Structure and electronic properties of the polar ZnO-GaN (0001) interface

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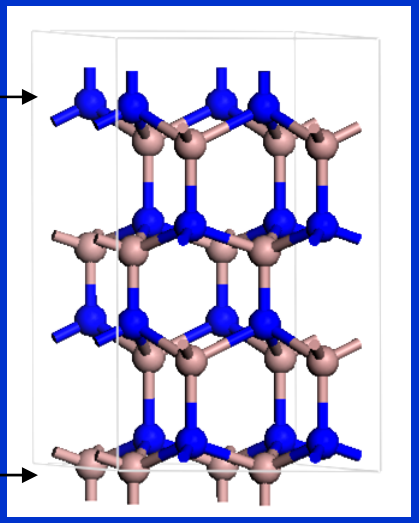
Properties of GaN

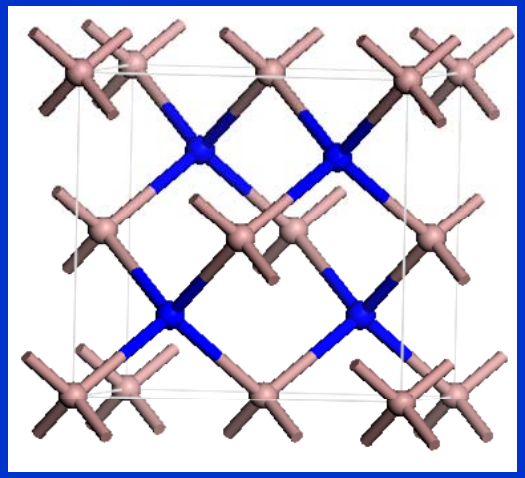
Structure

N-face

Ga-face



wurtzite
global minimum
a,b = 3.189 Å
c = 5.185 Å



zincblende
Metastable
a = 4.52 Å

- Both zincblende and wurtzite material important
- Note polarity of wurtzite GaN along (0001) direction

Properties of GaN

Electronic Properties

- Large direct band gap of 3.44 eV that can be tailored to anything between 1.9 eV (650 nm) and 6.2 eV (200 nm) by alloying with In and Al respectively. Entire visible spectrum can be covered.
- Ideal for optoelectronic devices
- high breakdown field of 3×10^{-6} V cm^{-1} – allows for high power operation
- high RT electron mobility of 1350 cm^2 V^{-1} s^{-1}

Other important Properties

- strongly bonded with bond energies of 2.5 eV; reflected in high melting point (> 2500 K)
- both n- and p-type material available

Applications of GaN

Optoelectronic Devices

- Light Emitting diodes in green/blue region of spectrum.
    - no viable alternative to GaN
    - traffic lights, energy-saving domestic lighting
    - LED-based white lighting by colour mixing (red, blue, green)

- Laser diodes - high frequency
    - High density optical storage devices
    - Predicted 4-fold increase in amount of information storable on a disk.

Other Applications

- FETs and UV detectors.

Growth of GaN

The need for heteroepitaxy

- Bulk growth of GaN extremely difficult due to high MP of GaN. Only viable method is HNPS (Ga melt at 1700 ˚C under 20,000 atm of N_2).
- Limited to very small crystallites.
- Also electronic properties of crystallites rather poor.
- hence foreign substrates have to be used

Substrates for GaN Epitaxy

- Sapphire • basal-lattice constant mismatch of ~20 %,
  • thermal expansion coefficient > GaN
  → dislocation density ~ 10^{10} cm^{-2}

- SiC • better lattice matched (3.1 %)
  • thermal expansion coefficient < GaN
  • expensive

Alternative Substrates for GaN epitaxy

- Need lower dislocation densities for more sophisticated devices, operating at more extreme conditions of temperature, voltages and current densities.

Choice of substrate

- Important substrate properties that have to be considered for growth of high quality epilayers
  - Structure and lattice constant,
  - Composition and reactivity,
  - Thermal and electrical properties.

- Many different materials have been tried, but no ideal substrate has been found so-far.

