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Do all screw dislocations cause leakage in GaN-based devices?

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ABSTRACT

Screw dislocations are generally considered to be one of the main causes of GaN-based device leakage, but so far, nearly no reports have focused on the effects of open-core screw dislocations on device leakage currents experimentally. In this paper, we use a conductive atomic force microscope to characterize the electronic properties of threading dislocations (TDs) in the GaN layer. The full-core screw dislocations and mixed dislocations are found to provide conductive paths for device leakage currents. In terms of the contribution to device leakage currents, the edge and open-core screw dislocations have smaller effects than the full-core screw dislocations and mixed dislocations. We use isotropic linear elasticity theory and density functional theory calculations to model the core atomic structures of TDs and calculate the corresponding electronic structures. The results show that screw dislocations with full-core structures are found to introduce both deep and shallow energy states within the energy gap dispersedly, while the open-core screw dislocations and the most edge dislocations introduce only shallow energy states. The calculated electronic structures of each type of dislocation are systematically compared and correlated with experimental observations. Our findings demonstrate that full-core screw dislocations and mixed dislocations in the GaN layer have a far more detrimental impact on device leakage than edge and open-core screw dislocations.

III-nitride semiconductors and their alloys, especially GaN, are promising materials made in the fabrication of optoelectronic and high power electronic devices due to their unique properties such as wide direct bandgap, high saturation velocity, and thermal, chemical, and mechanical stability.[1–5] However, it is difficult to obtain a low dislocation density and residual strain GaN film because of the large lattice misfit and thermal mismatch between the GaN crystal and the foreign substrate, which results in lowering of the performance of devices.[6–10]

It has been reported that threading dislocations (TDs) in luminescent devices are usually acting as strong non-radiative recombination centers for electrons and holes and thus bring down the luminescence efficiency, where the activity of screw and mixed dislocations is more important than that of edge dislocation in GaN based devices.[6,7] TDs can also lower charge mobility by scattering charge carriers in AlGaN/GaN high-electron-mobility transistors when they get charged.[8] Reynolds *et al.* have found that TDs can act as electrical shorts in Schottky devices because they provide leakage paths along their dislocation lines.[9] Hsu *et al.* have demonstrated that screw dislocations are the dominating source for gate leakage current in GaN samples.[10] However, the effect of open-core type screw dislocations on leakage currents was not mentioned. To date, most studies have found that screw dislocations in the GaN layer are a major cause of leakage currents, but there is no further study on the influence of different types of screw dislocation on device leakage currents. The deeply physical mechanism of device leakage caused by TDs in GaN based devices remains unclear.

The GaN epitaxial film was grown on sapphire by metal organic chemical vapor deposition (MOCVD). A 25-nm thick GaN buffer layer was first grown on the substrate at 635 °C, and the reactor pressure during the process was set to 400 mbar. Then, an undoped 4.5-μm thick GaN layer was grown at 1080 °C.

We constructed 5/7-atom core ring configurations for atomic structures of edge dislocation calculations and single/double 6-atom

ring and open-core configurations for screw dislocation calculations because they are the most stable configurations in GaN.[11] Atom positions of the screw dislocation core were formed by the slippage of atoms with a perfect crystal structure along the [0002] direction based on isotropic linear elasticity theory. The displacement of atoms was acquired by the displacement field expressed as[12]

$$u_z(x,y) = \frac{b}{2\pi}\left[arctan\left(\frac{y}{x}\right) + \frac{\pi}{2}sign(y)[1 - sign(x)]\right], \quad (1)$$

where b is the magnitude of the Burgers vector and sign(x) is the sign function with x = −1, 0, and 1 for positive, null, and negative values to make sure that the displacement is a discontinuous form.

Our atomistic calculations are based on density functional theory (DFT) as implemented in the QuantumATK software.[13] The atomic positions of configurations were fully relaxed until forces lower than 0.02 eV/Å.[14] We performed the geometry optimization of the GaN bulk configurations using Perdew–Wang functional with the local density approximation (LDA).[15] As the generalized gradient approximation (GGA) and LDA usually underestimate the bandgap, the LDA-1/2 method was employed for a more accurate bandgap, which corrects the DFT self-interaction error by defining an atomic self-energy potential that cancels the electron-hole self-interaction energy.[16] A well conserved Monkhorst–Pack 1 × 1 × 15 k-point mesh was employed for the determination of electronic properties. The density mesh cutoff energy was set to 300 Ry.

