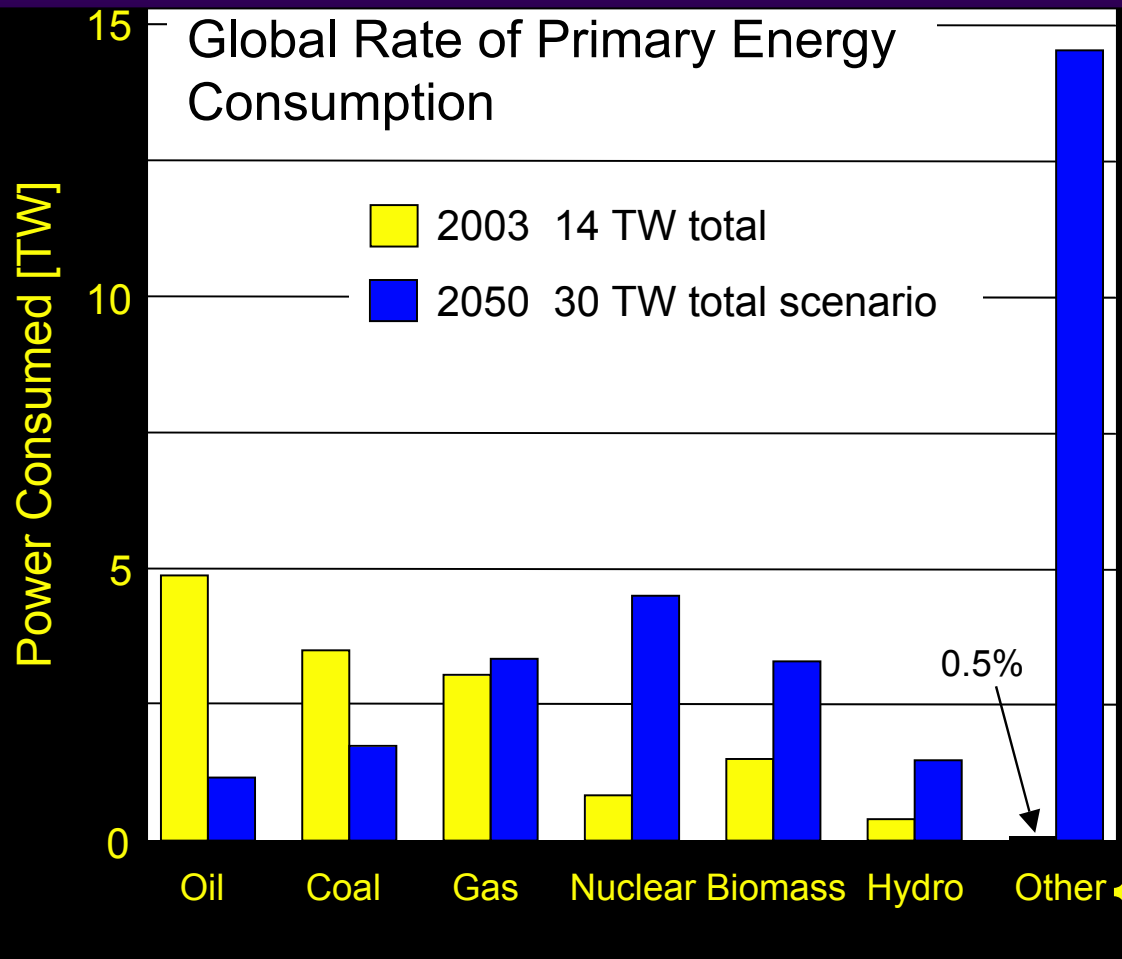
BNC Research Symposium

2 April 2007

Overview of Energy-Related Research at the Birck Nanotechnology Center

The Terawatt Challenge



Primary source for 2003 data: International Energy Agency

Adapted from Richard Smalley's presentation on "Our Energy Challenge" at the 2004 International Electron Devices Meeting (IEDM), San Francisco, CA 12/14/04

Slide courtesy of T. Sands

Energy Consumption Rate per Capita

- **In 2003:**
  - World: 2.24 kW/person (6.268 B people)
  - US: 10.4 kW/person (0.291 B people)
  - If everyone consumed at the US rate, the global rate of primary energy consumption would be ***65 TW***.

