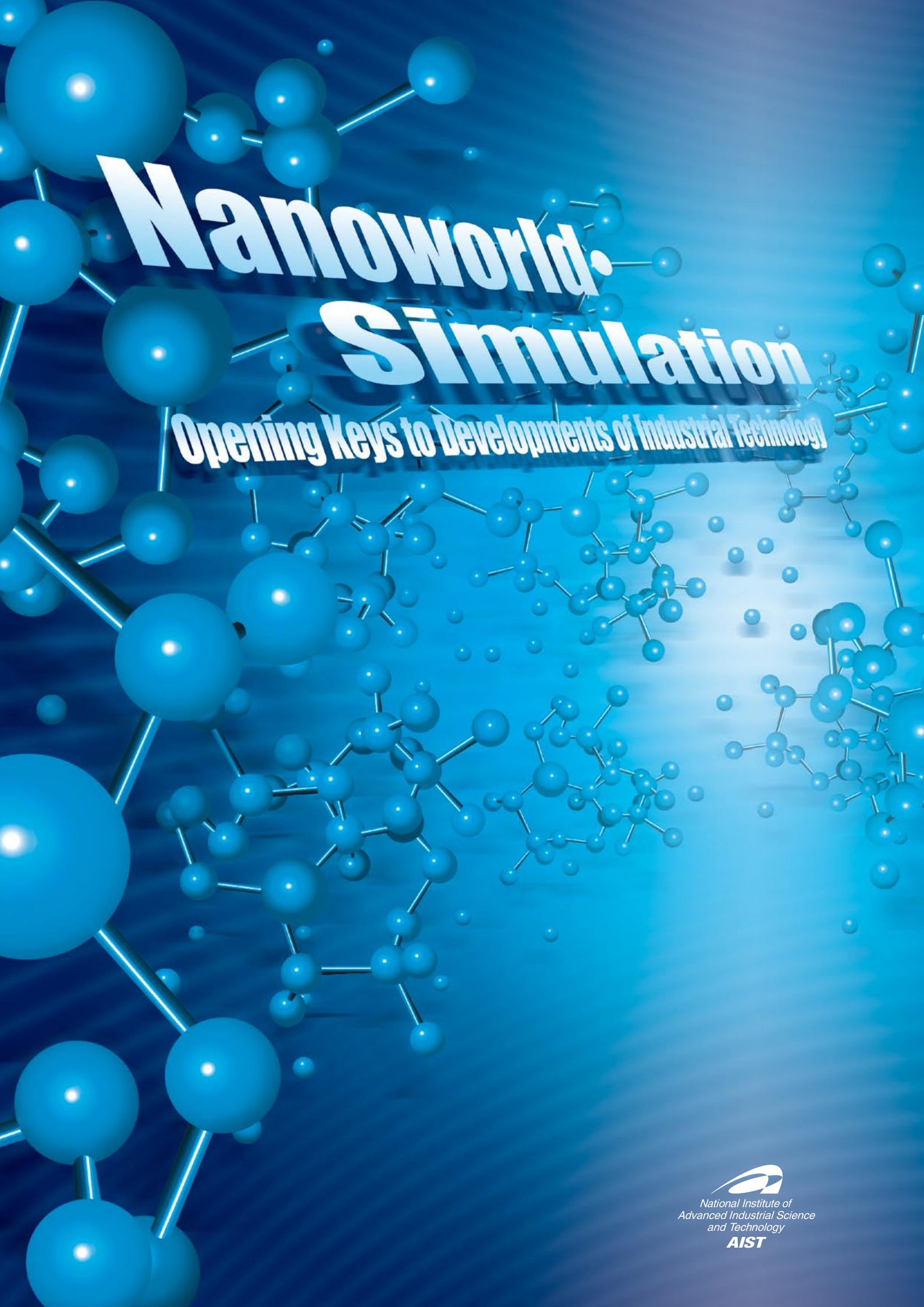

National Institute of
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and Technology
AIST

Computational Science that Supports the Development of Industrial Technology

Computational science and industry

The simulation technology has supported the advanced industrial technologies, and has promoted innovation in these fields. In the 21st century, with the emphasis on developing a sustainable society as well as enhancing the industrial competitiveness, the importance of simulation technology has grown even stronger. Especially in the leading technological fields as nanotechnology and biotechnology, the simulation technology has become indispensable. In the nanoregion, the quantum effect and phenomena specific to nanosize dominate. As a developing tool, simulation is indispensable in understanding these phenomena and in formulating materials and devices that are usable in industry.

Simulation technology that leads the high-tech industry

In the semiconductor industry where the microfabrication technology is advancing, there is a demand for a break-through technology for processing the surface and the interface. The simulation technology is essential for the formation of a nanoscale structure and for high-precision functional predictions, especially with the next-generation semiconductor nanodevice.

In advanced molecular electronics, basic knowledge is still being accumulated and it is important to observe and to understand various phenomena of interaction of molecules with the surrounding electrodes. Here, the simulation technology is also a prominent developing tool. It is needed, not only in molecular electronics, but also in many industrial areas as organic electronics, spin-electronics, areas of membrane and electrode reaction of fuel cells and others.

In the bio field, there is a demand for clarification of the functional expression mechanism of RNA and protein, and for designing and developing drugs or biodevice based on this knowledge. The fragment molecular orbital method developed by AIST (Figure 1) is expected to become a powerful tool for development.

A Beacon which points the path of innovation

As the computational performance evolves from the present tera (10^{12}) FLOPS to peta (10^{15}) FLOPS, the simulation technology will also advance and will be able to handle a more realistic system. Of course, this does not mean that we can totally simulate the real system, but in the development of industrial technology, this achievement is important. In countries all over the world, effort is poured into innovative creation for enhancing industrial competitiveness and for the construction of a sustainable society. The nanosimulation technology which is opening new doors in the nanoregion is expected to strongly promote innovation.

With all the needs and importance considered, at AIST, we intend to energetically develop simulation technology including software development with the Research Institute of Computational Science at the center. We aim to become the beacon of innovative creation in industrial technology development. (Simulation examples are shown in Figure 2.)