Figure 1 shows the profile diagram of three kinds of screw dislocation defects in the GaN layer, named α-, β-, and γ-type pits. The β-type pit is considered to be the mixed screw dislocation, and the rest belong to the pure screw dislocations.[17] In more details, the α- and γ-type pits belong to the full-core and open-core screw dislocations, respectively. It can be seen that the current was generated mostly through the sidewalls of α- and β- type pits, as shown in Figs. 2(a)–2(d). Only a noise level current signal of several pA was measured at the plane surface of the GaN layer due to a large Schottky barrier between the AFM probe and the GaN surface.

Currently, many studies have claimed that the increased current flow within the V-defects of the GaN samples is attributed to a smaller Schottky barrier formed inside the V-defects than that formed on the planar area outside the V-defects.[18–21] Our experimental results also confirm that the work function of plane $[10\bar{1}0]$ is smaller than that of plane GaN [0002] (see Fig. S1 in the supplementary material). It should be noted that the six surfaces $[10\bar{1}0]$ of the V-shaped pit are equivalent. So, similar results should be obtained when measuring the current of the V-shaped pit. However, it is obvious that the distribution of current on these six surfaces is uneven, and there is no certain

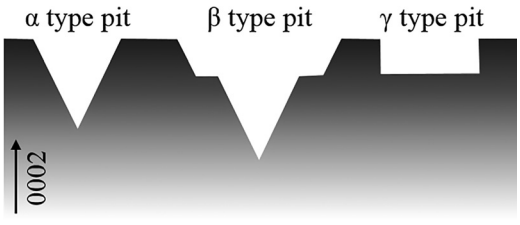

FIG. 1. The profile diagrams of three kinds of screw dislocation defects in the GaN layer.

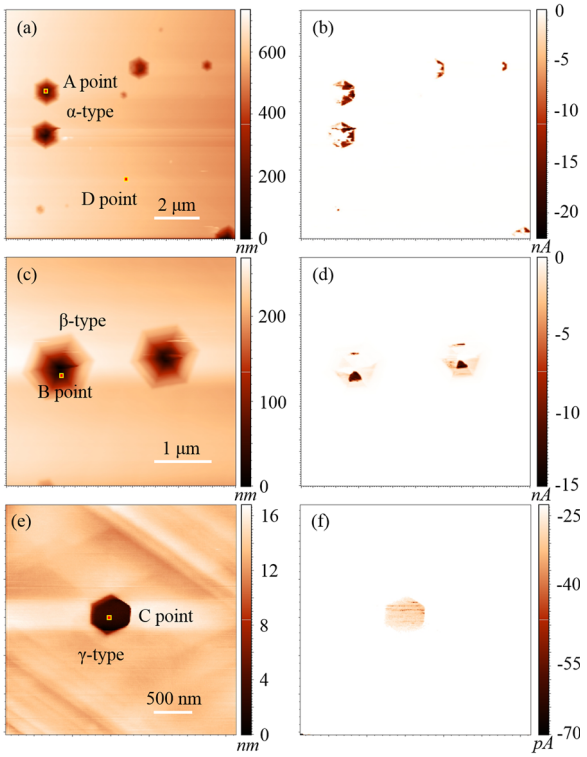

FIG. 2. Topographical (a), (c), and (e) and corresponding current (b), (d), and (f) maps measured at −10 V on the GaN surface at different pits.

rule to follow, which has been overlooked by most of the pervious papers. Therefore, the increase in current at the V-shaped pits cannot be simply ascribed to the lowering of the barrier.

In addition, we find that the current in the γ-type pit is also increased as compared to the plane surface of GaN, although only several-fold, as shown in Figs. 2(e) and 2(f). It should be pointed out that the conduction characteristics of open-core screw dislocation have never been reported in III-nitride materials. As for γ-type pit, the crystal orientation of the pit bottom is consistent with that of the plane surface. Thus, the Schottky barrier should be identical when the probe scans the plane surface and the γ-type pit bottom. Therefore, the increase in the current at the open-core screw dislocation can be attributed to the leakage current caused by the material defect.

