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Microscopic Reason for the Leakage Current due to the Mg-Attached Dislocation in GaN

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Abstract

Threading dislocations with segregated impurities such as Mg are suspected to induce leakage currents, thus leading to the degradation of GaN-based electronic devices. However, the microscopic reason for the segregation and the leakage currents is totally unknown. We here focus on the Mg impurity near the screw dislocation in GaN and perform the density-functional (DFT) calculations that clarify the reason. We find that segregated Mg to the particular shape of the dislocation core is energetically favorable and induces the electron states in the gap, thus being responsible for the leakage currents.

1. Introduction

GaN attracts great attention for the use in a wide range of power semiconductor devices due to its superior characteristics compared with silicon [1]. During the crystal growth of GaN, however, threading dislocations appear with high density (10^8-10^9 cm^{-2}) due to the lattice mismatch with the substrates [2,3]. Even on the GaN substrate, the dislocation density is still high (10^4 to 10^7 cm^{-2}) [4], and those threading dislocations degrade the performance of GaN-based electronic devices [5]. A recent study has shown that pure screw dislocations are responsible for the leakage currents [4], and other studies have reported that certain impurities are segregated around the dislocations in GaN [6-8].

Also, it is reported that Mg atoms gathers around pure screw dislocations at high concentration, and pure screw dislocations with Mg atoms are related to the leakage currents [9]. However, it is not clear that the affinity between Mg impurity and pure screw dislocation at an atomic level, and the electronic structure of the screw dislocation with Mg impurity is not fully understood. It is very important to clarify those points for the fabrication of power-saving GaN electronic devices having low leakage currents. In this study, we focused on [0001] pure screw dislocations in GaN.

2. Models and Calculation method

Before examining the dislocation with Mg atoms, we clarified the core structures of the pure screw dislocations with no impurities. First, we prepared initial atomic structures of the screw dislocation in GaN. Then, these model structures were optimized. We constructed a supercell containing about 800 atoms for threading dislocations (Fig. 1(a), (b)). The model had a periodic boundary condition in the [0001] direction, parallel to the dislocation line. The model was terminated by fictitious hydrogen atoms and surrounded by a vacuum region in the [11-20] and [-1100] directions.

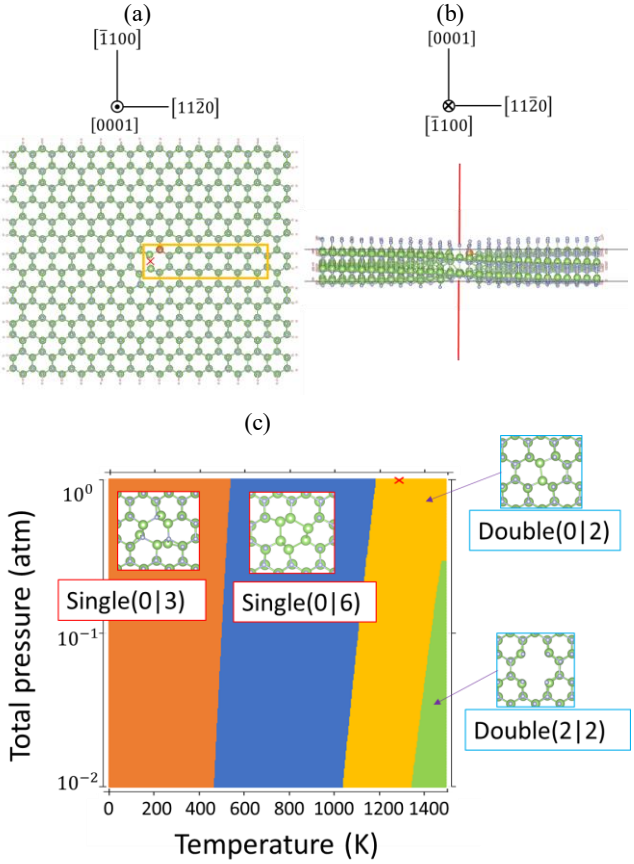

Fig. 1 (a) Top and (b) side views of the [0001] screw dislocation with Ga-filled core model (Double(0|2) model, see Fig. 2). Green, blue and light orange balls indicate Ga, N, and H atoms, respectively. (c) Most stable structures in [0001] screw dislocations with no impurities considering the crystal growth conditions. Each region shows the most stable core structures considering the free energies. The horizontal axis is substrate temperature and the vertical axis is total pressure. Our current experimental conditions (shown by red cross marks) are included within the region of Double(0|2) model.

For the screw dislocations, the core types are mainly classified into the closed core model, the open core model,

and Ga-filled core or N-filled core model [10]. We examined these all core configurations for the screw dislocations. Structural optimization and electronic state calculations were performed using VASP (Vienna Ab-initio Simulation Package) [11], which is a first principles calculation code based on density functional theory (DFT).