Research Coordinator
(Nanotechnology, Materials & Manufacturing)
Kazuo Igarashi

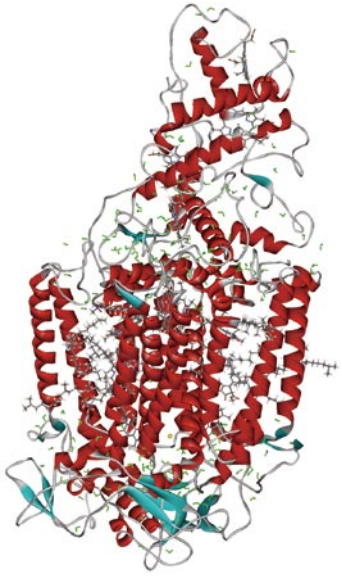


Figure 1: Simulation of a protein with 20,000 atoms (a photosynthetic reaction center complex of purple bacteria) done by computation with the fragment molecular orbital method

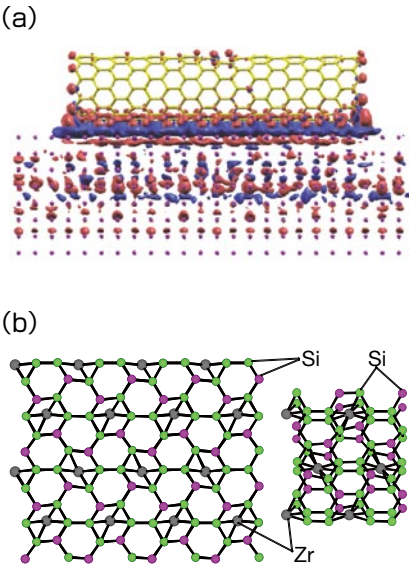
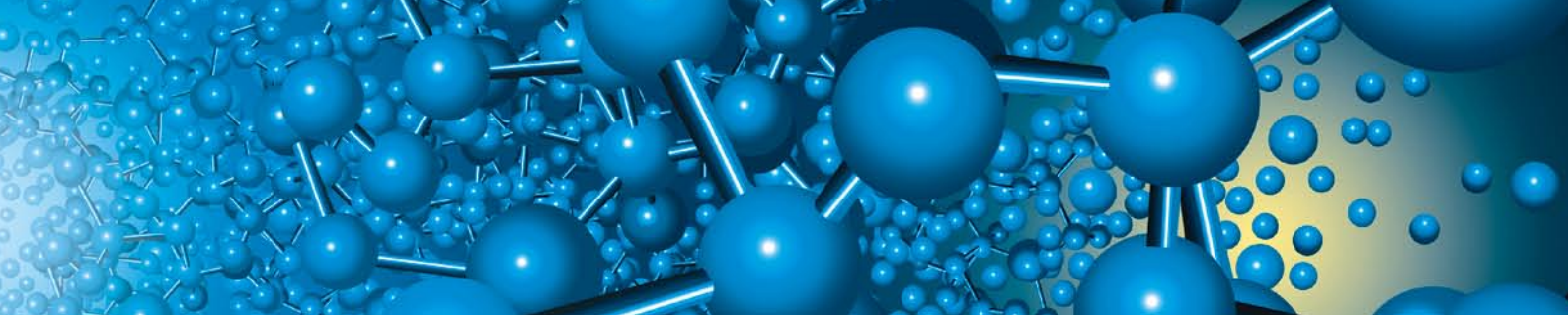


Figure 2: (a) Simulation of the difference of electron density of a zigzag carbon nanotube (10,0) on the aluminum (001) surface using the Order N method (OpenMX)
(b) Simulation of a silicon ultra-thin film semiconductor suggested with the ultimate miniaturization of MOS transistor in mind



Simulation of Nano-spin-electronics Device

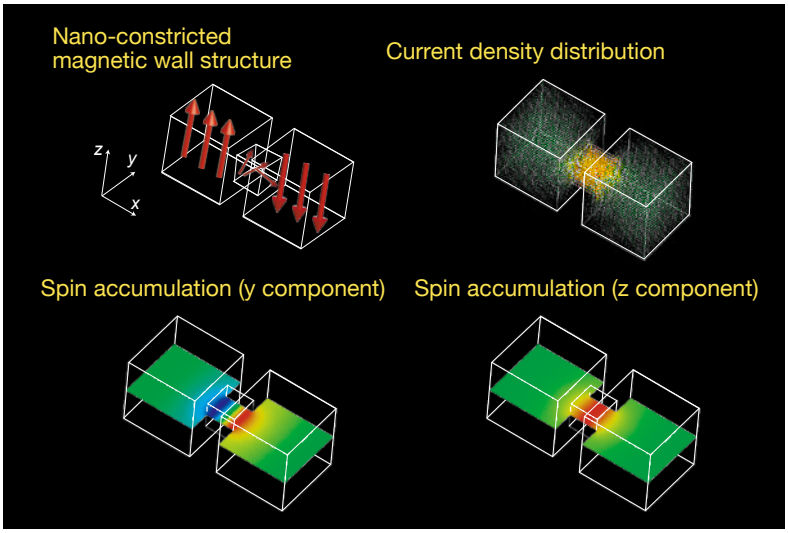
What is “nano-spin-electronics” ?

Electron has two kinds of degrees of freedom, the electric charge which has an electric property, and the spin which has a magnetic one. In conventional electronics, only the degree of freedom of the charge has mainly been used in semiconductor devices such as transistor, and only the degree of freedom of the spin has been mainly used in magnetic devices as hard discs.

In recent years, with the rapid progress in microfabrication technology, it has become possible to create a device that uses semiconductor and magnetic materials in a nanometer scale. Thus a new field called “nano-electronics” was born. When the device is made on a nanometer scale, it becomes possible to maneuver the electron at a higher level as in handling the spin using electric current or electric field and in manipulating the electric resistance of a nanosize spin structure. In nano-spin-electronics, we skillfully control the electron’s degree of freedom of both the charge and the spin in nanoscale microscopic structure, and develop advanced information processing devices. We are presently developing such devices as quantum repeater, spin transistor, nonvolatile magnetic memory, and a readout head for ultra high-density magnetic recording.

Simulation of a nano-spin-electronics device using the finite element method (FEM)

In collaboration with Toshiba Corporation and Tohoku University, we are developing a readout head for ultra high-density magnetic recording using the magnetoresistive effect which arises with a nano-constricted structure. Specifically, we aim to realize a new device which uses the giant magnetoresistive effect of ferromagnetic metal atom thin line which is presently detected only in basic research.



The current distribution and spin buildup of a nano-constricted magnetic wall structure

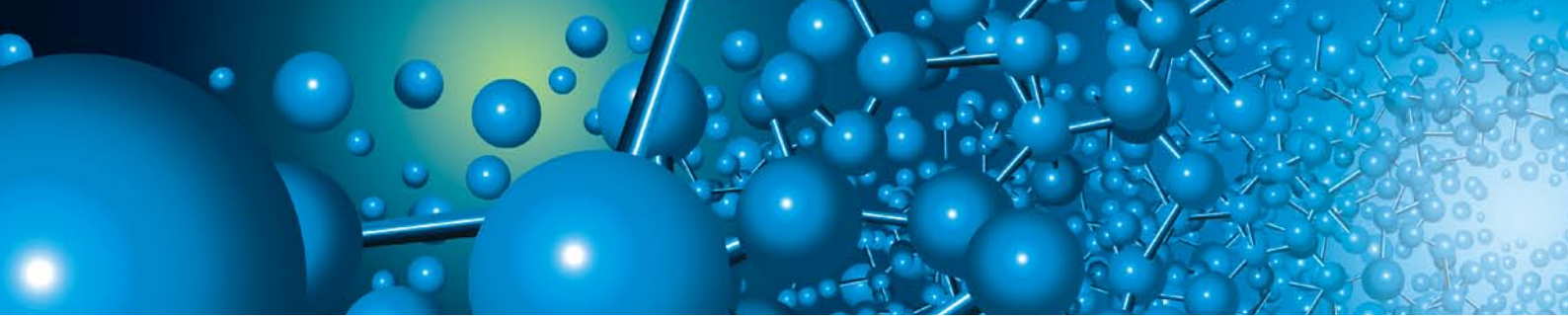
The realization can be done by stably building a nano-constricted structure of ferromagnetic metal in oxide insulator film by using the self-assembly method. With computer simulation, we elucidate the operating mechanism of the device, predict its operation properties, and design high-performance devices.

