First-Principles Calculation on CMP Process of Glass Surface by CeO_2 Particle and Design of Alternative Abrasive Grain

N. Ozawa, M. Nakamura, K. Kawaguchi, Y. Higuchi, M. Kubo*

Fracture and Reliability Research Institute, Graduate School of Engineering, Tohoku University,
6-6-11 Aoba, Aramaki, Aoba-ku, Sendai 980-8579, Japan

*Corresponding author for momoji@rift.mech.tohoku.ac.jp

1. Introduction

CeO_2 abrasive grains are employed for high-precision smoothing of glass in various electric appliances. Since Ce yields in only a few regions, development of alternative materials of CeO_2 abrasive grains is necessary. In this study, to clarify chemical mechanical polishing (CMP) mechanism of a glass surface by a CeO_2 abrasive grain, we investigated the polishing processes of the SiO_2 surface by the CeO_2 particle via first-principles calculation. Furthermore, based on our revealed CMP mechanism, we propose the design principles for the alternative abrasive grain of CeO_2 and theoretically design a new abrasive grain.

2. Method

We employed the first-principles calculation package, "DMol^3" to calculate the electronic states and structure of the abrasive grain and SiO_2 surface.

3. Results and discussion

To clarify the chemical reaction of the CeO_2 particle with the SiO_2 surface under water environment in the CMP process, we initially calculated the Ce atom charges of the CeO_2 particle and Si-O bond length of the SiO_2 surface by the first-principles calculation, when the particle was pushed down to the surface (Fig. 1). Here, we have revealed that Ce atoms of the commercial CeO_2 abrasive grains are exposed on the surface and take a valence value of +III. Then, we adopted the Ce_2O_3 cluster model since this model expresses the surface state of the abrasive grain. The calculation results show that the charges of the Ce atoms increases by pushing down the Ce_2O_3 cluster to the SiO_2 surface. In addition, the two Si-O bond lengths of the SiO_2 surface increase by the contact with the Ce_2O_3 cluster (Fig. 1(b)). These indicate that the Ce^{3+} donates electrons to the Si-O bonds and it leads to the weakening of the Si-O bonds. Next, we investigated the structural change of the SiO_2 surface which the Ce_2O_3 cluster contacts by approach of a H_2O molecule via the first-principles calculation. After the H_2O molecule dissociates to H^+ and OH^-, the Si-O bond is stretched due to the binding with H^+ and OH^-. We found out that the Si-O bond is broken and the SiO_2 surface is softened due to the chemical reaction by the H_2O molecule. The mechanical polishing of the softened glass surface occurs later.

Then, we suggest that these chemical reactions by the Ce^{3+} atoms and H_2O molecule enhance the mechanical polishing processes on the glass surface in the CMP process (Fig. 2). Thus, we can propose that low-valent metal atoms exposed on the surface have chemical reactivity and are efficient for the polishing of the glass surface as a design principle for the alternative materials of CeO_2 abrasive grain.

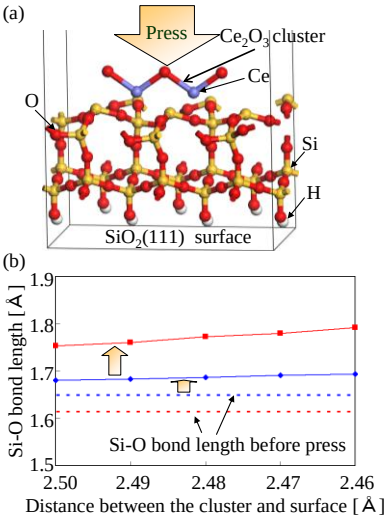

Fig.1 (a) SiO_2(111) surface model pressed by Ce_2O_3 cluster. (b) Change in the Si-O bond length of the SiO_2(111) surface during the press process by Ce_2O_3 cluster.

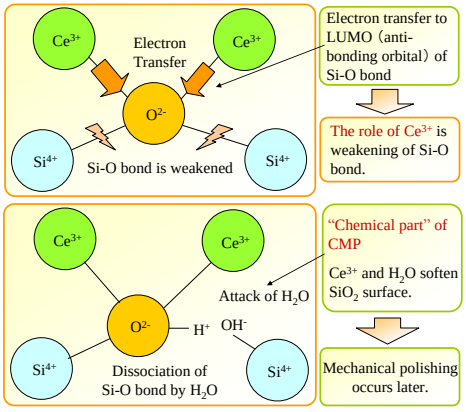

Fig.2 Chemical mechanical polishing mechanism of SiO_2 by CeO_2 abrasive grains.

Based on our established design principle, we proposed $CaCeO_3$ with the perovskite structure as the alternative materials, in which the more low-valent Ce atoms are exposed on the surface than the CeO_2 abrasive grain. The details of the CMP property of $CaCeO_3$ will be explained in the conference.