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Atomic and Electronic Structures of the Complex of Mg and Screw Dislocations in GaN

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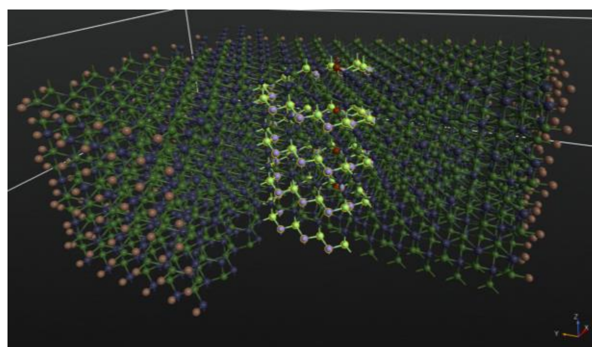
Graphical Abstract



p-type

Mg + dislocation
(n-type)

Abstract

GaN is attracting great attention as next-generation power semiconductor devices. In order to improve device performance in GaN power semiconductor devices such as a p-n diode, reliability requirement is the most important issue. To solve the reliability issue, clarification of the physical origin of leakage current is mandatory. Usami et al. has shown that a leakage spot correlates with the placement of a threading screw dislocation in a p-n diodes [**1**]. Also, Mg impurities with higher concentration (1019 cm-3) more than doping concentration are observed around the screw dislocation by atomic probe observation [**2**]. These results suggest that the aggregation of Mg impurities to a screw dislocation causes the leakage current. The atomic and electronic structures were obtained using VASP (Vienna ab initio simulation package) code, which is based on density functional theory with the generalized gradient approximation [**3**]. All atoms were relaxed until the Hellmann-Feynmann force becomes smaller than 10meV/Å for structural optimization. Spin polarization and spin orbital coupling does not include in our calculations. First, we investigated where a Mg atom is stable around the screw dislocation. We found that the closer to the dislocation core the Mg position is, the more stable the system formation energy becomes. This result coincides with the experiments that Mg impurities are gathering around a screw dislocation. Next, we examined the electronic structure of each system with Mg replacement around the screw dislocation. As the Mg position becomes closer to the dislocation core, the highest occupied level elevates toward conduction band minimum. This indicate that Mg impurities are gathering around a screw

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dislocation, which leads to form the n-type region near the dislocation core even in the p type GaN. Therefore, the aggregation of Mg impurities around a screw dislocation is a possible origin of leakage current. In the presentation, we also discuss the effect of leakage current from the electronic structure in more detail.

Keywords: GaN, Mg impurity, screw dislocation. first principles calculation.

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Biography of Presenting Author

Kenji Shiraishi received the B.E., Master and Doctor. degrees in physics from the University of Tokyo and worked in the research of science and technology of semiconductors for 13 years in NTT. After NTT he joined University of Tsukuba and he worked in the research of semiconductor devices for 13 years. He is now a Professor of Institute of Materials and Systems for Sustainability, Nagoya University and continue semiconductor device researches. Since joining NTT, he has developed new physical concepts of surfaces, interfaces and nano-structures of semiconductors which are very important for semiconductor devices. He has also been engaged in research on semiconductor devices more than 30 years. He has authored and coauthored more than 270 papers.

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