Supporting Information

The effect of interface polarity on the basal dislocations at the GaN/AlN interface

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The convergency of parameter settings in DFT calculations of GaN/AlN supercell have been tested using the interfacial energy (γ):

$$\gamma = \left[E(interface) - \left(E_{bulk}(GaN) + E_{bulk}(AlN)\right)\right]/S, \quad (1)$$

where $E(interface)$ is the energy of the GaN/AlN interface supercell. $E_{bulk}(GaN)$ and $E_{bulk}(AlN)$ are the energies of the bulk GaN and bulk AlN, respectively. The sizes of bulk GaN and bulk AlN are the same as the parts of GaN and AlN in the GaN/AlN interface supercell. S is the total interfacial area in the GaN/AlN interface supercell.

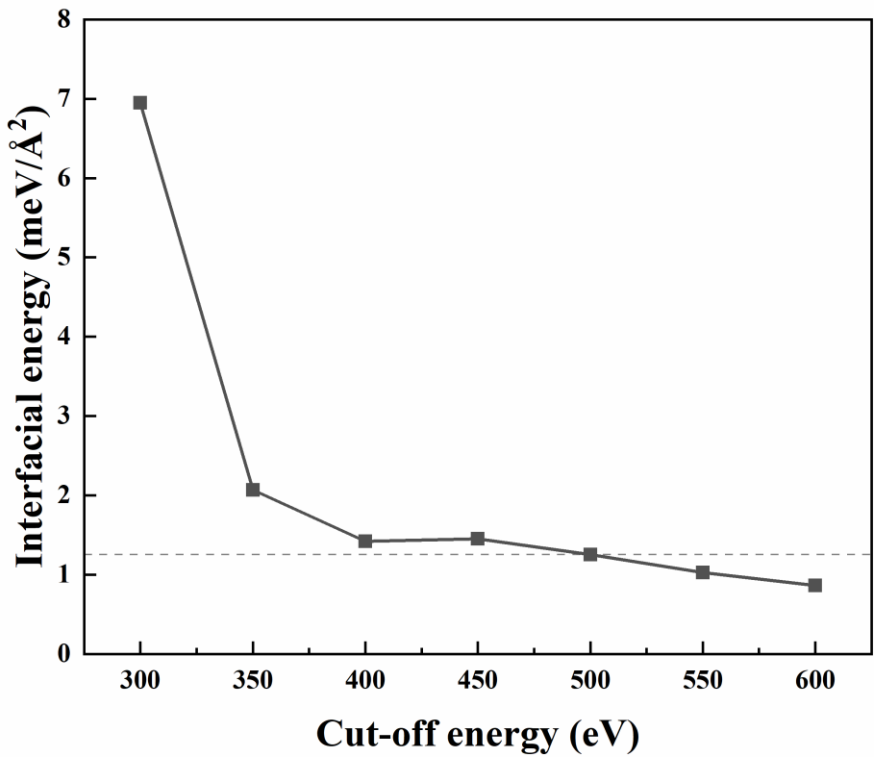

Fig. S1 Cut-off energy converge test of GaN/AlN interface using the interfacial energy.

