First principles XPS calculation for the B defects in SiC

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We investigate X-ray photoelectron spectroscopy (XPS) binding energy of boron (B) defects in silicon carbide (SiC) using the first principles calculation. Since 1990s, many studies based on the density functional theory had been carried out for surfaces and molecules. For lattice defects, however, few reliable first principles calculations have been reported. This is because the evaluation of the boundary condition for the electrostatic potential as a common energy origin is not enough to compare the energies between the different defect models and fairly large supercell size is required to obtain the reliable results [1].

So far, such calculations with special care for the boundary condition were reported for the monoelemental semiconductors: Si and Ge. The main aim of this work is to extend the core-level XPS calculation technique to the compound semiconductor SiC, which has been attracting the researchers’ interest as the efficient power device. Unlike Si and Ge, the SiC has the many crystalline structure called polytypes. It is interesting to investigate the effect of the polytypes on the boundary conditions.

We examine the following B defects: Si substitutional site (B\textsubscript{Si}), C substitutional site (B\textsubscript{C}), the hexagonal interstitial site (B\textsubscript{H}), the silicon-coordinated tetrahedral interstitial site (B\textsubscript{ITSi}) and B\textsubscript{Si} with a C vacancy (B\textsubscript{Si} + V\textsubscript{C}). For the XPS calculation, we adopt ΔSCF method based on the density functional theory with screened core hole pseudopotentials [2]. Figure 1 shows the dependence of supercell size on the chemical shifts of the B1s XPS binding energy in 3C-SiC (zincblende structure). The energy origin is that of B\textsubscript{Si} for each supercell size. It is found that the supercell of 1000 atoms reveals the accuracy within 0.1 eV. The results of defects in other polytypes will be also discussed in the conference.