ZnO as a Substrate for GaN epitaxy

Properties – similar to GaN

- isomorphic; close match in lattice constant (1.8 %);
- S/C, large band gap ~ 3.3 eV, applications in high frequency LEDs
- strongly bonded – high melting point (2248 K)
- bulk material available

Experimentally

- high quality GaN has been grown on ZnO (and vice versa).
- Recently LEDs based on the the GaN/ZnO interface have been reported.

Study Outline

- Study atomic and eletronic structure of GaN/ZnO interface
- In particular effect of interfacial compensation on stability and electronic properties of the interface was considered.

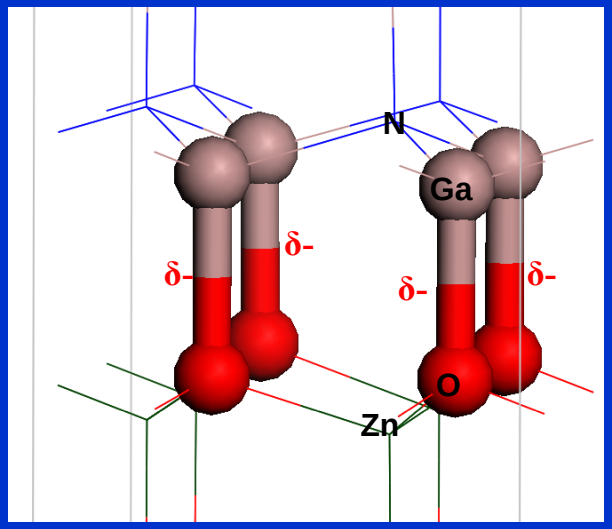
Method

- PW DFT - CASTEP
- PBE functional – exchange correlation
- Periodic boundary conditions
- Ultrasoft Pseudopotentials to model ion-electron interaction

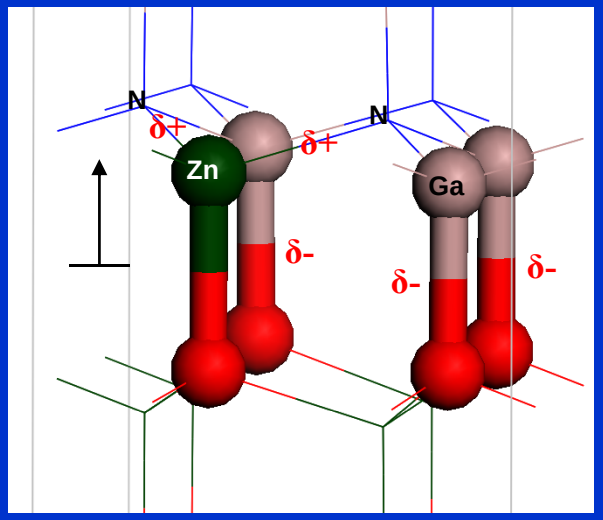
The ZnO/GaN interface

Heterovalent Interface

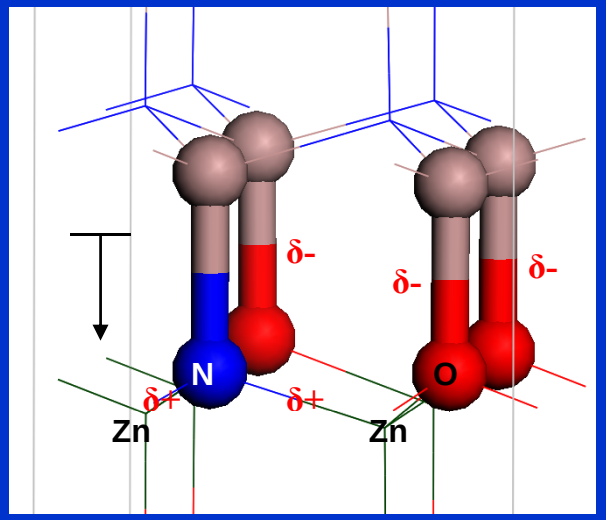
- considering cation/anion interfaces only, got Ga-O and Zn-N interfaces
- Abrupt Ga-O interface will contain an excess of ¼ of an electron/bond; Zn-N interface will be deficient by ¼ of an electron/bond → substantial electric fields, destabilising interface.
- charge build-up can only be avoided by atomic mixing of interfacial layers, such that number of electron-rich bonds equal to electron deficient bonds
- opposite directions of dipoles for cation and anion compensation