Figure shows an example of the current distribution and the spin accumulation of a nano-constricted magnetic wall structure derived by simulation. The simulation was done by numerically solving the transport equation of the electron by using the FEM method with consideration of the spin structure. In our simulation, the variation of electric resistance from the change in the spin structure is induced by the shift in the spin accumulation around the magnetic wall. The experimentally observed dependence of magnetoresistance on the resistance area product is well reproduced by the simulation, we think that the cause of the magnetoresistive effect is the spin accumulation around the magnetic wall.

In order to apply this device to the readout head of ultra high-density magnetic recording, we need to simulate the movement of the magnetic wall induced by electric current, as well as the noise that it causes. We will do research on the dynamics of such device, and not only promote its practical use but also propose a new nano-spin-electronics device.

The development that is introduced here is done as a consignment of “Development of nano-constricted magnetic wall type HDD magnetic head device by using self-assembled nanopatterning method” NEDO Research and Development of Nanodevices for Practical Utilization of Nanotechnology. I would also like to thank Akira Tezuka of the Advanced Manufacturing Research Institute of AIST for his useful advice.

Nanotechnology Research Institute
Hiroshi Imamura

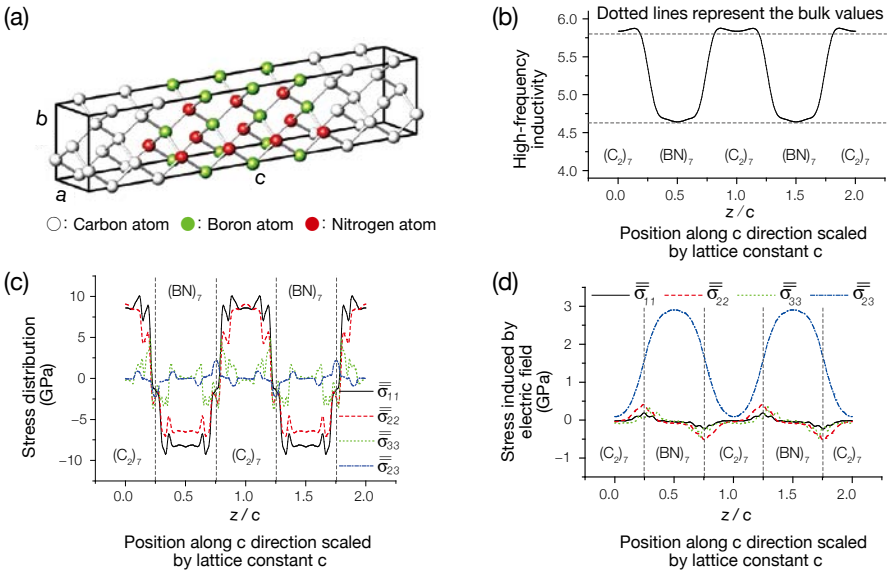


Simulation Software Accelerates the Device Industry

Research background

A device is basically a stacking structure of heterogeneous materials. Not only the constituent materials themselves but also the bonded surface or interface plays an important role. With our in-house software, QMAS[1], as a platform, we have been developing and improving unique computational tool for studies of systems including interface. We are also performing practical application studies.

Here, we introduce functions of several tools and examples of apllication studies for a model substance, a superlattice consisting of diamond and cubic BN (boron nitride) that are regarded promising as future device materials (Figure (a)).



The distribution of dielectric constant

Dielectric constant is one of the most important physical properties for electronic devices. With QMAS, electronic-structure calculations under a uniform electrostatic field can be performed. From the polarization induced under the field, the dielectric constant and its one-dimensional distribution can be obtained with high precision. As shown in Figure (b), the high-frequency dielectric constant has a modulation that corresponds to the superlattice period, and the increase of dielectric constant can also be confirmed in the area around the interface.

The distribution of stress and the influence of electric field[2]

As the lattice constant of diamond is 1.4 % smaller than that of cubic BN, it is predicted that the tensile stress exists in the diamond area, and the compressive stress exists in the BN area, within the plane that is perpendicular to the stacking direction of the superlattice.

With QMAS, the distribution of stress can be computed. The behavior of the inplane stress component of $\bar{\bar{\sigma}}_{11}$, $\bar{\bar{\sigma}}_{22}$[3] shown in Figure (c) confirms the prediction. The moment electrostatic field is applied parallel to the stacking direction, forces are applied on the polar boron and nitrogen atoms as well as carbon atoms at the interface. This corresponds to the shear stress field existing mainly in BN layer (Figure (d)). After the atomic-position relaxation, this shear stress field spreads almost uniformly throughout the superlattice. When a device is prepared and when electric field is applied, stress is induced within the device. Another characteristic of QMAS is that the magnitude and distribution of such stress components can be computed.

Future development

On the development of semiconductor devices, various difficulties lie in the path of further refinement for better performance. One possible breakthrough is the introduction of new functional materials such as transition metal compounds. With such materials, more precise descriptions are required concerning the magnetism and the electron correlation. We intend to deal with whatever problems that may arise by using the most advanced computational technologies with QMAS as a platform.

Research Institute for Computational Sciences

Shoji Ishibashi

Related information

[1] QMAS (Quantum MAterials Simulator): *ab initio* simulation software package based on the plane-wave basis set, the Projector Augmented-Wave method and the LDA/GGA. Aiming for future public release, the following people are involved in the development: Shoji Ishibashi, Tomoyuki Tamura (Research Institute for Computational Sciences, AIST), Shingo Tanaka, Masanori Kohyama (Research Institute for Ubiquitous Energy Devices, AIST), Kiyoyuki Terakura (Research Center for Integrated Science, Japan Advanced Institute of Science and Technology). We are receiving cooperation from other members of the research institutes mentioned above, as well as from National Taiwan University and Tamkang University.

[2] Relevant article published in Phys. Rev. B **76**, 153310 (2007).

