



Inidium Nitride: A potential material for hot carrier solar cells?



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- **Current Limitations in Solar Cell Efficiency**
- **Nitrides in Solar: Next Generation PV**
- **Hot Carrier Solar Cells *and* InN**



Seminar, July 14th, 2021





RENEWABLE ENERGY

Terawatt-scale photovoltaics: Trajectories and challenges

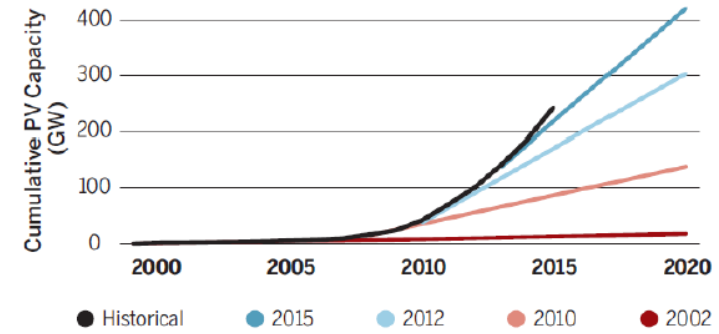
Coordinating technology, policy, and business innovations

By Nancy M. Haegel, Robert Margolis, Tonio Buonassisi, David Feldman, Armin Fritzscheim, Raffi Garabedian, Martin Green, Stefan Glunz, Hans-Martin Henning, Burkhard Holder, Izumi Kaizuka, Benjamin Kroposki, Koji Matsubara, Shigeru Niki, Keiichi Sakurai, Roland A. Schindler, William Tumas, Eicke R. Weber, Gregory Wilson, Michael Woodhouse, Sarah Kurtz



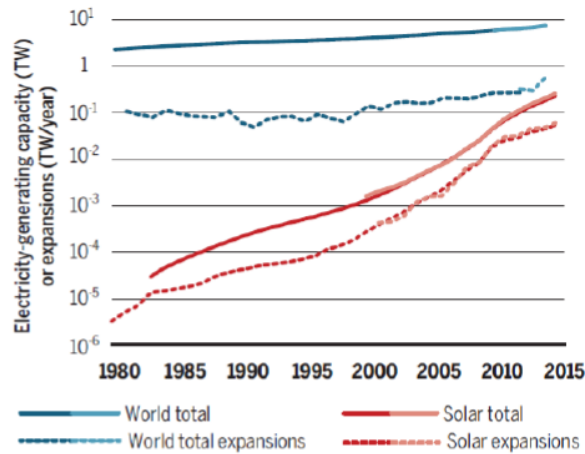
Cumulative PV installations

Projected (labeled by year of IEA publication) versus actual (labeled as "historical"). See supplementary materials for data sources and discussion.



Global electricity-generating capacity

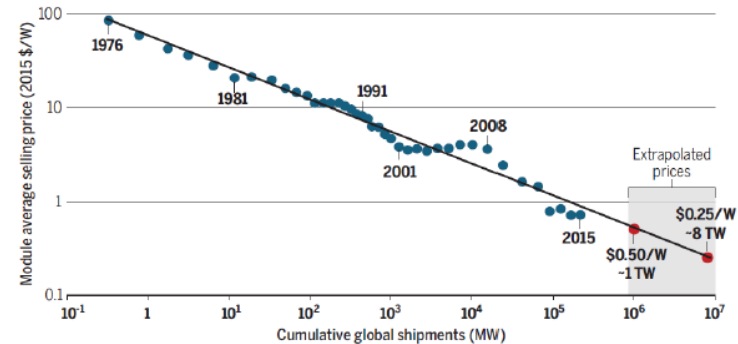
See supplementary materials for data sources.



Science 356 (6334), 141-143.
DOI: 10.1126/science.aal1288

PV module experience curve

Historically, module prices have decreased as a function of cumulative global shipments (blue dots reflect historical data, red dots reflect extrapolated prices for 1 TW and 8 TW based on the historical trend line). See supplementary materials for data sources.



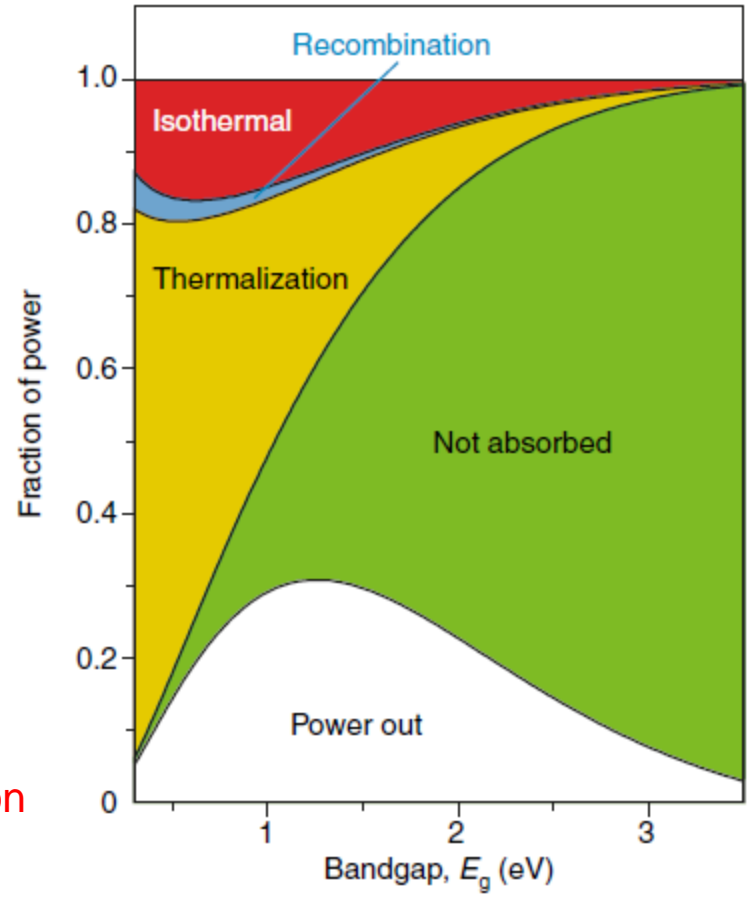
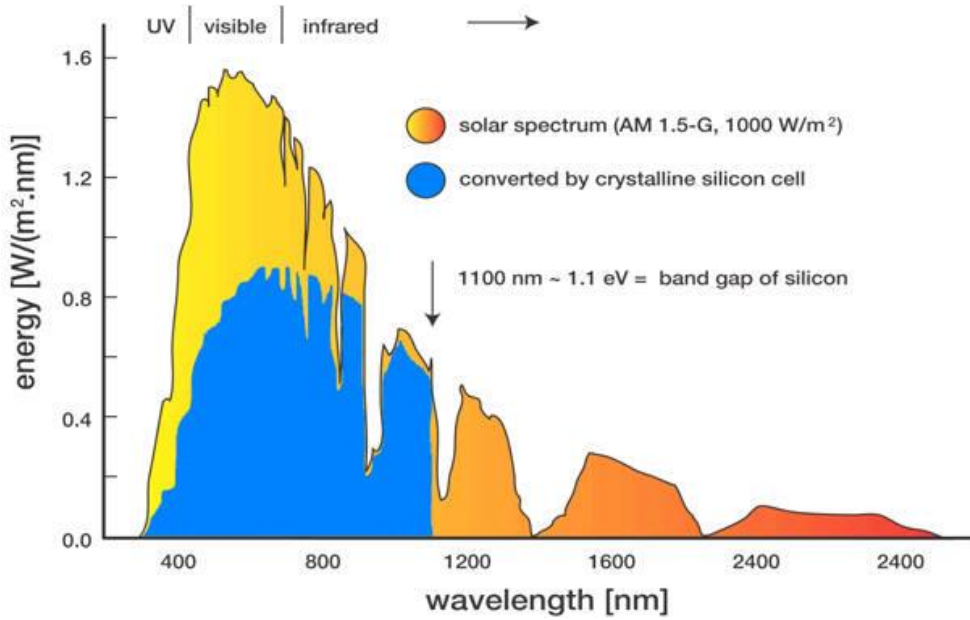
Photovoltaics Materials & Device Group, University of Oklahoma: <http://www.nhn.ou.edu/~sellers/group/index.html>

DoE SETO: "Net zero emissions no later 2050."