abrupt



Zn-compensated

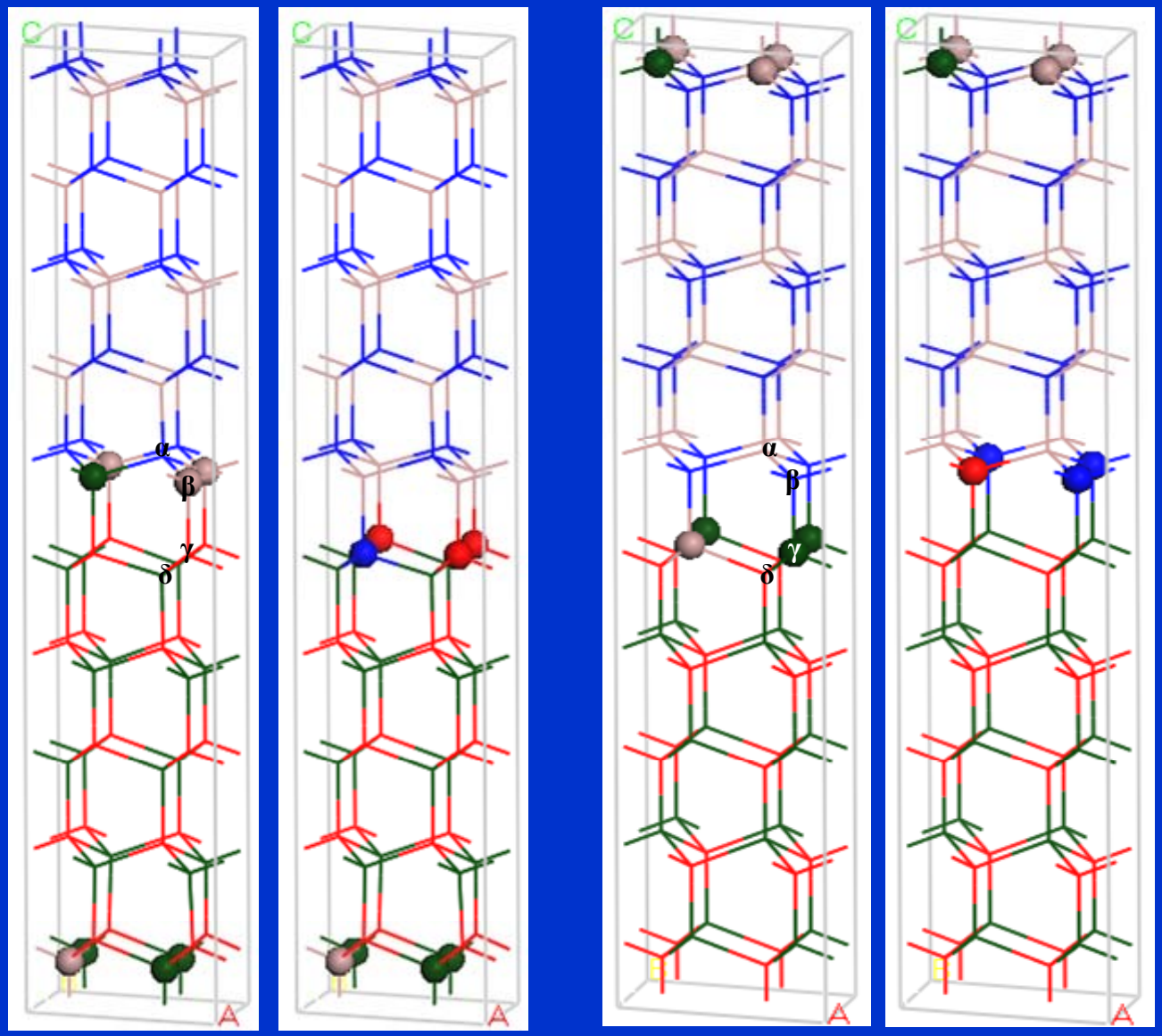


N-compensated

Interfaces Considered

Ga-O interface

Zn-N interface



Reference Interface

Reference Interface

Interfacial Formation Energy

- Interfacial formation energy defined as

$$E_f^{\text{int}} = \frac{1}{2}(E^{tot} - n^{GaN}\mu^{GaN} - n^{ZnO}\mu^{ZnO})$$

