switching between quantized conductances. Recently, we found that the atomic switch can be formed at each crossing point when an Ag_2S wire is crossed by Pt wire. The crossbar structure was fabricated with a conventional nanofabrication method for semiconductor devices, and this demonstrates that manufacturing the atomic switch as a practical application device is feasible.

In conclusion, we have developed a new type of nanoelectronic device, an atomic switch that is operated by exploiting a new principle. We believe that its simple structure, ease of operation, and unique function will enable its use as an element in future nanodevices, and that the developed atomic switch will make possible conceptually new electronics that will be part of a new computer architecture.

References

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