Photovoltaics Materials & Device Group, University of Oklahoma: <http://www.nhn.ou.edu/~sellers/group/index.html>



Fundamental Losses in Solar Cells



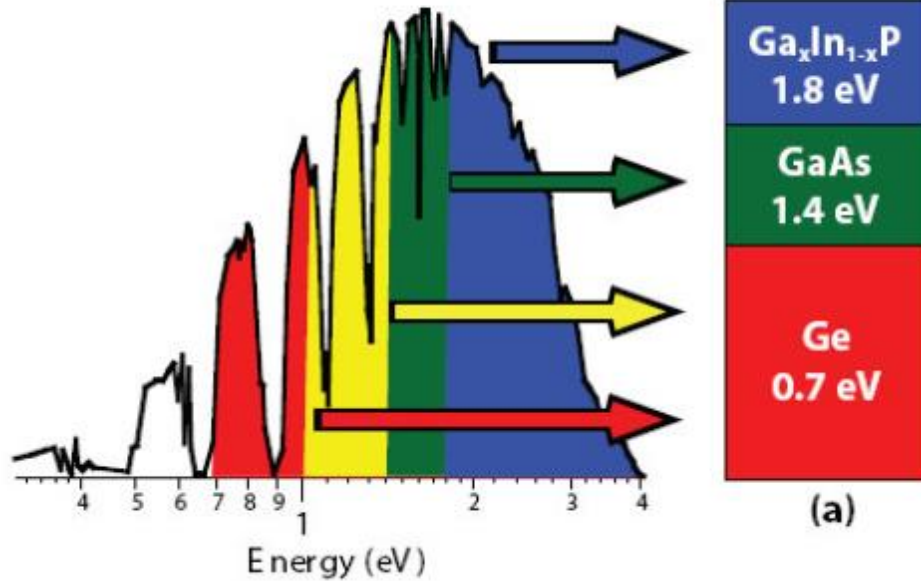
- Photocurrent determined by the photon absorption
- Photovoltage determined by the energy gap

Guillemoles *et al.*, Nature 13, 501 (2019)

Shockley-Queisser limit predicted max efficiency ~ 30% (J. Appl. Phys. 1961)

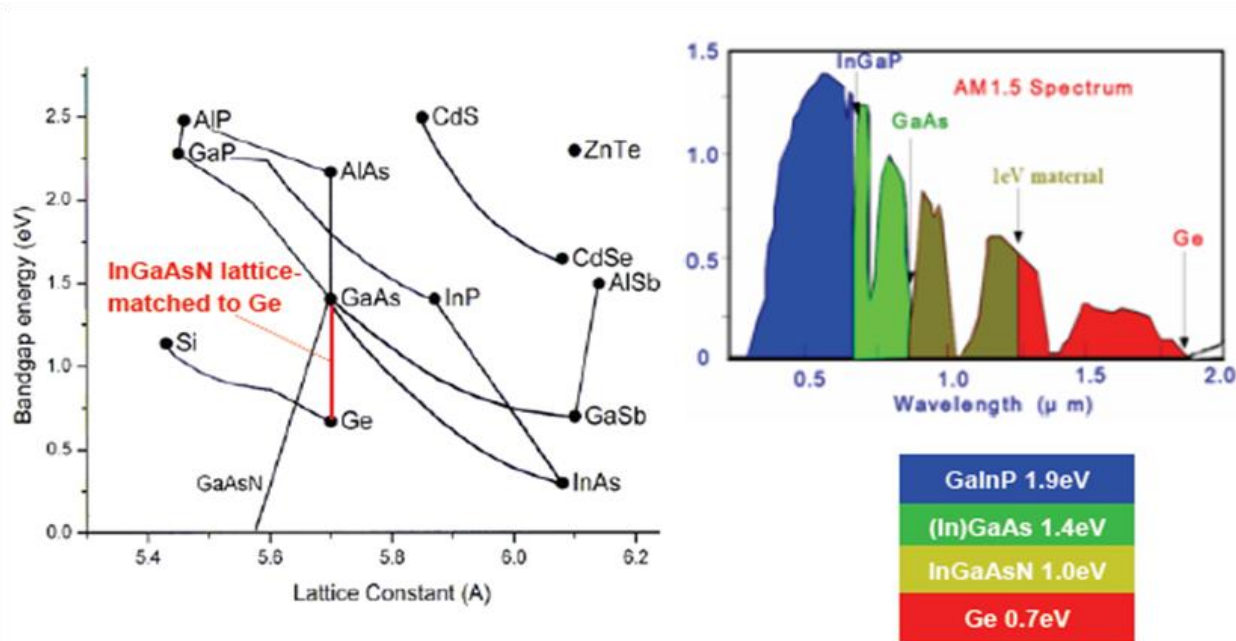


Multi-junction Solar Cells





GaNAs: potential, but issues!



GaNAs lattice matched to GaAs/Ge potential for > 50 %

Materials Quality Serious Problem

- Low Nitrogen Solubility
- Phase Segregation

J. F. Geisz & D. J. Friedman. Semicond. Sci. Technol. 17 (2002) 769-777

SHARP

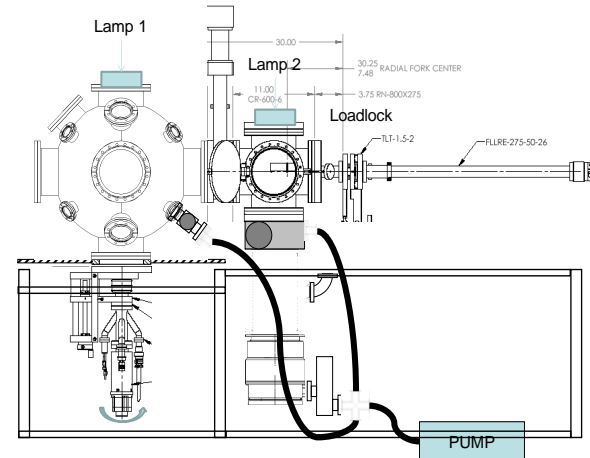
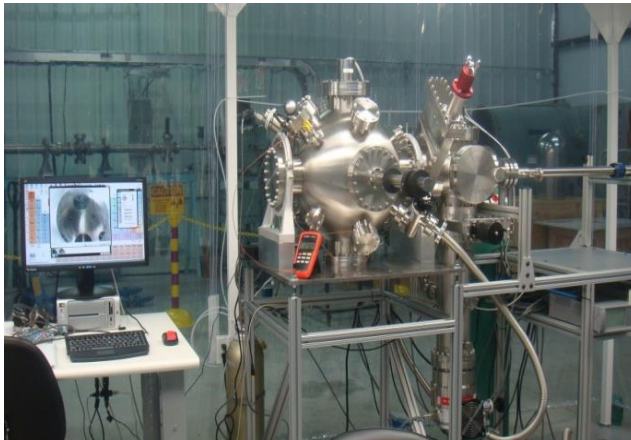


