Supporting informations

Zn-dopant Dependent Defect Evolution in GaN Nanowires

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S1 Crytalline structure of undoped GaN nanowires

Figure S1 shows the undoped GaN nanowires are crystallized in perfect wurtzite structure. The SAED pattern and HRTEM image indicate no stacking faults are present.

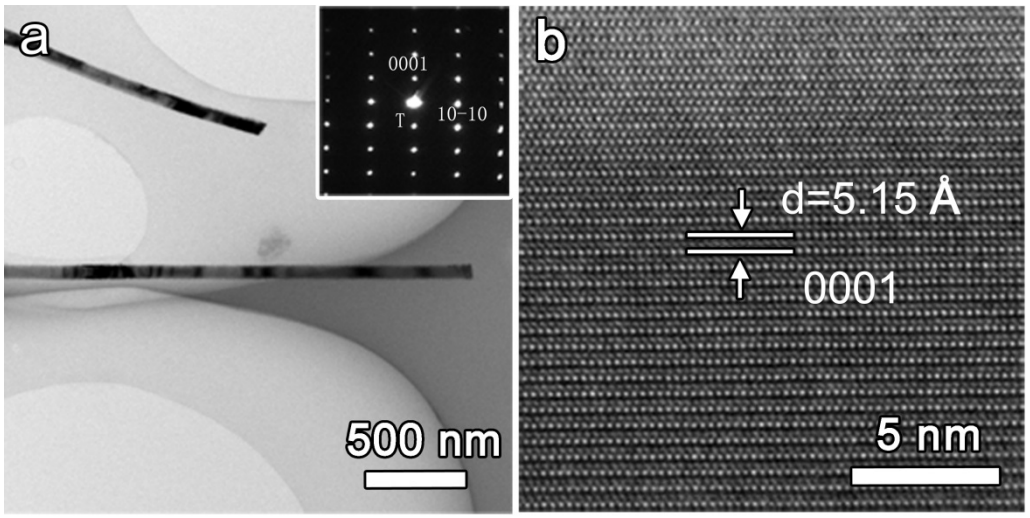

Figure S1 (a) A typical TEM image of undoped GaN nanowires, in which the inset of SAED pattern indicating the nanowire crystallized in perfect wurtzite structure; (b) HRTEM image of the GaN nanowire without any defects inside.

S2 First-principles calculations of Zn doped GaN nanowires

In the calculation of stacking fault energies (SFE), we used somewhat small supercells of $1 \times 1 \times 7$. To demonstrate that this kind of supercell is sufficient, we performed the following calculations. A supercell composed of 48 Ga and 48 N atoms ($2\sqrt{3} \times 3 \times 2$ of a unitcell) was constructed as the background for doping. A series of

models were built where two Zn atoms were introduced to substitute two Ga atoms. In all models, one Zn atom was placed in a specific Ga site in a (0001) atomic plane, which was nominated as Layer 0, while the other Zn atom was placed at any other possible Ga sites, both in Layer 0 and other layers (Figure S2a). It is found that the total energies of models with two Zn atoms located at the same layer are the lowest, as displayed in Figure S2b. It implied that Zn atoms would segregate along the (0001) layer in GaN lattice. Therefore, it is reasonable to assume that Zn atoms occupy a whole (0001) layer, that is, one unit cell in the base plane is enough for the calculation of SFE.

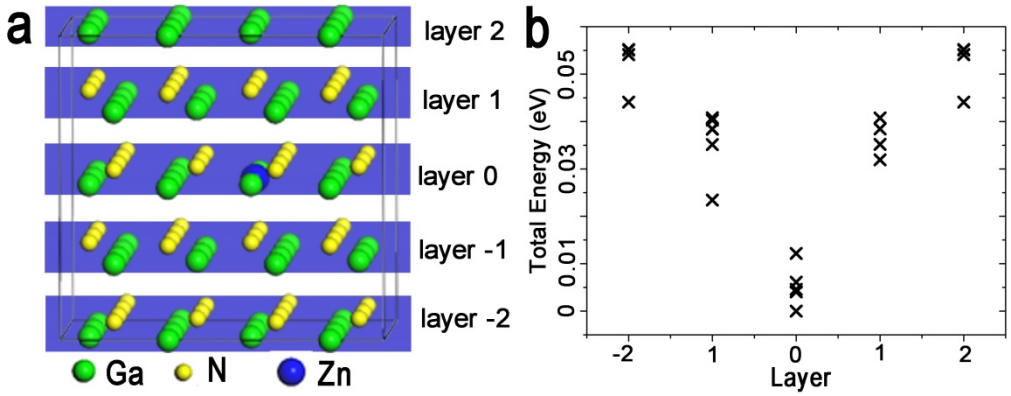

Figure S2 First-principles calculations of Zn doping in hexagonal GaN lattice: (a) the atomic model with one Zn atom occupied at a specific Ga site at Layer 0 (the blue one), while the other Zn atom positioned at different layers marked by blue rectangles; (b) total energies of models with different Zn occupation. The reference is the one with the lowest energy.