[3] The double line over the symbols indicates that planar and microscopic averages are taken for the corresponding quantity. For details, see the above reference.

Development of the Order N Method

What is the *ab initio* calculation / first-principles calculation?

In recent years, a new calculation method called "*ab initio* calculation" is widely used. With this method, it is possible to calculate various physical quantities such as energy, stable structures, vibrational spectra, diffusion constant and so forth of a system from only basic equations of quantum mechanics, without using the parameter attained by experiments. Now we can normally deal with systems of around 500 atoms at most.

On the other hand, "molecular dynamics" has been widely known as the study of the behavior of a large number of atoms by numerically solving the Newton equation of the atoms. By using the *ab initio* calculation to compute "the force applied to each atom", it is possible to combine the two methods, and this is called "*ab initio* molecular dynamics".

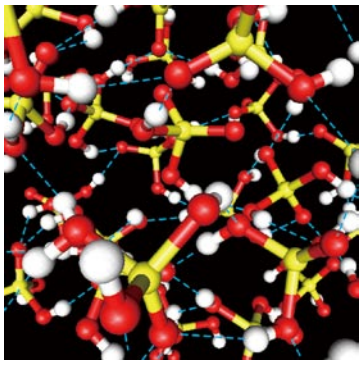
We have been successful in obtaining much information by *ab initio* molecular dynamics calculations, of mainly systems that are related to fuel cells as concentrated phosphoric acid, sulfuric acid solution, and Nafion / water interface. Especially, with such phenomenon as the proton transfer in solution, it is extremely difficult to handle with other calculation methods. However, with *ab initio* calculation, we are able to understand it at an atomic level.

The problem with *ab initio* calculation

Although *ab initio* calculation is an extremely useful method, the biggest problem it has is that the work load is huge. For example, the time needed for one step to calculate the molecular dynamics of about 500 atoms is about 2 or 3 minutes, even if we monopolize a parallel computer of a large scale of about 100 desk top PCs. In order to acquire enough data accuracy, we need at least 10,000 steps, and, including the preparatory calculations, it often takes over a month. Moreover, the work load increases in proportion to the cubed number of atoms in a system, and therefore, even a computer of a speed ten times as fast, can only deal with a system of twice the comparative size. On the other hand, if we want to make an exact model of complex systems that are often targeted in nanotechnology and biotechnology, ability to deal with 500 atoms is not enough. For example, if enough number of water molecules is arranged around a macromolecule, there would be thousands of atoms.

The appearance of the order N method

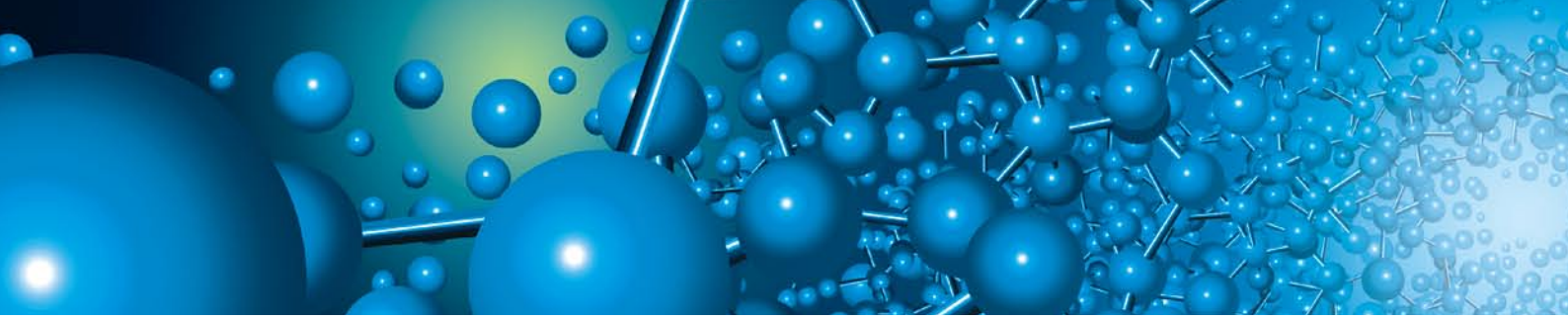
In order to avoid such problems with *ab initio* calculation, a new algorithm was proposed called "the order N method" in the 90s. This method was revolutionary as its computation time was relatively in proportion to the number of atoms with equal results. Many researchers became interested in this method and several algorithms as the divide and conquer method and the density matrix method were proposed. However, gradually it became clear that none of the methods were sufficiently reliable or their performance satisfactory. The situation was stagnated for a long time. Recently, however, with advancement of the algorithm including ours, the order N method has finally reached a practical level. Part of it is shown in the publication by Dr. Ozaki (presently associate professor of Japan Advanced Institute of Science and Technology) incorporated in Open MX which uses atomic basis. (ref. Figure 2 (a) p.2)[3] Furthermore, we have added a new order N idea to FEMTECK, the *ab initio* calculation program that we have been developing which uses the finite element basis. Using this program, we have already proven that the order N method can be applied to systems with about 3,000 atoms maximum. We are presently carrying out several of such demonstration computations at a large scale.



The state of hydrogen bond in concentrated phosphoric acid is shown in broken line.

Research Institute for Computational Sciences
Eiji Tsuchida

Reference
[1] http://staff.aist.go.jp/eiji.tsuchida/jp_index.htm
[2] "The Nano-Simulation Handbook", Nano-Simulation Handbook Committee edit., Kyoritu Shuppan Co., Ltd. (2006)
[3] http://www.openmx-square.org/



Prediction of Physical Property of Film Materials for Biosensors

Introduction

Molecular film has various structures and properties from artificial biosensor molecular film to natural cell membrane.

What determines these structures and properties is the molecular structure of a single molecule that composes the molecular film, the intermolecular interaction, and the thermal fluctuation. The structure of a single molecule can be determined experimentally with X-ray structural analysis, but it is difficult to measure the intermolecular interaction and the thermal fluctuation directly through experiments. As the most appropriate method for analyzing the intermolecular interaction, there is *Ab initio* molecular orbital method which is the numerical method in quantum mechanics. Moreover, using the intermolecular interaction, molecular simulation, which is the numerical method in statistical mechanics, is the best way to analyze the structure and the physical property of the molecular aggregate.

Here, I would like to present how useful molecular simulation is in the development of tetraether-type lipid membrane, which is regarded promising as a device for bioreactor, biosensor and others. For the calculations presented here, the high-precision high-speed general purpose molecular simulation program (MPDyn) [1] was used.

The development of lipid membrane and the molecular simulation

The structural stability of the lipid membrane and the permeability of low molecules and ions change drastically, depending on the structure of the lipid molecule that forms the membrane. This indicates that there is a possibility that a lipid membrane with a new function can be formed by using a new synthetic lipid molecule. The development of materials using synthetic lipid is actively promoted in the field of biotechnology in which such devices as bioreactor, biosensor are constructed.

