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Theoretical investigations of the defects in bulk 4*H*-SiC and its influence on the (0001) surface properties

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【Introduction】

The silicon carbide (SiC) material, being known for its wide bandgap, high thermal conductivity, and high electrical breakdown field strength, is becoming the material of preference for high power devices. Presence of defects, however, has been a major restraint in the commercialization of SiC. It has been found experimentally [1] that atomically observed defects contribute to the high density of interface traps. To mitigate this problem, understanding of the defect energetics at the atomic scale is necessary. Several defect configurations have been proposed [2]. In this study, intrinsic defects of 4*H*-SiC were considered. The 4*H* polytype is particularly considered because among the various polytypes, it has the highest bandgap suitable for SiC-based MOSFET devices. The influence of these defects on (0001) surface properties was also explored along with the possible passivation mechanisms.

【Method】

We employed density functional theory (DFT) methods to understand the energetics of these defects. Geometry optimization and energy calculations were carried out within the GGA framework using the PW91 functional. The DND basis set is used to expand the valence wave functions. Calculations were carried out in a 2x2x2 supercell containing 64 atoms. Surface calculations involve 12 alternating planes of Si and C atoms in a crystal structure with a vacuum thickness of 10 Å.

【Results】

The defect-free 4*H*-SiC structure was first fully relaxed until the forces on each atom were less than 0.1 eV/Å. Various defect configurations and their possible passivated forms were then incorporated into the structure. Fig. 1 shows the DOS of bulk 4*H*-SiC with no defects and with a Si vacancy (V_{Si}). Energy levels caused by the dangling bonds can be observed just above the valence band. The DOS of the fully passivated V_{Si} defect as shown also in the inset of Fig. 1 suggests that H atoms can effectively reduce the trap density by minimizing the energy levels within the bandgap. The size of the void left out by the Si atom allowed for full passivation of the defect by H atoms. In contrast, other defects such as a C vacancy (V_C) cannot be fully passivated by H atoms since the void created by this vacancy is much smaller than that by a V_{Si}. Steric repulsion between multiple H atoms is prevalent. Analyses on the DOS revealed that active states remain in the middle of the bandgap even after partial passivation.

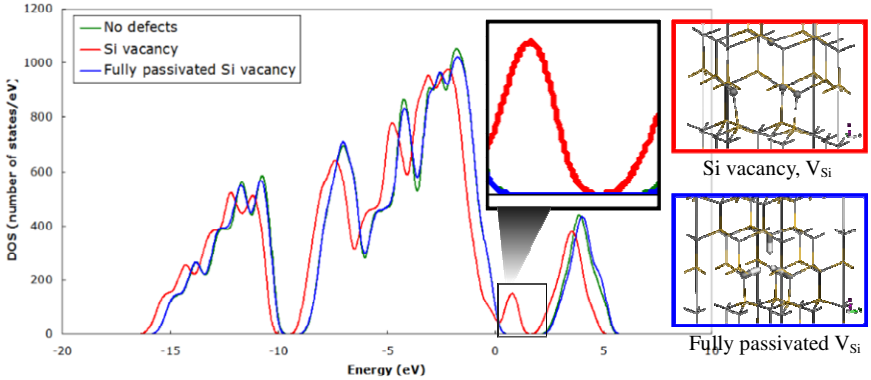

Fig. 1 DOS of 4*H*-SiC with no defects (green line), with one V_{Si} (red), and with fully passivated V_{Si} (blue); (insets) V_{Si} defect structure (upper-right) and its full passivation (lower-right).

These and other results on the influence of defect structures on the properties of the 4*H*-SiC(0001) surface will be presented in the conference.

References

[1] V.V. Afans'ev *et al.*, *Phys. Stat. Sol.*, **162** (1997) 321.
[2] F. Gao *et al.*, *Nucl. Instr. and Meth. in Phys. Res. B*, **267** (2009) 2995.