Effects of incorporating Si into Al_2O_3 gate oxides in GaN-MOSFETs

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There has been a growing interest in gallium nitride (GaN) as a material for next-generation power conversion devices. In order to realize GaN-MOSFETs, it is important to determine the most suitable gate oxide. Among the various materials for gate oxides, Al_2O_3 is one of the best owing to its relatively large conduction band offset (CBO) for GaN. However, the CBO of Al_2O_3 is smaller than that of SiO_2, which means the leakage current of GaN devices with Al_2O_3 gate oxides are higher than those with SiO_2 gate oxides. Leakage current can lead to instability of the threshold voltage. Kikuta et al. have reported that $Al_{1-x}Si_xO_3$ mixed oxides deposited by plasma-enhanced atomic layer deposition might achieve high reliability MOSFET devices with reduced leakage current.[1] In this study, we investigated the effect of incorporating Si at oxygen vacancies in Al_2O_3. We calculated the atomic and electronic structures of oxygen vacancies in amorphous $Al_{1-x}Si_xO_y$ using first-principles calculations.

The calculations were performed using the VASP code[2], which is based on density-functional theory with the Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation.[3] We prepared amorphous Al_2O_3 with 120 atoms and constructed $Al_{0.8}Si_{0.2}O_3$, $Al_{0.46}Si_{0.54}O_3$ and $Al_{0.23}Si_{0.77}O_3$ models. Next, we removed an oxygen atom and calculated the atomic and electronic structures. In Al_2O_3, we found the well-known oxygen vacancy structures. However, a new Si-Si bond was formed in $Al_{0.8}Si_{0.2}O_3$, $Al_{0.46}Si_{0.54}O_3$ and $Al_{0.23}Si_{0.77}O_3$. As a result, no deep defect levels were formed in the bandgap with the $Al_{1-x}Si_xO_3$ mixed oxides, although deep defect levels originating from oxygen vacancies were formed in amorphous Al_2O_3 (Fig. 1 (a)-(d)). These results indicate that gate leakage would be reduced in MOSFETs with $Al_{1-x}Si_xO_y$ mixed oxides. Thus, $Al_{1-x}Si_xO_3$ is one of the best candidates for GaN-MOSFETs.

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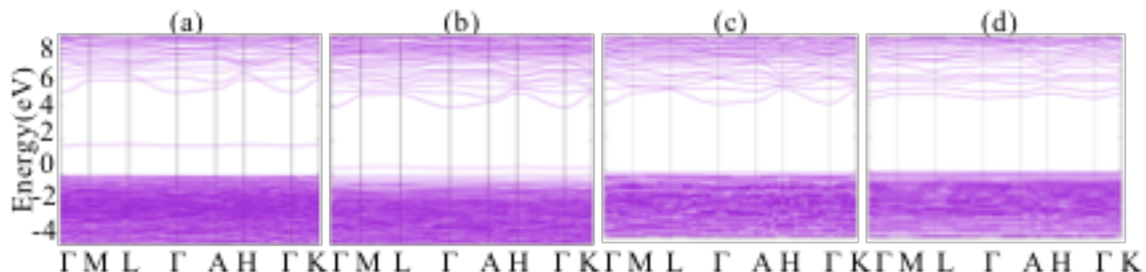

Figure 1: Band structures of $Al_{1-x}Si_xO_3$ mixed oxides with an oxygen vacancy, (a)Al_2O_3, (b)$Al_{0.8}Si_{0.2}O_3$, (c)$Al_{0.46}Si_{0.54}O_3$ and (d)$Al_{0.23}Si_{0.77}O_3$.

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