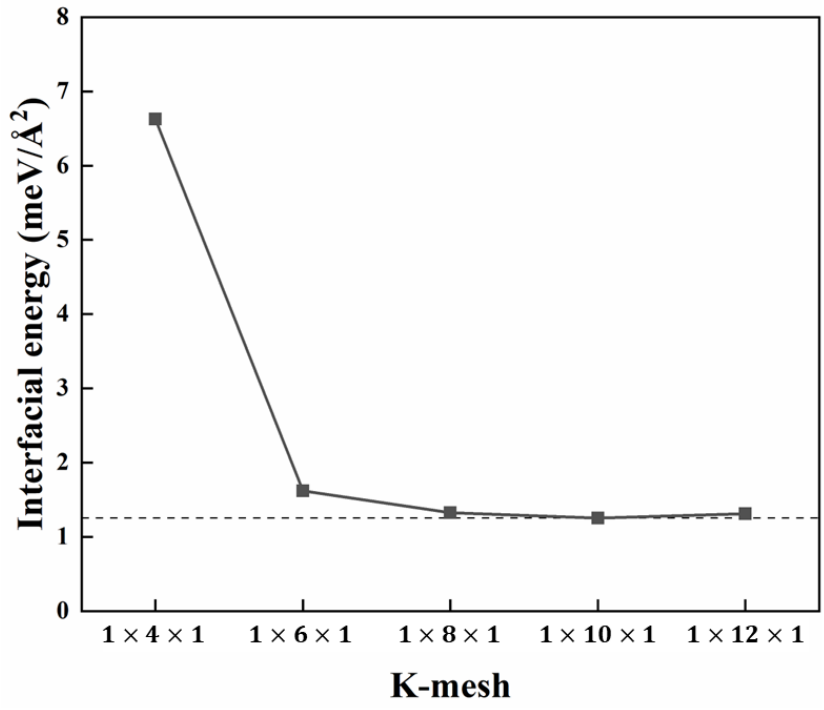

Fig. S2 K-mesh converge test of GaN/AlN interface using the interfacial energy.

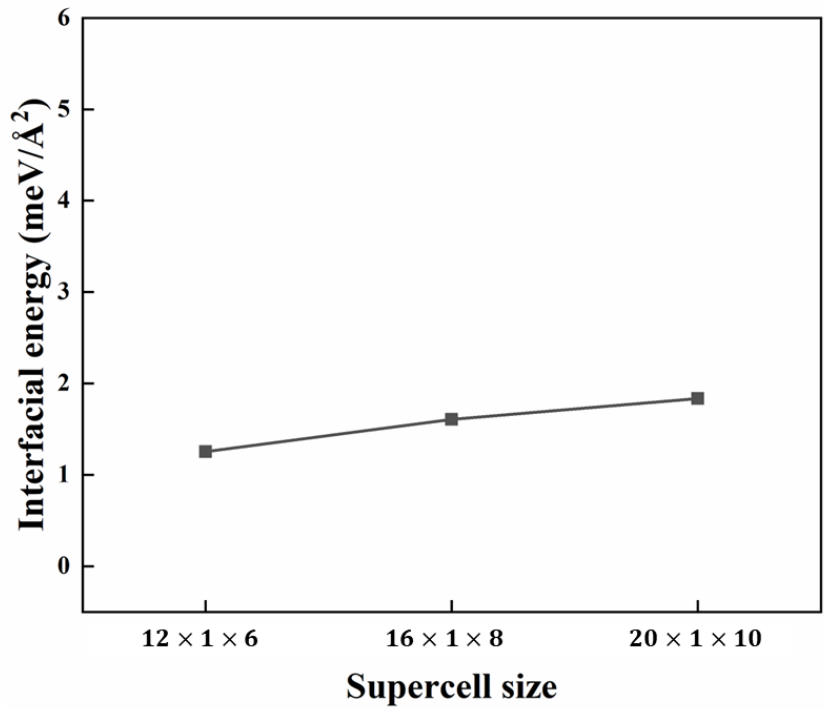

Fig. S3 Supercell size converge test of GaN/AlN interface using the interfacial energy.