- **In 2050:**
  - The projection of 30 TW in 2050 corresponds to an average of 3 kW/person for 10B people…very conservative in light of the rapid changes in the developing world.

Slide courtesy of T. Sands

Summary of Energy Research Topics & Investigators

- **Solar**
  - Rakesh Agrawal & Hugh Hillhouse (ChemE): nanocrystal-based solar cells
  - Kyoung-Shin Choi (Chemistry): photoelectrochemistry
  - Dick Schwartz & Jeff Gray (ECE): multi-junction photovoltaics
- **Direct Thermal Energy Conversion (DTEC)**
  - Hugh Hillhouse (ChemE): nanowire thermoelectrics
  - Tim Fisher (ME) & Ron Reifenberger (Phys): vacuum thermionics
  - Xiulin Ruan (ME): laser cooling
  - Tim Sands (MSE/ECE): nanowire thermoelectrics
- **Hydrogen**
  - Timothee Pourpoint (AAE), Tim Fisher, Issam Mudawar, Yuan Zheng (ME): nanoparticulate metal hydrides for hydrogen storage
  - Jerry Woodall (ECE): Al-Ga alloys for hydrogen storage & water splitting
- **Energy Utilization**
  - Tim Sands (MSE/ECE), Edwin Garcia and Eric Stach (MSE): solid-state lighting

Multi-Junction Photovoltaics

Sponsor: DARPA

Students: Alex Hass
Jeff Wilcox (ECE)
Faculty: Dick Schwartz,
Jeff Gray, Jerry Woodall (ECE)

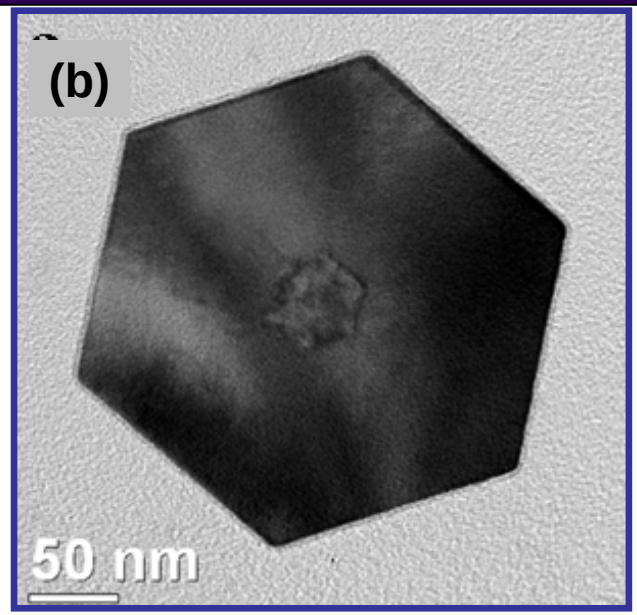
- Part of DARPA's Very High Efficiency Solar Cell Program which is working toward producing a multi-junction solar cell with a 50% operating efficiency. Purdue's part of the program involves detailed numerical modeling of the cells.
  - $200k/yr for up to five years

