8.10 FIRST-PRINCIPLES CALCULATIONS OF CHARGE STATES AND FORMATION ENERGIES OF Mg, Al, and Be TRANSMUTANTS IN 3C-SiC – S.Y. Hu, W. Setyawan, W. Jiang, C. H. Henager, Jr. and R. J. Kurtz (Pacific Northwest National Laboratory)

OBJECTIVE

To investigate the charge states and formation energies of Mg, Al and Be transmutants in 3C-SiC.

SUMMARY

The Vienna Ab-initio Simulation Package (VASP) is employed to calculate charge states and the formation energies of Mg, Al and Be transmutants at different lattice sites in 3C-SiC. The results provide important information on the dependence of the most stable charge state and formation energy of Mg, Al, Be and vacancies on electron potentials.

PROGRESS AND STATUS

Introduction

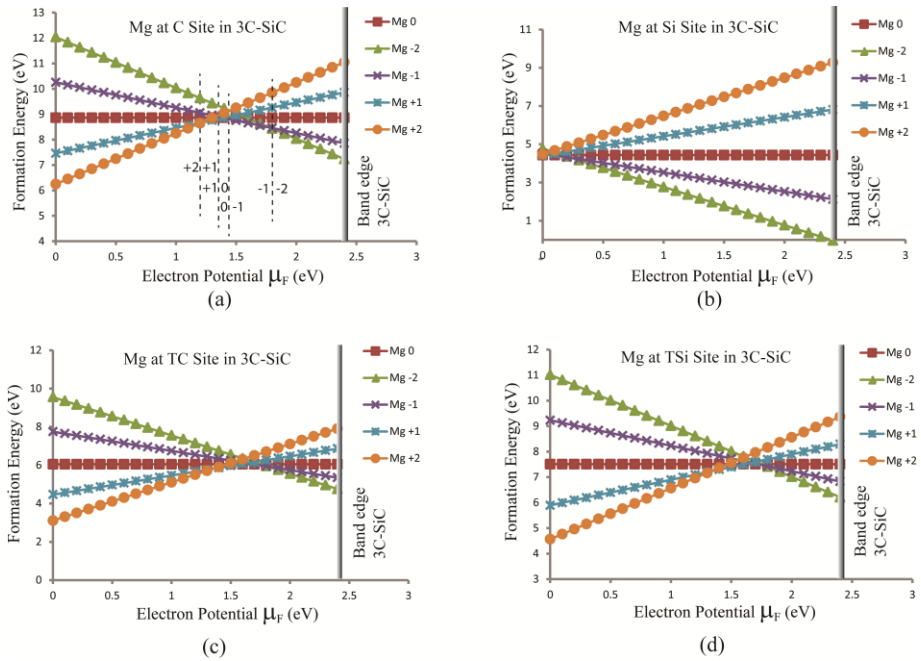
Theoretical calculations by Sawan, *et al*. [1] have predicted that at a fast neutron dose of ~100 dpa, there are ~0.5 at% Mg, ~0.15 at% Al, and ~0.2 at% Be generated in SiC through nuclear transmutation. These transmutants are expected to have potentially significant effects on phase stability, oxidation, transport properties (electrical and thermal conductivity), and elevated temperature mechanical properties. As we know, defects in semiconductor materials such as SiC might have different charge states, which depend on the local electron potentials. In order to determine thermodynamic and kinetic properties of defects in SiC, it is necessary to identify the charge states of defects and evaluate their effect on defect properties. This progress report presents possible charge states and formation energies of Mg, Al, and Be transmutants in 3C-SiC, calculated from density functional theory (DFT).

