GaN 평면결함의 구조와 형성에너지에 관한 연구

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Atomic structures and Energies of Planar defects in w-GaN

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Abstract

We investigate the structures and the formation energy of inversion domain boundaries (IDBs) using the Tersoff empirical potential. Four kinds of IDBs (A and B types for IDB* and Holt) are considered. The IDBs with A type are energetically favorable compared to B type with the structural instability. The IDB* is also more stable than the Holt type in spite of fourfold and eightfold rings of bonds. We calculate the atomic configurations of the Holt IDBs induced by the interactions of the IDB* with the stacking faults I_1 and I_2. The stacking fault I_2 interacted with I_1 on the IDB induces the structural transformation from IDB* to Holt type.

I. Introduction

Defects such as point, line, and planar defects in w-GaN play an important role in high temperature optoelectronics and high power, high frequency devices. Many experimental and theoretical investigations for defects, which affect the structural, electrical, and optical properties of GaN, have been reported in the literature. In the case of planer defects in GaN, inversion domain boundaries (IDBs) in particular have been much studied, though their characteristics and origin are still a controversy. The understanding of IDBs is important to characterize GaN films, because these affect the quality of GaN such as the surface structure and morphology.

In this paper, the structures and the formation energy of IDBs are investigated using a molecular -dynamics method. We calculate the atomic configurations of the Holt IDB induced by the interactions of the IDB* with the stacking faults.

II. Results and discussion

For the structural property of planar defects in w-GaN, we use a classical molecular-dynamics (MD) method based on the Tersoff empirical potential. Details of the Tersoff potential are described elsewhere. Although these empirical methods cannot give accurate results compared to first principles methods, they can be applied to complex systems, which require a large number of atoms or longer calculations, such as the mutual interaction and the movement of defects. We previously proposed the Tersoff potential parameters for GaN [1].

To investigate IDBs in w-GaN, the structures and the formation energy of (10-10) IDBs are first calculated. We consider four kinds of IDBs, which are grouped into IDB*-A, IDB*-B, Holt-A, and Holt-B. The optimized structures of IDB* and Holt type IDBs are shown in Fig. 1. The Holt IDBs show wrong bonds (Ga-Ga or N-N) by the exchange of anion and cation at the boundary, without any other translations in structure. The atomic structure of the IDB* is characterize by a c/2 translation to avoid the less favorable homoelemental bonds. As a result of simulations, the B type of IDBs leads to the geometrical distortion of w-GaN and has the structural instability, compared to the A type. Table 2 shows the formation energy of IDBs. These results are in agreement with other

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theoretical predictions.

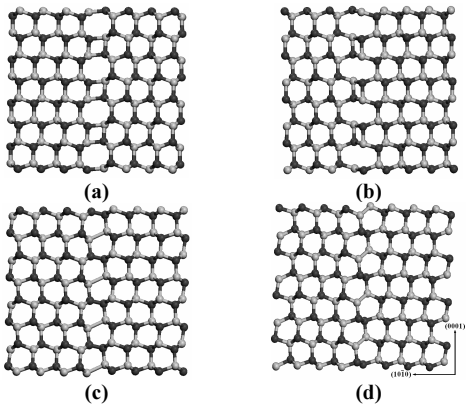

Fig. 1 Optimized structure of IDBs in w-GaN. (a) IDB*-A, (b) IDB*-B, (c) Holt-A, and (d) Holt-B.

Table2. Defect formation energy (eV/Å^2) of IDBs in w-GaN.

	present	calculation
IDB*-A	0.074	0.037, 0.025
IDB*-B	0.127	
Holt-A	0.194	0.250, 0.167
Holt-B	0.372	

It is found that the structure of the A type is energetically more stable than that of the B type. However, Ruterana and Nouet have reported that the boundary plane can move from one type to the other of the same model despite the instability of the B type [2]. As compared the Holt type with the IDB*, the latter is energetically favorable in spite of fourfold and eightfold rings of bonds. Northrup et al. have also proposed that most of the IDBs correspond to the IDB* type and the formation energy for the IDB* is much less than for the other structures [3]. This indicates that the high energy cost of homoelemental Ga-Ga and N-N bonds may outweigh the cost of the structural transformation by fourfold and eightfold rings. Nevertheless, Holt IDBs, which are electrically active, are also observed experimentally.

Many investigations for the formation mechanism of Holt IDBs have been reported in the literature [4]. First, the accommodation of the shift created by the substrate step showed the possibility of the formation of Holt IDBs. This step can reduce the energy barrier for the formation of IDBs, especially Holt type. Other mechanism is that Holt IDBs are formed through the interaction of IDB* with stacking faults. In particular, the stacking fault I_1 terminated on the IDB induces the structural transformation from IDB* to Holt type, while if the stacking fault crosses the IDB then no structural change occurs. In the case of the stacking fault I_2, it generally has not been reported in GaN layers grown on a sapphire. However, Iwamoto et al. have observed that the stacking fault I_2 with two stacking violations was introduced in the inversion domain while the stacking fault I_1 in the matrix in GaN film grown on the sapphire [5]. They proposed that the origin of the termination of inversion domains is related to the formation of Holt IDBs by the stacking faults. The presence of I_2 at the vicinity with the interface on the sapphire substrate has also been proposed by Ruterana and Nouet.

We calculate the atomic configuration of IDBs to investigate the formation of Holt IDBs through the interaction of the IDB* with stacking faults. Figure 2 (a) shows the atomic structure of the Holt IDB induced by the interactions of the IDB* with the stacking fault I_1. Also, the stacking fault I_2 interacted with I_1 on the IDB can introduce the structural transformation from IDB* to Holt type, shown in Fig. 2 (b). As the stacking fault I_2 terminates on or passes through the IDB, the IDB structure is not transformed.

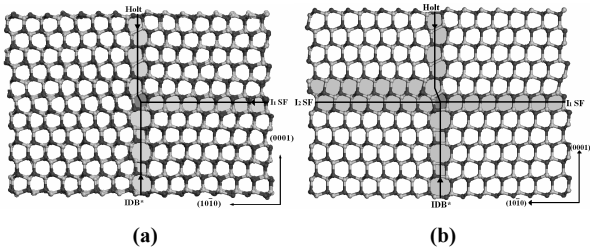

Fig. 2 Atomic configuration of IDBs to investigate the formation of Holt IDBs through the interaction of the IDB* with stacking faults (a) I_1 and (b) I_2.

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