First-Principles Calculations of Energy Levels in Metal-Doped Silicon Nitride for Charge Trap Memory Applications

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Introduction Silicon nitride-based three-dimensional (3D) NAND flash memory has become one of the rapidly evolving technologies in semiconductor memories [1]. The recent development of multi-level cell technology in NAND flash memory has offered a high-bit density and reduced cost per bit. However, this technology demands a large threshold voltage shift, which basically depends upon the amount of charge stored by deep trap levels distributed in silicon nitride. Thus, the introduction of point defects capable of inducing deep trap levels in silicon nitride is needed to realize high-bit density flash memories. In the present work, we investigate the energy levels caused by metal defects (Mg, Ti, Hf, V, Mn, and Al) in silicon nitride using first-principles calculations.

Calculation details A 168-atom supercell ($Si_{72}N_{96}$) was formed by expanding a unit cell of β-Si_3N_4 phase in a 2x2x3 matrix on a-axis, b-axis, and c-axis, respectively. The six different supercells were formed by substituting a Si-atom in the bulk region of the supercell $Si_{72}N_{96}$ by each metal listed in the previous section. The supercells thus obtained was named as the supercell $Si_{71}N_{96}Mg$, $Si_{71}N_{96}Ti$, $Si_{71}N_{96}Hf$, $Si_{71}N_{96}V$, $Si_{71}N_{96}Mn$, and $Si_{71}N_{96}Al$. The structure optimization and self-consistent field (SCF) calculations were performed using Advance/PHASE ver. 3.5 software. The generalized-gradient approximation (GGA-PBE) functional was used as exchange-correlation energy in calculations. The kinetic energy cutoffs for wavefunctions and charge density were 40 and 400, respectively, in the calculations. 2x2x4 k-points sampling in the Monkhorst-Pack grid was used to perform SCF calculations. Besides, we have also calculated the total energy of the supercell $Si_{71}N_{96}Mn$ for different cutoff energies for wavefunctions (52, 64, 76, and 88 Ry) and charge density (520, 640, 760, and 880 Ry).

Results and Discussion Figures 1(a) and 1(b) show the total DOS calculated for the supercell $Si_{71}N_{96}Ti$ and $Si_{71}N_{96}Mn$, respectively. In the case of Ti, some energetically shallow levels could be seen near the conduction band edge as shown in Fig. 1(a). On the other hand, in the case of Mn, we have found five different defect levels of energy 1.59, 1.91, 2.03, 3.00, and 3.12 eV below the bottom of the conduction band. From Atomic Layer DOS (ALDOS) calculation results, we have observed that all five trap levels are mainly localized at the Mn atom. Some of these trap levels would be able to behave as deep electron trap levels.

References [1] S. Inaba, *2018 IEEE International Memory Workshop (IMW)*, Kyoto, 1 (2018).

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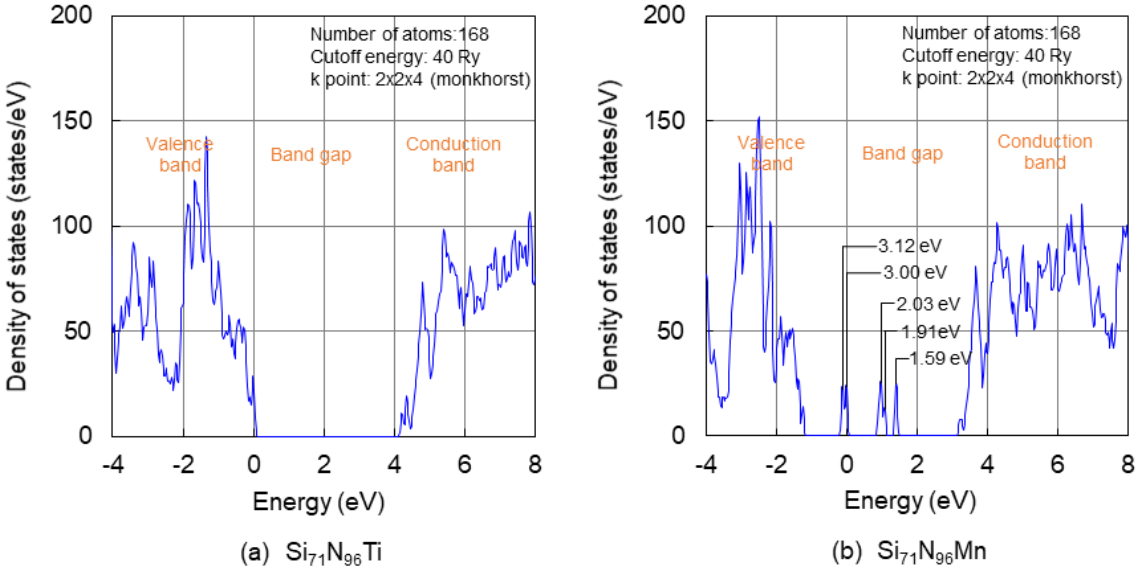

Fig. 1. Density of states (DOS) for supercell $Si_{71}N_{96}Ti$ (a) and supercell $Si_{71}N_{96}Mn$ (b).