To further understand that the increase in current at the TDs is associated with material defects, we test the current at different points, as shown in the Fig. 3. As for α- and β-type pits, the current of V-pits is significantly increased at voltages lower than −4 V. It should be noted that there exists an obvious shift in I–V curves under the forward and reverse biases. The current in the V-pits is significantly reduced in the after reverse scanning, indicating the possibility of charge trapping effects or defect levels in the GaN layer. However, there is only a slight difference in the current of forward and reverse scanning at the plane surface of GaN, as shown in Fig. 3(d). Only noise level currents around pA can be observed at the plane surface. As for γ-type pits, the conductivity of the measured point does not change significantly during the forward and reverse scans as compared to

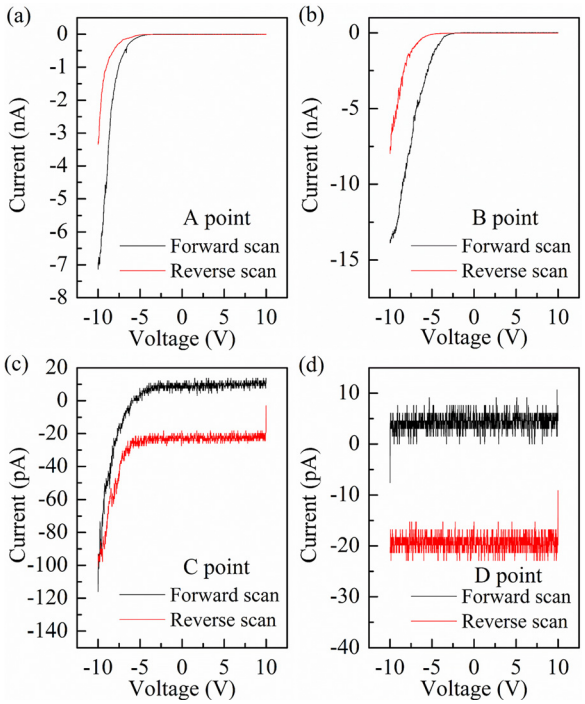

FIG. 3. I–V curves measured at different points as indicated in Fig. 2.

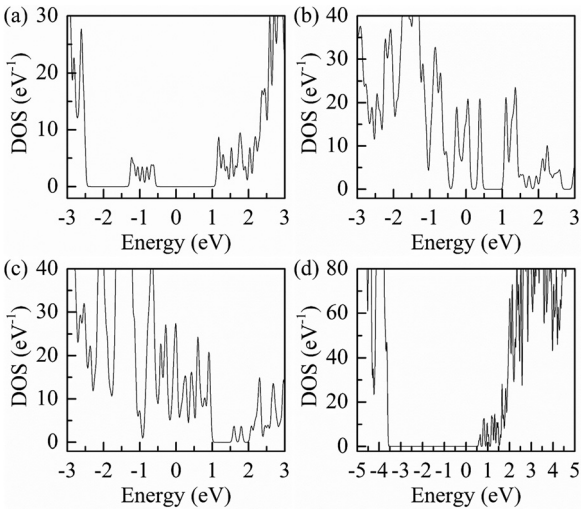

FIG. 4. Density of state curves associated with atomic core structures of various TDs. Edge dislocation: (a) the 5/7 core configurations. Full-core screw dislocations: (b) single 6-atoms ring configurations and (c) double 6-atoms ring configurations. (d) Open-core screw dislocation configuration.

α- and β-type pits. This obvious discrepancy can result from different electronic structures between full-core screw dislocations and open-core screw dislocations, as will be shown later. We did not mention the edge dislocations in the preceding discussions because we cannot directly observe the small trace of edge dislocations by scanning the morphology with the AFM probe due to the large platinum tip radius.[22] Thus, the effect of edge dislocation on the electronic properties of GaN is investigated by the DFT theory in the next paragraph.

We present the ball and stick models for the typical edge and screw dislocations in Fig. S2 and the corresponding density of states (DOS) in Fig. 4. Hydrogen passivation was used to saturate the outermost atoms to ensure the structural integrity. The effect of hydrogen on the electronic properties of the whole structure can be negligible (see Fig. S3 in the supplementary material). It can be seen that the 5/7-atom ring core structure introduces some deep occupied levels below the Fermi level. The deep occupied levels are mainly ascribed to Ga-Ga bonds in the core structure (see Fig. S4 in the supplementary material). We also present the DOS of configurations with 4- and 8-atom ring structures in Fig. S5. Largely different from the 5/7-atom ring core structure, the DOS results show that single and double 6-atom ring structures bring in both shallow and deep energy levels into the original bandgap, which are dispersed in the GaN bandgap, which originates from the uncoordinated atoms within the cores. Therefore, these two structures of screw dislocations show metallic behavior. As for the open-core screw dislocation, the bandgap of the GaN cluster has not changed much, but the position of the peak has shifted significantly. Such a large deviation is due to the limitation of calculating the size of the structure. It can be seen that there are no shallow or deep energy levels dispersed in the GaN bandgap, which is largely discrepant from the full-core screw dislocations. This is a good explanation for the phenomenon that the discrepancy in I–V curves between forward and reverse scans in the γ-type pit is significantly smaller than that of other two dislocation pits.