3. Results and Discussions

First, we calculated the formation energy of each core in the screw dislocations with no impurities. Fig. 1(c) shows the most stable core structures under crystal growth conditions. In Fig. 3(c), each region shows the most stable core structure by comparing free energies. Our current experimental conditions are included within the region of Double(0|2) model, which is Ga-filled core model. Therefore, Double(0|2) model appears during the crystal growth.

Next, we investigated where Mg substitute Ga site around the dislocation by comparing formation energies. Formation energy E_f was defined as follows :

$$E_f = E_{\mathrm{dis/Mg}} - E_{\mathrm{dis}}. \quad (1)$$

$E_{\mathrm{dis/Mg}}$ is total energy of the Mg substation for the Double(0|2) dislocation model, E_{dis} is total energy of without impurity model for the Double(0|2) dislocation model. The less the formation energy is, the more stable the model becomes. Fig. 2 shows the formation energy differences between each Mg substitution position. In our experiments, we conducted high temperature annealing after Mg ion implantation (700 ℃) when forming p-GaN layer [9]. We found that the closer the substitution position is to the dislocation core, the more stable each model becomes. Moreover, the most stable Mg substitution model is near the dislocation core.

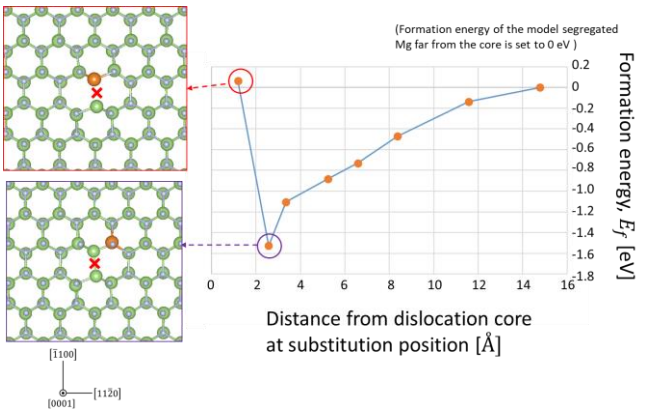

Fig. 2 The relationship between the distance from the dislocation core of the Mg substitution position and the formation energy in each system. Mg substitution occurs in the light blue areas. Green, blue and orange balls indicate Ga, N and Mg atoms, respectively.

Finally, we examined the density of states of the most stable model for Mg substitution to the Double(0|2) (Fig. 3 (a)). In Fig. 3(a), there are no defect peaks near the bottom of the conduction band, and the model have a certain width of band gap. We also examined the Mg substitution model closest to the dislocation core (see Fig. 2). As it can be seen in Fig. 3 (b), there are defect levels under the conduction band for the model. Therefore, the Mg substitution model at Ga site closest to the dislocation core causes the leakage currents in n-type GaN.

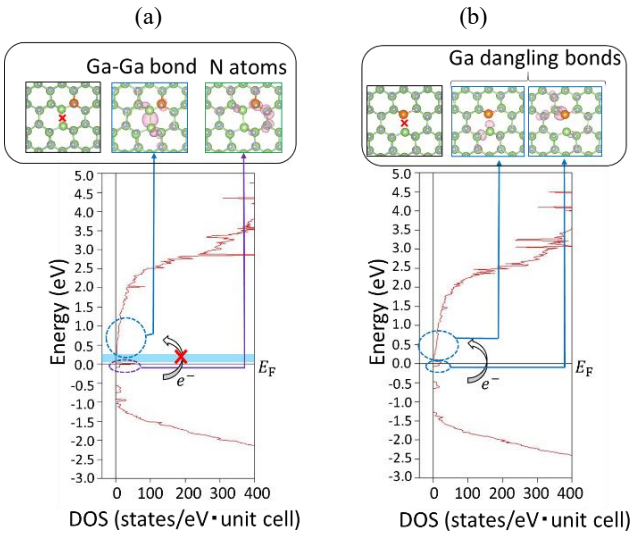

Fig. 3 Density of states of (a) the most stable model for Mg substitution to Double(0|2) (shown by green circle in Fig. 2), and (b) Mg substitution model closest to the dislocation core of Double(0|2) model (shown by red circle in Fig. 2) in the screw dislocations.

4. Conclusions

We have examined the affinity between Mg and the [0001] screw dislocations and its electronic properties. The closer to the dislocation core the position of Mg substitution for the Ga site is, the more stable the system becomes (Fig. 2). Therefore, it is possible that Mg atoms are gathering near the dislocation core. This Mg substitution model closest to the dislocation core have defect levels under the conduction band (Fig. 3(b)). These results show that the screw dislocations with the Mg substitution are possible origin of leakage currents.

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