

Computational Physics Technologies for Developing Novel Functional Nanostructures

Hiroyuki Kageshima[†]

Abstract

This paper presents an overview of recent progress in computational physics technologies. In developing novel functional nanostructures, it is necessary to take into consideration the fact that all materials consist of atoms. Computational physics technologies enable us to study the motion of the fundamental components of atoms, their nuclei and electrons, based on quantum dynamics.

1. Introduction

New functional nanoscale devices, or nanodevices, are now being studied intensively because nanostructures are expected to exhibit novel physics. Their extremely small size, however, makes nanodevice formation and observation difficult for experimental researchers. Moreover, it is not clear what physics really appears in experiments or how it appears. Nanodevice research and development are, therefore, currently expected to advance via theoretical methods. Nanodevices cannot be described by traditional treatments based on Newtonian dynamics and classical electromagnetism with continuum models. It is necessary to take into consideration the fact that all materials consist of separate particles, namely atoms. Computational physics technologies enable us to study the motions of the fundamental components of atoms, their nuclei and electrons, on the basis of quantum dynamics.

NTT Basic Research Laboratories has a long history of developing such computational physics technologies. Among these technologies, first-principles calculations are the most powerful tools for studying the physics of nanostructures [1]-[6]. They enable us to calculate the electronic states that govern the physical properties of materials, such as the bonding of atoms and the energy gaps of the valence and conduction bands, by inputting the position and element

number of each atom constituting the material. In the calculations, the movements of electrons are calculated using the Schrödinger equation, which is the quantum dynamics counterpart of the Newtonian equation in classical mechanics. We can also change any parameters at will, which we generally cannot do in experiments, so we can thus create virtual experiments in computers and obtain ideal results.

In the early days, first-principles calculations strained the limits of available computational resources because they calculate the complex coupled motions of the huge number of electrons in a material, so they could be applied to only very limited materials and physical properties. NTT Basic Research Laboratories started developing technologies based on first-principles calculations in the 1980s and has been developing and improving them for about 20 years. During this period, the first-principles calculation methods were merged with supercomputer technologies, and the possible targets were extended from simple crystals to defects, surfaces, interfaces, nanostructures and so on. Similarly, the introduction of new technologies extended the methods to include materials with a second row and transition metal elements, such as diamond, oxides, nitrides, iron, manganese, and palladium. They were also extended to evaluate optimized atomic structures and reaction energies as well as to calculate the density of states and band structures.

2. Approaches for nanodevices

We are studying how to develop novel functional

[†] NTT Basic Research Laboratories
Atsugi-shi, 243-0198 Japan
Email: kages@nttbl.jp

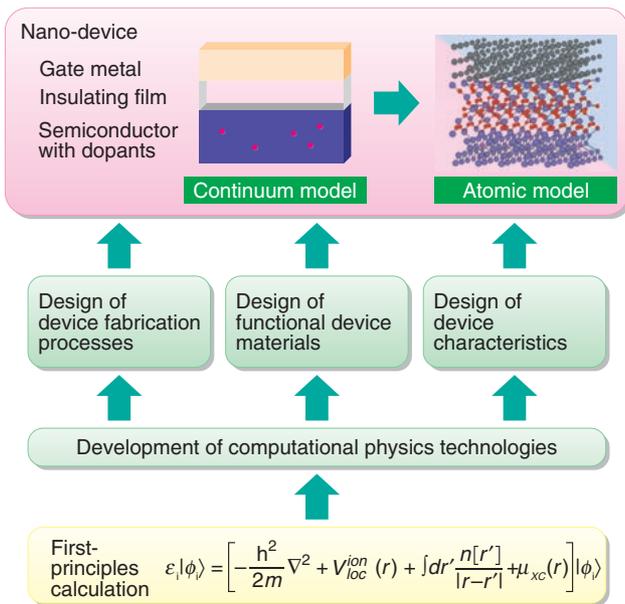


Fig. 1. Approaches to the design of novel functional nanodevices.

nanodevices by four approaches: designing device fabrication processes, designing functional device materials, designing device characteristics, and developing computational physics technologies to support the three design approaches (**Fig. 1**). As a typical example of nanodevices, let us consider one that uses a metal-insulator-semiconductor field-effect transistor (MISFET). This device is formed by stacked layers: the semiconductor, insulating film, and gate metal layers. The semiconductor layer might include dopants or impurities. Since the thickness of the insulating film layer is on the atomic scale, the roughness of the upper and lower interfaces and the uniformity of the insulating film layer are the key factors. This means that it is very important to control the fabrication of such structures. The design of the fabrication processes is thus important for nanodevices.