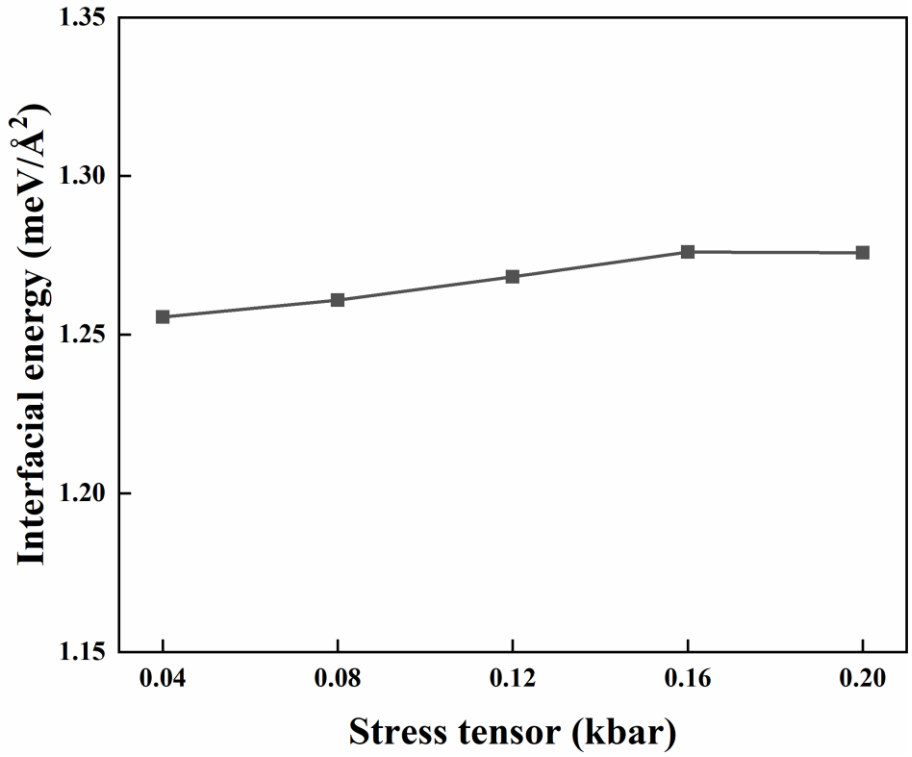

Fig. S4 Stress tensor converge test of GaN/AlN interface using the interfacial energy.

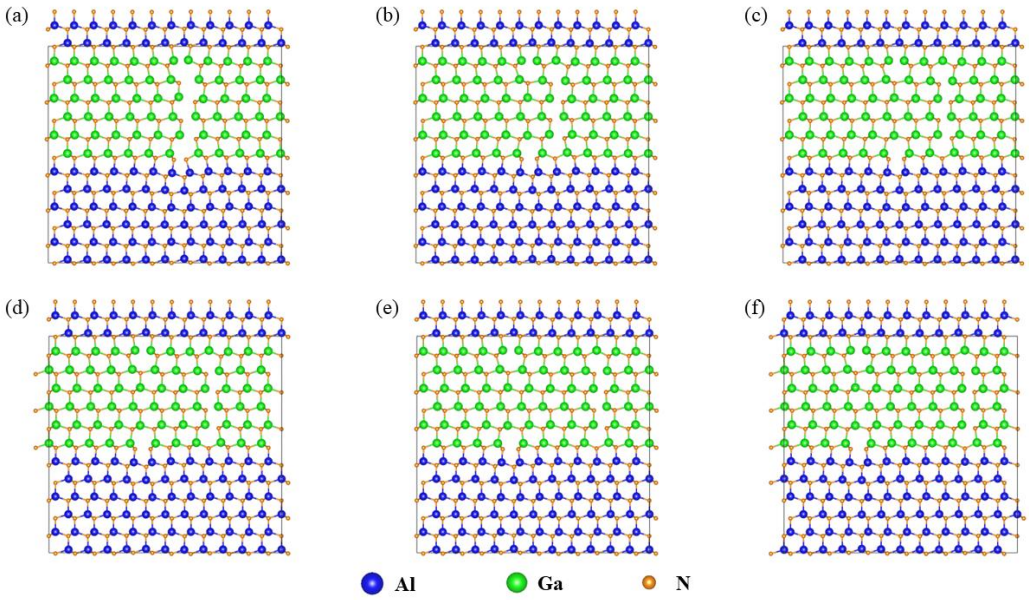

Fig. S5 Combinations of basal dislocations (Glide-Glide) at the GaN/AlN interface after relaxation (Density functional theory calculations). Fig. a-f correspond to different initial dislocation distances d: (a) d = 0 Å, (b) d = 3.127 Å, (c) d = 6.254 Å, (d) d = 9.381 Å, (e) d = 12.508 Å, (f) d = 15.635 Å.