- two interfaces are not identical → cannot derive *absolute* stability of different interfaces

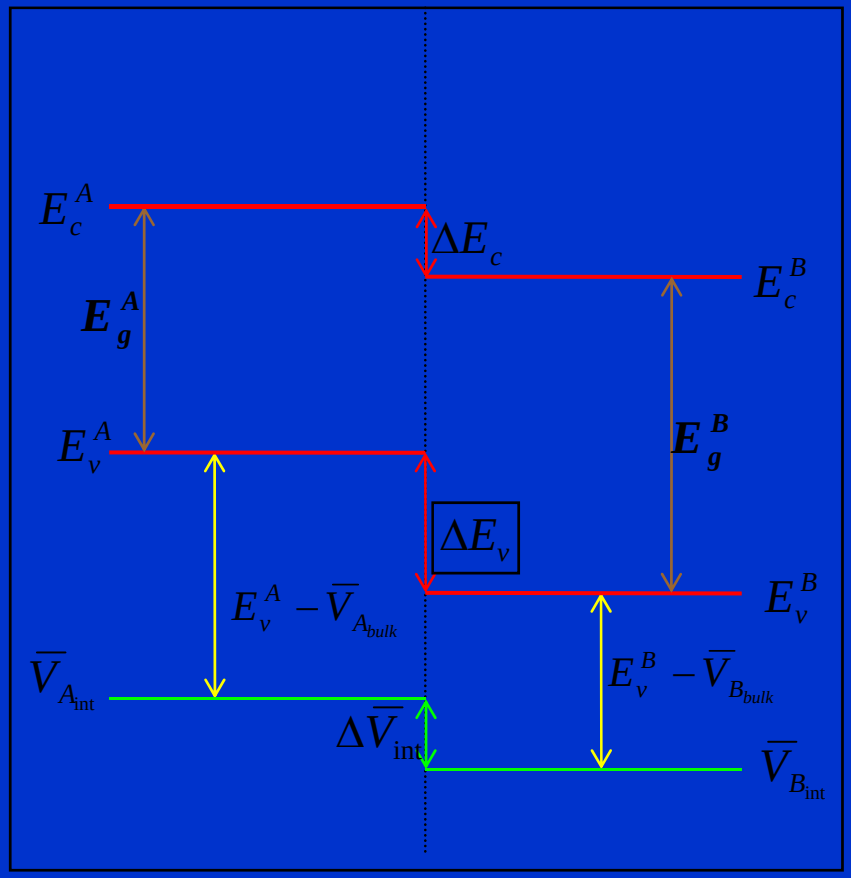
- by introducing reference interface can determine relative stabilities of various interfaces of same polarity; i.e relative stability of 4 different Ga-O interfaces and relative stability of 4 different Zn-N interfaces, using

$$\Delta E_f^{\text{int}} = E_f^{SL_1} - E_f^{SL_2}$$

where

$$E_f^{SL_x} = (E_x^{tot} - n_x^{GaN}\mu^{GaN} - n_x^{ZnO}\mu^{ZnO})$$

Determining the Valence band off set



Align

Bulk band structure of ZnO and GaN

to

average electrostatic potential of semiconductor slabs in supercell containing the interface

$$\Delta E_v = \Delta \bar{V}_{\text{int}} + (E_v^A - \bar{V}_{A_{bulk}}) - (E_v^B - \bar{V}_{B_{bulk}})$$

Results

- Compensated interfaces are about twice as stable as non-compensated interfaces
- Cation-compensated interfaces are by about 15 meV more stable than corresponding anion-compensated interfaces
- Position of interface in wurtzite cell does not significantly affect its formation energy
- The valence band offset at the cation- and anion-compensated interfaces were found to be 1.0 eV and 0.5 eV, respectively.

Further Work on the ZnO/GaN interface

Consider strain effects – used average basal lattice constant of GaN and ZnO so-far. Due to large piezoelectric constant of GaN and ZnO, expect dependence on strain state of heterojunction system. Rerun calculations using basal lattice constant of GaN and ZnO.

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