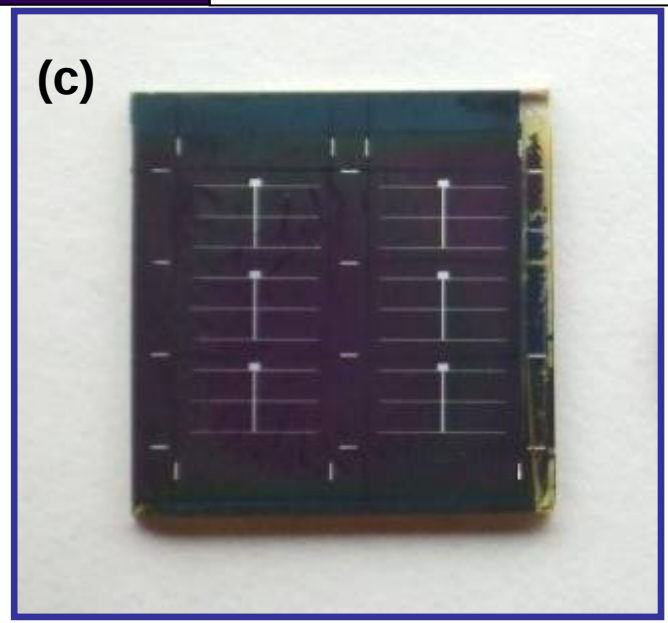
- Publications
  - R. J. Schwartz, "The Contributions of Numerical Modeling to Improved Understanding of Solar Cell Performance," 2nd World Conference on Photovoltaic Solar Energy Conversion," Vienna, Austria, July 6-10, 1998. Plenary IEEE Cherry Award Address.
  - R.J. Schwartz, "The Evolution of High Intensity Photovoltaic Cells from Thermophotovoltaic Applications to High Concentration Solar Applications: Lessons Learned," International Conference on Solar Concentrators for the Generation of Electricity or Hydrogen, Scottsdale, AZ, May 1-5, 2005. [Invited]
  - A. Barnett, C. Honsberg, D. Kirkpatrick, S. Kurtz, D. Moore, D. Salzman, R. Schwartz,J. Gray, S. Bowden, K. Goossen, M. Haney, D. Aiken, M. Wanlass, K Emery, "50% Solar Cell Architectures and Designs," 2006 IEEE 4th World Conference on Photovoltaic Energy Conversion, Waikoloa, HA, May 7-12, 2006.
  - R. J. Schwartz, Chair, M. L. Bowden, H. P. Davis, R. L. Kline, M. K. Macauley, L. D. Peterson, K.C. Reinhart, R.R. Rhodes, "Laying the Foundation for Space Solar Power: An Assessment of NASA's Space Solar Power Investment Strategy," National Research Council Report, National Academy Press, 2001.

- Recognition
  - Fellow, IEEE, "For contributions to the design and analysis of high efficiency silicon solar cells", 1987.
  - IEEE William Cherry Award, "For outstanding contributions to the advancement of photovoltaic science and technology", July 1998, Vienna, Austria.
  - Fellow, International Engineering Consortium, "For pioneering work in the field of photovoltaics cells and contributions to engineering education", October 2002, Boca Raton, FL.

Nanocrystal "Ink" Based Solar Cells

Prof. Rakesh Agrawal and Prof. Hugh Hillhouse





Summary: A unique solution chemistry route has been developed that yields an ink composed of nanocrystals of copper indium diselenide. A photograph of the ink is shown in (a) while an electron micrograph of one of the crystals is shown in (b). These crystals may be coated on a substrate, sintered, and used as the active layer of a solar cell. The completed solar cell, Purdue's first nanocrystal based solar cell, is shown in part (c). This cell was measured to have an efficiency of 2% under standard conditions.

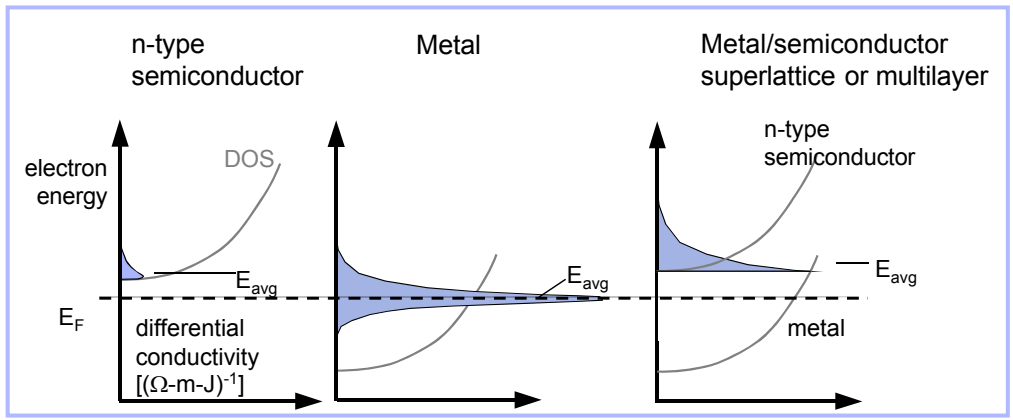
Grants: Energy Center Seed Grant (2006-2007)

