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Modeling of the Leakage Current in GaN mediated through the Dislocation-Impurity Complex

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Abstract

The leakage current is occasionally observed in semiconductor devices and its suppression is crucial to guarantee the reliability of the devices. Recent experimental studies on GaN p-n diodes have revealed that the leakage spot is the dislocation core decorated with Mg impurities. Our first-principles calculations have indeed clarified that deep levels are induced by the dislocation-impurity complex in the gap of GaN. We here construct a microscopic model in which an electron hops among spatially distributed deep levels along the dislocation core, thus leading to the leakage current. By simplifying the electron spectrum near the gap, we obtain an analytical formula for the hopping conduction which may be a basis to consider the leakage current microscopically.

1. Introduction

Development of materials for next generation power device is crucial to realize future energy saving society. GaN has been attracting a great attention as one of the alternatives for Si which is the conventional power device material. However, reliability problems of GaN power devices have not been solved yet. This is due to the fact that physical origin of leakage current has not been clarified.

Recently, Usami et al. found that a leakage spot correlates with the existence of threading screw dislocation in the GaN p-n diodes [1]. Moreover, Mg impurities segregate near the dislocation cores with much higher concentration than the intentional doping concentration by atomic probe observations [2]. These results imply that the dislocation-Mg complexes generate leakage paths.

In this study, we propose a physical model for leakage current of GaN power devices with dislocation-Mg complexes. We found that dislocation-Mg complexes drastically modify the electronic structures. The highest occupied level depends on the relative position of Mg from the dislocation core and we take account of the distribution of the level for our physical model. We simplify the distribution as a rectangular distribution and solve the equation for the hopping current analytically. The obtained physical model can describe the current-voltage characteristics from low field to high field seamlessly. Then, we demonstrate the behavior of the obtained analytical formula with realistic model parameters.

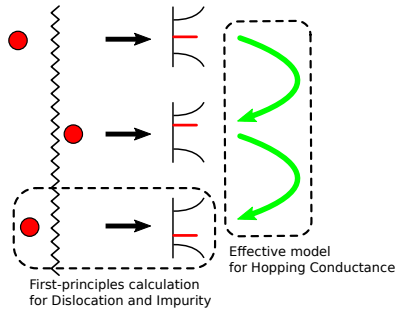

Fig. 1 Schematic picture of the approach to analyze the hopping conductance in the system with dislocation and impurities. Red circles in the left denote impurities and zigzag line denotes dislocation. The middle shows density of states in the systems with dislocation and an impurity. Red bars denote the localized level formed due to the dislocation and an impurity. The hopping conductance occurs among the localized states shown as green arrows in the right. The density of states is derived from first-principles calculation and we construct a model based on the density of states.

2. Models

We assume that physical origin of leakage current is hopping conduction. In this assumption, we formulate the calculation method of hopping conduction. The schematic illustration of our physical model is given in Fig. 1.

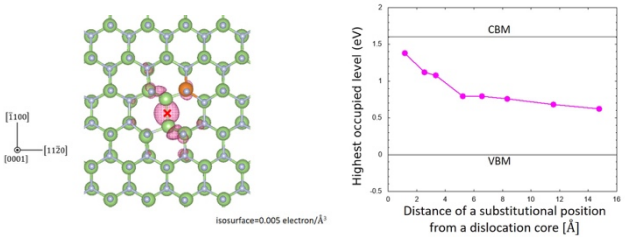

Fig. 2 (left) An example of the isosurface of the localized states at Fermi level in GaN (Ga:green sphere, N:gray sphere) with screw dislocation and Mg impurity (orange sphere). A red cross is the dislocation center. (right) Mg position dependence of highest occupied level. CBM and VBM denote a conduction band minimum and a valence band maximum, respectively. The origin of the energy is set to VBM of the bulk system.

3. Results

First-principles calculation results

We performed first-principles calculation by using VASP (Vienna Ab-initio Simulation Package)[3]. An example of a model structures for the dislocation is shown in Fig. 2. Mg yields a compensation and hopping levels are generated near the highest occupied levels. The states are localized at the dislocation center. Thus, the hopping is one dimensional.

Hopping conductance

The hopping conductance consists with the following four physical factors. (i) hopping distance R; (ii) overlap of envelope functions defined by width of the envelope function α^{-1}; (iii) distributions of occupied and unoccupied levels ρ_o and ρ_u; (iv) transition probability $e^{-\beta[(E_2-E_1)-eRF]}$ for $(E_2-E_1) \geq eRF$ and 1 for $(E_2-E_1) < eRF$[4,5]. Consequently, we get an expression of the hopping current as,

$$j = e\nu_{e-ph}n^2VS\int dR\, Re^{-2\alpha|R|}\int dE_1dE_2 \rho_o(E_1)\rho_u(E_2)\begin{cases} e^{-\beta[(E_2-E_1)-eRF]}, & (E_2-E_1) \geq eRF \\ 1, & (E_2-E_1) < eRF, \end{cases} \quad (1)$$

where e, ν_{e-ph}, n, F are an electron charge, an electron-phonon frequency, a concentration of hopping sites, and external electric field, respectively. As mentioned above, the hopping is one dimensional while Mg distribute in three dimensional space. V is effective volume in which the impurities distribute and corresponding effective area is S. (These values have ambiguity due to a region of a local concentration for inhomogeneously distributed impurities.)