Selective Defects Passivation in Solar Cell Materials



OCAST

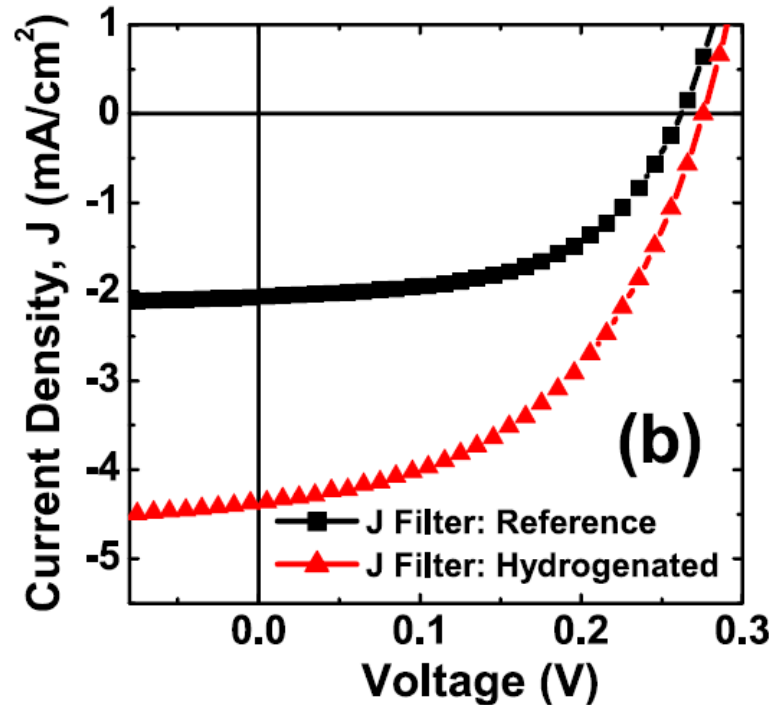
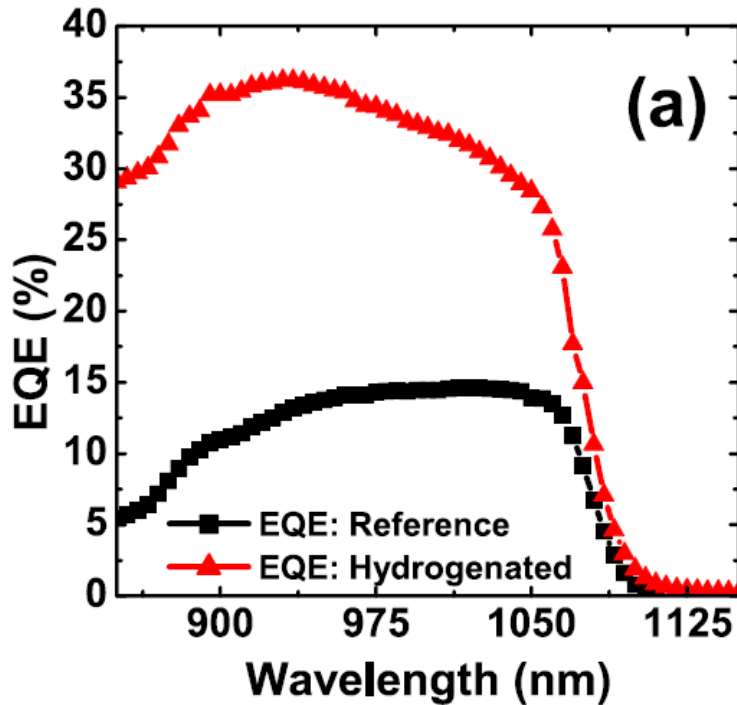
Oklahoma Center for the Advancement of Science and Technology



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



Solar Cell Characterization

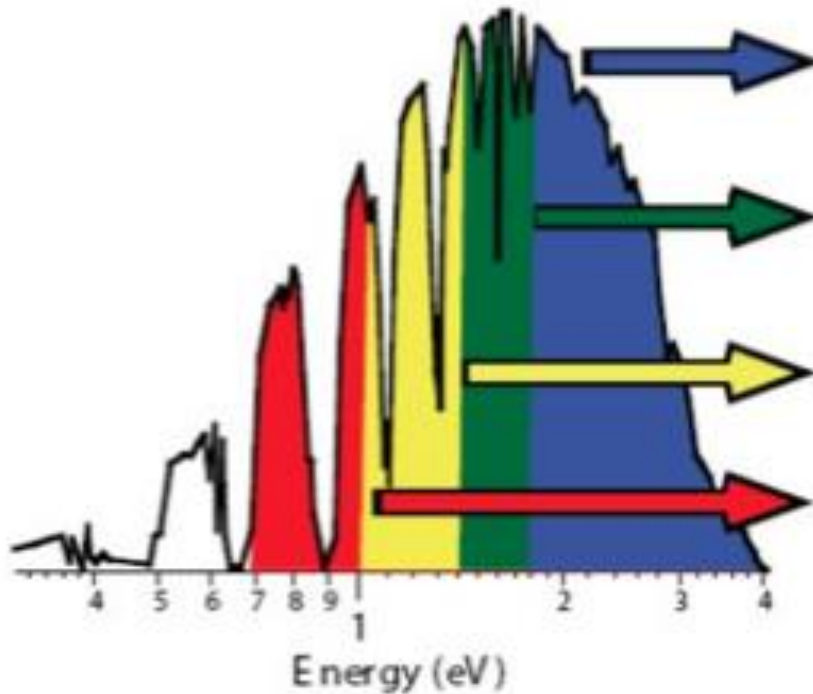


- Increase in performance of the solar cell after hydrogenation
- No visible effect on the substitutional Nitrogen – *selective passivation*

Fukuda *et al.* *Applied Physics Letters* **106**, 141904 (2015)



3G PV: Harnessing the solar spectrum



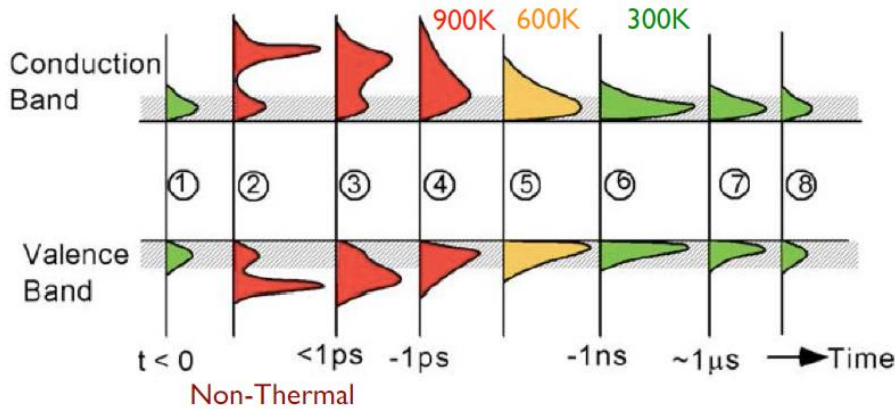
Hot Carriers
2, 3x E_g - MEG
 ΔE_{IC} - IBSC

Fundamental Gap
 $\sim 0.7\text{eV}$

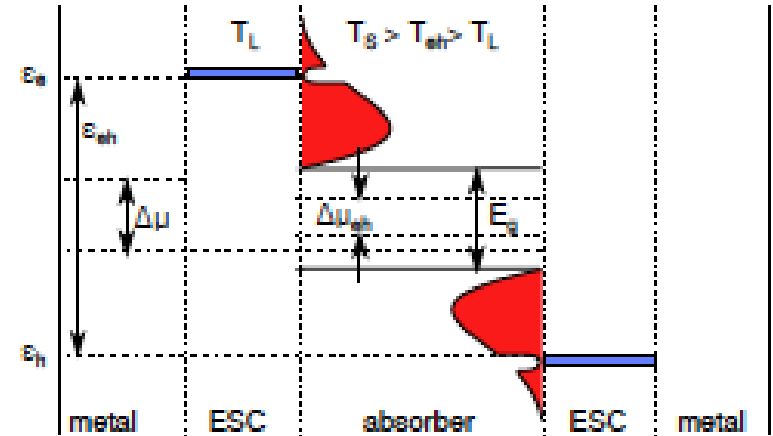
To harness the solar spectrum effectively Energy-gap is lowered slightly to $\sim 0.7\text{eV}$



Hot Carrier Losses and Solar Cells



Green, M.A., Third Generation Photovoltaics, Springer 2003



Wurfel, Sol. Energ. Mat. Sol. C, 46, p.43 (1997)

- “Hot carriers” rapidly transfer energy to the lattice – *thermalization*
- Rapid extraction of higher energy carriers via energy selective contacts has potential to increase power conversion:
 - **selective energy extraction**
 - **inhibited electron-phonon relaxation pathways**
 - **phonon bottleneck**