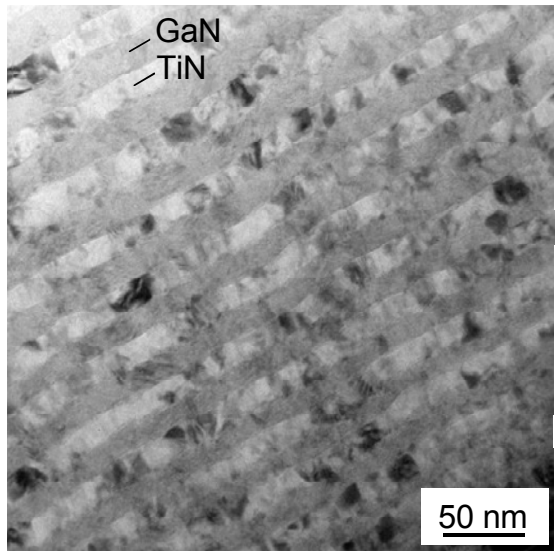
Publications: Guo, Jun, Agrawal, Hillhouse, Stach, "Facile Solution Synthesis of Chalcopyrite Structure CuInSe2 Nanocrystals," In preparation.

Metal/Semiconductor Multilayers for Solid-state Thermionic Energy Conversion

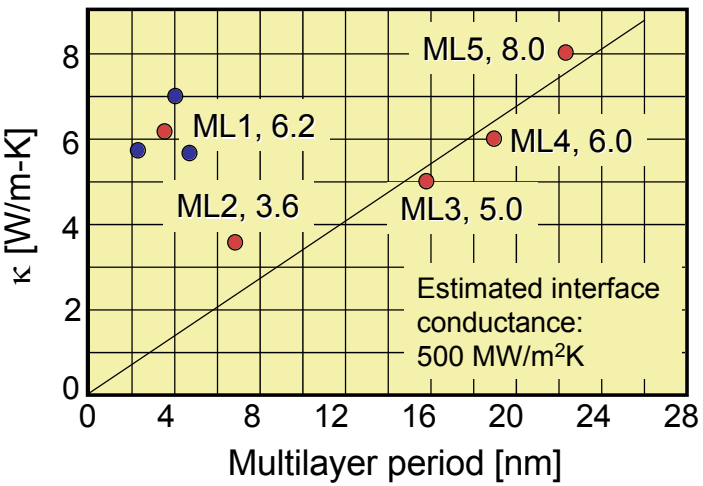
Prof. Tim Sands; Students: Vijay Rawat, Himanshu Mishra, Kalapi Biswas, Robert Wortman

Metal/semiconductor thermionic multilayers are “artificial” thermoelectric materials that convert heat flux into electrical power through energy filtering





TiN/GaN multilayers grown by reactive PLD at Purdue



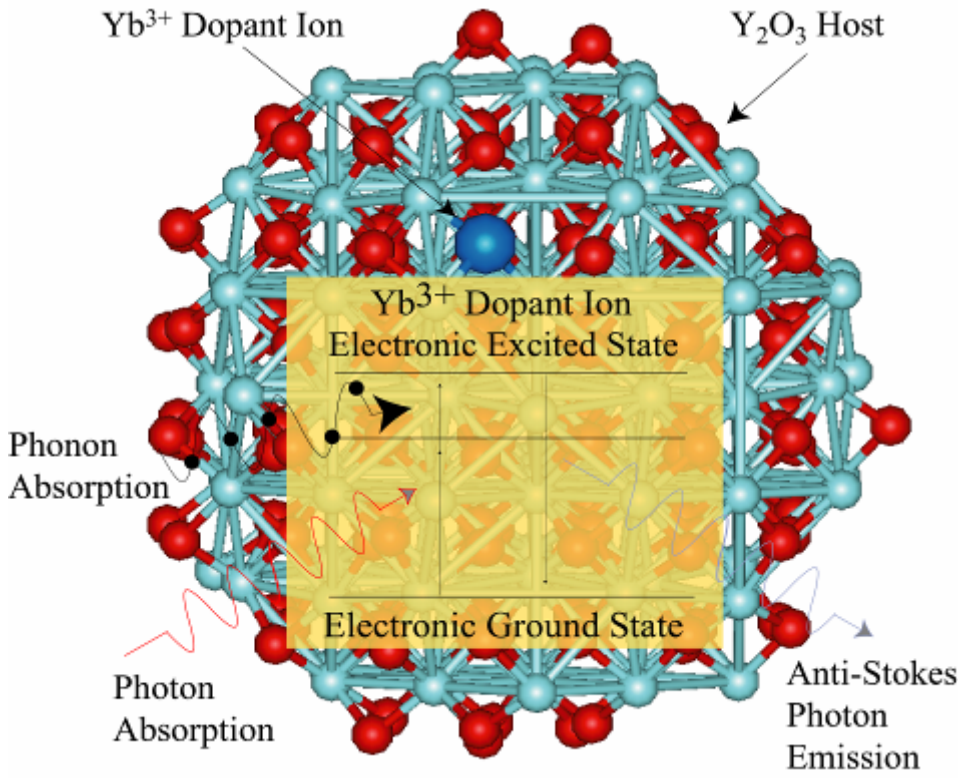
Thermal conductivity reduced by a factor of 40, dominated by interface resistance down to periods of about 5-10 nm

