

Atomic Structures and Chemical States of Dopants in Ga₂₀3

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(Ga₂O₃におけるドーパントの原子構造及び化学状態)

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論 文 内 容 の 要 旨

Gallium oxide (Ga₂O₃) has attracted a significant amount of interest due to its excellent properties, such as a large bandgap of 4.5–5.3 eV (depending on the crystal polymorphs), high thermal stability, and high breakdown electric field. Ga₂O₃ has six crystal polymorphs, α , β , γ , δ , ϵ , and κ . Among these polymorphs, β -Ga₂O₃ is the most thermodynamically and chemically stable. The high-quality β -Ga₂O₃ film can be homoepitaxially grown on the β -Ga₂O₃ substrate. The other polymorphs of Ga₂O₃ (α , γ , δ , ϵ , and κ), on the other hand, are thermodynamically metastable phases. Among the metastable polymorphs, κ -Ga₂O₃ is expected to exhibit significant spontaneous polarization and ferroelectric properties. Due to its spontaneous polarization property, κ -Ga₂O₃ is expected to be used in devices with high-mobility two-dimensional electron gas systems.

For Ga₂O₃-based devices, Si and Sn are usually used as dopants. These dopants are formed as shallow donors. However, it has not been clarified how many chemical states exist in Ga₂O₃ and which of the substitutional and/or interstitial sites is the active dopant one. In addition, the atomic structures and chemical states of the inactive dopant sites should be clarified because the inactive dopant sites are the additional carrier scattering sites. The additional carrier scattering sites decrease the carrier mobility. Determining the atomic structure and chemical state of the active and inactive dopant sites in Ga₂O₃ is a necessary step to control the properties of Ga₂O₃-based devices. Therefore, it is important to clarify the active dopant sites in Ga₂O₃. Once the active and inactive dopant sites are revealed, a strategy for eliminating the inactive sites of dopants is established.

In the doctoral course study, I aim to clarify the atomic structures and chemical states of active and inactive dopant states of Ga₂O₃. The dopants in β - and κ -phase Ga₂O₃ are selected in this doctoral thesis because they are considered as the most suitable of the Ga₂O₃ polymorphs for device applications. To clarify the atomic structures and chemical states of the active and inactive dopant sites of β - and κ -Ga₂O₃, photoelectron spectroscopy (PES), photoelectron holography (PEH), x-ray absorption near-edge structure (XANES), and extended x-ray absorption fine structure spectroscopy (EXAFS) are employed. The present results are useful for the improvement of doping efficiency and the preparation of Ga₂O₃-based devices with high performance.

This doctoral thesis consists of five chapters and is structured as follows.

Chapter 1 introduces the general background of Ga₂O₃, polymorphs of Ga₂O₃, the dopants for Ga₂O₃, the current issues for Ga₂O₃, and the research purpose of this thesis.

Chapter 2 introduces the experimental part of this thesis, including the sample preparation and

characterization methods used in this thesis. The principle of the characterization methods used in this thesis is also explained.

Chapter 3 describes the clarification of the chemical states and the atomic position of the active dopant sites of the Sn dopants for Sn-doped β -Ga₂O₃ using PES, XANES, and EXAFS.

Chapter 4 presents the results of the chemical states and the atomic position occupancy of the Si dopants for Si-doped κ -Ga₂O₃ using PES, chemical state-discriminated PEH, and EXAFS.

Chapter 5 describes the conclusions and the outlook of the thesis. The conclusions summarize the most important results in this thesis.