Hot Carrier Relaxation – Heat Generation

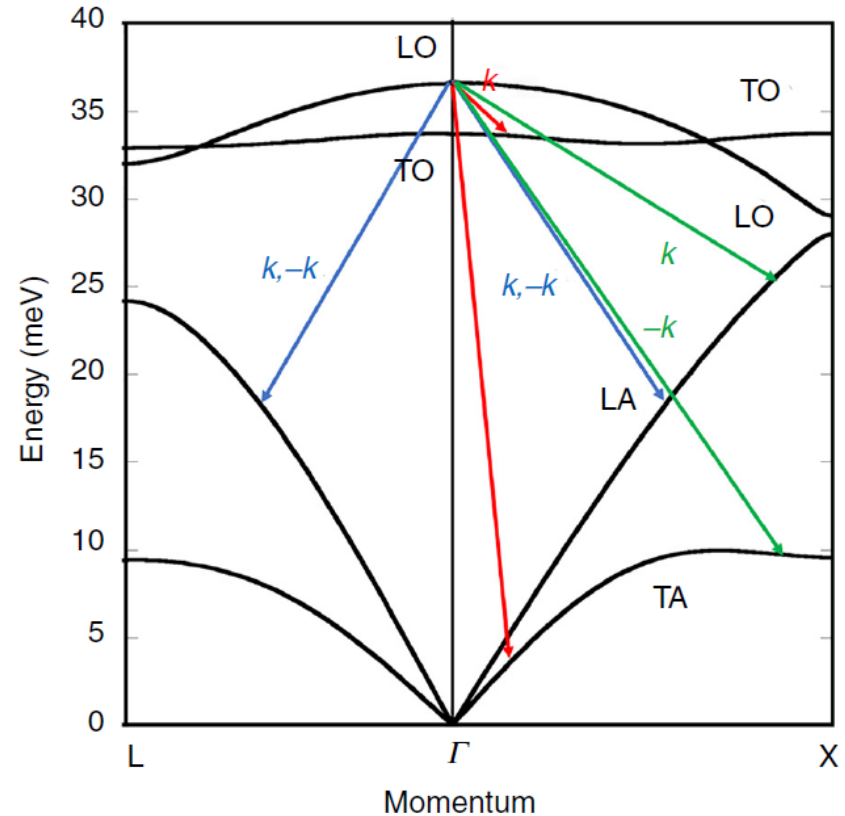
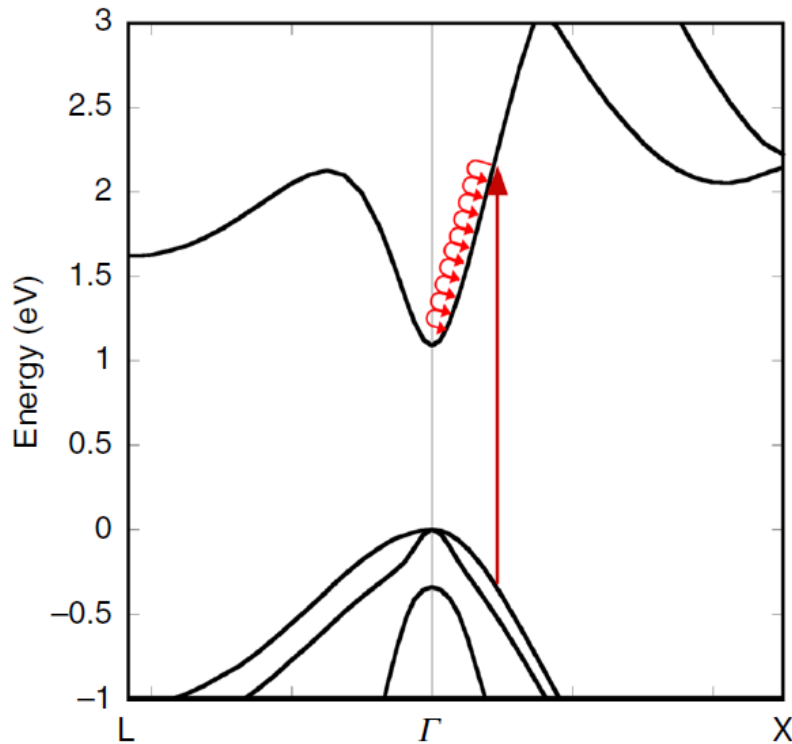


Phonon Bottleneck: Klemens versus Ridley

Non-equilibrium longitudinal optical phonons and their lifetimes

Cite as: Appl. Phys. Rev. **8**, 021324 (2021); <https://doi.org/10.1063/5.0044374>
Submitted: 15 January 2021 . Accepted: 21 May 2021 . Published Online: 29 June 2021

 David K. Ferry



- Klemens LO \rightarrow 2LA
- Ridley LO \rightarrow TO + LA



Hot-Carrier Effects in Semiconductor Devices



Several papers suggesting hot carriers are most robust in quantum confined systems:

- J. F. Ryan *et al.* PRL **53**, 1841 (1984)
- J. Shah *et al.* PRL **54**, 2045 (1985)
- N. Balkan *et al.* Semi. Sci. Techn. **4**, 852 (1989)
- K. Leo *et al.* PRB **38**, 1947 (1988)

Potential for Solar Cells:

Energy & Environmental Science

Dynamic Article Links

Cite this: DOI: 10.1039/c2ee02843c

www.rsc.org/ees

PAPER

Thermalisation rate study of GaSb-based heterostructures by continuous wave photoluminescence and their potential as hot carrier solar cell absorbers†

A. Le Bris,^{*,abc} L. Lomez,^{*,abc} S. Laribi,^{*,abc} G. Boissier,^d P. Christol^d and J.-F. Guillemoles^{*,abc}

Received 6th October 2011, Accepted 15th December 2011

DOI: 10.1039/c2ee02843c

IEEE JOURNAL OF PHOTOVOLTAICS

Enhanced Hot-Carrier Effects in InAlAs/InGaAs Quantum Wells

Louise C. Hirst, Michael K. Yakes, Christopher G. Bailey, Joseph G. Tischler, Matthew P. Lumb, María González, Markus F. Führer, N. J. Ekins-Daukes, and Robert J. Walters

Progress in PHOTOVOLTAICS

PROGRESS IN PHOTOVOLTAICS: RESEARCH AND APPLICATIONS

Prog. Photovolt: Res. Appl. 2016, 24:691–699

Published online 26 February 2016 in Wiley Online Library (wileyonlinelibrary.com). DOI: 10.1002/pij.2763

ACCELERATED PUBLICATION

Suppression of phonon-mediated hot carrier relaxation in type-II InAs/AlAs_xSb_{1-x} quantum wells: a practical route to hot carrier solar cells

Hamidreza Esmailpour¹, Vincent R. Whiteside¹, Jinfeng Tang¹, Sangeetha Vijayaragunathan¹, Tetsuya D. Mishima¹, Shayne Cairns¹, Michael B. Santos¹, Bin Wang² and Ian R. Sellers^{1*}

¹ Homer L. Dodge, Department of Physics & Astronomy, University of Oklahoma, 440 W. Brooks Street, Norman, OK 73019, USA

² School of Chemical, Biological and Materials Engineering, Sarkeys Energy Center, University of Oklahoma, East Boyd Street-T301, Norman, OK 73019, USA

Progress in PHOTOVOLTAICS

PROGRESS IN PHOTOVOLTAICS: RESEARCH AND APPLICATIONS

Prog. Photovolt: Res. Appl. (2013)

Published online in Wiley Online Library (wileyonlinelibrary.com). DOI: 10.1002/pij.2444

ACCELERATED PUBLICATION

Demonstration of a hot-carrier photovoltaic cell

James A. R. Dimmock^{*}, Stephen Day, Matthias Kauer^{*}, Katherine Smith and Jon Heffernan

Sharp Laboratories of Europe Ltd, Edmund Halley Road, Oxford Science Park, Oxford OX4 4GB, UK

Le Bris *et al.* APL **97**, 113506 (2010)

