III-Nitrides for Photovoltaic and Photoelectrochemical Energy Conversion
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Motivation and Design Principles
- The band gap tunability and material properties of these alloys makes them ideal candidates for photovoltaic and photoelectrochemical applications.
- Higher precision growth with molecular beam epitaxy allows for higher indium incorporation and p-type doping.

Photovoltaic cell design: p-i-n versus p-n junction
- Use p-type GaN easier to grow than p-type InGaN
- Record for cell of this type: V_oc, of 2.4 eV under UV enhanced illumination (limited by phase-separation of the InGaN)
- Growth of lattice mismatched GaN on InGaN causes polarization issues
- No issues with conduction band discontinuities
- Latent strain induced polarization effects less likely to affect performance
- P-type doping of InGaN not yet demonstrated across entire composition range
- Surface accumulation layers form limiting contact efficiency

Photoelectrochemical cell design: material property requirements
There are 3 key requirements for materials in PEC cells:
- Optimum band gap
- Tunable through visible spectrum
- Correct alignment of conduction and valence bands
- GaN is one of few possibilities to fulfill this requirement
- Corrosion resistant

A better understanding of the reaction of InGaN alloys with water is necessary to prove their potential as photoelectrodes.

Synthesis of III-Nitride Alloys
Buffer Layer Growth
Given the lattice mismatch between GaN and sapphire, development of an appropriate buffer layer scheme has been imperative.

Buffer Layer Growth Sequence
- GaN growth on buffer layers
- RMS roughness ~ 20 nm

Demonstration of InGaN Alloy Growth
- Successful growth of films with up to 27% in composition has been demonstrated with no apparent phase separation
- Challenges that remain include demonstration of doping and increased indium incorporation
- Threading dislocations must be mitigated via thicker buffer layer growth to improve film quality

Density Functional Theory Study of H_2O on GaN(0001)

Computational Details
- Ultra-soft pseudo-potential Density Functional Theory (DFT) simulation within the Generalized Gradient Approximation (GGA) performed by Vienna Ab-initio Simulation Package (VASP) code.
- Exchange and correlation function: PW91
- Valence electrons of Ga atom with 3d^104s^2 and N atom with 2s^22p^3.
- Plane wave cutoff energy is 400 eV
- Monkhorst-Pack scheme for generating the special k points in the irreducible part of the Brillouin zone (BZ): [4x4x2] mesh for bulk and [2x2x1] mesh for 2x2 surface.
- Periodically repeated slab model: 6 layers of GaN, vacuum region of 11 Å, one side of the slab is saturated with hydrogen atoms, and the bottom layer of the slab is fixed.
- Electronic band structure calculation: 10 k-points per line connecting high symmetry points.

Molecular Adsorption at 0.25 ML
- At 0.25ML, water molecules prefer to adsorb on top of Ga atoms.
- Molecular water adsorbates thermodynamically prefer to form dissociative adsucts, HO-Ga and H-Ga.

Future Work
- Successful doping of both GaN and InGaN alloys will be demonstrated
- Simulation of both p-i-n and p-n junction structures will be used to determine growth requirements
- Understanding of device requirements and growth restrictions will be used to develop high indium multiphase solar cell design
- Further study of oxygen or hydrogen generating redox reactions on a variety of GaN surfaces will be performed using DFT

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