Lattice Constant and Band Gap Tuning in BInGaN Alloys for Higher-Efficiency LEDs

ENGINEERING HONORS PROGRAM
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Background

InGaN Light-Emitting Diodes (LEDs)

- Possess the useful property of a band gap that is tunable throughout the visible spectrum
- Enable cost and energy savings over incandescent and fluorescent lighting because of their high efficiency
- Suffer from an efficiency droop while operating at high power
  - Related to the loss of charge carriers to Auger recombination, which is especially prevalent at high charge-carrier densities[1,2]
  - Charge-carrier density can be reduced by increasing active region volume

$$\eta = \frac{Bn^2}{An + Bn^2 + Cn^3}$$

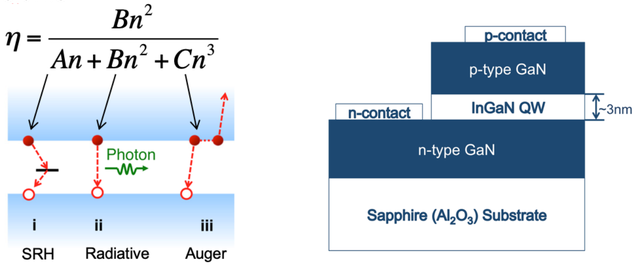

Figure 1: Left: The ABC model of internal quantum efficiency (IQE), where A, B, and C are material-dependent coefficients that control the three recombination mechanisms. Right: Single InGaN quantum well structure on GaN.

Strategies for Increasing Active Region Volume

- Multiple quantum wells (MQWs) – current predominant strategy
- Single, thicker layers of InGaN
  - Theoretically more efficient than MQW structures
  - Performance-degrading defects form when InGaN grown beyond a certain critical thickness on GaN
- Co-alloying with boron nitride to form BInGaN[3]
  - Same tunable band gap as InGaN
  - Structural properties could be matched to GaN if we find proper B to In ratio for the more stable structure (wurtzite vs. zincblende)

Methodology

1. Generate Special Quasi-random Structures (SQSs) to approximate a random alloy in a small unit cell (for computational efficiency)
   a. Repeat for various compositions across $B_yIn_xGa_{1-x-y}N$ composition space for both wurtzite and zincblende structures
2. Density functional theory (DFT) calculations to explore the thermodynamic, structural, and electronic properties
   a. Included Van der Waals forces in calculations to obtain structural properties
   b. Used a hybrid functional to overcome well-known limitations of DFT with respect to underestimating band gaps.

Results and Discussion

Thermodynamic and Electronic Properties

- Enthalpy of mixing Increases as B content increases
- B incorporation has stronger effect on enthalpy of mixing than indium

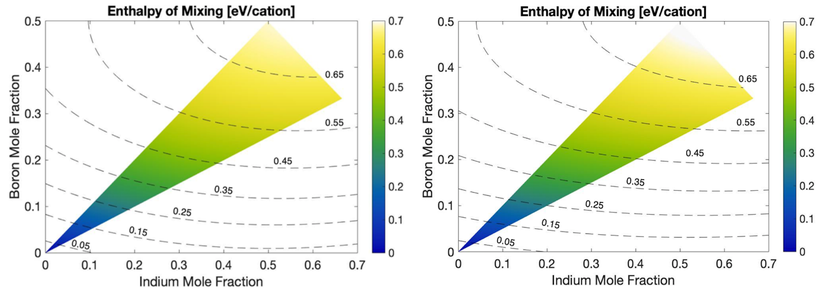

Figure 2: Enthalpy of mixing per cation as a function of composition for wurtzite (left) and zinc blende (right) $B_yIn_xGa_{1-x-y}N$ alloys.