When we develop novel functional nanodevices, we expect to alter the semiconductor layer by means of a layer with novel functional materials, such as magnetic materials, strongly correlated materials, organic materials, or superconducting materials. As shown by the dilute magnetic semiconductor GaMnAs, for example, dopants in the semiconductor layer are expected to show new functionality. It may be possible to integrate such new functional materials into nanodevices. For this, the design of such materials is another important issue.

Even if we fabricate nanostructures appropriately

and integrate novel materials into the nanodevices, the characteristics of the fabricated nanodevices may still not be clear because novel physics is expected to appear in nanostructures. Thus, designing and clarifying the device characteristics is also an important step. Moreover, to design all these things theoretically, we must develop new methods based on computational physics technologies because new physics can be much more efficiently studied if the new physical properties can be calculated.

3. Design of fabrication processes

The thermal oxidation process of silicon is very important in the fabrication of silicon-based devices. This process forms a silicon oxide insulating film layer on the semiconductor layer of the MISFET device structure. Despite its importance, the atomic-scale details of the process have not yet been clarified. The surface of the silicon substrate is covered with the silicon oxide film, so an oxygen molecule must first diffuse through the oxide film before it can react with the silicon. Since this process is thus an interfacial reaction process and the volume of newly formed oxide is much larger than that of the reacted silicon substrate, a large expansion in volume should occur at the interface. Furthermore, it is known that the interfacial reaction rate changes with the strain at the interface. Thus, it is important to clarify how the interfacial reaction process occurs and how it is affected by interfacial strain.

Using computational physics technologies, we evaluated the path and the energy landscape for the interfacial reaction of the oxygen molecule with the silicon substrate (**Fig. 2**) [7],[8]. The results show that the process consists of two stages. Initially, the oxygen molecule is situated in a cage formed by the bond network of the silicon oxide film. In the first stage, it rotates as it approaches the substrate and is adsorbed on the substrate at the interface. Then, in the second stage, the oxygen molecule breaks up and each oxygen atom separately penetrates into the silicon substrate to form new silicon oxide. The first stage of this reaction emits a reaction heat of about 3 eV per oxygen molecule or 70 kcal/mol and the second stage emits about 7 eV per oxygen molecule or 160 kcal/mol.

With the help of macroscopic simulation based on a continuum approximation, these results can be closely compared with experimental results, giving us useful information for designing the process [9].