V. Rawat and T. Sands in collaboration with the groups of A. Shakouri (UCSC), A. Majumdar (UC Berkeley) and D. Cahill (UIUC)

Fundamentals of Laser Cooling of Solids and its Enhancement using Nanopowders

Faculty: Xiulin Ruan (ME)

- Ab initio calculations are used to identify materials with strong photon-electron-phonon couplings
- Maxwell's equations and molecular dynamics are used to study photon and phonon localization in nanostructures
- Nanopowders are proposed to enhance the cooling performance to the cryogenic temperature range (i.e., less than -150^{o}C).



Direct Thermal Energy Conversion by Vacuum Electron Emission

Sponsor: NSF, Nanoscale Science and Engineering Program

Student: Tyler Westover
Faculty: Tim Fisher, Ron Reifenberger

Motivation and Goals

- Vacuum structures provide inherent thermal insulation
- Apply the Non-Equilibrium Green's function (NEGF) method to investigate nanoscale effects on energy conversion with experimental validation

Technical Challenges

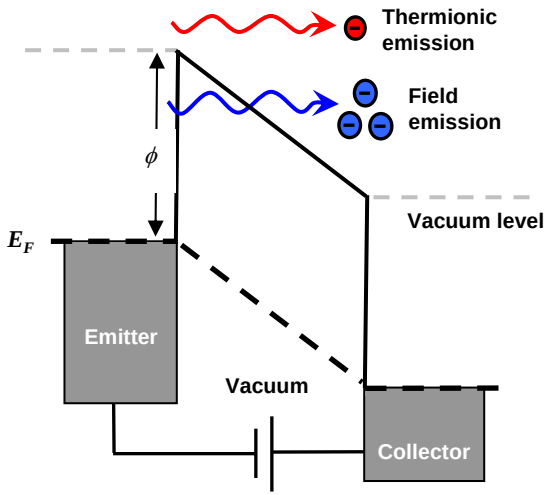
- Requires low work function (≈1 eV) emitters capable of stable emission
- Minimizing Joule heating is critical because of large electric currents

Nanoscale emitter structures and vacuum gaps offer the possibility of direct refrigeration and power generation devices capable of operating at efficiencies approaching the Carnot limit

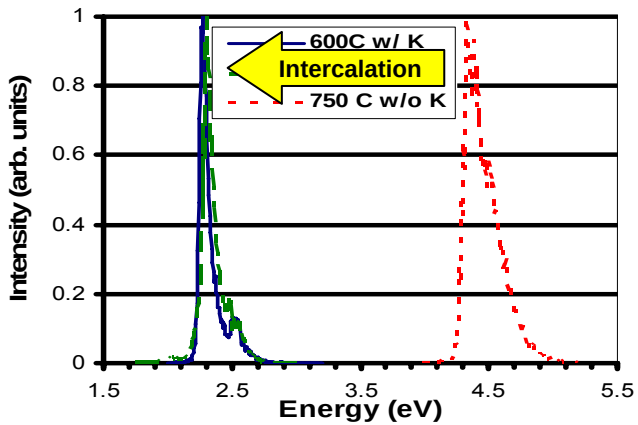
Technical Approach

- NEGF modeling approach provides accurate modeling of quantum effects
- Experimental results obtained from carbon nanotube emitters intercalated with cesium and potassium
- Experimental apparatus is capable of resolving cooling powers as low as 1 μW, and electron energies below 5meV