Simulation Method

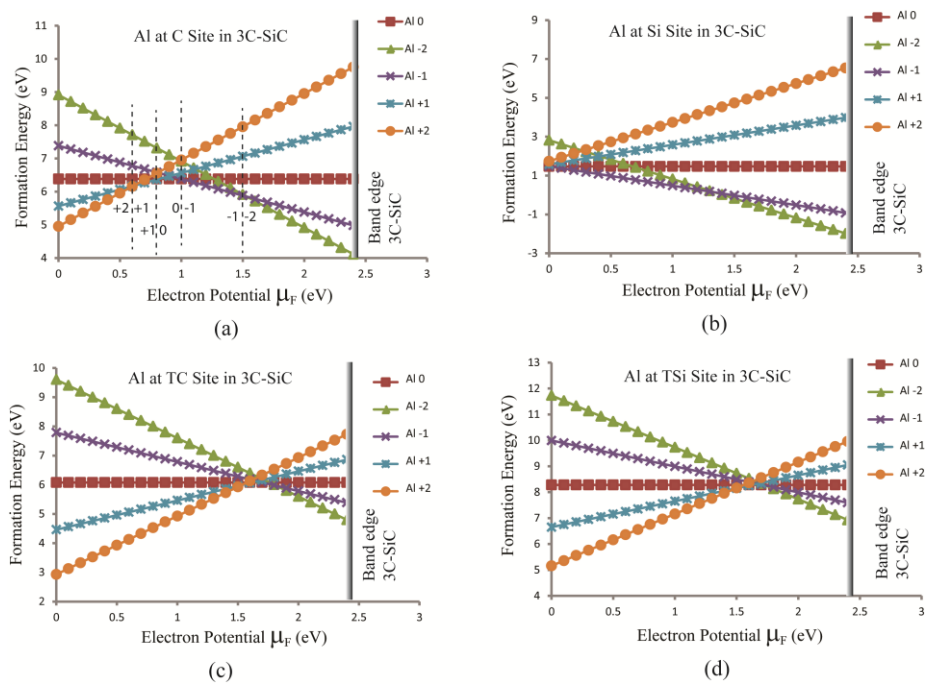
The method of calculating the formation energy of a charged defect is described in our previous report [2]. In the present simulations, a large supercell $3a_0 \times 3a_0 \times 3a_0$ (about 216 atoms) with a $3\times3\times3$ Monkhorst-Pack k-point mesh for Brillouin-zone sampling is used to minimize the spurious interactions between images of charged defects in periodic simulation cells.

Results

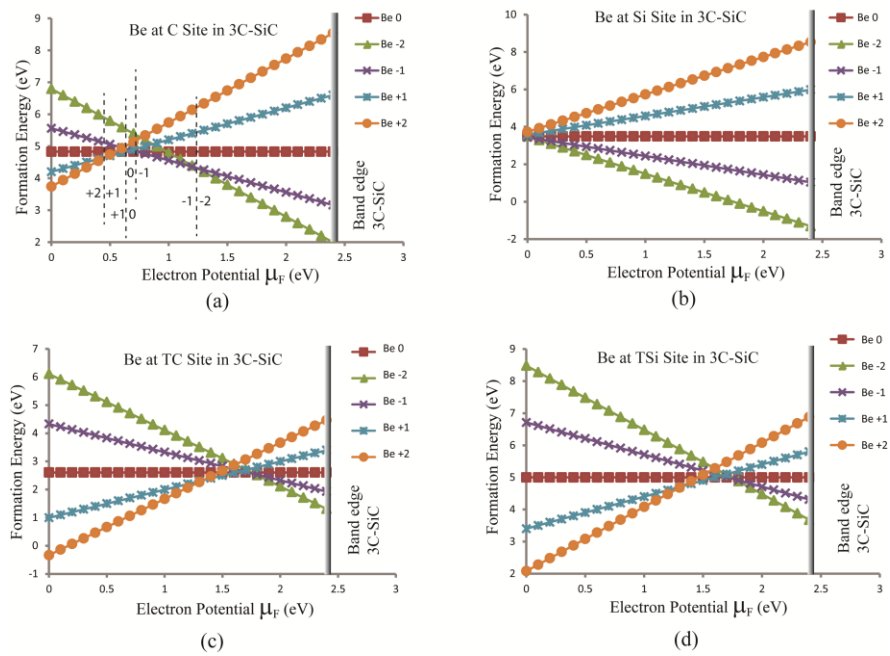
The defect energies of Mg, Al, Be and a vacancy with different charges $(q=-2,-1,0,+1,+2)$ at different lattice sites [Si, C, the tetrahedral center of carbon atoms (TC), and the tetrahedral center of Si atoms (TSi)] in 3C-SiC have been calculated. Figure 2 plots the formation energy $E^f(q)$ with different charge states at different lattice sites as a function of electron potential μ_F. The ionization level ($q/q\pm1$) can be determined by the intersection between two linear formation energy curves with charge q and $q+1$ $(\text{or } q-1)$, respectively. The vertical dashed lines in Figure 2 indicate the ionization levels for different defects. The segments defined by the intersections at ionization levels show the formation energy of the most stable charged defect for a given electron potential. Table 1 summarizes the most stable charge state, the formation energy, and lattice site of Mg, Al, Be and a vacancy for given electron potentials: 0.2, 1.0 and 2.0 eV, respectively.



