Estimation of breakdown electric-field strength reflecting local structures of SiO₂ by using first-principles molecular orbital calculation technique

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1. Introduction

Dielectric breakdown of gate SiO₂ films in advanced MOSFETs is one of major concerns. It is known that breakdown electric-field strength $E_{\rm BD}$ decreases due to the presence of defects in the film. The decrease in $E_{\rm BD}$ is widely discussed by the percolation theory [1], which is illustrated in Fig. 1. Defects are produced in SiO₂ by continuous electric stress and connected with each other so that a percolation path is formed. Finally, a current path is irreversibly formed after breakdown occurs through the percolation path. It is thus important to investigate the effects of locally-distributed defects on $E_{\rm BD}$.

Although the value of the bandgap is a potential parameter for $E_{\rm BD}$ estimation because it has a correlation with $E_{\rm BD}$, this bandgap-based approach is inapplicable to our targets. The bandgap parameter does not reflect effects of defects locally distributed. In the present study, we propose a method for $E_{\rm BD}$ of SiO₂ films that contain locally-distributed defects such as atomic-scale strains and vacancies, that is, $E_{\rm BD}$ reflecting local structures.

2. $E_{\rm BD}$ estimation method

The approach that we propose in this study is based on an inner electric-field model, which we developed and demonstrated its applicability to dielectric constant estimations [2].

Inner electric-field model

Through the first-principles molecular orbital calculations employed with the DV-X α code [3], in this inner electric-field model, we analyze a cluster model for a target material, an example of which for SiO₂ is illustrated in Fig. 2. From an inner orbit of the center atom of the cluster, we remove electrons and thus create core holes so as to generate inner electric field in a radial fashion. This electric field results in the dielectric response: valence charge of the neighbor atoms moves to the center one. The amount of the moved charge Δn is recorded. We have found that this value is an interesting parameter that indicates various physical properties of materials, as shown in Fig. 3, for example; for a wide variety of Si and Al compounds, a universal straight-line relationship is observed between a function of the dielectric constant and the dipole moment given by $\Delta n \bullet r$, in which "r" represents a bond length. In this study we expand the concept of this inner electric-field model to the $E_{\rm BD}$ estimation.

Parameter of "Recovery rate" and its application to E_{BD} estimation

This study reveals that a parameter deduced from a Δn analysis is applicable to $E_{\rm BD}$ estimation. Figure 4 shows a relationship for Si compounds between Δn and the charge quantity originally removed. The gradient of Δn with respect to the removed charge for each material is a parameter indicating how strongly the studied sample recovers to the original state. We have thus named it "recovery rate" and found that this value has a good correlation with $E_{\rm BD}$ for Si and Al compounds, as demonstrated in Fig. 5, where $E_{\rm BD}$ given by literatures [4-10] are plotted as a function of the recovery rate that we calculated. From this result, we conclude that it is possible to estimate $E_{\rm BD}$ from recovery-rate calculations for various structures through these straight-line relationships.

3. Estimation in strained and defective SiO₂

We have applied the proposed method to SiO₂ films that have defects. We have studied two types of defects: atomic-scale strain and oxygen vacancies. For the strained SiO₂ case (Fig. 6), we have analyzed SiO₂ cluster with inter atomic distances changed by -3%~9%. It is found that $E_{\rm BD}$ decreases with inter atomic distance increases. In the oxygen vacancy case (Fig. 7), we have built a cluster model illustrated in Fig. 7. Note that the model is energetically relaxed. It is found that $E_{\rm BD}$ is lower compared to SiO₂ without oxygen vacancies. These results also suggest that the dielectric breakdown occurs with an aide of defects, which is consistent with the basic concept that underlies in the percolation theory.

4. Conclusion

We propose an estimation method of breakdown electric-field strength reflecting local structures of SiO₂. The method is based on an inner electric-field model, which is analyzed in a computation system associated with the first-principles molecular orbital calculations. From a parameter named "recovery rate", which is given by the analysis, it is possible to estimate the breakdown electric-field strength of SiO₂ even with defects locally distributed. Results of case models exhibit trends expected from the percolation theory.

References

[1] J. H. Stathis, J. Appl. Phys., 86, 5757 (1999).

[2] K. Hirose, D. Kobayashi, H. Suzuki, and H. Nohira, *Appl. Phys. Lett.* **93**, 193503 (2008).

[3] H. Adachi, et al., J. Phys. Soc. Jpn., 45, 875 (1978).

[4] E. Harai, Appl. Phys. Lett., 30, 601 (1977).

[5] S. M. Sze, "Semiconductor Devices: Physics and

Technorogy, 2nd Edition" (2002).

[6] S. Yaginuma, et al., Thin Solid Films, **486**, 218 (2005).

[7] M. Levinshtein, et al., "Handbook Series on Semiconductor Parameters in 2 Volumes", Wold Scientific Pub. Co. Inc. (1996).

[8] S. Adachi, "Properties of group IV, III-V, semiconductors", John Willy and Sons (2005).

[9] Fujikura Technical Journal No.114 "Single Crystal of Aluminum Nitride" in Japanese, Fujikura (2008).

[10] K. Arai, S. Yoshida, "The Foundation and Application of SiC Devices" in Japanese, Ohmsya (2005).



Fig.1 Conceptual drawing of the percolation theory.



Fig.2 Cluster model of SiO₂.



Fig.3 Relationship between the function of dielectric constant ε and the dipole moment $\Delta n \bullet r$, where r is the inter atomic distance.



Fig.4 Observed relationship between the amount of removed charge and Δn , for Si compounds.



Fig.5 Correlation between recovery rate and breakdown electric-field strength.



Fig.6 Estimated E_{BD} for strained SiO₂.



Fig.7 Estimated E_{BD} for SiO₂ with an oxygen vacancy.