Our calculations show that the screw dislocations with full-core structures are more electrically active than the edge and open-core screw dislocations because the former introduce more energy levels near the Fermi level of GaN than the latter. These shallow and deep energy levels originate from the wrong bonds, dangling bonds, strained bonds, and twisted bond angles. Our theoretical results can well explain why full-core screw dislocations have higher conductivity than open-core screw dislocations. In addition, our theoretical result is also in line with previous experimental phenomenon that the screw dislocations have stronger activity as non-radiative recombination centers than edge dislocations.[6,7]

In order to further understand the influence of different TD types on the leakage of GaN-based Schottky devices, we put forward the Schottky band diagrams of metal-GaN contacts. We ignore the thermionic emission and thermionic field emission in this diagram because these two physical mechanisms could not cause a high level of leakage current in the GaN layer.[23] The tunneling leakage current can be significantly increased with the help of TDs through the deep energy levels. As mentioned above, the screw dislocations with full-core structures introduce more energy levels near the Fermi level than the edge and open-core screw dislocations. Therefore, the dispersed shallow and deep energy levels of full-core screw dislocation introduce a leakage path along the dislocation line, resulting in a narrower depletion width at the Schottky contact than that on the flat surface, edge dislocations, and open-core screw dislocations, as indicated in Fig. 5(a). As for metal-V-pit contact, the Schottky barrier will be lower than that of the metal-GaN [0002] plane because the work function of the GaN [$10\bar{1}0$] plane is lower than the GaN [0002] plane, as shown in

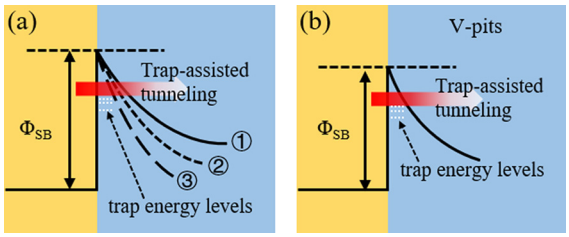

FIG. 5. Model for the Schottky band diagram between the metal and (a) different threading dislocations (①GaN plane surface, ②open-core screw dislocations, and ③full-core screw dislocations and mixed dislocations) and (b) V-pits.

Fig. 5(b). In addition, the V-pits can also have a narrower depletion width because the V-pits are considered to be the full-core screw dislocations.

In summary, the electrical conductivity of screw dislocation and mixed dislocation in GaN was measured using a conductive atomic force microscope (C-AFM). The results show that full-core screw dislocations are responsible for the GaN-based device leakage. Screw dislocations with full-core structures are found to introduce both deep and shallow energy states within the energy gap, while the open-core screw dislocations and the most edge dislocations introduce only shallow energy states. More importantly, the electronic structures of the GaN cluster show that the energy levels introduced by full-core screw dislocations are more dispersed within the GaN bandgap than those introduced by the open-core screw and most edge dislocations. Experimental and theoretical results demonstrate that the full-core screw dislocations are the main cause of GaN-based device leakage, while the open-core screw dislocation has little effect on device leakage.

See the supplementary material for the surface potential image of the V-pit, Ball and stick models for the core configuration of the TDs, the effect of H atoms, and the partial density of states (PDOS) of edge core configurations.

