First-principles study on complexes of impurity and dislocation in GaN p-n diodes

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The development of power semiconductor devices is one of the key issues for the realization of a sustainable society. GaN has properties suitable for power devices, such as a large band gap, and is expected to be a candidate for next-generation power semiconductor materials. On the other hand, the threading dislocations generated during the synthesis of GaN become a source of leakage current, which impairs the rectifying effect, an important characteristic of the device. It has been reported that the leakage current is related to the type of threading dislocation and the condensation of impurities around the dislocation, but the microscopic mechanism of leakage current generation has not been clarified.

Power semiconductor devices consist of a combination of p-type and n-type layers, with impurities such as Si and Mg doped to each layer. To understand the mechanism of leakage current generation, it is necessary to understand the electronic state in each layer. The electronic structure of the complex of Mg and screw dislocations doped to make the p-layer has been clarified by our previous studies using first-principles calculations and atom probe tomography. [1] The purpose of this study is to analyze the interaction between Si impurities doped to make the n-layer and dislocations, and to clarify the properties of the complex consisting of Si and dislocations.

The effective mass of electrons is smaller than that of holes in GaN, and the effective Bohr radius, which indicates the width of the impurity states, is larger. Therefore, it is necessary to consider larger systems. For larger system size calculations, we use RSDFT[2, 3], a highly parallelized and efficient first-principles code. In this study, we consider a screw dislocation with the Burgers vector [0001]. The dislocations break the periodic structure and we use a supercell. In order to avoid these strains affecting each other at the periodic boundary, a vacuum layer is inserted in the lateral directions of c-axis.

We consider a 21 Å $\times$ 27 Å $\times$ 30 Å supercell, which includes about 800 atoms. An Si atom is substituted at a Ga site. In order to analyze the binding energy of Si, we performed calculations for several substitutional sites. We optimized the atomic positions and obtained the stable structures of the complex. We are analyzing the results for the binding energy of Si to the screw dislocation.

References

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