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Article

Computational R&D for Industrial Applications

by Prof. Feng Liu

Department of Materials Science & Engineering, Center for Computational Design & Testing of Novel Nanomaterials, University of Utah

Recent advances in high-speed supercomputer and computational algorithms have brought us into a new era of computational materials science. These advances make it possible to investigate many existing materials systems that were previously considered intractable and also predict and design novel materials that did not exist in nature but possess desirable and superior properties. Computer modeling and simulation has not only emerged as an additional method for scientific research in parallel to experimentation and theory, but has also become a new and effective method for industrial design, testing, and development. Most exciting, computational research and development (R&D) has been rapidly emerging in many sectors of industry, with increased hiring of graduate students with computational backgrounds.

The need for computational R&D becomes even more prominent in view of the emergence of nanotechnology. The continued miniaturization of electronic and optoelectronic devices is increasing the need for nanoscale structural assemblies to perform the function of computer, laser, data storage, sensor, and satellite communication. However, the nanostructured materials and devices are generally not existing themselves in nature and thus have to be designed and made in laboratories. Also, their properties are not *a priori* known. Therefore, the fabrication and characterization of novel nanostructured materials and devices are both exciting and challenging. To this end, computational R&D has obvious advantages over the conventional experimental R&D in terms of the cost effectiveness, repetitiveness, and versatility.

For the materials industry, the cost effectiveness, the repetitiveness, and the versatility of computational prediction and design of novel materials prior to laboratory synthesis and production have shown great commercial potentials. "Computational experimentation" may now develop products that would otherwise be too costly to develop in the laboratory. Therefore, to meet the demands of the broad interests of materials industries, reliable and efficient state-of-the-art computational packages that are capable of characterizing a wide spectrum of material properties of technological interest must be developed. They must produce results that compare accurately with known properties in the representative existing materials systems and hence be applied to predict and design yet-to-be-explored novel materials. Also, such computational packages themselves possess a great market value

First-principles computational methods based on density functional theory (DFT) have been well established for predicting materials properties. They are capable of predicting the equilibrium structural and mechanical properties as well as dynamic diffusion energy barriers with an accuracy within a few percent of the experimental values and have been successfully applied to a variety of materials systems of semiconductors, metals, and ceramics. They have also made it possible to predict the non-equilibrium materials properties, such as electrical transport, from first principles by performing DFT analysis within the framework of nonequilibrium Green's function (NEGF) formalism. Such quantum mechanics-based computations are also becoming more and more efficient due to the recent advance in high-speed parallel computers and computational algorithms. The Center for High Performance Computing (CHPC) at the University of Utah hosts one of the largest parallel computational platforms for such computations.

In 2002, we established "The Center for Computational Design and Testing of Novel Nanomaterials" (CCDT, http://ccdt.coe.utah.edu/) as part of the Utah Centers of Excellence Program sponsored by the Governor's Office of Economic Development. The mission of CCDT is to develop and commercialize computational packages for materials design and testing and license designs of novel nanostructured materials and device components. Two first-principles computational engines have been developed: a "Materials Designer" (**MaDes**) for predicting the structural, mechani-

cal, and dynamic properties and a "Device Simulator" (**DeSim**) for predicting the electrical transport properties. In addition, a Web-based interface has been developed for visual, interactive, and on-line computational applications. In 2003, a spin-off company, Visual Interactive Scientific Computing, Inc. (VISCO), was founded to commercialize and market our center's technologies.

Recently, **Fairchild Semiconductor Corp.**, the world's leading silicon wafer supplier and the largest semiconductor firm in the Salt Lake valley, has granted a service contract to our center for computational characterization of oxygen diffusion in heavily arsenic (As) doped silicon (Si) to help optimize their Si wafer processing technology. It demonstrates a unique industrial application for computational materials characterization, as we briefly discuss below.

Heavily doped Czochralski-grown silicon wafer is a substrate used most frequently in power discrete devices. Arsenic has been used as one of the most important doping species for source and drain in deep submicron complementary metal oxide semiconductor (CMOS) technology. For the node smaller than 90 nm, the concentration of As in the ultra shallow source and drain is approaching a range of 10^{20}~10^{21} cm^{-3}. Knowledge about the interaction between interstitial oxygen (Oi) and As dopant and diffusion of Oi in such a heavily As-doped Si substrate will help us to better understand this system, so as to optimize the Si wafer processing for current leakage reduction.

When we computationally characterized the Oi-As interaction and diffusion barrier in the heavily As-doped Si, we found that the direct As-O bond formation is prohibitive with a large energy cost, and the optimal lowest-energy configuration is for As and O to be at the second nearest-neighbor positions forming a -Si-O-Si-As- complex, as shown in Fig. 1. Oi can therefore be trapped by As to form such a complex when Oi diffuses in As vicinity. Also, we found that Oi can easily diffuse around As with a low barrier from one complex structure to another (see Fig. 1). But it must overcome a larger barrier to escape from As. Thus, the overall Oi mobility is decreased in comparison with that in intrinsic Si. Our findings have provided key information for Farichild Semiconductor Corp. in explaining the retardation of Oi diffusion and precipitation observed in their heavily As doped Si wafer samples, and provided important guidance for improving their Si wafer process. Currently, we are extending such computational characterization to other types of dopants, including phosphorus (P), boron (B), and antimony (Sb).