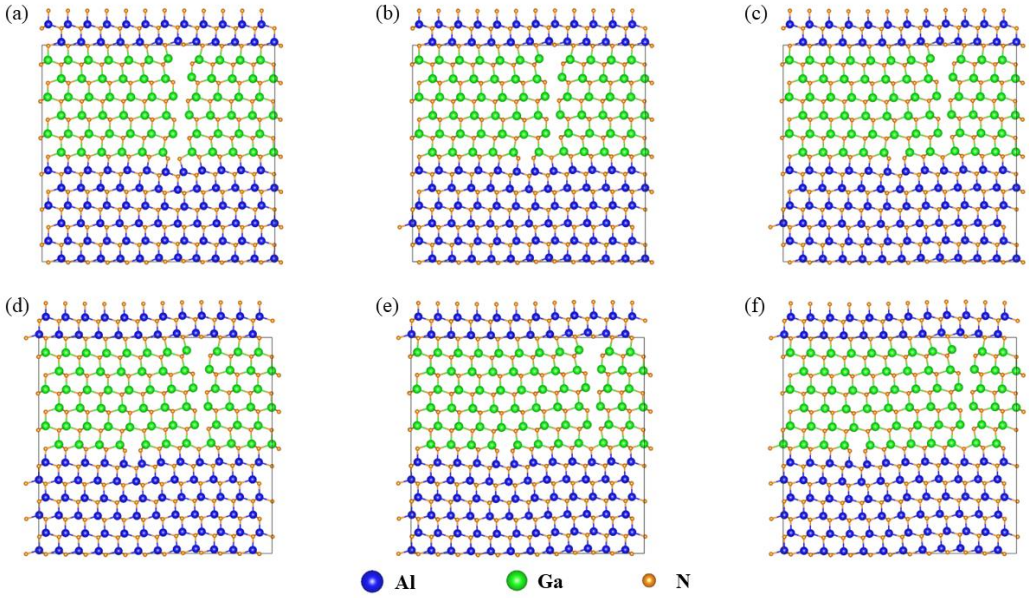

Fig. S6 Combinations of basal dislocations (Glide-Shuffle) at the GaN/AlN interface after relaxation (Density functional theory calculations). Fig. a-f correspond to different initial dislocation distances d: (a) d = 0 Å, (b) d = 3.127 Å, (c) d = 6.254 Å, (d) d = 9.381 Å, (e) d = 12.508 Å, (f) d = 15.635 Å.

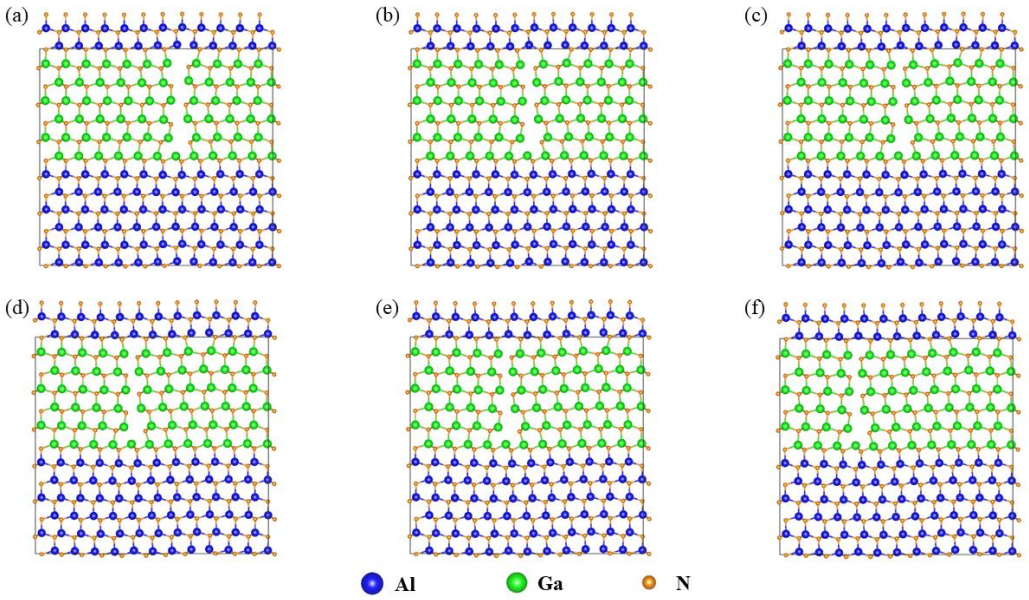

Fig. S7 Combinations of basal dislocations (Shuffle-Glide) at the GaN/AlN interface after relaxation (Density functional theory calculations). Fig. a-f correspond to different initial dislocation distances d: (a) d = 0 Å, (b) d = 3.127 Å, (c) d = 6.254 Å, (d) d = 9.381 Å, (e) d = 12.508 Å, (f) d = 15.635 Å.