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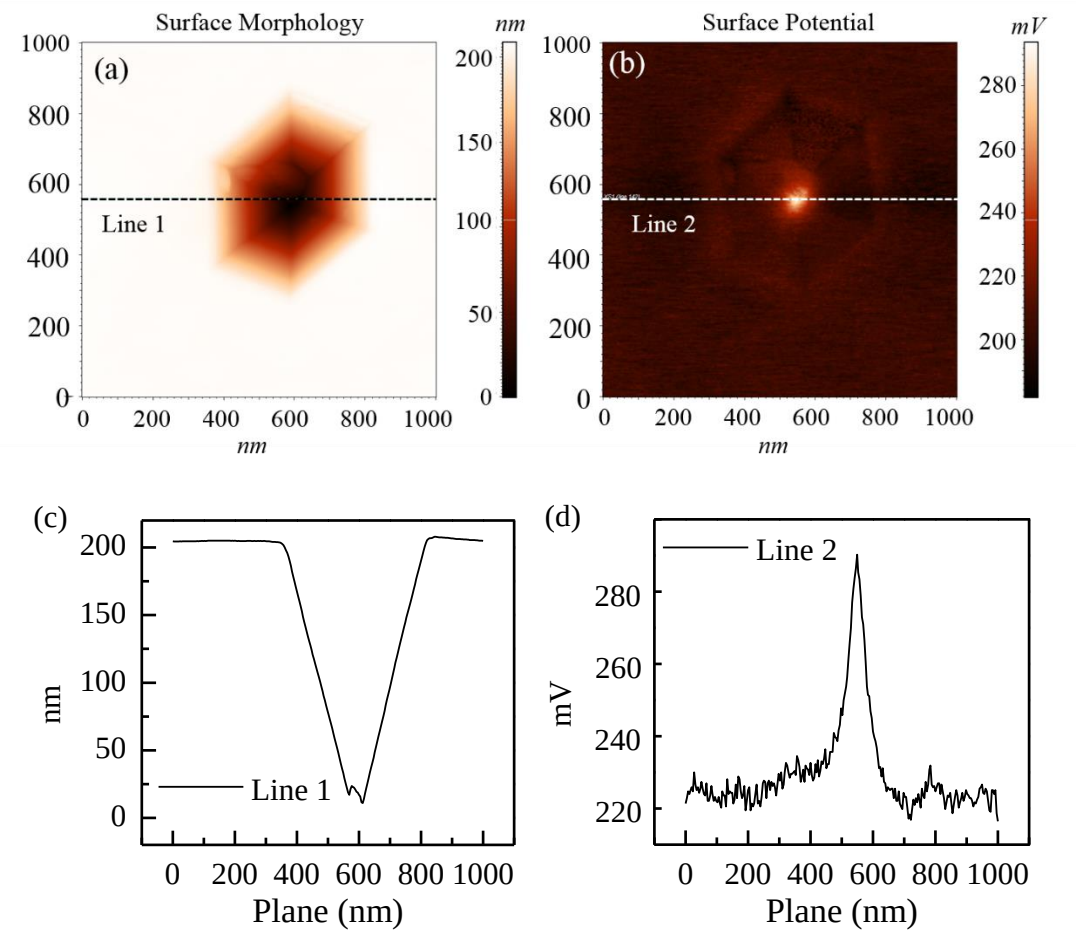

Figure S1 (a) AFM image and (b) Surface potential image of the V-pit; (c) and (d) are section profile along the lines crossing the V-pit.

The relationship between the surface potential (V_{sp}) and work functions of the sample (ϕ_{sample}) and the tip (ϕ_{tip}) can be expressed as:

$$V_{sp} = V_{sample} - V_{tip} = \frac{\phi_{tip} - \phi_{sample}}{e} \quad \text{(S1)}$$

It can be seen that the value of the ϕ_{sample} is inversely proportional to the surface potential. The surface potential band upward bends at the center of pit and the value obviously larger than that at the planar surface, leading to lower work function at the pit defects ($\phi_{pit} < \phi_{planar}$).

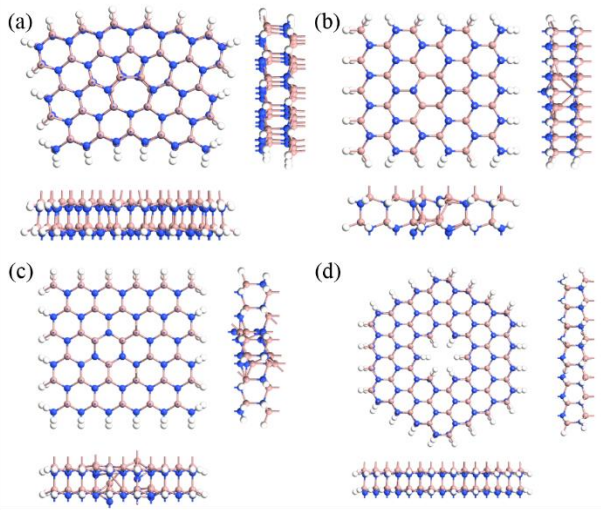

Figure S2 Ball and stick models for core configuration of the edge a-type: (a) the 5/7 core configuration; full-core screw dislocations: (b) single 6-atoms ring configuration and (c) double 6-atoms ring configuration; and (d) open-core dislocation configuration.