Electron Emission



Real Work Function Reduction



PURDUE UNIVERSITY | Discovery Park | Birck Nanotechnology Center

Hydrogen Storage in Nanoparitculate Metal Hydrides

Sponsor: General Motors

Students: *Varsha Velagapudi, Kyle Smith, Scott Flueckiger*

Faculty/Staff: *T. Pourpoint, T.S. Fisher, I. Mudawar, Y. Zheng*

Motivation and Goals

- Enhanced heat transfer needed for hydrogen storage in high pressure metal hydride systems
- Build an experimental apparatus to test hydriding-dehydriding processes in nanoscale metal hydrides

Technical Challenges

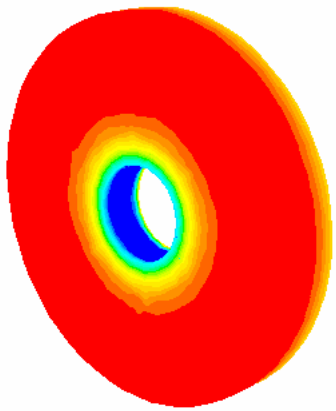
- Ultra-high heat fluxes (~1 MW) must be dissipated in short periods of time
- Designing and working with pyrophoric materials at large scales in high-pressure systems

This project is the first of its kind to be undertaken by a university at this scale. The results of the project will enable the rapid development of vehicle-scale metal hydride storage systems.

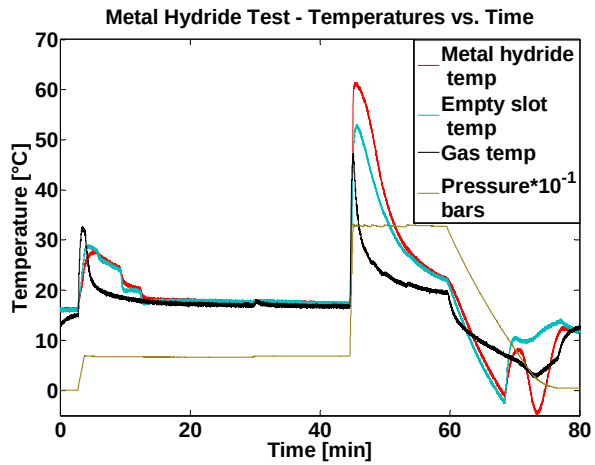
Technical Approach

- Development of large-scale high-pressure systems
- Use of nanoparticulate metal hydrides
- Pyrophoric material handling in inert environment
- Modeling chemical reactions and heat transfer
- Optimization of heat exchanger design
- Use of Fluent, LabVIEW

Modeling of Nanopowders



Large-scale Testing (Energy Center)



Toward Phosphor-free White LEDs

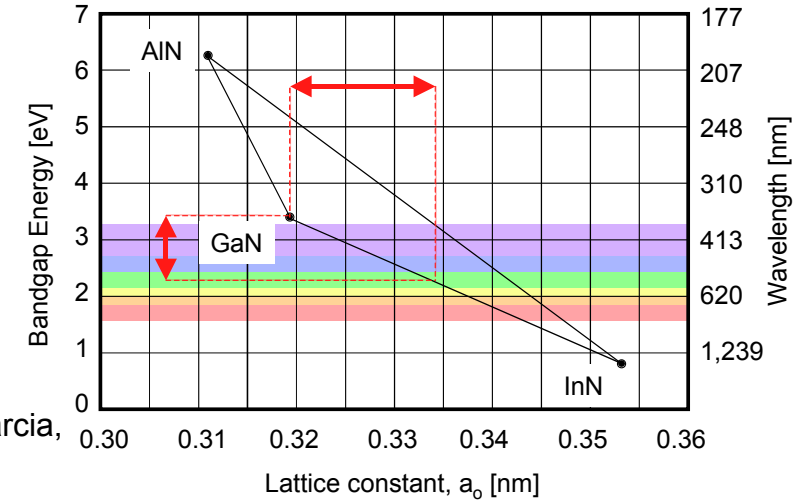
Sponsor: DoE

***Students**: Mark Oliver, Parijat Deb, Robert Colby, Ho Gyoung Kim, David Ewoldt, Isaac Wildeson, Zhiwen Liang, Patrick Cantwell*
***Faculty**: Tim Sands, Edwin Garcia, Eric Stach*

Lattice misfit strain limits (In,Ga)N emission to uv, blue and green
Solution: lateral strain relief in nanostructures