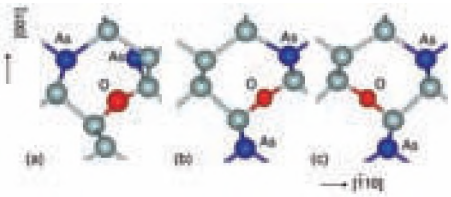

***Fig. 1**: Computational characterization of binding and diffusion of interstitial O (red) in heavily As (blue) doped Si (grey), illustrating the formation of a -Si-O-Si-As- complex*

Computational R&D can be applied not only for industrial materials characterization (which is what we are doing for Fairchild Semiconductor Corp.) but also for industrial design of new materials and devices. For example, an invention disclosure on "in situ continuous human organ pressure monitor" has been filed at University of Utah Technology Commercialization Office and a patent of "carbon nanotube electromechanical pressure sensor" has been filed through Hon Hai Precision Industry Co., both based on our center's computational R&D.

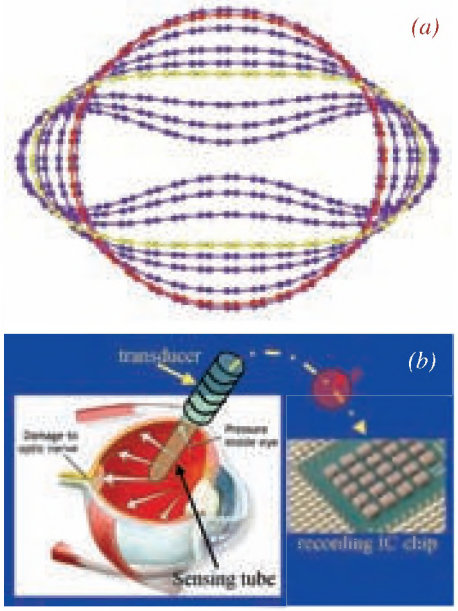

***Fig. 2**: (a) Simulated cross-sections of a carbon nanotube under pressure, displaying a series of shape transitions from circle to oval (red) and then to peanut (yellow); (b) Schematic illustration of an in situ continuous IOP monitor, based on the discovery of pressure induced tube shape transition and P-V relations*

Using Materials Designer, we have discovered novel pressure induced shape transitions and a universal constant defining such transitions for carbon nanotubes, as shown in Fig. 2a. Such a transition is further found to be universal, not limited to carbon nanotubes but apply to tubes made of any materials and of any size. Because of the derivation of a quantitative pressure-volume (P-V) relation of such transitions and its applicability to very small size, the discovery has stimulated some unique designs of minute pressure devices that can be put inside human body for medical applications. This has led to the invention of "in situ continuous human organ pressure monitor", as illustrated in Fig. 2b for an intraocular pressure (IOP) monitor for diagnosis of Glaucoma.

Using the Device Simulator, we discover also the pressure induced shape transition of carbon nanotubes in turn induces an electrical transition: the original metal tube becomes a semiconductor beyond a critical transition pressure. Such correlated mechanical and electrical response of carbon nanotube to external pressure provides an effective method for designing nanoscale electromechanical pressure sensors. The critical pressure is found to decrease with in- creasing tube radius, which allows sensing of different pressures by using different radii of tubes. Figure 3

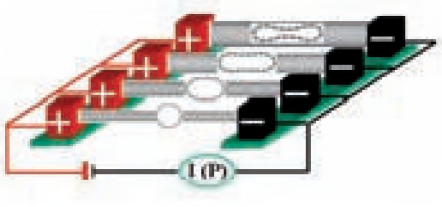

***Fig. 3**: Schematics of a tunable electromechanical pressure sensor consisting of an array of different sizes of tubes, sensing a broad range of pressures*

shows the principle-of-design of such a pressure sensor. Under a given pressure, each tube transforms into different shapes and hence exhibits different conductance. By measuring the current under a given voltage, it will be capable to detect a wide range of pressures. A patent of this pressure sensor has been filed.

To make the computational R&D a viable industrial sector, one must make the computational engines user-friendly. To this end, we have been developing a web laboratory for visual interactive on-line computational applications. An on-line 'DEMO" is available at our center's web site: http://ccdt.coe.utah.edu/. The virtual laboratory is built by integrating web interface programs with materials computational engines to provide an on-line interactive environment for computational R&D. The architecture of the web laboratory is shown in Fig. 4. It consists of a client-side interface program, a web server, a server-side interface program, an archive of computational engines, and a database server.

Fig. 4: Schematic illustration of the architecture of the web laboratory for computational R&D

The client side interface works as a gateway for users to log in, manage accounts, upload input files, submit jobs, run simulations, monitor the simulation process, view results in 2D and 3D graphics, and download reports. The server-side interface will perform account management, pass client-side messages to simulation programs or the database server, activate simulation programs, process simulation results, prepare reports, and pass messages from simulation programs or database server back to client-side interface. The web laboratory can be customized for individual industrial applications.

In summary, computational R&D saves time and money! We foresee that computational R&D will have broad applications in future industries, especially those industrial sectors derived from emerging nano and biotechnologies.