Extended Abstracts of the 2001 International Conference on Solid State Devices and Materials, Tokyo, 2001, pp. 424–425

P-1-13

Development of New Tight-Binding Molecular Dynamics Program to Simulate Chemical-Mechanical Polishing Processes

Toshiyuki Yokosuka, Hitoshi Kurokawa, Seiichi Takami, Momoji Kubo,
Akira Miyamoto and Akira Imamura[1]

Department of Materials Chemistry, Graduate School of Engineering, Tohoku University,
Aoba-yama 07, Sendai 980-8579, Japan.
Phone: +81-22-217-7233, Fax: +81-22-217-7235, E-mail: miyamoto@aki.che.tohoku.ac.jp
[1]Department of Mathematics, Faculty of Engineering, Hiroshima Kokusai Gakuin University,
6-20-1 Nakano, Aki-ku, Hiroshima 739-0312, Japan.

1. Introduction

Recent advancement of the silicon technology requests the ultimate integration technique for the development of new devices. Especially, the global planarization technique of the silicon wafer is strongly demanded for new device development. Recently, the chemical-mechanical polishing (CMP) process has gained much attention as a key technology to realize the planarization of the silicon wafer, and has already used in the industrial processes.

The CMP utilizes both the mechanical polishing and chemical reaction. The CMP is expected to solve all problems related to the roughness of the silicon surface such as the aspect ratio, focus depth, and so on. The damascene interconnection architectures can be constructed by the CMP technique, which can not be realized by the other planarization techniques. Therefore, CMP is considered to be a key technology of the Giga bit devices. Although a lot of experimental results related to the CMP processes have been accumulated, the detailed mechanism of the CMP process has not been clarified on atomic and electronic level.

Recently, computational chemistry has been applied to a lot of silicon technology, however no simulation studies on the CMP processes have been performed to the best of our knowledge, because of the lack of the software which can simulate the CMP processes. In the present study, we developed a new computational chemistry program which can realize the atomistic and electronic level simulation of the CMP process.

2. Development of New Program

First-principles molecular dynamics method cannot simulate the CMP processes since it requests huge calculation time. On the other hand, recently we developed a new accelerated quantum chemical molecular dynamics program "Colors" based on our original tight-binding theory [1][2]. It is more than 5,000 times faster than the regular first-principles molecular dynamics program.

In the present study, we developed a new program which can simulate the CMP processes, based on the above Colors program. In this program, the shear process on the silicon wafer can be simulated by sliding the polishing particles. Figure 1 shows the flow chart of the Colors program as well as the improvement points for the CMP simulation.

3. Results and Discussion

In order to confirm the effectiveness of our new program, we constructed simple models of the silicon surfaces as shown in Figure 2. We employed a SiO_2 particle as a polishing material. Two types of the silicon surfaces, clean Si(100) surface and H-terminated Si(100)2×1 surface were constructed to clarify the effect of the surface structure on the CMP processes. The bottom part of the silicon surface was fixed. Calculation condition is shown in Table 1. Velocity of the polishing particle is 100 m/s in the X direction and 0 m/s in the Y direction. We applied a constant force of -1.0×10^{-9} N/atom to the SiO_2 particle in the Z direction. Under the periodic boundary conditions, the calculations were performed for 10,000 steps with a time step of 2.0 fs at 300 K.

Figure 3 shows the final structures of the two models at 10,000 steps. Both models were polished by the SiO_2 particle. It indicates that our program is effective to simulate the CMP processes. To the best of our knowledge, this is a first simulation of the CMP processes in the world. We also investigated the bond population of the polished silicon atom. Table 2 shows the typical result for one silicon atom. In both cases, the bond population of the silicon atom decreased by the CMP process. It indicated that the electronic state of the silicon wafer was unstable by the mechanical polishing.

From Figure 3, we confirmed the desorption of the hydrogen atoms from the H-terminated Si(100)2×1 surface. The dynamic process of the hydrogen desorption is shown in Figure 4. One hydrogen atom bonded to the silicon atom of the wafer transferred to the SiO_2 particles at 490 steps. At that time the hydrogen atom was bonded to the oxygen atom of the SiO_2 particle. At 500 step, a hydrogen desorption from the oxygen atom was observed. At 490 step, the O-H bond distance was 0.90 Å, which

is shorter than the regular O-H bond length. Therefore, the strong repulsive force worked between the hydrogen and oxygen atoms. It may produce the hydrogen desorption from the SiO_2 particle.

4. Summary

In this study, we developed a new quantum chemical molecular dynamics program, which can simulate the CMP process, and applied to the planarization process of the silicon wafer by the SiO_2 particle. We observed the electronic changes of the silicon atoms and the desorption of the hydrogen atoms after the CMP processes. Since the atomic and electronic information on the CMP processes can not be obtained by the experiments, we confirmed the effectiveness of our new program.

