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A Novel Methodology for the Electrical Breakdown of Insulator and Semiconductor Materials Based on Tight-binding Quantum Chemistry Theory

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【Introduction】

Dielectric breakdown has always been of serious reliability concern in the electric industry, particularly in semiconductor field, because of the continuous trek towards smaller and smaller devices. In the present work, we addressed a dielectric breakdown simulation on atomic scale, by using a novel methodology combined with tight-binding quantum chemistry theory and molecular dynamics.

【Method】

Firstly, New-Ryudo, molecular dynamics (MD) program developed in our laboratory was employed to obtain the crystal structures under various electric fields. Next, our original tight-binding quantum chemical dynamics program, Colors, was used to calculate the electronic structures for each obtained crystal structure mentioned above. Finally, based on the electronic structure information, electrical conductivity for a given system is estimated by Monte Carlo simulation [1].

【Results and discussion】

One of dielectric material investigated in our study is amorphous SiO_2, which have been extensively studied. Calculation model of amorphous SiO_2 as shown in Fig. 1(a), contains 62 oxygen atoms and 31 silicon atoms. In order to determine the validity of the potential parameters accepted in our MD calculation, the cohesive energies of some SiO_2 molecular clusters were calculated and these values were compared with the density functional theory (DFT) calculation results. The cohesive energy values of two, three, and four SiO_2 molecules calculated with the accepted potential parameters were 574.7, 871.6, 1229.1 kcal/mol, respectively. These values were in good agreement with the DFT values of 586.5, 916.9, 1232.1 kcal/mol for two, three, and four SiO_2 molecules, respectively. In the following, MD simulation was performed at 300K and the total time is 10 ps with a time step of 0.5 fs. Electric field was applied parallel to the z-axis, which is perpendicular to the x-y plane. Fig. 1(b) is the obtained SiO_2 structure from dynamics calculation when the electric field reached to 5.0×10^{10} V/m. It is clear that the regular geometry of amorphous SiO_2 was almost destroyed compared with the Fig. 1(a). Fig. 2 is the simulation results for effect of electric field on the electrical conductivity of Amorphous SiO_2. It indicates that transformation of insulator to conductor for amorphous SiO_2 occurs when electric field strength is very high. The detailed description of simulation procedure will be present at the conference.

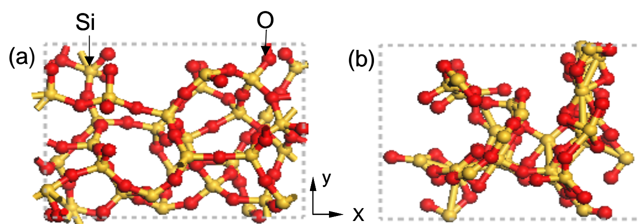

Fig. 1 Amorphous SiO_2 structure obtained from MD calculation at 300K. (a) under no electric field (b) under electric field of 5.0×10^{10} V/m (electric field is perpendicular to the x-y plane)

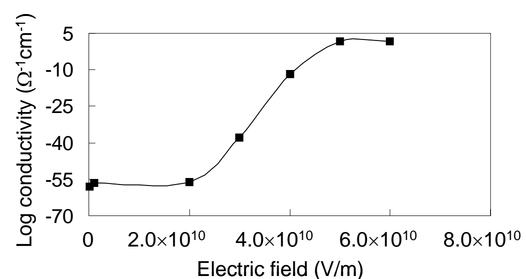

Fig. 2 Effect of electric field on the electrical conductivity of amorphous SiO_2

[1] H. Tsuboi *et al., Jpn. J. Appl. Phys.*, to be published.