First principles study on leaking current at a dislocation in doped semiconductors

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In the second half fiscal year of 2019, we have revealed the following results related with the performance of gallium nitride (GaN) power devices [1].

- The threading screw dislocations attract Mg impurities, and the electronic levels in the energy gap induced by the threading dislocations elevate towards the conduction band as the Mg approaches the dislocation line.

This results suggest that the leakage current which degrade the performance of the devices is induced by the presence of the Mg and the screw dislocation complexes.

GaN is one of the most promising compounds for the power devices since it has a large band gap. For the realization of the device, suppressing the leakage current is an important issue. The leakage current has been observed at the position of the threading dislocation. Recent experimental study suggests that the Mg impurities are condensed around the dislocation. The electronic structure of the Mg-dislocation complexes should be related with the origin of the leakage current, and it is important to guarantee the device reliability.

In this study, we systematically perform first-principles total-energy calculations for possible 16 core structures of the screw dislocations as shown in Fig. 1. The core structures are expressed as D(n | m) or S(n | m). The first capital letter denotes the position of the dislocation line. One is called single core,

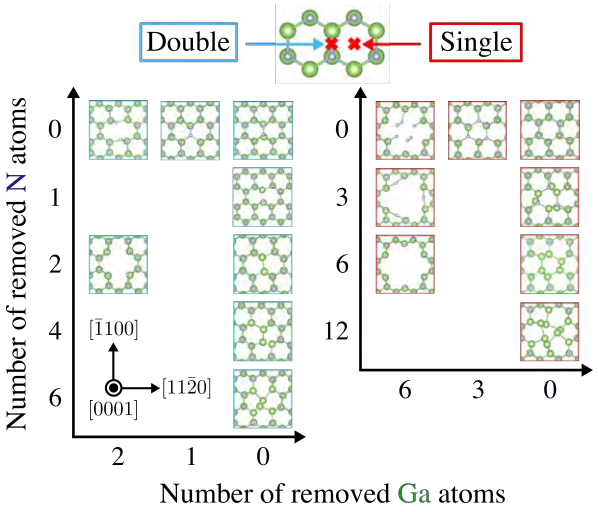

Figure 1: The 16 core types of the screw dislocations. A red cross in the top panel denotes the position of the dislocation line. The left is for D(n | m) and the right is for S(n | m), where n is the number of removed Ga and m is that of N.

in which the dislocation line is at the center of the single hexagon; Another is called double core, in which the dislocation line is at the middle of the bond of hexagon. n and m represent the numbers of Ga and N atoms removed from the fully filled structures. An example of D(0 | 0) is shown in Fig. 2

Those first-principles calculations are done by using the Vienna Ab initio Simulation Package (VASP) [2] which is based on the projector augmented-wave (PAW) method. The exchange-correlation energy is treated within the generalized gradient approxima-

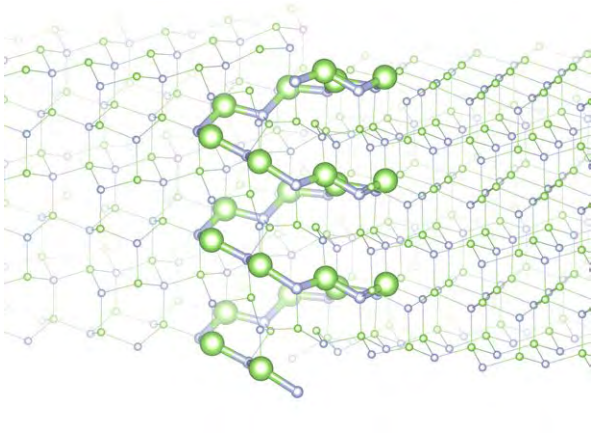

Figure 2: The core structure D(0 | 0). Green and blue spheres denote Ga and N, respectively. The atoms surrounding the dislocation line are enlarged to emphasize the position.

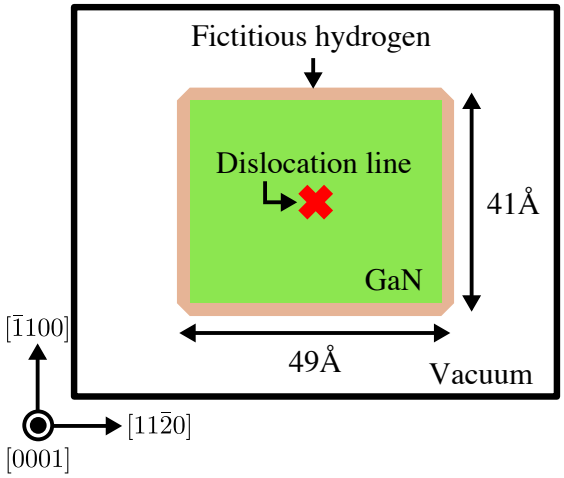

Figure 3: A schematic picture of the [0001] plane of the unit cell. The green region denotes GaN and it is terminated by the fictitious hydrogen atoms. The outermost region is the vacuum. A red cross denotes the position of the dislocation line.

tion (GGA) with the Perdew-Burke-Ernzerhof functional. We also use the Heyd-Scuseria-Ernzerhof (HSE) hybrid functional to evaluate more accurate electronic levels in the band gap. The unit cell contains about 800 Ga and N atoms in total. The GaN pillar is surrounded by the vacuum on the lateral directions perpendicular to the [0001]. We expect that this vacuum relaxes artificial strain caused by rounding the lateral surfaces. The dangling bonds on the lateral surface of the GaN pillar are terminated by $\approx$ 100 fictitious hydrogens. The schematic picture of the unit cell on the [0001] plane is shown in Fig. 3. The integration over Brillouin zone is taken with 4 sampling points along the [0001] direction. The structural optimization is performed for each core structures.

We found that D(0 | 2), S(0 | 3), and S(0 | 6) are stable. Then we replace one Ga atom in these three core structures with an Mg atom. The relative position of the Mg from the dislocation line is sampled. The resultant binding energy of the Mg shows that Mg is attracted by the screw dislocation and the electronic levels in the gap elevate towards the conduction band, as mentioned above.

References

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[2] G. Kresse and J. Furthmuller: Phys. Rev. B **54**, 11169 (1996).