The role of N-H complexes in the control of localized center recombination in hydrogenated GaInNAs

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Multijunction Solar Cells: Divide and Conquer

- Three junctions: 44% efficient
- Four junctions: Up to 52% efficient
- Power wasted by Ge due to poor current matching

We need a material with 1 eV band gap, correct lattice spacing

J.F. Geisz and D.J. Friedman, Semiconductor Science and Technology 17, 769 (2002)

http://www.pvmeasurements.com/
GaInNAs is a Promising but Problematic Candidate for the Fourth Junction

Growth Problems:
- High temperature—phase separation, clustering
- Low temperature--defect formation, low nitrogen inclusion

Regardless of sample quality, substitutional N is locally different electrically than As, causing low diffusion lengths.

Effects of Annealing

Post – growth annealing improves material quality
- Ga-vacancies removed
- N – As exchange increase nitrogen incorporation
- Low temperature PL dominated by localization centers

Effects observed in the performance of GaInNAs solar cells
Hydrogenation Has Shown Passivation of Substitutional Nitrogen

- Restoration of original band gap
- Process reversible through annealing
- Favorable due to small, electronegative nitrogen


Selective Defects Passivation in Solar Cell Materials

- UV-activated hydrogenation – Deuterium based
  - Typical 100 °C – 350 °C
  - Pressures ranging from $10^{-6}$ – $10^5$ Torr
Passivation in Solar Cell

Reference

Lowest Hydrogenation

Highest Hydrogenation

Proc. 40th IEEE PV Specialists, Denver 2014
Solar Cell Characterization

- Increase in performance of the solar cell after hydrogenation
- No visible effect on the substitutional Nitrogen – *selective passivation*

Samples Used

-Bulk $\text{Ga}_{0.91}\text{In}_{0.09}\text{N}_{0.028}\text{As}_{0.972}$
grown via MBE using RF plasma source for nitrogen
annealed at 800°C for 30s

UV-Activated hydrogenation, 2 μm penetration

Three samples:
• Reference – Unhydrogenated
• #9 – Intermediate hydrogenation
• #8 – High hydrogenation
Hydrogenation of GaInNAs Mitigates Localization Effects, Retains Band Gap

Reduction in intensity of low-energy “shoulder”
Hydrogenation of GaInNAs Mitigates Localization Effects, Retains Band Gap

Reference PL by T

Hydrogenated (#8) PL vs T

Peak now has reduced ‘s-shape’ with temperature
• Individual Peaks $E_G$, $E_L$, and $E_D$ are tracked and intensities are fitted
  • $k(l \alpha P^k)$

• $k < 1$ - Defect/localized states
• $1 < k < 2$ - Band to band recombination
Selective Passivation: Effect of excitation intensity

Reference - unhydrogenated

Hydrogenated – $1 \times 10^{15}$ cm$^{-2}$

Acknowledgement: Joseph Tischler and Chase Ellis
Density Functional Theory Results

- Supercell of 64 atoms used
  - 29 Ga, 32 As, 3 In
  - 1 N replaces an As atom for GaInNAs, giving 3% Nitrogen

- As Hydrogen concentration increases Ga-H$_2$-N complexes form. The feature related to nitrogen is pushed into the continuum. However the scattering center still remains.

Acknowledgement: Dr. Bin Wang – CBME, University of Oklahoma
Further Testing of Samples is Needed

- Annealing at different temperatures breaks certain N-H complexes, may be used to identify hydrogenation type
- Hall measurements will more directly ascertain effects of centers on carriers
- Thermopower measurements will qualitatively ascertain degree of doping change due to hydrogenation
- Transport Measurements
- Electrical Characterization - DLTS
Summary

- The hydrogenated samples exhibit lessened effects of localization centers while retaining substitutional nitrogen.
- Further studies will be conducted to verify which N-H complexes are forming and to analyze their effect on the band structure and carriers.

Acknowledgements

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DFT calculations performed at OSCER at the University of Oklahoma.