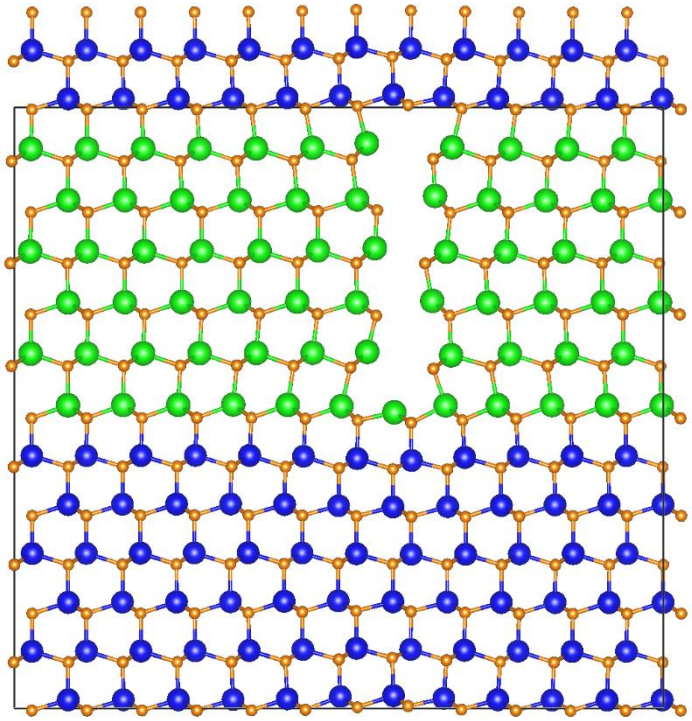

Fig. S8 Combinations of basal dislocations (Shuffle-Shuffle) at the GaN/AlN interface after relaxation (Density functional theory calculations).