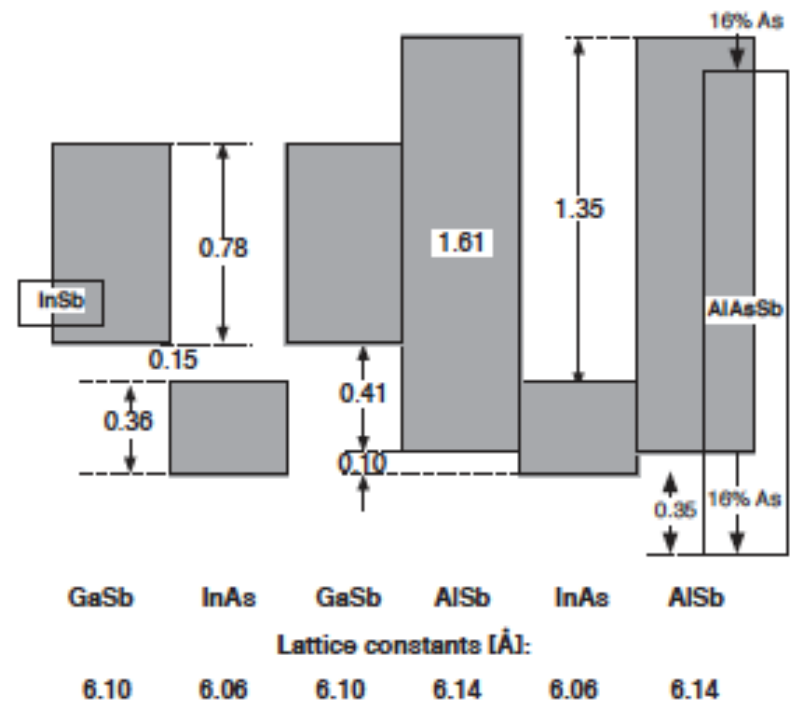
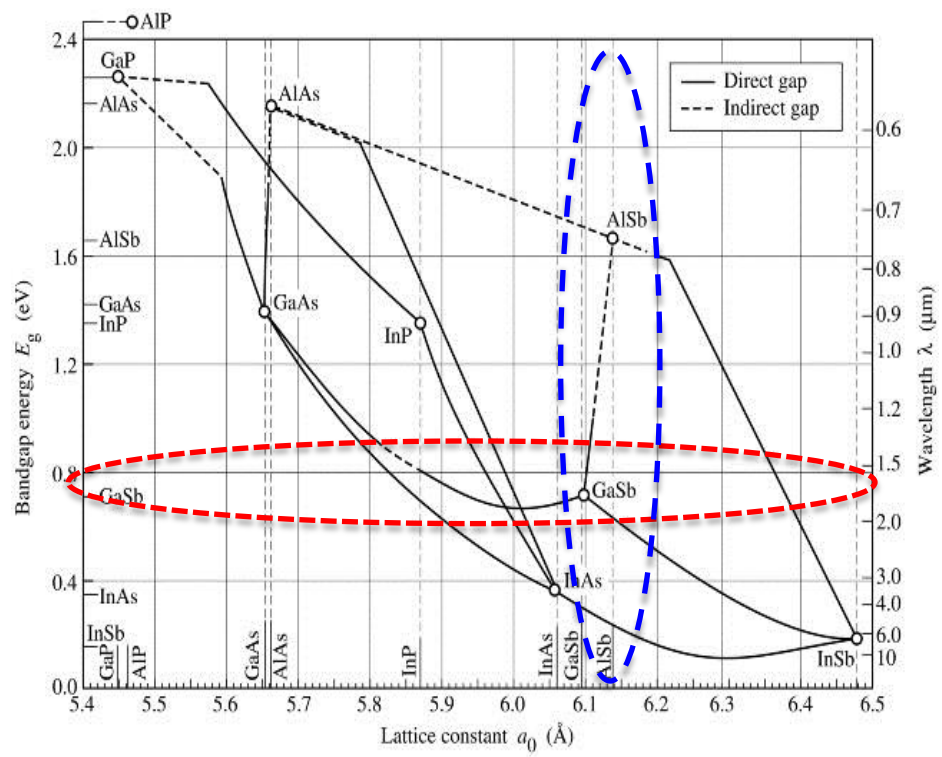
Hirst *et al.* IEEE JPV **4**, 244 (2014)

Hirst *et al.* APL **104**, 231115 (2014)

Tang, IRS, *et al.* APL **106**, 061902 (2015)



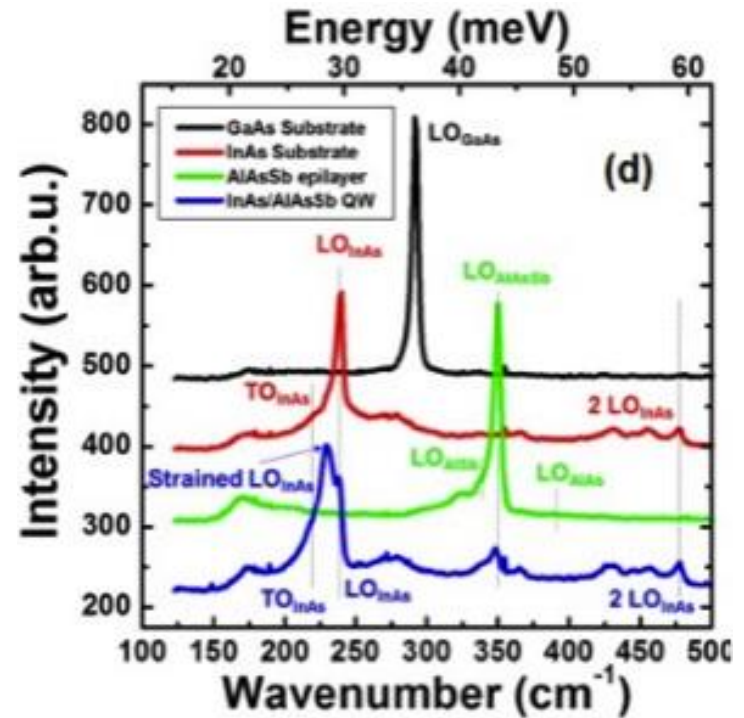
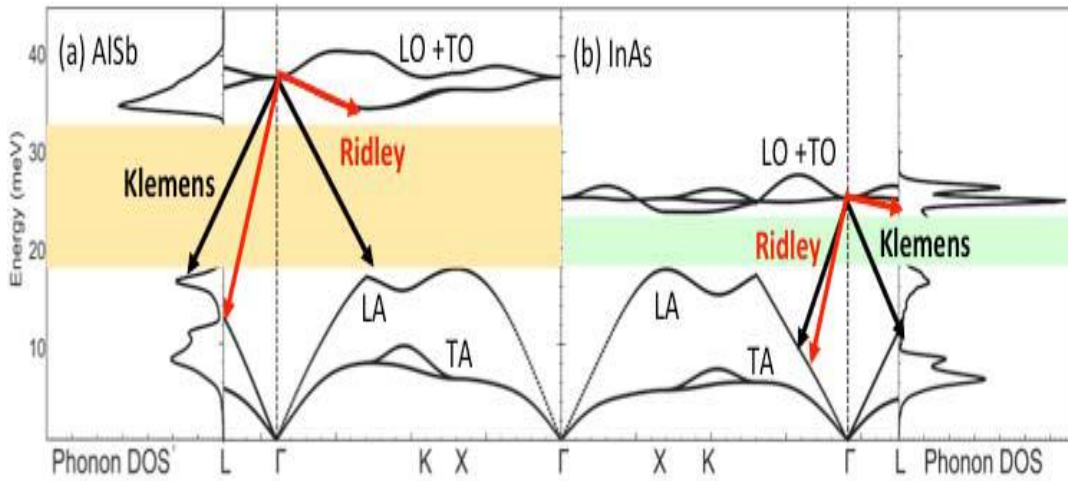
InAs/Al_xAs_{1-x}Sb quantum wells: an interesting potential system for hot carriers solar cells



Kroemer *et al. Physica E* **20**, 196 (2004)