Meanwhile, the membrane of archaebacteria that survives in harsh environments of high temperature, low pH, high-salt concentration etc., is thought to have high stability and low permeability. These properties are needed in the above mentioned devices. Therefore, archaebacteria-type synthetic lipid has been developed, and, the membrane made of this material has proven to actually be stable against outside stress and to be difficult for protons to penetrate through.

The molecular structure of lipids that form the archaebacteria membrane has distinct characteristics of: 1) its hydrophobic chain having many methyl branches, 2) the hydrophobic chain and glycerol being ether-bonded, 3) the membrane containing transmembrane-type lipid molecules with two polar groups. It is important to know what influence these characteristics have on the stability and the permeability of the membrane when designing the synthetic lipid molecule. To attain such information, the molecular simulation, which builds a model based on the molecular structure and analyzes the physical property of the molecular aggregate, is one of the most effective research tools.

Here, we will introduce our research based on the molecular dynamics (MD) simulation of the archaebacteria lipid membrane [2]. The aim of this research is to provide a guideline for designing synthetic lipid by studying the influence of the lipid molecule structure on the physical property of the membrane.

The physical property prediction of lipid membrane for biosensor

Natural tetraether-type lipid, tetraether phosphatidylcholine (TEPC), has a cyclic structure (TEPC of Figure 1) and forms not a bilayer but a monolayer film. Cyclic tetraether-type lipids are rigid and, therefore, often difficult to use in devices. Thus, in the field of bio materials, the pseudo-cyclic-type lipids (acyclic tetraether phosphatidylcholine: a -TEPC) is anticipated to show physical properties intermediary of diether-type lipid, diphytanyl phosphatidylcholine (DPhPC), and cyclic tetraether-type lipid. However, the physical property pseudo-cyclic-type lipid membrane has not been sufficiently predicted.

In this study, as shown in Figure 1, the physical properties of membrane made of DPhPC, a - TEPC, and TEPC have been predicted by MD simulation.

The MD simulation was done with isothermal isobaric conditions (298 K, 0.1 MPa). To reach equilibrium, the MD calculation of 2 ~ 5 ns was first performed, and then was followed by the long time MD calculation of 25 ns. Figure 2 shows the probability distribution and the time-dependeuce of the surface area of the lipid membrane. Compared to DPhPC, TEPC and a - TEPC show smaller surface area as their thermal motion of the hydrophobic chain is restricted. TEPC also shows a surface fluctuation of extremely long time constant (>10 ns). When the elastic modulus is calculated from the fluctuation,

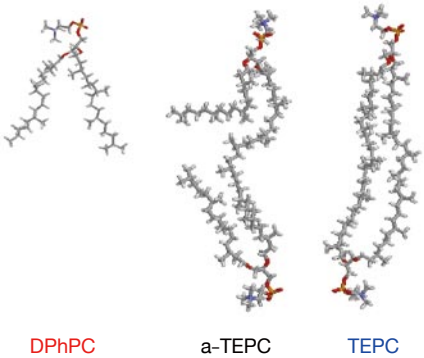


Figure 1: Structure of lipid molecule

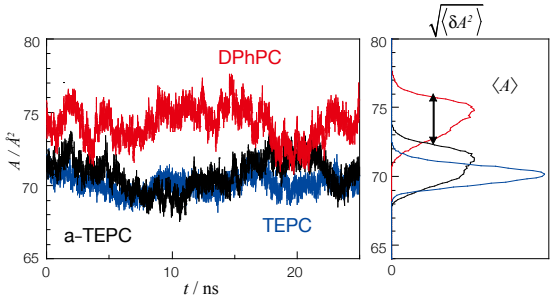


Figure 2: Time variation of film surface area of each lipid molecular film

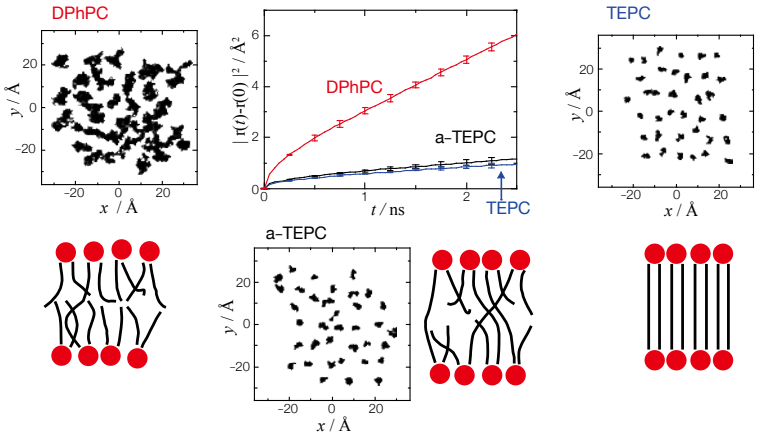


Figure 3: MSD of centroid of each lipid molecular film, and the type drawings of the molecular centroid tracing within the film surface and also the schematic molecular film structure

DPhPC is 0.67, a – TEPC is 0.71, TEPC is 2.02 N/m^2, which shows that TEPC solely has three times the elastic modulus than the others.

Figure 3 shows the mean square displacement (MSD) of the molecular centroid and the tracing of the molecular centroid. Again, compared to DPhPC, the MSD of a – TEPC and TEPC show values one fifth or less, and therefore, proved to be stable.

From the results, we can see that, of the transmembrane tetraether-type lipid, compared to TEPC, a – TEPC has a film elasticity closer to DPhPC which forms a normal bilayer film and has a mechanical property of being softer. Furthermore, a – TEPC is as stable as TEPC. The conventional cyclic type lipid has been considered as too hard and too breakable to be used for experiments. Now, this research has shown that the pseudo cyclic type ripid has a low elastic modulus. These results suggest that a – TEPC is a possible ideal membrane material that has both the necessary flexibility and the stability.

Summary

The elastic modulus can be calculated precisely with MD simulation, and this has enhanced the possibility of actual membrane design by molecular simulation. We think that such membrane designing by molecular simulation will be put to practical use.

Molecular simulation is not only limited to the development of membrane for biosensor. Recently we are advancing "The Research and Development of a Drug Delivery System (DDS) Simulator", a project of Basic Research Program of Japan Science and Technology Agency. With this project, the multi-scale simulation technology for drug delivery system that uses liposome (a technology that combines molecular simulation with molecular orbital method and fluid simulation) is being developed.

Acknowledgements

The research on lipid membrane mentioned here is the result of a collaborative research done with Dr. Wataru Shinoda, Dr. Keiko Shinoda of Research Institute for Computational Sciences (Now Dr. K.Shinoda is at Mitsubishi Chemical Group Science and Technology Research Center, Inc) and with Dr. Teruhiko Baba of Research Center of Advanced Bionics, AIST. I would like to express my gratitude to all three.