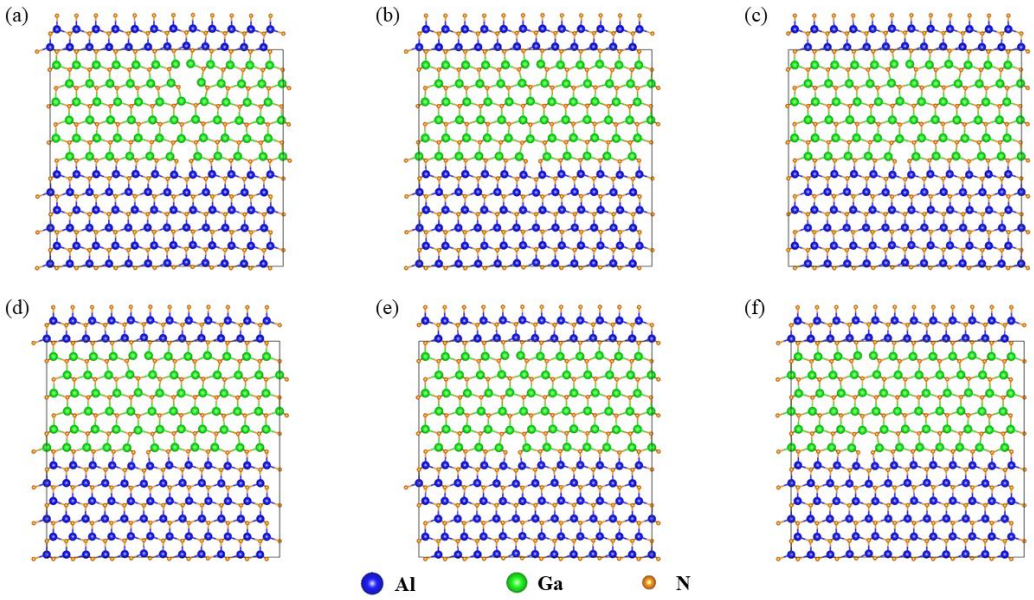

Fig. S9 Combinations of basal dislocations (Glide-Glide) at the GaN/AlN interface after relaxation (Molecular dynamic calculations at 1300K). Fig. a-f correspond to different initial dislocation distances d: (a) d = 0 Å, (b) d = 3.127 Å, (c) d = 6.254 Å, (d) d = 9.381 Å, (e) d = 12.508 Å, (f) d = 15.635 Å.

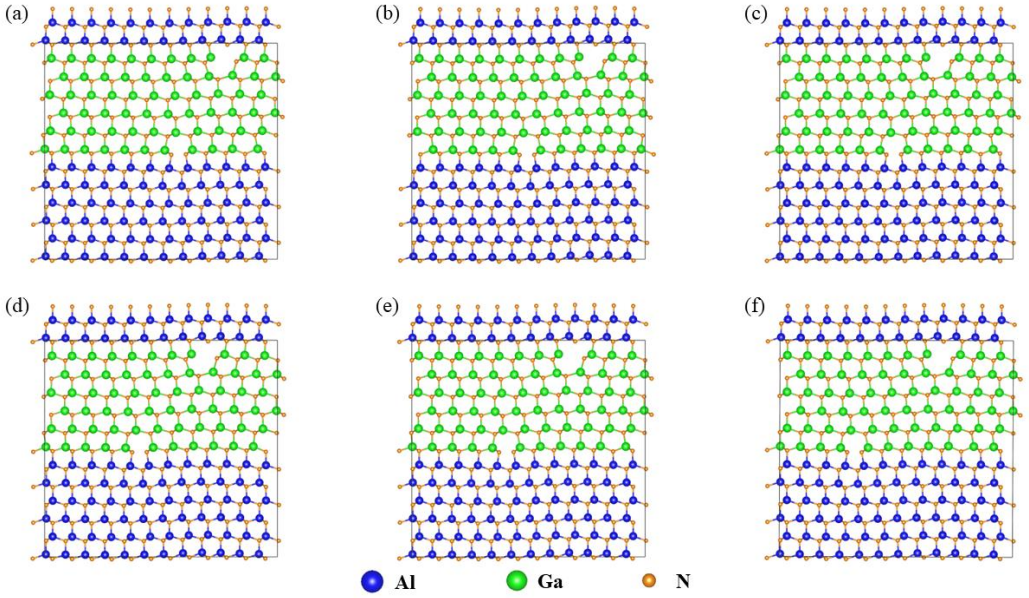

Fig. S10 Combinations of basal dislocations (Glide-Shuffle) at the GaN/AlN interface after relaxation (Molecular dynamic calculations at 1300K). Fig. a-f correspond to different initial dislocation distances d: (a) d = 0 Å, (b) d = 3.127 Å, (c) d = 6.254 Å, (d) d = 9.381 Å, (e) d = 12.508 Å, (f) d = 15.635 Å.

