Interface states in abrupt epitaxial Al/GaN(001) contacts

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Using *ab-initio* pseudopotential calculations, we investigate the nature of the electronic states with energies within the semiconductor bandgap in abrupt, defect-free N-terminated Al/GaN(001) junctions. The interface is modeled using the supercell technique considering GaN in the cubic fcc phase. For this system, we find a high density of interface states near the Fermi level.

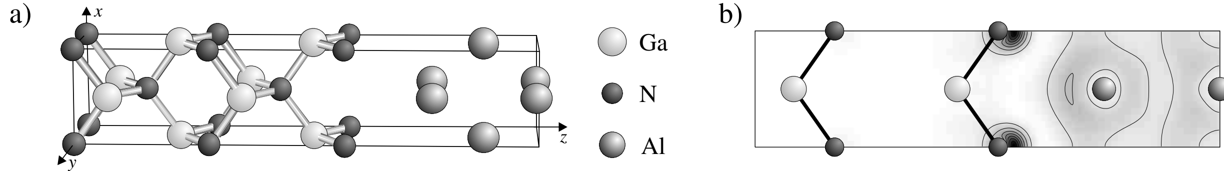

Figure 1: **a)** Atomic structure of the abrupt, N-terminated Al/GaN(001) interface. The x and y axes are rotated by 45° with respect to the conventional cubic axis of unit cell. **b)** Contour plot of the integrated probability density of all electronic states with energy in the range [E_F-1 eV, E_F+1 eV]. The basal plane shown above includes the interfacial Ga and N atoms while the interfacial Al atoms are in a different plane. Contour spacing is $6 \cdot 10^{-3} e/a_0^3$.