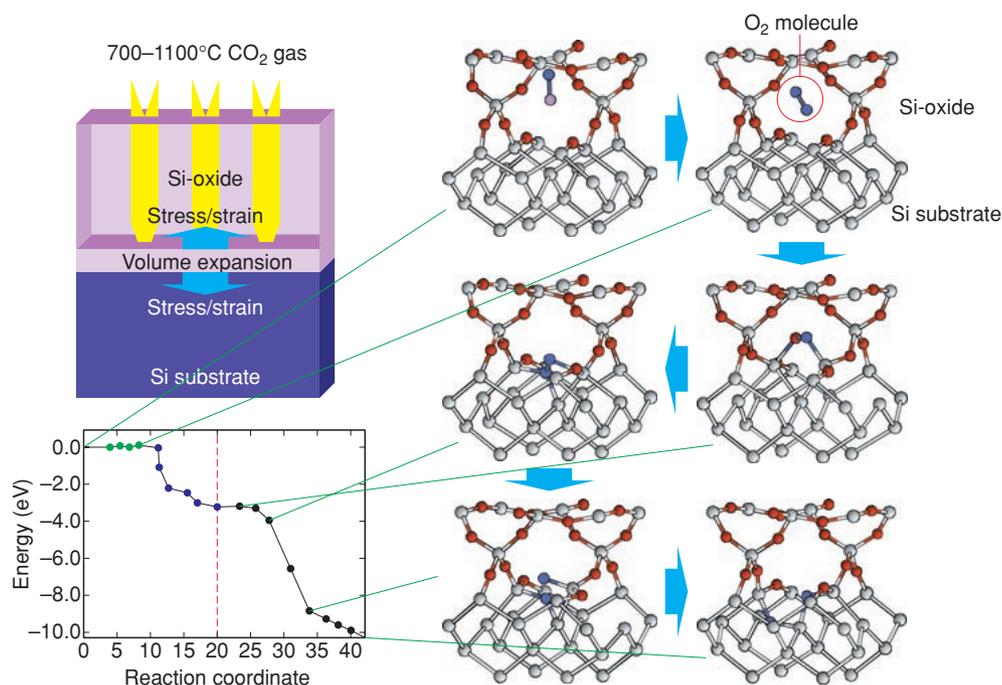


Fig. 2. Thermal silicon oxidation process clarified by computational physics technologies.

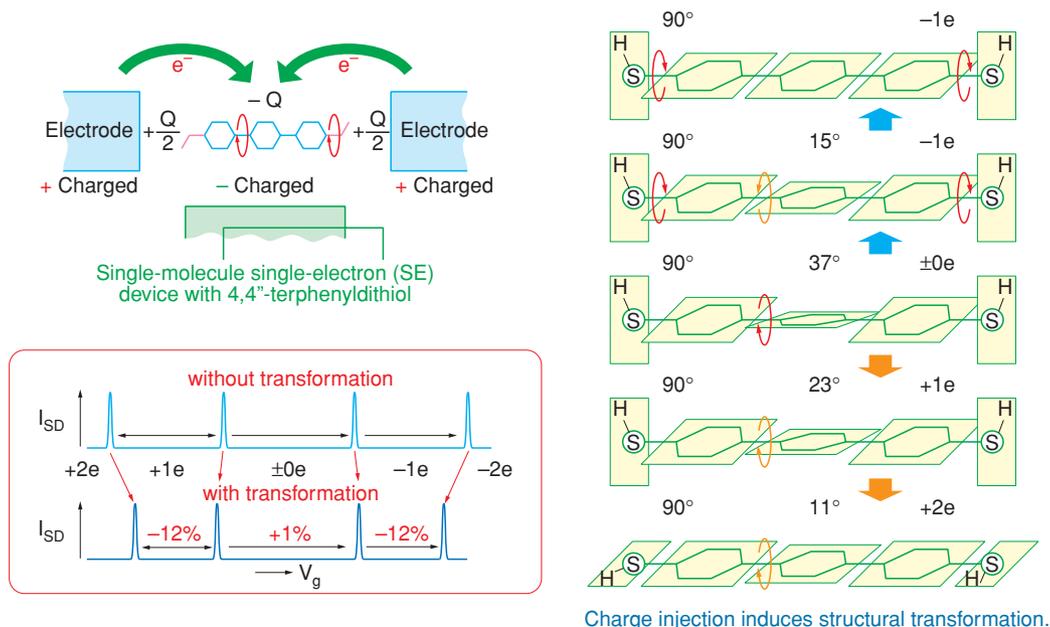


Fig. 3. Single-electron device characteristics of an organic molecule clarified by computational physics technologies.

4. Other approaches

Single organic molecules are very attractive materials for novel nanodevices of the future. Those molecules could be especially useful as the single-electron island of single-electron devices because the size of

the island, the key to the device characteristics, is definitely limited by the size of the molecule itself. To clarify the possibility of using a molecule as a single electron island, we evaluated the device characteristics (**Fig. 3**) [10]. The results on a single 4,4'-terphenyldithiol molecule show that the atomic struc-

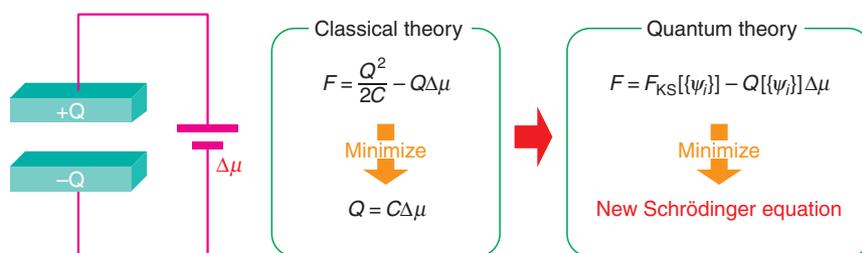


Fig. 4. Principle of newly developed EFED method.