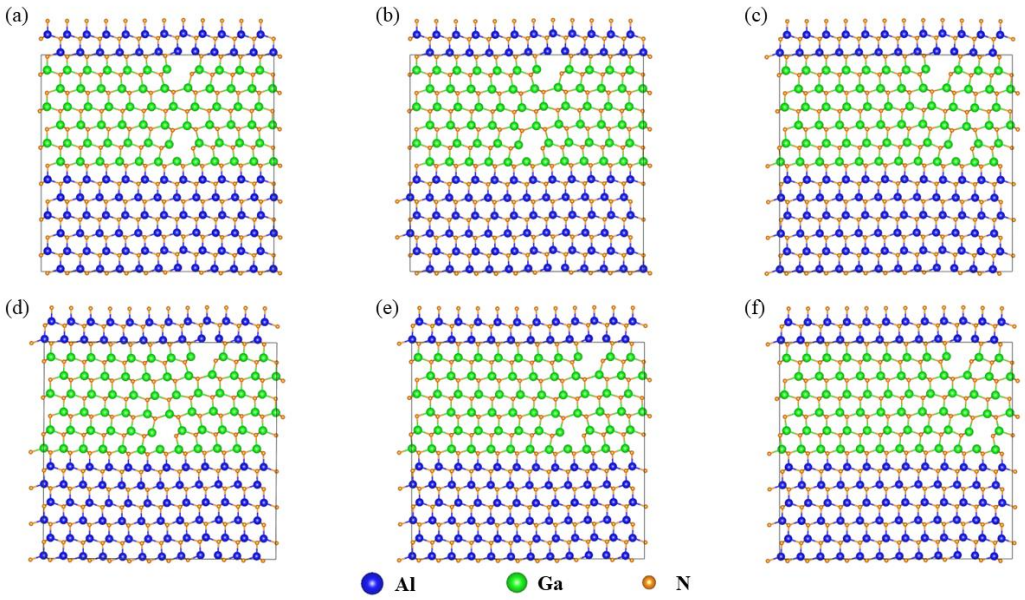

Fig. S11 Combinations of basal dislocations (Shuffle-Glide) at the GaN/AlN interface after relaxation (Molecular dynamic calculations at 1300K). Fig. a-f correspond to different initial dislocation distances d: (a) d = 0 Å, (b) d = 3.127 Å, (c) d = 6.254 Å, (d) d = 9.381 Å, (e) d = 12.508 Å, (f) d = 15.635 Å.

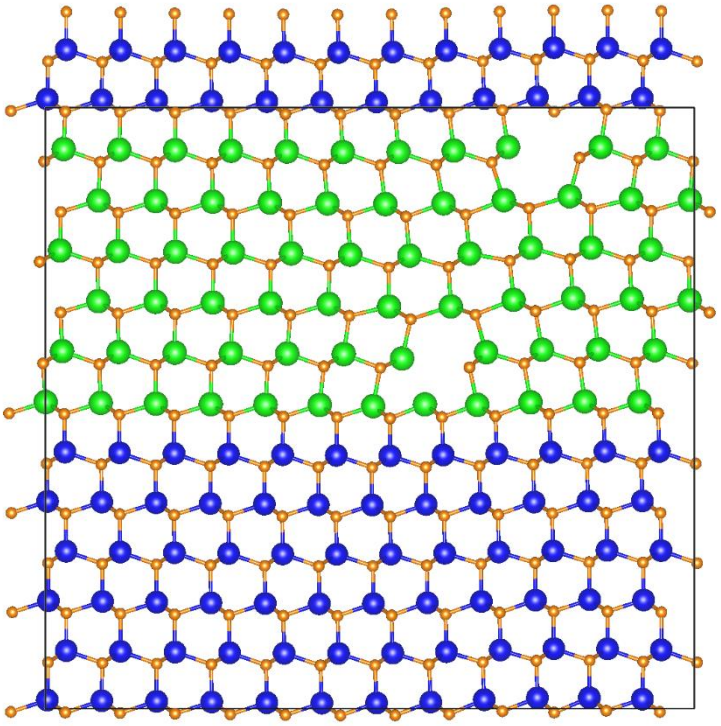

Fig. S12 Combinations of basal dislocations (Shuffle-Shuffle) at the GaN/AlN interface after relaxation (Molecular dynamic calculations at 1300K).