Research Institute for Computational Sciences
Masuhiro Mikami

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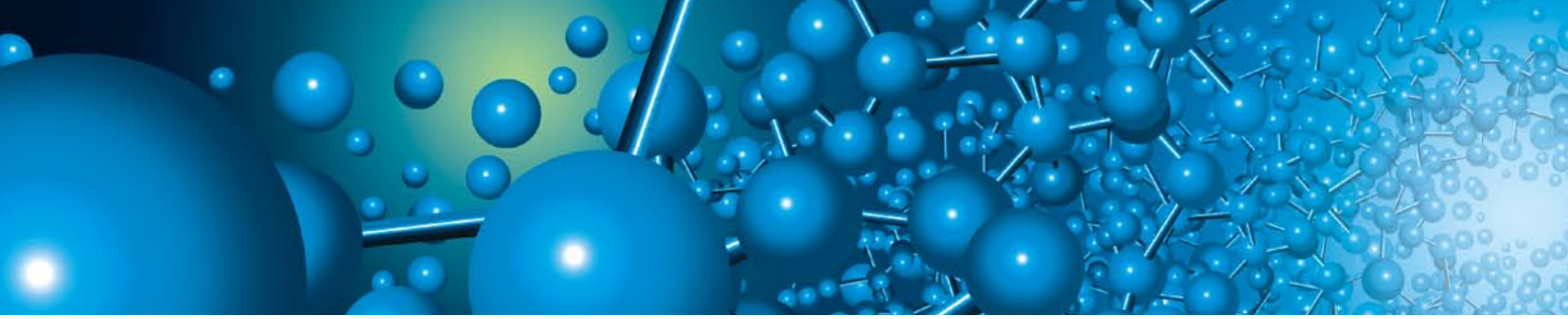

The Reaction and Conduction of Hydrogen Ion (Proton) —Fuel Cell and Beckmann Rearrangement Reaction—

Hydrogen ion (proton) H^+ whose concentration (more precisely, activity) is expressed by pH, plays an important role in various areas around us. In polymer electrolyte fuel cell which is regarded promising as energy source for cars, mobile electronics, etc., high proton conductivity and long life is expected of the polymer electrolyte membrane which separates positive and negative electrodes.

Proton relay

As a unique property, hydrogen ion in aqueous solution is known to have higher ionic conductivity of one figure more than other ions.

This is not because hydrogen ion is small in size, but is because its charge moves at extremely high speed by exchanging proton with surrounding water molecules as shown in Figure 1. This idea, which is called proton relay or proton hopping, was suggested by Grotthuss 202 years ago[1].

It was 10 years ago that this Grotthuss mechanism of proton transfer dynamics was visibly shown with first principles simulations[2]. Three years ago, we demonstrated by first principles simulations that proton in supercritical water induces Beckmann rearrangement reaction which is used in the manufacturing process of ε-caprolactam, the raw material for nylon[3].

By first principles simulations, we are now looking at the movement of hydrogen ion within the electrolyte film (Nafion) which is presently an essential element of fuel cell.

For chemical reaction within the fluid and for fluid itself, the dynamics of atomic level is important and thus, first principles simulation becomes effective.

The Beckmann rearrangement reaction in supercritical water and hydrogen bond network

The density of water at room temperature and at atmospheric pressure is 1 g/cm^3, and the water molecules are bound together by the hydrogen bond. The hydrogen bond is a weak bond between the hydrogen atom of the water molecule and the oxygen atom of a neighboring water molecule (this bond is weaker than a chemical bond but stronger than the usual intermolecular interaction). A hydrogen bond network is formed within the water. The hydrogen ion in aqueous solution exists as hydronium ion (H_3O^+) with one addition of water molecule. A hydrogen bond network exists around it as well, and therefore, hydrogen ion is at a stable state.

In supercritical water, the water density is smaller than 1 g/cm^3, and therefore, the hydrogen bond network becomes incomplete as is shown in Figure 2. Because of this, we have confirmed by first principles simulation that, triggered by hydrogen ion, Beckmann rearrangement reaction occurs. We have also confirmed by first principles simulation that, even at thermodynamically supercritical temperatures, if the density is 1 g/cm^3 (this is experimentally difficult to attain), hydrogen bond network is formed and Beckmann rearrangement reaction does not occur. We have finally confirmed that, although it is a reaction at high temperatures in supercritical state, the temperature is not the factor but the density is an important cause. At temperature lower than supercritical point, phase separation of liquid and gas occurs, and proton either becomes stable within the solution or it doesn't exist at all (within gas). Industrially, concentrated sulfuric acid which is a dangerous substance is often used. By first principles simulation, we know that the reaction can be regulated by controlling the hydrogen bond, without the use of dangerous substances.

Thus, we have reproduced on computer, by first principles simulation, the Beckmann rearrangement reaction in supercritical water which was discovered by the late Dr. Ikushima of AIST Tohoku[4]. We have also clarified its reaction mechanism.

First principles simulation of Nafion

In fuel cell, hydrogen is supplied to the negative electrode and hydrogen ions (protons) are produced. These move

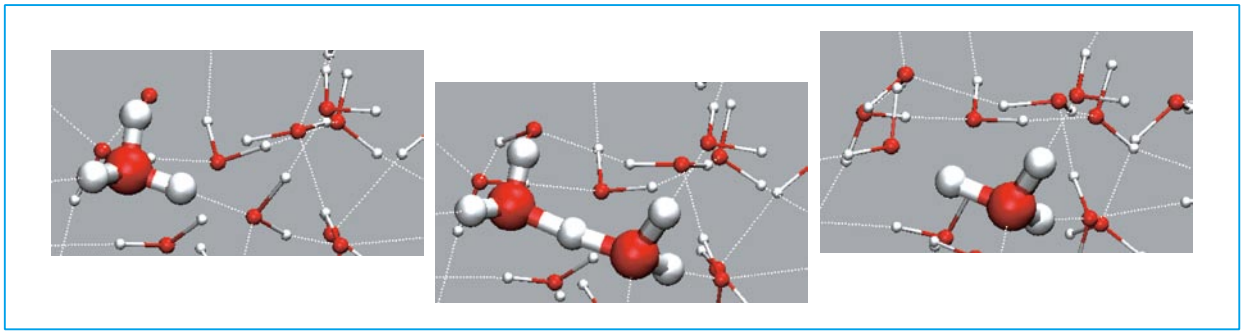

Figure 1: The scheme of proton conduction according to Grotthuss mechanism
● : oxygen ○ : hydrogen

through the proton conductive membrane to the positive electrode and reacting to the supplied oxygen, it produces water. As the proton conductive membrane which separates positive and negative electrodes, the fluorinated polymer electrolyte represented by Nafion, a product of DuPont, is used. There is a demand for a membrane that works in a larger temperature range of longer life-time, and of lower cost. Not only fluorinated polymer but hydrocarbon polymer is drawing attention. How does hydrogen ion conduct within such polymer? To know such mechanism is important in developing a new membrane.