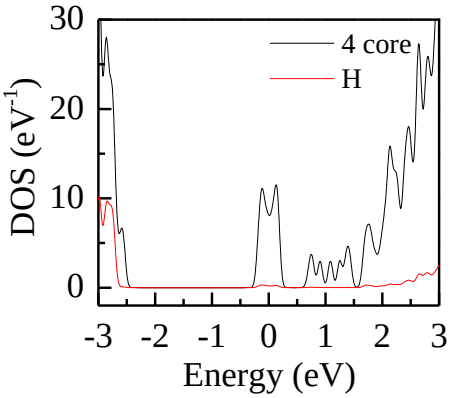

Figure S3 Partial density of states (PDOS, DOS on specified atoms and orbitals) of 5/7 core configuration. It can be seen that the effect of H atoms on the electrical properties near the Fermi level of the whole configuration is very small.

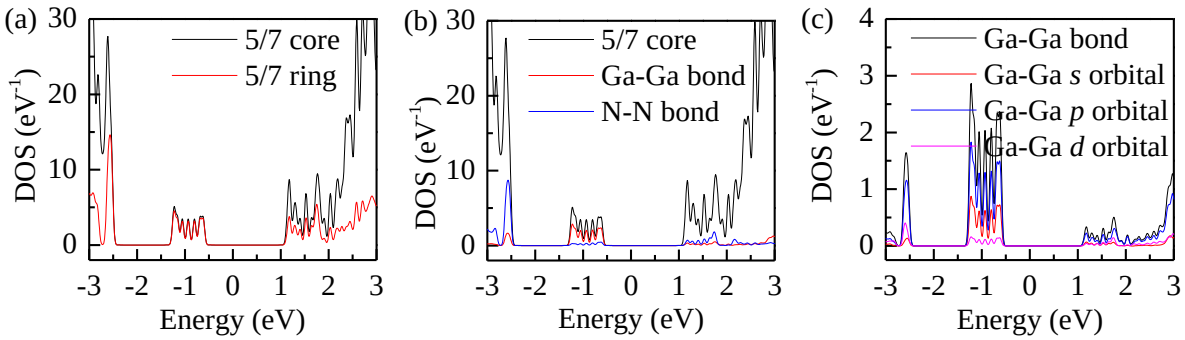

Figure S4 Partial density of states (PDOS, DOS on specified atoms and orbitals) of 5/7 core configuration. The deep occupied levels are contributed to these energy levels, which are due to the *p*-orbital states issued from the Ga–Ga bonds separating the 7- and 5-atoms rings.

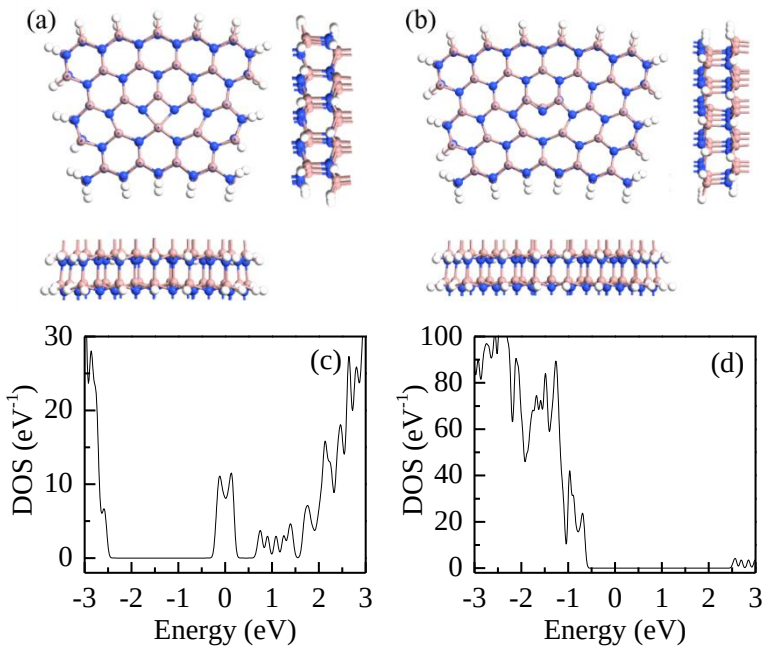

Figure S5 Density of states curves associated with atomic core structures of edge dislocations with the (a, c) 4-atoms core and (b, d) 8-atoms core configurations.