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Quantum Chemical Molecular Dynamics Studies on the Chemical Mechanical Polishing Process of Cu Surface

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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, a chemical-mechanical polishing (CMP) process has gained much attention as a key technology to realize the planarization of the semiconductor device, and has been 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, the CMP is considered to be a key technology for 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 study on the CMP processes has been performed, to the best of our knowledge, because of the lack of the software which can simulate the CMP processes. Hence, recently we have succeeded in the development of new simulation software for the CMP process, which is based on our accelerated quantum chemical molecular dynamics method [1]. In the present study, we applied the above new simulation software to clarify the CMP process of the Cu surface.

2. Theoretical Method

First-principles molecular dynamics method cannot simulate a large system since it requests huge calculation time. Hence, recently we developed a new accelerated quantum chemical molecular dynamics program "Colors" based on our original tight-binding theory [2]. It is more than 5,000 times faster than the regular first-principles molecular dynamics program. Moreover, we have developed a new simulation software for the CMP process [1], based on the accelerated quantum chemical molecular dynamics program. Hence, in the present study we employed the above new simulation software for the CMP.

3. Results and Discussion

We simulated the surface chemical reaction of the Cu-CMP process before the simulation of the mechanical polishing processes. In order to analyze the effect of pH, we constructed two different models (Figure 1). Model (a) has 13 H_2O molecules and 1 H_2O_2 molecule, while model (b) has 13 H_2O molecules and 3 H_2O_2 molecules. In both models, we used Cu(100) surface as a polishing target and fixed the bottom part of the surface during the simulation. Under the periodic boundary condition, all calculations were performed for 5,000 steps with a time step of 0.2 fs at 300 K.

Figure 2 shows the snapshots of two simulations for models (a) and (b). From this figure, we confirmed the different reactivity of the H_2O_2 molecules. In the model (a), we observed only the OH adsorption on the Cu surface, while in the model (b) we observed that the H_2O_2 molecules oxidized the Cu surface and produced H_2 molecules during the oxidation process.

For the model (b), we investigated the change in the atomic charges during the simulation (Figure 3). From this figure, we observed the electron transfer from the Cu substrate to the H_2O_2 solution at the first stage of the simulation. Moreover, we found that the atomic charges in the Cu atoms of the first layer changed more significantly compared to those of the second layer. This result indicates that the surface Cu atoms are very active to the H_2O_2 molecules. Moreover, we observed the production of the H_2 molecules around 3,500 steps.

We also paid attention to the trajectories of the oxygen atoms in order to analyze the oxidation process (Figure 4). First, oxygen atoms moved to the 4-fold site of the surface Cu atoms from 0 to 2500 steps. Second, oxygen atoms moved to the 4-fold site of the Cu atoms in the second layer. The above chemical reaction process can not be simulated by the other software, and hence we confirmed the applicability of our new simulation

software for the CMP process.

Moreover, we have simulated the mechanical polishing process of the Cu surface with H_2O and H_2O_2 solution, involving the chemical reactions. These results will be presented in the conference.

References

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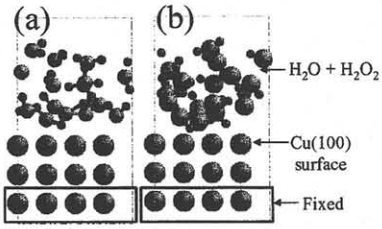

Fig. 1 Calculation models
(a) H_2O : 13 molecules, H_2O_2 : 1 molecule
(b) H_2O : 13 molecules, H_2O_2 : 3 molecule