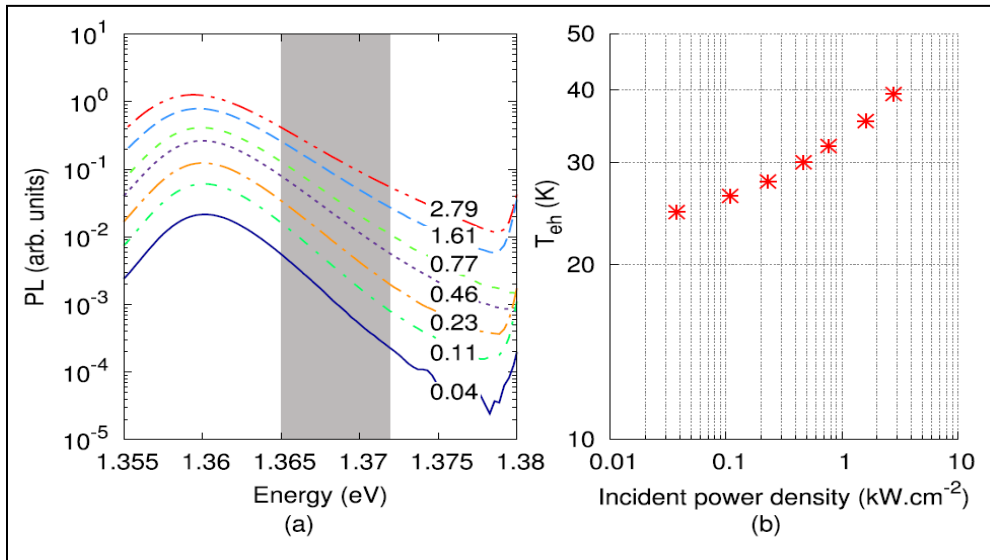
- Potential to produce type-I, II or quasi-type-II structures
- Extremely deep confinement potential: large proportion of solar irradiance absorbed directly in QWs

DFT Calculations: Bin Wang - OU

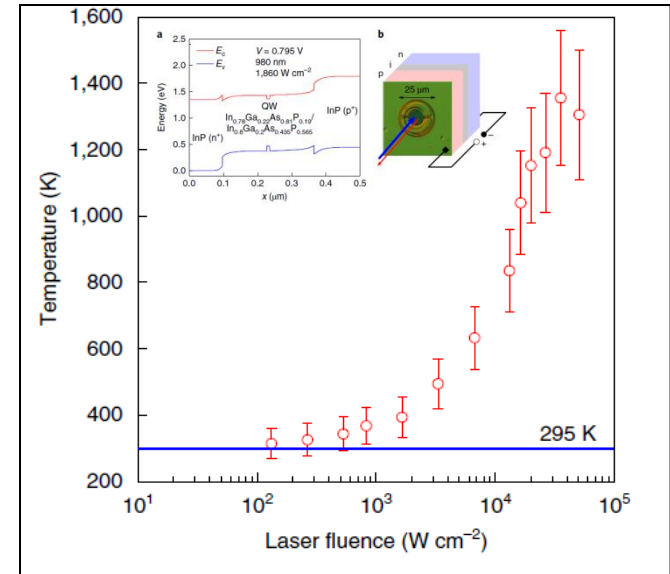


H. Esmailpour *et al.* Scientific Reports 8, 12473 (2018)

- Dominate relaxation processes: Klemens LO \rightarrow 2LA
Ridley LO \rightarrow TO + LA
- Large energy difference – Reflections, poor thermal dissipation
- Stable hot phonon bath



Hirst & Ekins-Daukes. *Appl. Phys. Lett.* **104**, 231115 (2014)



Nguyen, Lombez, Guillemoles *et al.* *Nature Energy* **3**, 231115 (2018)

Maxwell-Boltzmann like distribution of carriers:

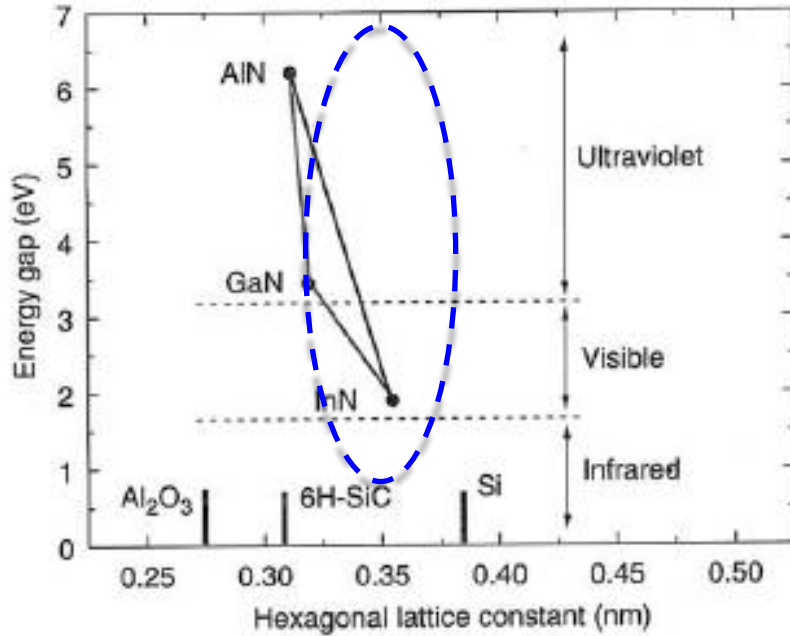
$$I(PL) \propto \exp\left(-\frac{h\nu}{k_B T_H}\right)$$

- Lasher & Stern, *Phys. Rev.* **133**, A553 (1964)
- De Vos & Pauwels, *Appl. Phys.* **25**, 119 (1981)
- P Wurfel, *J. Phys. C: Solid State Phys.* **15** 3967 (1982)

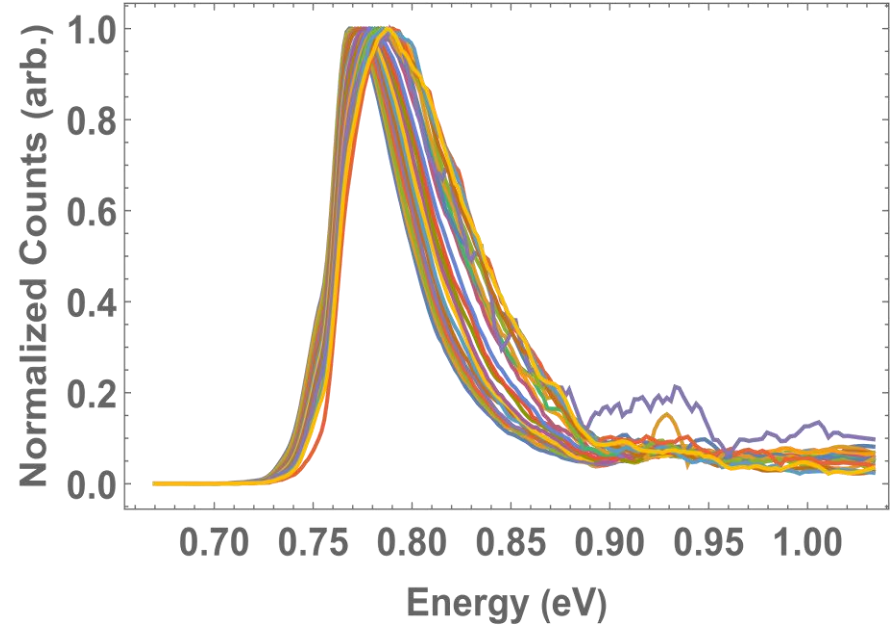
Proof of principle systems

- Very high-power excitation
- Monochromatic illumination
- Non-optimum architecture

Narrow-Gap Semiconductors



Y. S. Park, Optoelectronics Rev. **9**, 117 (2001)



Credit: Shashi Sourabh (OU)