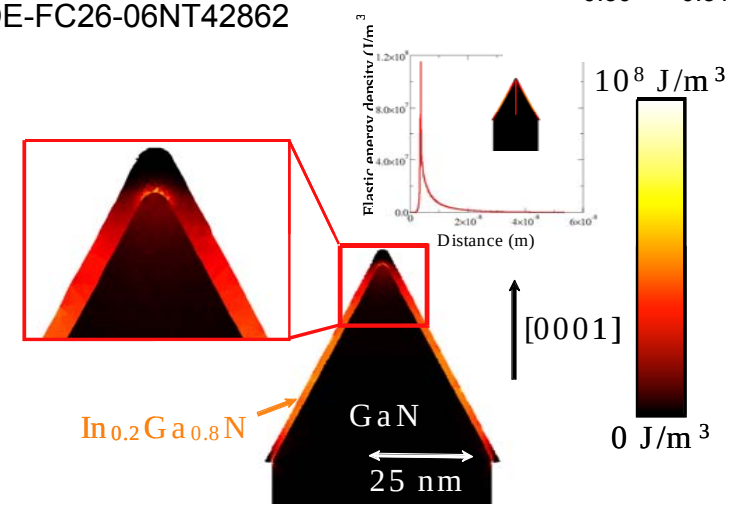
GaN blue lasers and green LEDs are used in optical recording and traffic lights, respectively. To fabricate efficient yellow and red emitters, the lattice strain associated with larger InN mole fractions must be relieved.

Tim Sands, Eric Stach and Edwin Garcia, DE-FC26-06NT42862

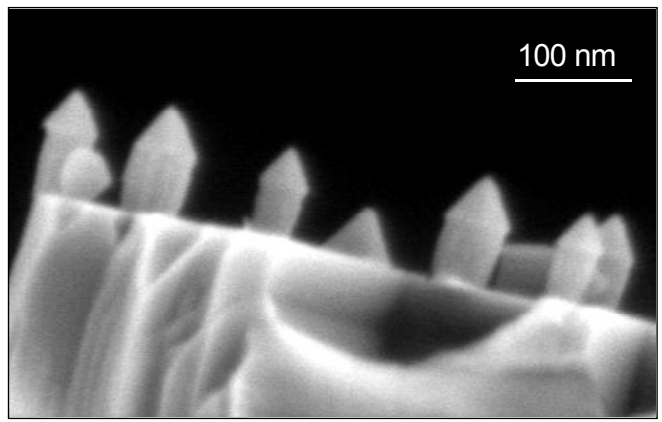


Deb, Kim, Rawat, Oliver, Kim, Marshall, Stach and Sands, *Nano Letters* (2005)

The Purdue group has developed a method for fabrication GaN nanorod arrays by selective epitaxy through a self-organized nanoporous template

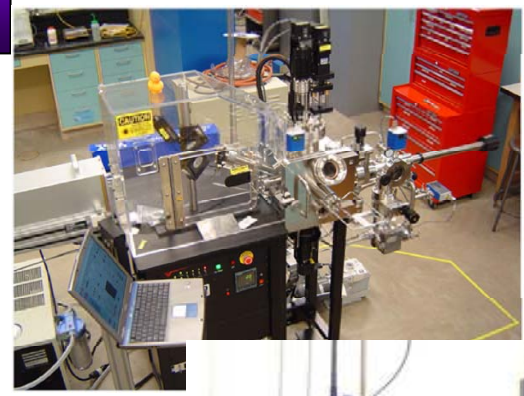


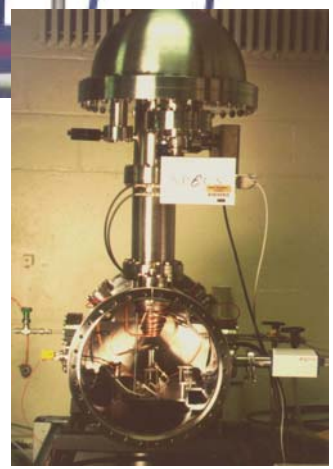
Finite element modeling shows that lattice mismatch strain can be effectively relieved in nanorods, and particularly at the apex of pyramidal caps



Facilities and Instrumentation (partial list)