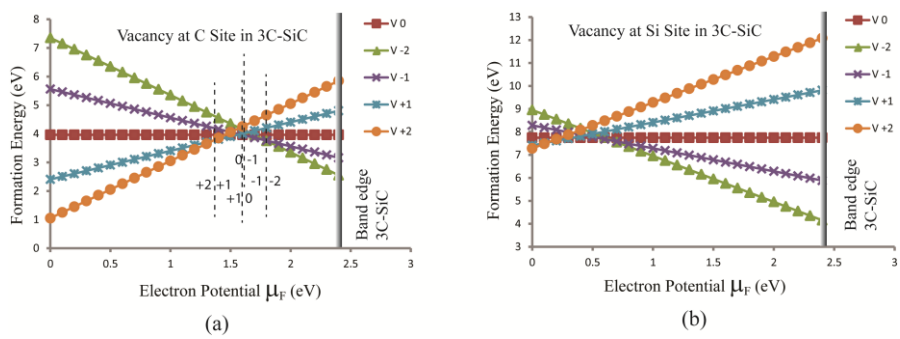
(A) Formation energy of charged Mg, (a) at C, (b) at Si, (c) at TC, and (d) at TSi.



(B) Formation energy of charged Al, (a) at C, (b) at Si, (c) at TC, and (d) at TSi.



(C) Formation energy of charged Be, (a) at C, (b) at Si, (c) at TC, and (d) at TSi.



(D) Formation energy of a charged vacancy, (a) at C, (b) at Si, (c) at TC, and (d) at TSi.

Figure 1. Formation energy of charged Mg, Al, Be and Vacancy at different lattice sites under different electron potential. The band gap value is taken as E_{band} = 2.39 eV,determined from experiment. [3]

Table 1. Most stable charged defect and formation energy of Mg, Al, Be and a vacancy under different electron potentials.

Electron potential	Mg		Al		Be		Vacancy	
	Stable defect	Formation energy	Stable defect	Formation energy	Stable defect	Formation energy	Stable defect	Formation energy
0.2eV	Mg_{TC}^{+2}	3.51eV	Al_{Si}^{-1}	1.28eV	Be_{TC}^{+2}	0.07eV	V_C^{+2}	1.45eV
1.0 eV	Mg_{Si}^{-2}	2.77eV	Al_{Si}^{-1}	0.48eV	Be_{Si}^{-2}	1.49eV	V_C^{+2}	3.05eV
2.0 eV	Mg_{Si}^{-2}	0.77eV	Al_{Si}^{-2}	-1.18eV	Be_{Si}^{-2}	-0.51eV	V_C^{-2}	3.35eV

FUTURE WORK

In the future work, we will examine the effect of charge states on migration energies of different defects by DFT calculations, and study the defect evolution kinetics in 3C-SiC by modeling and experiments.

Acknowledgements

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