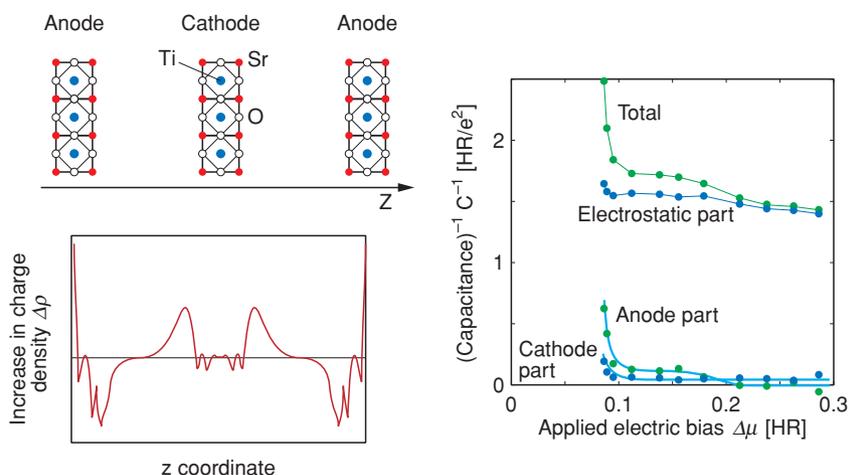


Fig. 5. Device characteristics of a nanocapacitor with repeated cathode-anode pairs made of atomically thin SrTiO_2 electrodes clarified by the EFED method. HR is Hartree (1 HR = 27.2 V) and e is the elementary charge.

ture of the molecule changes if the charge on the molecule is modified by the gate voltage. The two thiol groups at the ends and the phenyl group at the middle rotate independently when the charge changes. As a result, the separation of the source-drain current peak is greatly modified by these rotations in the atomic structure.

Among the device characteristics, capacitance is very important because the FET is essentially a capacitor. However, the capacitance characteristics cannot be calculated by current first-principles calculations. To overcome this difficulty, we have developed a completely new method, which we call the enforced Fermi-energy difference (EFED) method (Fig. 4) [11]. This method takes into account the external work ($Q\Delta\mu$) by the electric bias ($\Delta\mu$) to fix the polarized charge in the system. By adding this work to the quantum free energy of the system, we obtained a new Schrödinger equation for the system under electric bias.

Using the EFED method, we have been studying what characteristics appear in nanocapacitance (Fig.

5) [12]. When an electric bias ($\Delta\mu$) is applied, our method surely induces positive charges on the cathodes and negative charges on the anodes as shown in the bottom-left figure ($\Delta\mu$ is the increase in charge density). The results show that the capacitance is not constant as the classical theory would predict. Instead, it is governed by the electronic states of the electrodes as well as by their shapes and separation. The right figure shows that the inverse of the capacitance is the sum of electrostatic, cathodic, and anodic parts. The cathodic and anodic parts are governed by the density of states of the corresponding electrode. The electrostatic part is governed by classical electrostatics, but a detailed analysis shows that the charges on the electrodes expand to the vacuum and the estimated effective electrode separation changes with the applied electric bias while the real separation is fixed. This means that we can expect quantum effects in nanocapacitors. Since the EFED method is very simple and works well with any first-principles method, it should clarify the physics in many nanodevices in the future.

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**Hiroyuki Kageshima**

Senior Research Scientist, Nano-Devices Research Group, Physical Science Laboratory, NTT Basic Research Laboratories.

He received the B.S. degree in physics from Waseda University, Tokyo, in 1986, and the M.S. and D.S. degrees in physics from the University of Tokyo, Tokyo, in 1988 and 1991, respectively. Since joining NTT in 1991, he has been studying the physics of semiconductor nanostructures and computational physics technologies. He received the Best Poster Paper Award at the Fall Meeting of the Materials Research Society, Boston, USA, in 1997 and the JJAP Paper Award of the Japan Society of Applied Physics in 2000. He is a member of the Physical Society of Japan, the Japan Society of Applied Physics, and the Surface Science Society of Japan.