The fluorinated polymer membrane has a meso structure with phase separation between the water part and the back bone structure of the polymer molecule. To simulate this with first principles method is, by its real size, impossible. Therefore, we made an atomic geometry that has a structure similar to a partly-extracted meso structure by using the classical molecular dynamics simulation at Toyota Central R&D Labs. Inc., the lab having experience in meso-simulation. We first made the atomic geometry of two kinds of Nafion with different water content, and then made first principles simulations of about 20 ps. For the simulation, we used FEMTECK, the first principles molecular dynamics program with finite element method base introduced on Page 5 that we developed. Because the total number of atoms is around 400, and because it contains many fluorine atoms which have many electrons, the calculation load is very high. By using the 49 node (98CPU) of

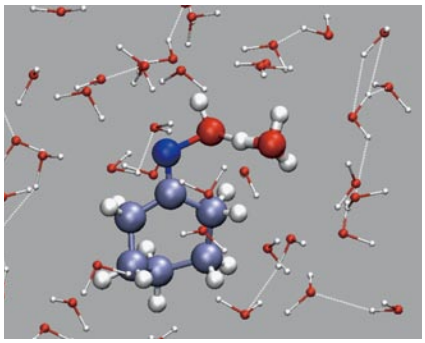

Figure 2: Cyclohexanone oxime and its surrounding hydrogen bonds in supercritical water
● : oxygen ○ : hydrogen ● : carbon
● : nitrogen

AIST Super Cluster P32, we were able to simulate about 2 ps in a week.

As a result, we now understand how hydrogen ion is transported in electrolyte membrane through the hydrogen bond network. With FEMTECK, a calculation with uniformly applied electric field is possible, and the ion movement can be directly followed. As a result of the simulation, how hydrogen ion conducts while interacting with sulfonic group has become clear. We now know that the movement is affected by the water content. Furthermore, we can grasp the behavior of water transport which is problematic in water control of fuel cell.

Of what has been presented here, the reaction simulation within supercritical water is from the collaboration with Dr. Boero Mauro, Associate Professor at Tsukuba University, and others. Concerning Nafion, the results are from the research, JST – CREST research project, " Nano-simulation of Electrochemical Two-Phase Interfaces", with Toyota Central R&D Labs. Inc., NEC Nano Electronics

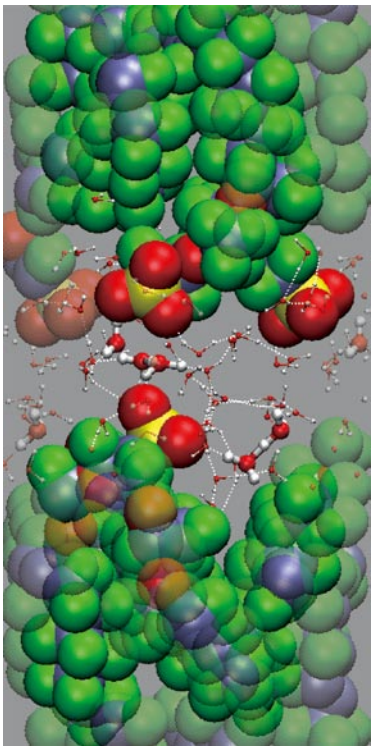

Figure 3: A snap shot of hydrogen ion conduction in Nafion
● : oxygen ● : sulfur ● : fluorine ● : carbon
○ : hydrogen. The water molecules are shown as small balls. Amongst them, the hydronium ion atoms are shown as larger balls. The pale parts express out of the unit cell under the periodic boundary conditions.

Research Laboratories, the Institute for Solid State Physics, University of Tokyo and the Institute of Scientific and Industrial Research, Osaka University. With the latter, we have been successful in simulating the electrode reaction under bias voltage by first principles method.

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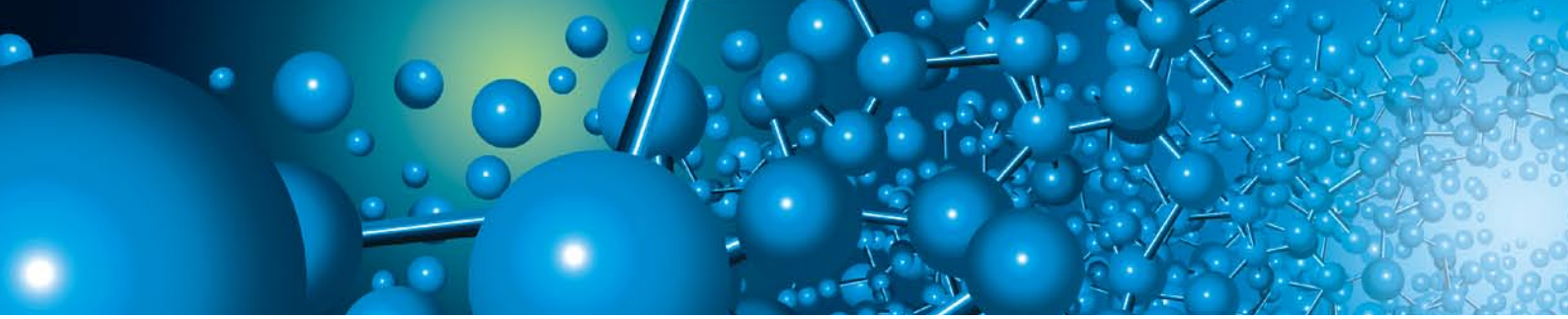


Basic Theories Expanding Realms of Simulations

Virtual observation of the transient phenomena in nano-space

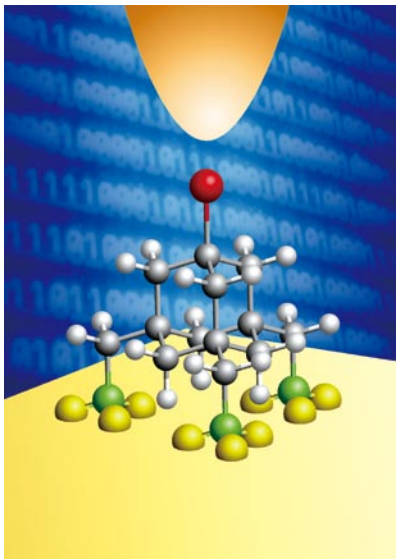
With the help of rapid progress in simulation method, the possibility of "virtual observation" of the transient phenomena of materials in nano-space becomes more and more realistic. Accordingly, computational science in nanotechnology will dramatically gain importance. In order to speed up such development, it is crucial to emphasize the importance of the basic theory of simulation, to promote large-scale high-accuracy calculation strongly, and to develop model theories for generalizing the obtained results.

