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Quantum Chemical Molecular Dynamics Simulations of Chemical Mechanical Polishing Processes for Silicon Wafer by SiO_2 Abrasive Grain

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1. Introduction

Chemical mechanical polishing (CMP) is one of the most effective methods to achieve ultra-smooth and non-damage surface in manufacturing silicon wafer. Miniaturized high-efficiency semiconductor devices have required more precise CMP technology to achieve the atomic-scale planarization. However, the CMP mechanism, such as material removal processes and influence of additives in slurry, has not been understood completely since it is difficult to obtain atomic-scale information on the wafer surface during polishing directly by experiments. In this study, in order to clarify the CMP mechanism of the single-crystal silicon surface, we investigated the polishing processes of a silicon surface by a silica abrasive grain in alkaline slurry via our tight-binding quantum chemical molecular dynamics (TB-QCMD) method [1].

2. Method

We employ our TB-QCMD code, Colors, for performing the polishing simulations of a Si(001)-2×1 surface terminated with H atoms by an amorphous SiO_2 abrasive grain terminated with OH groups in 10% aqueous NaOH solution. We applied a load of 4.5×10^{-10} N on the SiO_2 abrasive grain and forcibly slid it with 50 m/s as shown in Fig. 1(a). Temperature was set at 300 K.

3. Results and discussion

To reveal the chemical reactions on the Si surface and the surface structural change during polishing, we performed polishing simulation of the Si surface by the SiO_2 abrasive grain in aqueous NaOH solution via our TB-QCMD method. At first, relaxation calculation was performed for 10 ps. During this calculation, the chemical reaction on Si surface did not occur. Next, we applied the load on the SiO_2 abrasive grain and forcibly slid it. We observed that OH^- ions adsorbed on the Si surface by friction of the SiO_2 abrasive grain. Then, some Si-Si back-bonds were extended and dissociated as shown in Fig. 1(b). We observed condensation reactions between an OH group terminated on the abrasive grain and an OH group adsorbed on Si surface as shown in equation (1);

$$\text{Si-OH} + \text{HO-Si} \rightarrow \text{Si-O-Si} + H_2O \quad (1)$$

thereafter, $Si_{abrasive}$-O-$Si_{surface}$ bonds were generated. Then, the Si atoms were removed from the substrate with $Si_{abrasive}$-O-$Si_{surface}$ bonds as shown in Fig. 1(c). We revealed that the Si-Si back-bond was weakened and dissociated by OH^- ion adsorptions on the Si surface. Then, Si atoms were removed from the substrate with $Si_{abrasive}$-O-$Si_{surface}$ bonds. The friction of the SiO_2 abrasive grain enhances chemical reactions such as OH^- ion adsorptions on the Si surface and condensation reactions.

4. References

[1] Hayashi, K., Sato, S., Bai, S., Higuchi, Y., Ozawa, N., Shimazaki, T., Adachi, K., Martin, JM. and Kubo, M., "Fate of Methanol Molecule Sandwiched between Hydrogen-Terminated Diamond-Like Carbon Films by Tribochemical Reactions: Tight-Binding Quantum Chemical Molecular Dynamics Study", Faraday Discussions, 156, 2012, 137-146.

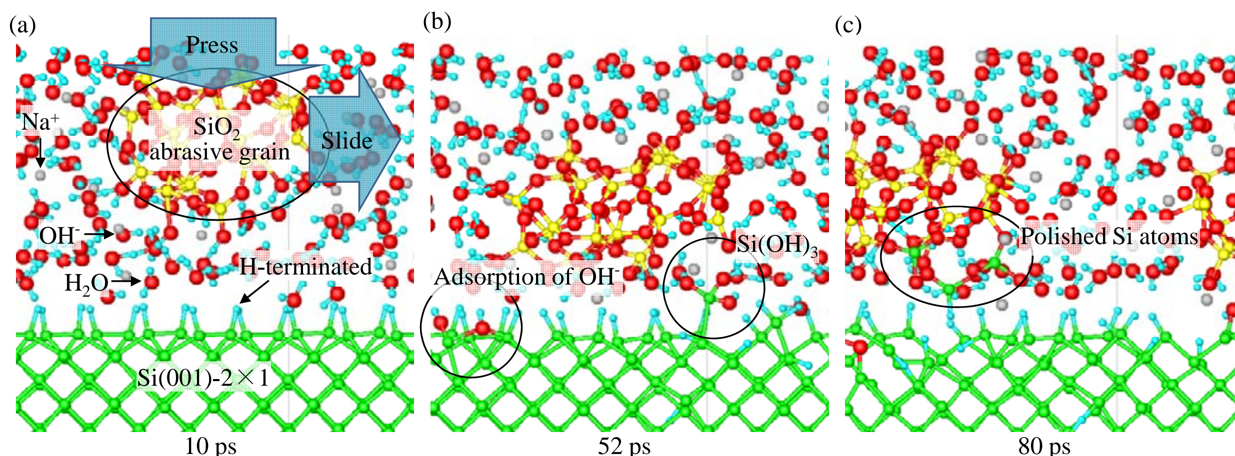

Fig. 1 Snapshots of the polishing simulation by abrasive grain in NaOH solution at (a)10, (b)52, and (c) 80 ps.