Surface properties of InN and InGaN alloys

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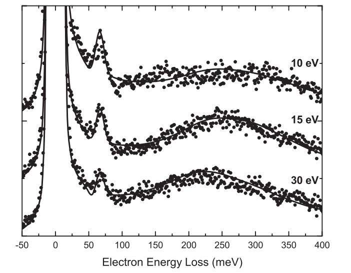
Introduction

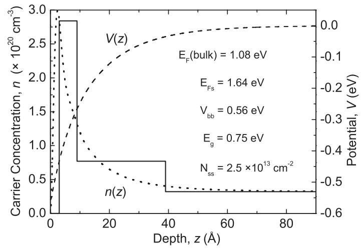
Indium nitride (InN) remains one of the least understood of the III-V semiconductor systems, despite its enormous potential for device applications. However, InN and In-rich III-N alloys are known to have a number of striking fundamental properties, particularly at the free surface. These surface properties are investigated here.

Electron accumulation at InN surfaces

Intrinsic electron accumulation at InN(0001) surface



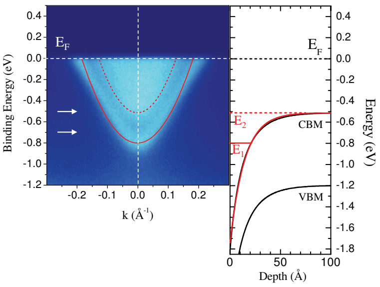
- HREEL spectra: Plasmon peak dispersion → surface electron accumulation
- Layered profile used to simulate HREELS spectra



- Realistic charge and potential profile determined by solving Poisson's equation within the MTFA including non-parabolicity

I. Mahboob *et al.*, Phys. Rev. Lett. **92**, 036804 (2004).

Quantized electron accumulation

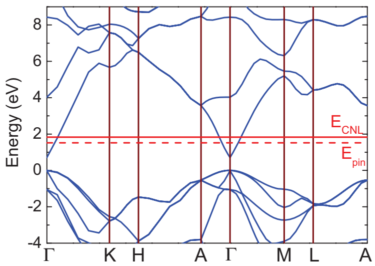


- Downward band bending causes 1D quantum well (approximately exponential) near surface
- CB states become quantized at surface (quasi 2DEG)
- Quantization direction is perpendicular to surface
- Subbands can be resolved by ARPES

L. Colakerol *et al.*, Phys. Rev. Lett. **97**, 237601 (2006).

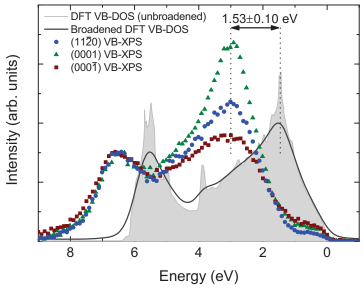
Origin of the electron accumulation

- Charge neutrality level (CNL) marks cross-over from donor-like (below) to acceptor-like (above) surface states
- Low Γ-point CBM → CNL high above CBM
- E_F at surface below CNL → unoccupied donor ViGS and positive surface charge
- Surface E_F pinned close to CNL: bands bend downwards, space-charge balances surface charge, extreme electron accumulation



I. Mahboob *et al.*, Phys. Rev. B **69**, 201307 (2004);
P. D. C. King *et al.*, Phys. Rev. B *(in press)*.

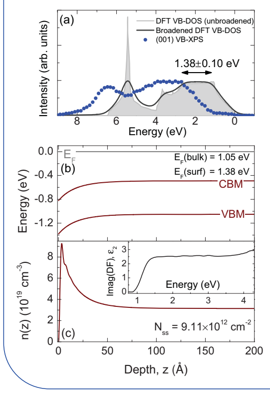
Universal electron accumulation



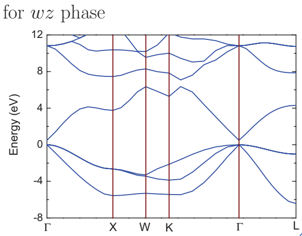
- Compare VB-XPS with quasi-particle corrected DFT VB-DOS [1]
- VBM to surface E_F is 1.53±0.10 eV for In– and N–polar *c*-plane and *a*-plane InN
- Surface E_F pinned in same place for different surface orientations
- $N_{ss} \approx 1.65 \times 10^{13}$ cm^{-2}
- Differences in intensity due to surface DOS [2]

P. D. C. King *et al.*, Appl. Phys. Lett. **91**, 092101 (2007).

Zinc-blende InN

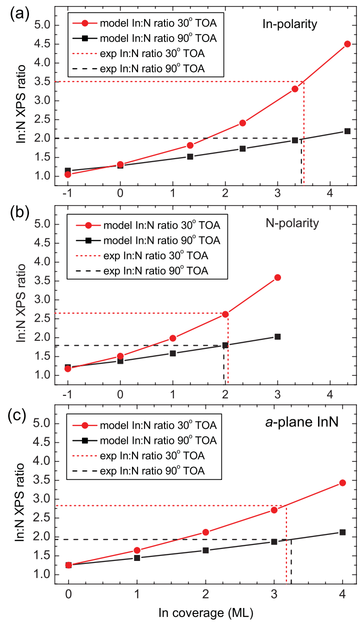


- MBE grown *zb* InN with only ∼5% *wz* inclusions [3]
- VB photoemission for surface E_F, ellipsometry (P. Schley & R. Goldhahn, TU Ilmenau) for bulk E_F
- Surface E_F > bulk E_F → surface electron accumulation
- *zb* surface E_F < *wz* surface E_F; surface state density may be lower for *zb* than for *wz* phase
- Γ-point CBM low for *zb*–InN as well as *wz*–InN
- CNL above CBM
- Surface electron accumulation as for *wz*–InN