- Aixtron 200HT MOCVD
- Homebuilt (In,Ga)N HVPE
- PVD Products NanoPLD
- Anodization and electrodeposition
- PVD Products reactive nitride sputter system
- FEI Titan environmental TEM
- FEI FIB
- Panalytical HRXRD
- FESEM, PL, EL, lithography, metallization, etc.
- CAFMs
- Seki microwave PECVD for carbon nanostructures
- PHOIBOS electron energy analyzer





Example External Projects

- Monolithic phosphor-free white LEDs for solid-state lighting (DOE, $900K, 3 years, May 2006 start) - Garcia, Stach and Sands
- Metal/semiconductor superlattices for solid-state thermionic generators (ONR MURI, $233K, 2-yr renewal, July 2006 start) - Sands
- CNT “dry solder” for joining thermoelectrics to microdevices (CTRC $100K, 2 years, Jan 2006 start) - Fisher and Sands
- Nanowire array composites for thermoelectric power generation (ONR, $296K, 3 years, May 2006 start) - Sands
- Acquisition of a custom nitride sputter deposition system for nitride multilayers (ONR, $300K, 1 year, May 2006 start) – Sands
- NIRT: Direct Power Generation by Electron Emission from Novel Carbon Nanostructures (NSF, $451K, 5 years, Sept 2002 start) – Fisher
- Optimization of Manufacturable High Pressure Metal Hydride Storage Systems (General Motors, $764K, 2 years, Apr 2007 start) – Pourpoint, Fisher, Mudawar, Zheng, Anderson (with Energy Center lead)

Other Example Publications

- V.S. Robinson, T.S. Fisher, J.A. Michel, C.M. Lukehart, "Work Function Reduction of Graphitic Nanofibers by Potassium Intercalation," Applied Physics Letters, Vol. 87, No. 6, art.no. 061501, 2005.
- P. Deb, H. Kim, V. Rawat, M. Oliver, S. Kim, M. Marshall, E. Stach and T. Sands, "Faceted and Vertically Aligned GaN Nanorod Arrays Fabricated without Catalysts or Lithography," Nano Letters, 5 (2005) pp. 1847-51.
- J. Zhang, T.S. Fisher, P.V. Ramanchandran, J.P. Gore, I. Mudawar, "A Review of Heat Transfer Issues in Hydrogen Storage Technologies," ASME Journal of Heat Transfer, Vol. 127, pp. 1391-1399, 2005.
- H. Kim, S. Kim, P. Deb and T. Sands, "Effect of KOH Treatment on the Schottky Barrier Height and Reverse Leakage Current in Pt/n-GaN," J. Electron. Mater. 35 (2006) 107.
- X.L. Ruan and M. Kaviany, Enhanced Laser Cooling of Rare-earth-ion-doped Nanocrystalline Powders, Physical Review B 73, 155422-1-15, 2006.
- V. Rawat and T. Sands, "Growth of TiN/GaN Metal/Semiconductor Multilayers by Reactive Pulsed Laser Deposition," J. Appl. Phys. 100 (2006) 064901.
- V.S. Robinson, Y. Show, G.M. Swain, R.G. Reifenberger, T.S. Fisher, "Thermionic Emission from Surface-Terminated Nanocrystalline Diamond," Diamond and Related Materials, Vol. 15, No. 10, pp. 1601-1608, 2006.
- H.G. Kim, P. Deb and T. Sands, "High-reflectivity Al-Pt Nanostructured Ohmic Contact to p-GaN," IEEE Transactions on Electron Devices 53 (2006) pp. 2448-53.
- P. Deb, H. Kim, Y. Qin, R. Lahiji, M. Oliver, R. Reifenberger and T. Sands, "GaN nanorod Schottky and p-n junction diodes," Nano Letters 6 (2006) pp. 2893-8.
- X.L. Ruan and M. Kaviany, Laser Cooling of Solids, Journal of Heat Transfer-Transactions of the ASME 129, 3-10, 2007.
- T. Westover, T.S. Fisher, F.E. Pfefferkorn, "Experimental Characterization of Anode Heating by Electron Emission from a Multi-Walled Carbon Nanotube," International Journal of Heat and Mass Transfer, Vol. 50, pp. 595-604, 2007.
- H. Kim, P. Deb, and T. Sands, "Nanopatterned Contacts to GaN," J. Electronic Mater. (2007) published online, February 2007.
- T. Westover, T.S. Fisher, "Experimental Study of Energy Exchange Attending Electron Emission from Carbon Nanotubes," in press.