- Wurtzite structure more stable at compositions closer to InGaN, zincblende more stable closer to BGaN
- Band gap still tunable throughout entire visible spectrum and displays bowing

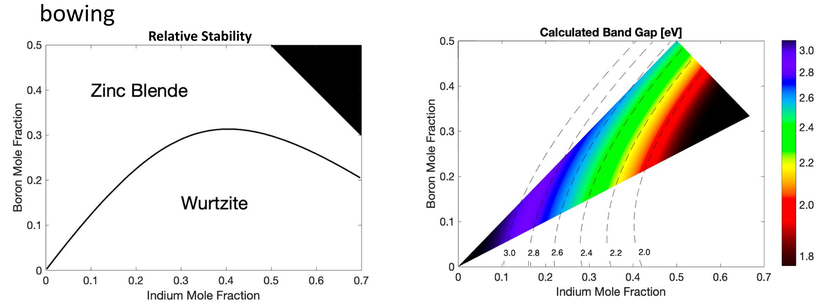

Figure 3: Left: Regions of relative stability for wurtzite and zinc blende $B_yIn_xGa_{1-x-y}N$ alloys. Right: Calculated band gap of wurtzite $B_yIn_xGa_{1-x-y}N$ as a function of composition.

Structural Properties

- Both wurtzite and zincblende can be lattice matched to GaN
- Wurtzite is more stable and lattice-matched simultaneously
- Ratio to 2 parts B to 3 parts In provides lattice match in wurtzite up to ~5% B (agrees with Vegard's law in dilute regime)

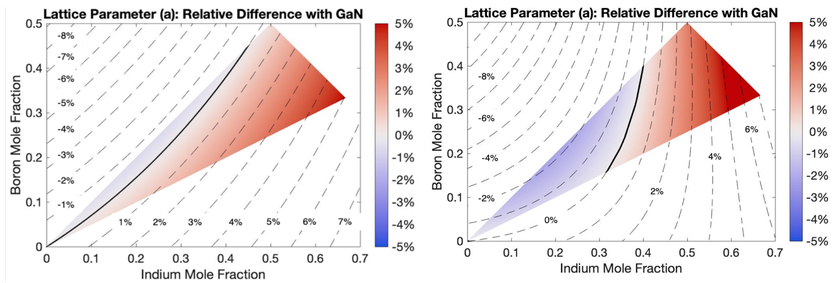

Figure 4: Relative difference between *a* lattice parameters of wurtzite (left) and zincblende (right) $B_yIn_xGa_{1-x-y}N$ and that of GaN.

Conclusions

BInGaN Alloys

- Have band gaps spanning entire visible spectrum
- Can be lattice-matched to GaN with an appropriate ratio of B to In
- Are more stable in the WZ phase at lattice-matched compositions
- Allow for growth of thicker active region that lowers charge carrier density and mitigates Auger recombination
- Enable higher-power, higher-efficiency LEDs

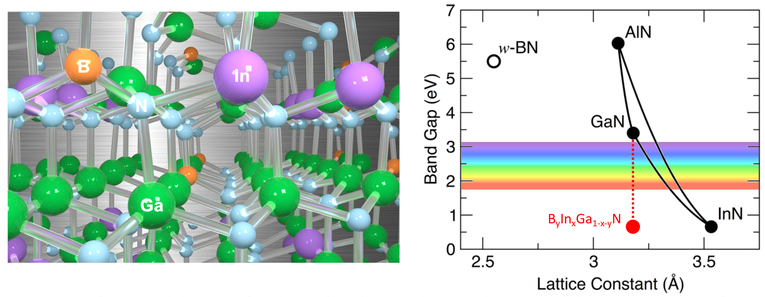

Figure 5: Left: Crystal lattice of a (BInGa)N alloy. Right: Band gaps and lattice constants of nitride compounds and their alloys (results of this work shown in red).

Future Work

- Experimental realizability
- Find ordered structures of BInGaN using cluster expansion and Monte Carlo techniques
- Create complete phase diagram of BInGaN

References

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Acknowledgements

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