The conventional simulation in material science has been limited to the ground state or the equilibrium state, and has never been applied to the behavior of materials under real dynamical environment where non-equilibrium effects are quite large. However, the situation has been changing.

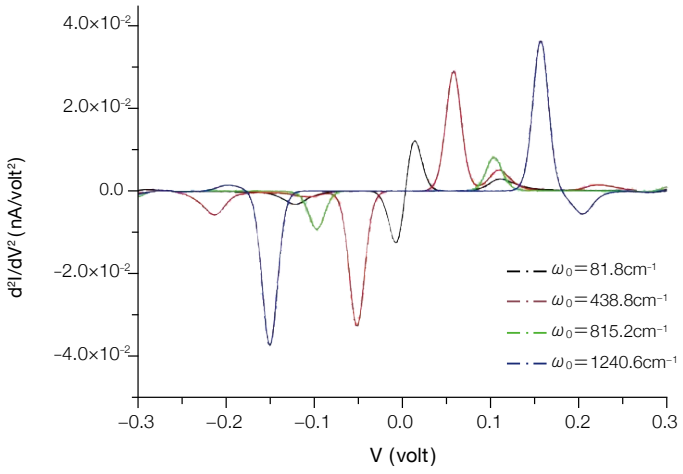
Ever since Gerd Binnig and Heinrich Rohrer invented the scanning tunneling microscope in 1982, the most important feature of nanotechnology is the measurement, the observation and the operation at atomic or molecular scale. In recent years, it has become possible to simulate non-equilibrium phenomena at atomic scale. The simulation technology thus developed may become an indispensable tool assisting nanotechnology research.

Transport properties through a single molecular bridge junction

Here are two examples. One example is the molecular vibrational excitation accompanying electric current through a single molecule. In bulk materials, a normal behavior, i.e., an increase in resistance when electrons are scattered by phonons, is observed. On the other hand, when electric current flows through a single organic molecule, it is known that an unconventional behavior appears of an increase in the electric current accompanied by the vibrational excitation of the molecule. It may be understood that conductive channels are forced to be opened at expense of vibrational excitations. Recently, it has become possible to predict theoretically under what conditions of molecules and electrodes, an increase of resistance or an increase of electric current is obtained. Moreover, *ab initio* calculations including such inelastic scattering effects in real molecules and electrodes have become possible. Such calculation is highly effective in the molecular electronics research which aims to construct electronics devices working at atomic scale by using electronic properties of single molecules. A single molecule is too small to be found by microscopes, it is not easy to confirm experimentally that it is really linked to the electrodes. However, if we use the specific feature of the electric current accompanied by the vibrational excitation, it can gives an evidence that electric current did actually pass over the molecule. The theoretical simulation is highly useful in analyzing this problem. All that has been discussed so far is related with the inelastic process accompanying electric current , namely the exchange of energy between electron and molecular vibration. As a result of such inelastic processes, heat is gererated during



Conceptual diagram of tunnel microscope
Molecule on substrate and the overhead probe

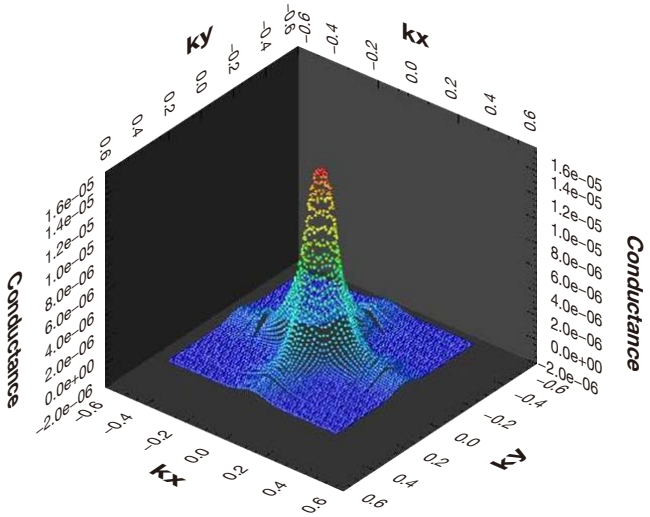


Voltage second-derivative of tunnel electric current through a molecule
The peak of positive value of molecular vibration energy means an increase of electric current accompanying the molecular vibration excitation.[1]

electrical conduction. How to release the gererated heat from the device, that may be related with the phonon heat transport problem, is another important issue. Recently, there is a progress in a theory discussing various aspects of this problem.

Single molecule chemistry is closely related with the inelastic problem. It is known that molecules react chemically when electric current dosing is made from scanning tunneling microscope. It has become possible to maneuver the chemical reaction freely by controlling the ways in which the voltage is applied. This problem, which is becoming of great interest, is closely related with the inelastic process, and the subsequent energy transfer processes among molecular vibrations and phonons.

In the molecular electronics research field, there are many possibilities of simulation research presented here to be applied. In addition to these, there are some other related problems. Simulating scattering resistances at interface between bulk materials and simulations of carrier injection efficiencies can be made without large alterations in theory. They have large influence on the performance of a device and, therefore, if the material design optimizing the properties is realized, then it would be highly useful in technology. Until now, there has not been any microscopic research on this problem because there are various factors involved in the complexity of the scattering resistance. The progress in the study of the quantum dissipation processes learned in single molecular bridge junction system may trigger the reexamination of scattering resistance problem at a nanoscale interface between bulk materials.



The flat surface wavenumber dependence of conductance of $SrRuO_3/SrTiO_3/SrRuO_3$ junction[2]

Spin transport

The second example is the spin transport problem. It has become possible to simulate, with high accuracy, spin dependent conduction across tunnel junction.

Here is such an example. It shows the surface wavenumber dependence of conductance of minority spin at zero bias of tunnel junction in nano capacitor $SrRuO_3/SrTiO_3/SrRuO_3$. One can see that the conductance at the gamma point is dominant. This calculation plays an important role in material design which aims for performance enhancement of TMR (tunnel magneto-resistance) device. In the development of TMR device of Fe(100)/MgO(100)/Fe(100) made in AIST which has broken a world record of the magneto − resistance ratio at the time, the surface band calculation published by Butler in 2001 played an important role. This is a good example where theory and simulation worked well.

Summary

Simulations in material science are more difficult than macroscopic simulations such like hydromechanics and continuum dynamics. They are still not mature. To overcome this, however, research of basic theory of simulation has been underway, and “real world” simulation of materials closer to the experimental environment is coming close to the reality. By using the new simulation methods thus obtained, the theoretical predictions will become more reliable.Simulations then will become able to provide valuable guide in the technology of nanoscale materials which are difficult to be “seen”.

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