InN has a favorable energy gap for Hot Carrier Solar Cells

Appl. Phys. Lett., Vol. 75, No. 21, 22 November 1999

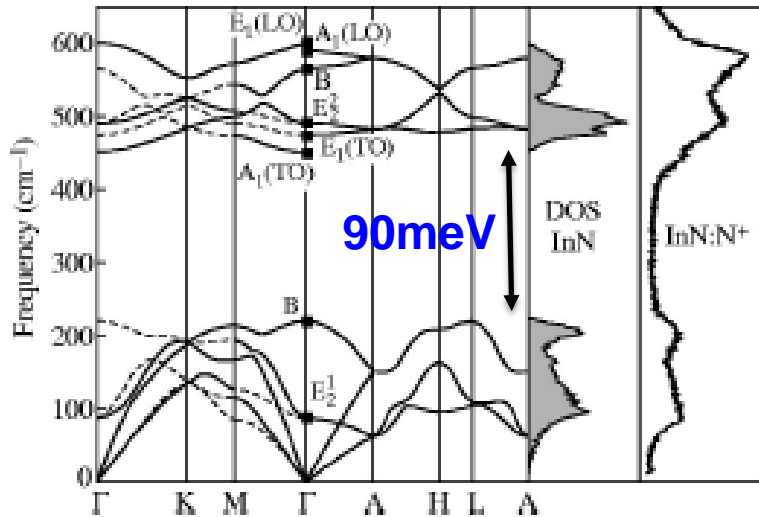
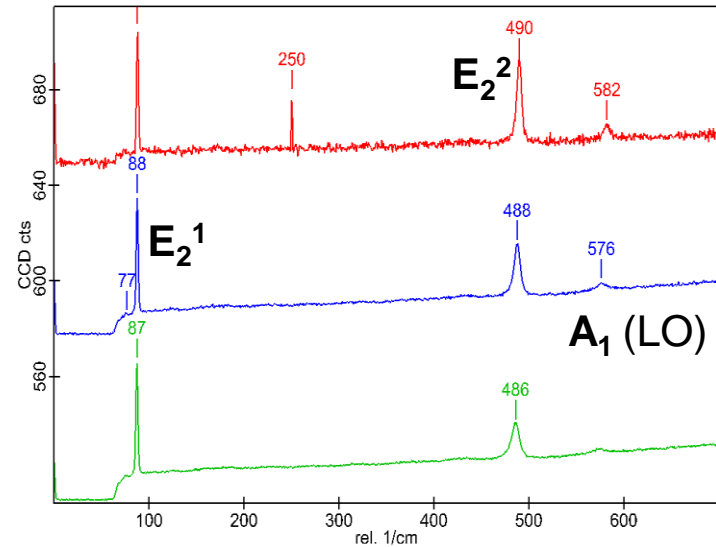


FIG. 4. Calculated phonon dispersion curves and phonon DOS function for hexagonal InN. The disorder-induced Raman spectrum obtained at 7 K for N⁺-implanted InN is also shown.

Davydov *et al* (1999)

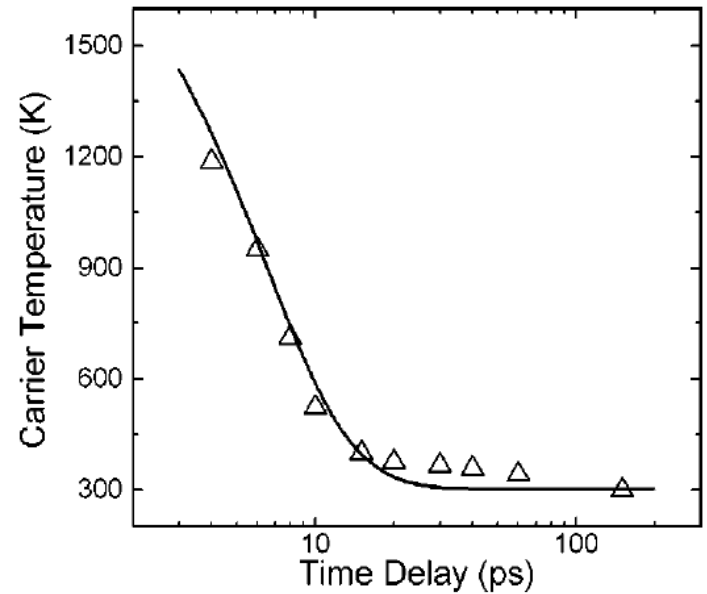
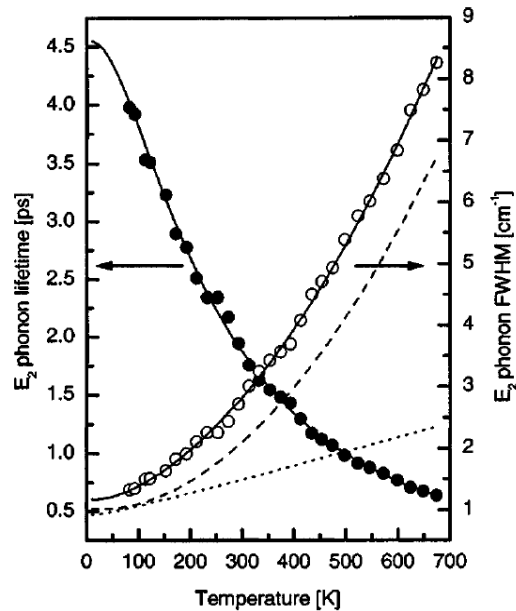
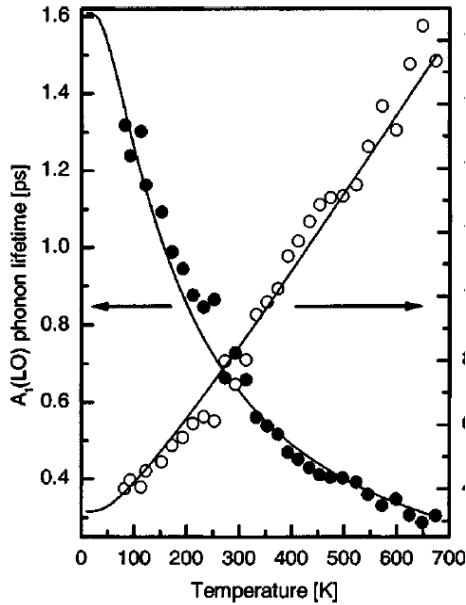


Acknowledgement: Nazli Sarabi (OU)

Extremely attractive “phononic” properties optimum Energy gap!



InN: Evidence of Carriers



Phonon lifetimes and phonon decay in InN

Cite as: Appl. Phys. Lett. 86, 223501 (2005); <https://doi.org/10.1063/1.1940124>
 Submitted: 18 January 2005 . Accepted: 21 April 2005 . Published Online: 24 May 2005

J. W. Pomeroy, M. Kuball, H. Lu, W. J. Schaff, X. Wang, and A. Yoshikawa

APPLIED PHYSICS LETTERS

VOLUME 83, NUMBER 24

15 DECEMBER 2003

Time-resolved spectroscopy of recombination and relaxation dynamics in InN

Fei Chen and A. N. Cartwright^{a)}
 Department of Electrical Engineering, University at Buffalo, State University of New York, Buffalo, New York 14260

Hai Lu and William J. Schaff
 Department of Electrical and Computer Engineering, Cornell University, Ithaca, New York 14853

(Received 18 June 2003; accepted 22 October 2003)

Early prediction *and* data suggested strong potential

Not the whole story.....

Acknowledgement: Gavin Conibeer (UNSW)



Phonon Bottleneck: Klemens versus Ridley

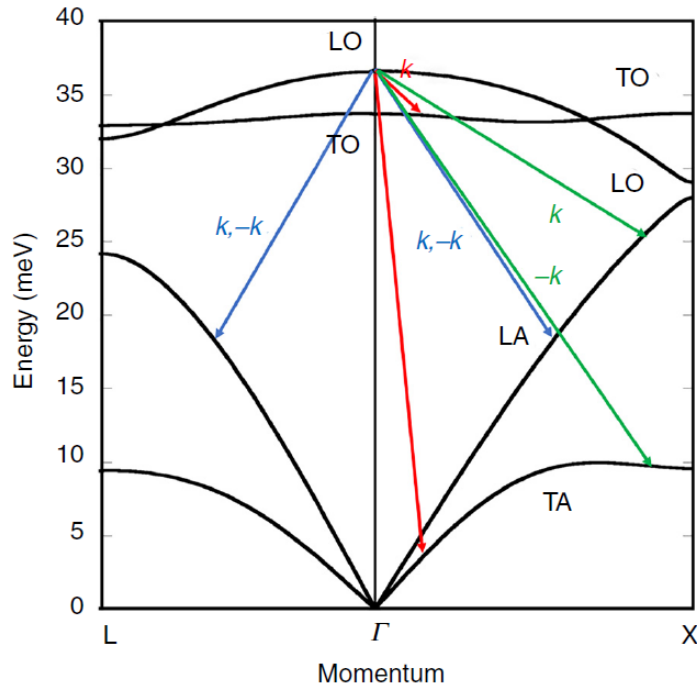


FIG. 13. The decay mechanisms suggested by Klemens⁷³ are shown in blue, Ridley-Gupta in red, and Vallée-Bogani in green. The indicated momenta are discussed in the text.