In this study, we simplify the distributions ρ_o and ρ_u as a rectangular distribution. This simplification is based on the following assumptions. (i) The hopping occurs between the levels just below and just above a level separating occupied and unoccupied states; (ii) There are a lot of hopping level in the band gap of GaN such that the distribution becomes continuous. From those distributions, we can derive a distribution of the energy difference $W = E_2 - E_1$ as following.

$$P(W) = \int dE_1dE_2\, P(E_1)P(E_2)\delta\big(W-(E_1-E_2)\big) = \begin{cases} \frac{1}{2D}\left(1-\frac{W}{2D}\right), & W \geq 0 \\ \frac{1}{2D}\left(1+\frac{W}{2D}\right), & W < 0 \end{cases} \quad (2)$$

D is width of the distribution, which can be extracted from the distribution of the Fermi levels given by first-principles calculation (see Fig. 2). From Eqs. (1) and (2), we derive an analytical expression of the hopping current as,

$$j \propto \left(\frac{2D}{eF}\right)^2\Big[h_2^{ff}(\alpha') + \left(\frac{1}{2}+t-t^2\right)h_2^{nf}(\alpha') + (1-t)h_3^{nf}(\alpha') - \frac{1}{2}h_4^{nf}(\alpha') + t^2e^{-\frac{1}{t}}h_2^{nf}\left(\alpha'-\frac{1}{t}\right) + \left(\frac{1}{2}+t+t^2\right)h_2^{nb}(\alpha') + (1+t)h_3^{nb}(\alpha') + \frac{1}{2}h_4^{nb}(\alpha') + t^2\left(e^{-\frac{1}{t}}-2\right)h_2^{nb}\left(\alpha'+\frac{1}{t}\right) + t^2\left(e^{\frac{1}{t}}+e^{-\frac{1}{t}}-2\right)h_2^{fb}\left(\alpha'+\frac{1}{t}\right)\Big], \quad (3)$$

$$\alpha' \equiv \frac{2D}{eF}2\alpha, \quad t \equiv \frac{k_BT}{2D}, \quad (4)$$

$$h_n^{ff}(y) \equiv (n-1)!\sum_{m=1}^{n}\frac{y^{-m}}{(n-m)!}e^{-y}, \quad (5)$$

$$h_n^{nf}(y) \equiv -(n-1)!\left[\sum_{m=1}^{n}\frac{y^{-m}}{(n-m)!}e^{-y}-y^{-n}\right], \quad (6)$$

$$h_n^{nb}(y) \equiv (-1)^{n-1}h_n^{nf}(y), \quad (7)$$

$$h_n^{fb}(y) \equiv (-1)^{n-1}h_n^{ff}(y). \quad (8)$$

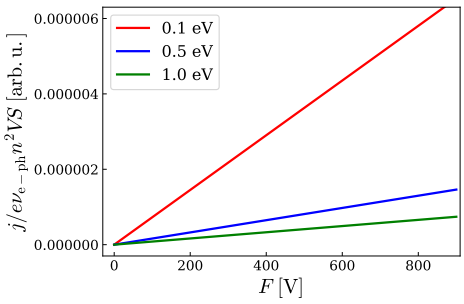

Fig. 3 Field dependence of Eq. (3) other than prefactors. D=0.1, 0.5, and 1.0 eV. α^{-1} = 0.1 nm and T = 300 K.

We demonstrate the behavior of the leakage current, Eq. (3), with D=0.1, 0.5, and 1.0 eV (Fig. 3). α^{-1} is 0.1 nm which seems to be reasonable by seeing the left panel of Fig. 2. From Fig. 3, we found that larger width D decreases the current. The decrease of the current is caused by a large energy difference in a wider distribution. Once an electron occupies a lower level in a distribution, it has to overcome a large energy difference to move to a next hopping site. This indicate that high Mg concentration in the dislocation core corresponds to the appearance of leakage path which coincides with the experiments [2].

4. Conclusions

We constructed a physical model for the leakage current of GaN power devices by considering the electronic structures of dislocation-impurity complexes obtained by first principles calculations. We assume that leakage current is governed by the hopping conduction. We extract the width of the distribution of the Fermi levels and construct a physical model with approximation of a rectangular shape distribution. We found an analytical formula for the hopping conductance and demonstrate the behavior of the model. Our obtained results are consistent with the recent experimental reports [2].

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