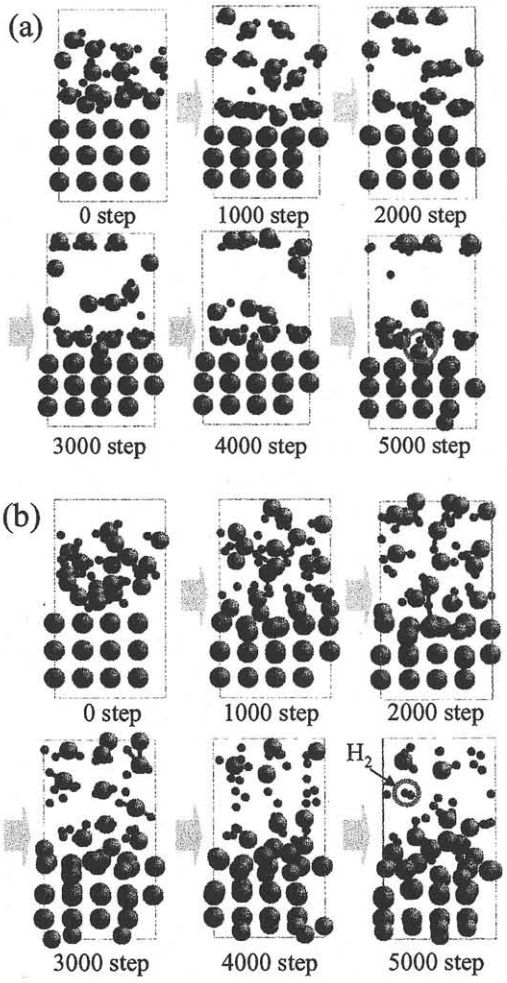

Fig. 2 Snapshots of oxidation process of Cu surface - Model (a) and Model (b)

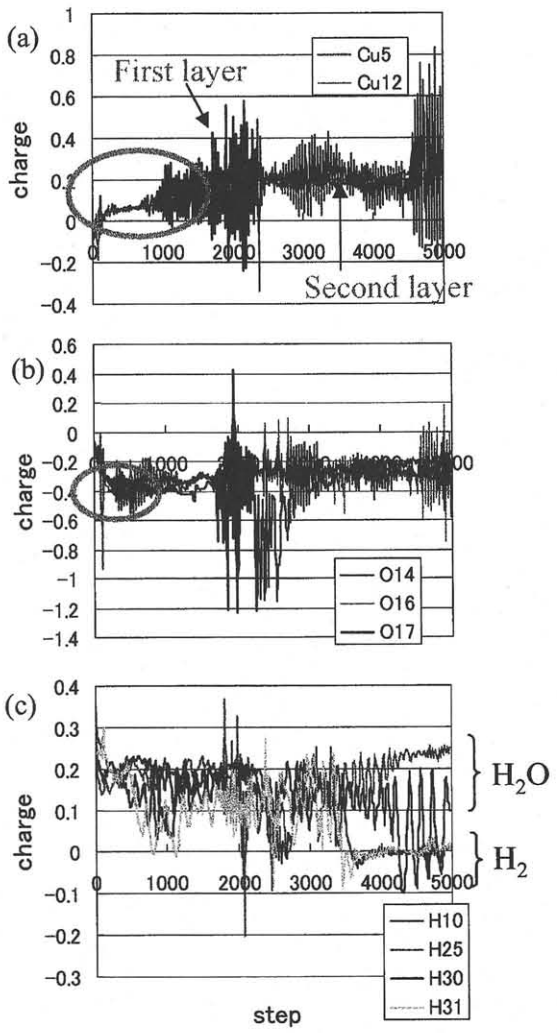

Fig. 3 Change of atomic charges in the model (b)
(a) Cu, (b) O and (c) H

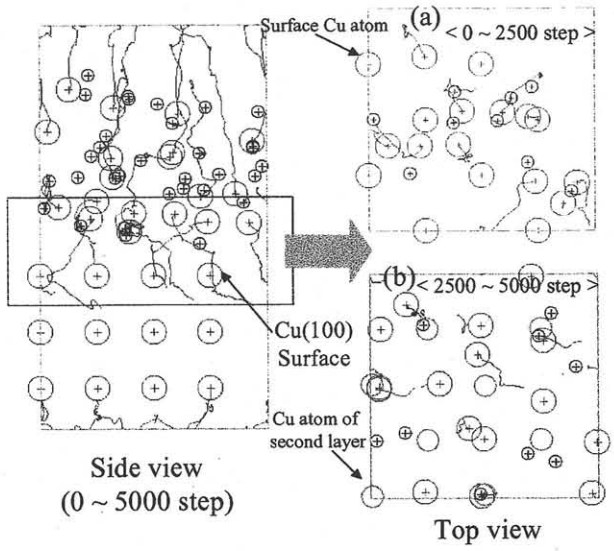

Fig. 4 Trajectories of the oxygen atoms for model (b)
(a) 0 ~ 2500 steps and (b) 2500 ~ 5000 steps