

不純物ドーピングによる 4H-SiC の低抵抗化

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***Ab initio* calculations of dopant energy levels in 4H-SiC**

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We have calculated structure, formation energies, and activation energies of substitutional group- II , III, V and VI impurity in 4H-silicon carbide (SiC). It is shown that a carbon site has lower formation energies than a silicon site for nitrogen, oxygen, and sulfur regardless of the crystal growth condition whereas favorable sites boron and selenium depend on the composition. Impurities except for the above elements are always reside on a silicon site. We also found that antimony forms a quite shallow donor level in 4H-SiC. The calculated activation energy of antimony atoms is 41 meV. The results suggest that antimony is the most promising as an n-type dopant for the formation of a doped layer with low resistivity in 4-SiC.