References

[1] K. Lassonen and R. M. Nieminem, J. Phys. Condens. Matter, 2,1509(1990).

[2] A. Yamada, A. Endou, H. Takaba, K. Teraishi, S. Salai Cheettu Ammal, M. Kubo, K.G. Nakamura, M. Kitajima and A. Miyamoto, Jpn. J. Appl. Phys., 38, 2434 (1999).

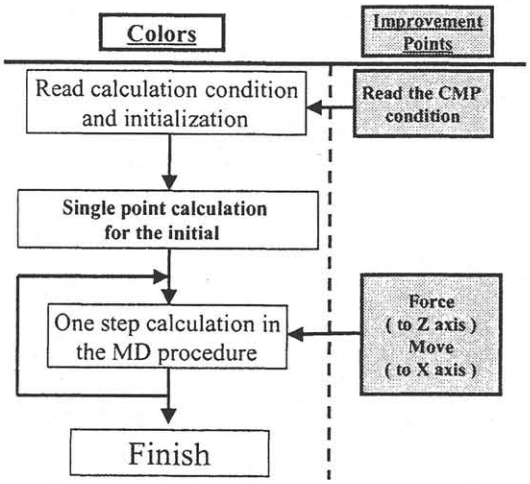
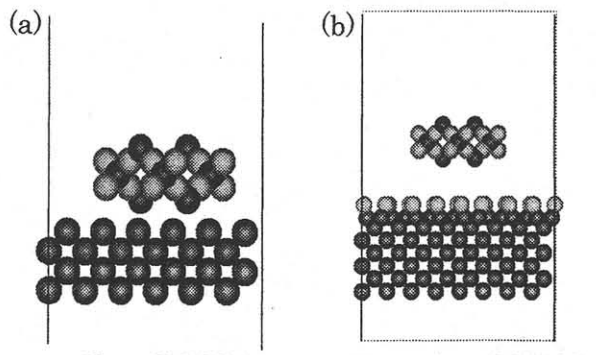


Figure 1 Flow chart of the "Colors" program and the improvement points for CMP process



Clean Si(100) surface

H-terminated Si(100) 2×1 surface

Figure 2 Calculation models

Table 1 Calculation condition

Velocity (x-direction)	100 (m/s)
Velocity (y-direction)	0 (m/s)
Force (z-direction)	-1.0×10^{-9} (N/atom)
Temperature	300 (K)
Integration time	2.0 (fs)
Total step number	10,000

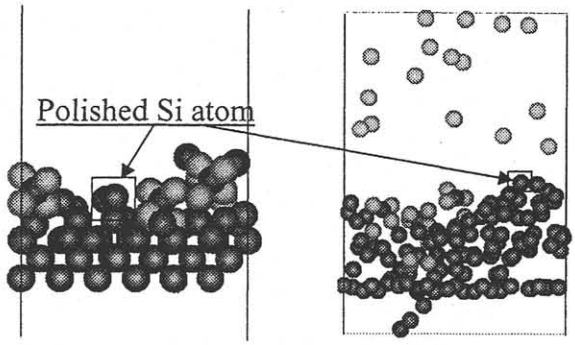


Figure 3 Structures of the silicon wafer with SiO_2 polishing particle at 10,000 step

Table 2 Bond population of the polished Si atom

Clean surface		H-terminated surface	
0 Step	10000 Step	0 Step	10000 Step
2.857	2.097	2.896	2.311
4 coordinations	2 coordinations	4 coordinations	2 coordinations

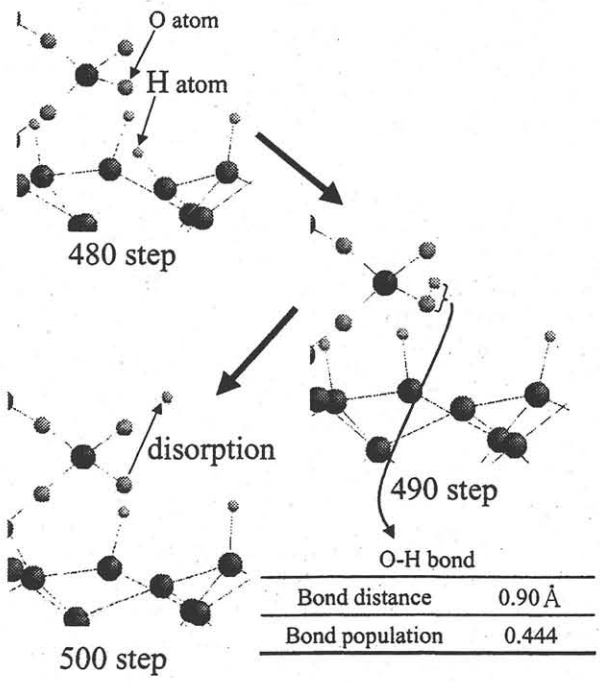


Figure 4 Desorption process of H atoms from the H-terminated Si(100) 2×1 surface