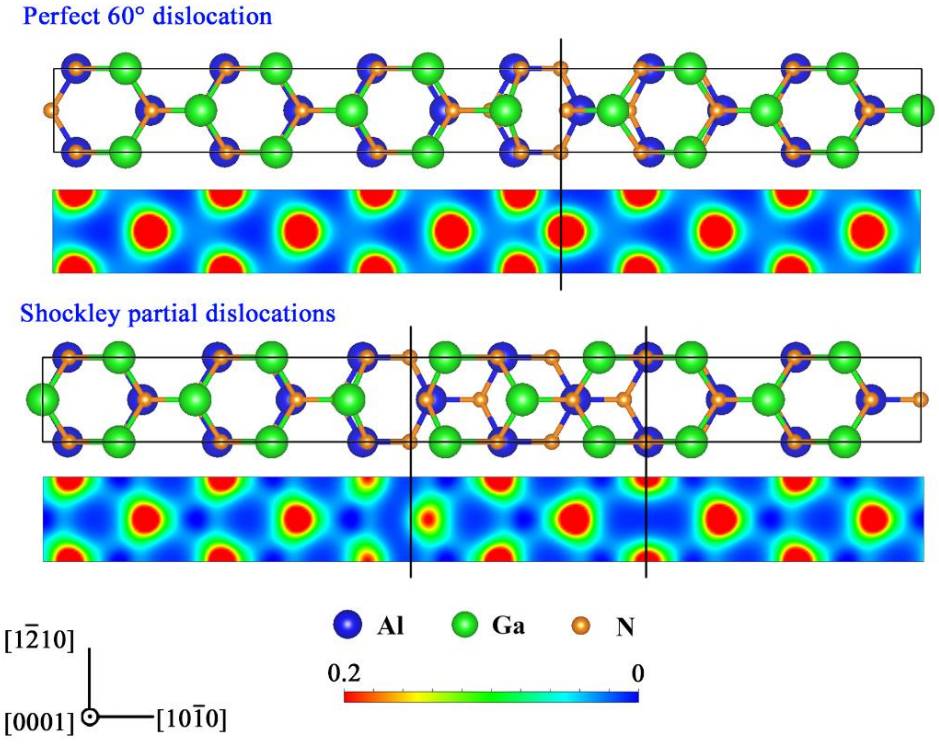

Fig. S13 The structure and charge density of different dislocations at Al polar GaN/AlN interfaces on the (0001) plane. The black lines along $[1\bar{2}10]$ correspond to the dislocation lines of different dislocations.

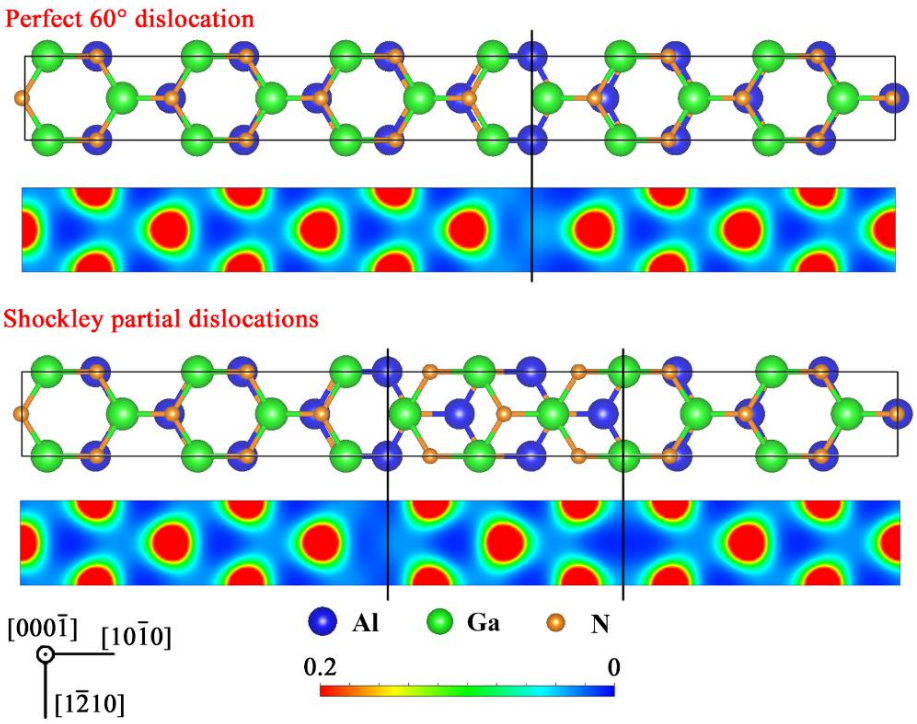

Fig. S14 The structure and charge density of different dislocations at N polar GaN/AlN interfaces on the $(000\bar{1})$ plane. The black lines along $[1\bar{2}10]$ correspond to the dislocation lines of different dislocations.