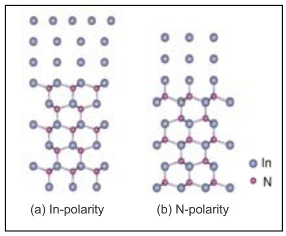
In-adlayers

Recent first principles calculations predict In-adlayers are the most favourable surface reconstruction for InN [4], similar to GaN under Ga-rich conditions. In–In bonds in an In-adlayer have been suggested as the microscopic origin for the electron accumulation [5].

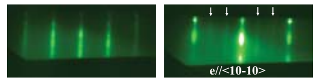


T. D. Veal *et al.*, Phys. Rev. B **76**, 075313 (2007);
T. D. Veal *et al.*, Physica B **401–402**, 351 (2007).

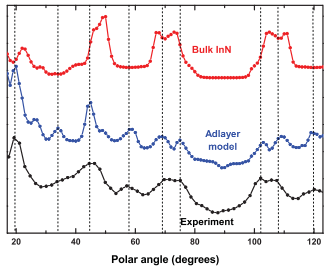
- XPS In:N ratio → ∼3.4 ML (∼2.0 ML) of In on In– (N–) polarity *c*-plane InN
- Both 1 ML more than for Ga adlayers on *c*-plane GaN under Ga-rich conditions

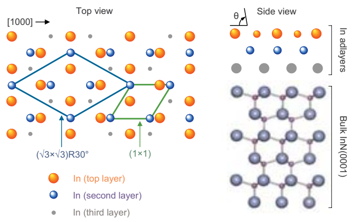


- *a*-plane InN has ∼3 ML In above non-polar bulk-like termination
- Fractional In-adlayer coverage for InN(0001) implies laterally contracted toplayer
- RHEED of an InN(0001) sample shows 1× and 3× → $(\sqrt{3}\times\sqrt{3})$R30° reconstruction

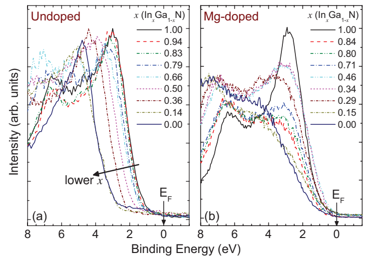


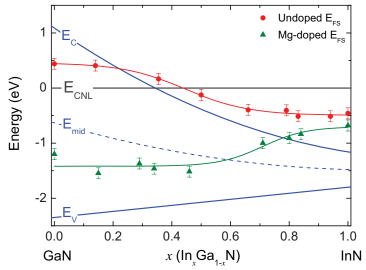
- Co-axial impact collision ion scattering spectroscopy supports this





InGaN alloys





- For undoped alloys, transition from electron accumulation (In-rich) to depletion (Ga-rich) occurs at $x \approx 0.43$ with a change in direction of band bending
- For Mg-doped alloys, downward band bending across composition range, but transition from inversion (In-rich) to hole depletion (Ga-rich) occurs at $x \approx 0.59$
- Form of space charge regions and difference in barrier height of undoped and Mg-doped alloys give evidence for *p-type bulk conductivity across the composition range*

T. D. Veal *et al.*, Appl. Phys. Lett. **89**, 202110 (2006); P. D. C. King *et al.*, Phys. Rev. B **75**, 115312 (2007); P. D. C. King *et al.*, Phys. Stat. Sol. *(submitted)*.

Conclusions

- Intrinsic electron accumulation at InN surfaces due to low Γ-point CBM
- Extreme downward band bending → quantized CB states at surface
- Core-level XPS and ion scattering reveal In-adlayer termination for *wz*–InN
- Transitions in space-charge type observed with InGaN alloy composition

References

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[5] D. Segev and C. G. Van de Walle, Europhys. Lett. **76**, 305 (2006).

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Acknowledgements
P. H. Jefferson & S. A. Hatfield – University of Warwick; F. Fuchs, J. Furthmüller & F. Bechstedt – Friedrich-Schiller-Universität; Hai Lu & W. J. Schaff – Cornell University; C. E. Kendrick, C. H. Swartz, P.A. Anderson & S.M. Durbin – University of Canterbury; H. Naoi, D. Muto & Y. Nanishi – Ritsumeikan University; L. Colakerol, T. C. Chen, T. D. Moustakas & K.E. Smith – Boston University; J. Schörmann, D. J. As & K. Lischka – Universität Paderborn.