D. K. Ferry, Appl. Phys. Rev. 8, 021324 (2021)

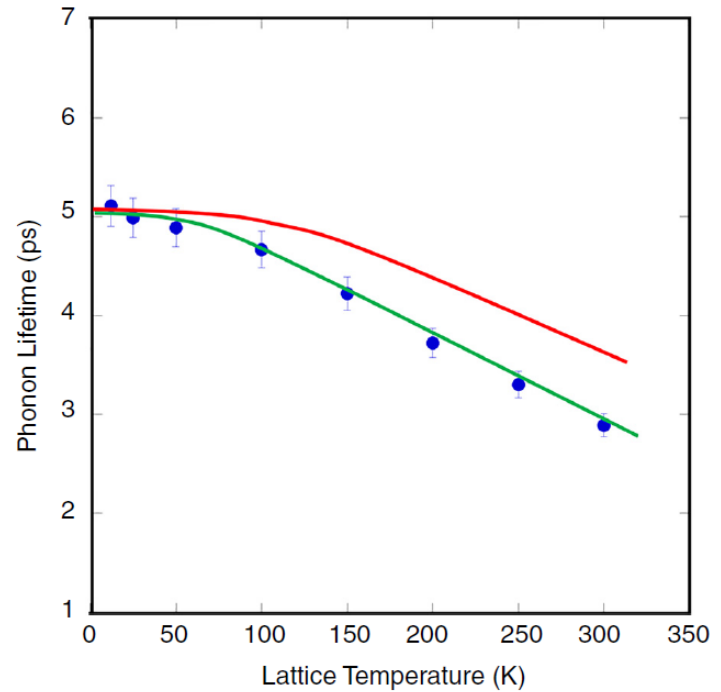


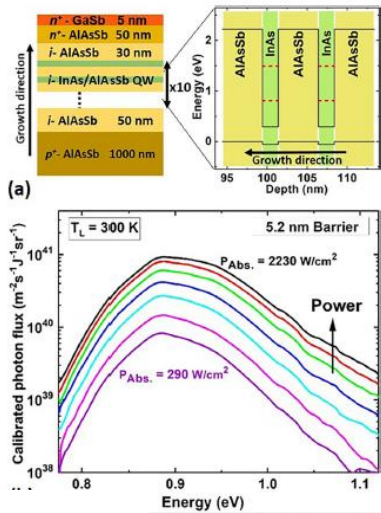
FIG. 14. The phonon lifetime, as deduced from Raman scattering, as given as a function of temperature for wurtzite GaN. The blue curve is the Klemens⁹⁹ channel while the green curve is the Ridley-Gupta¹⁰² channel. The data are adapted from K. T. Tsen *et al.*¹⁰⁵

Ridley channel is very effective in nitrides (in all III-V's)

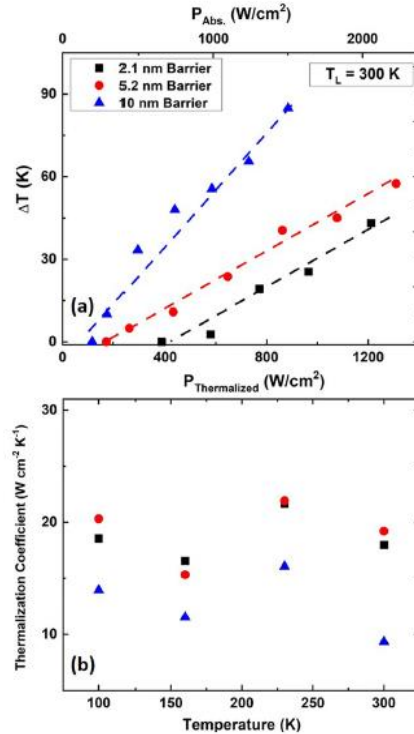
Strain and piezoelectric fields also facilitate hot carrier relaxation

M. D. Yang *et al.*, J. Appl. Phys. 105, 013526 (2009)

Phonon management in QWs

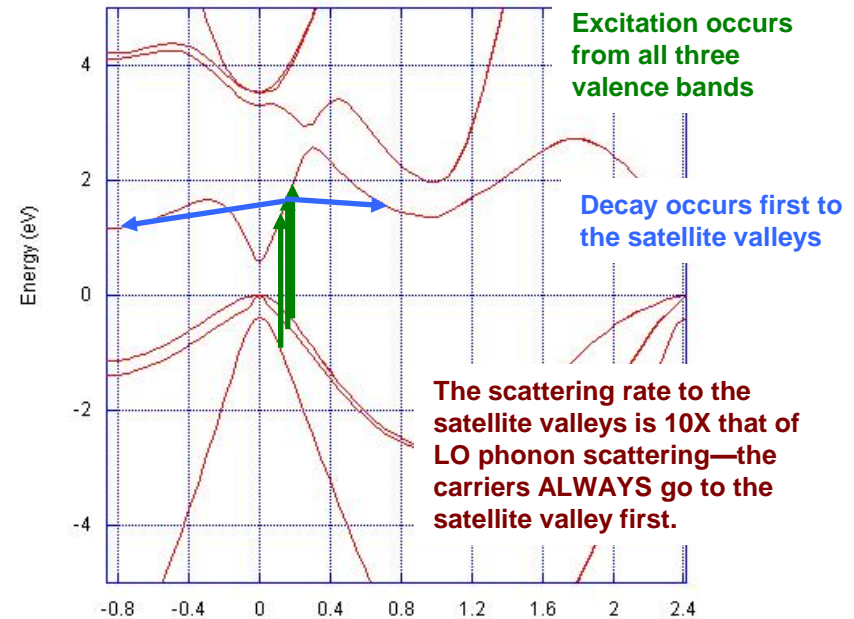


H. Esmailpour *et al.*
Appl. Phys. Lett. 118, 213902 (2021)



Valley Photovoltaics

Consider a typical direct gap III-V



D. K. Ferry *Semi. Sci. Techn.* 34, 044001 (2019)
H. Esmailpour *et al.* *Nature Energy* 5, 336 (2020)
D. K. Ferry *et al.*, *J. Appl. Phys.* 128, 220903 (2020)

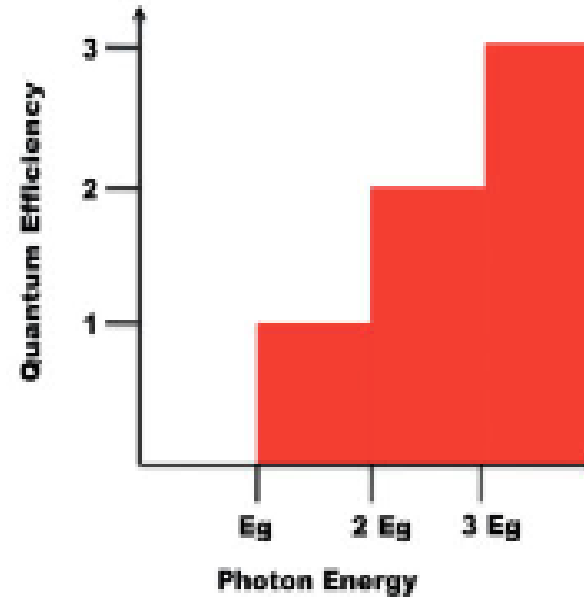
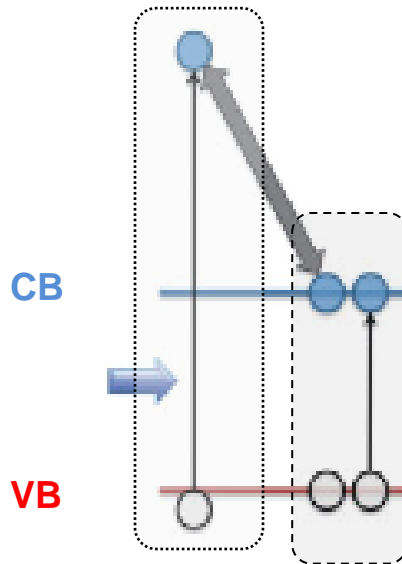
It is well established that thermalization can be inhibited in quantum wells

Intervalley scattering is now being considered as a method for HCSCs

Multi-Exciton Generation or Carrier Multiplication

Initial photon absorbed
one electron – hole pair

Energy relaxation with
second photon absorbed:
two electron – hole pairs

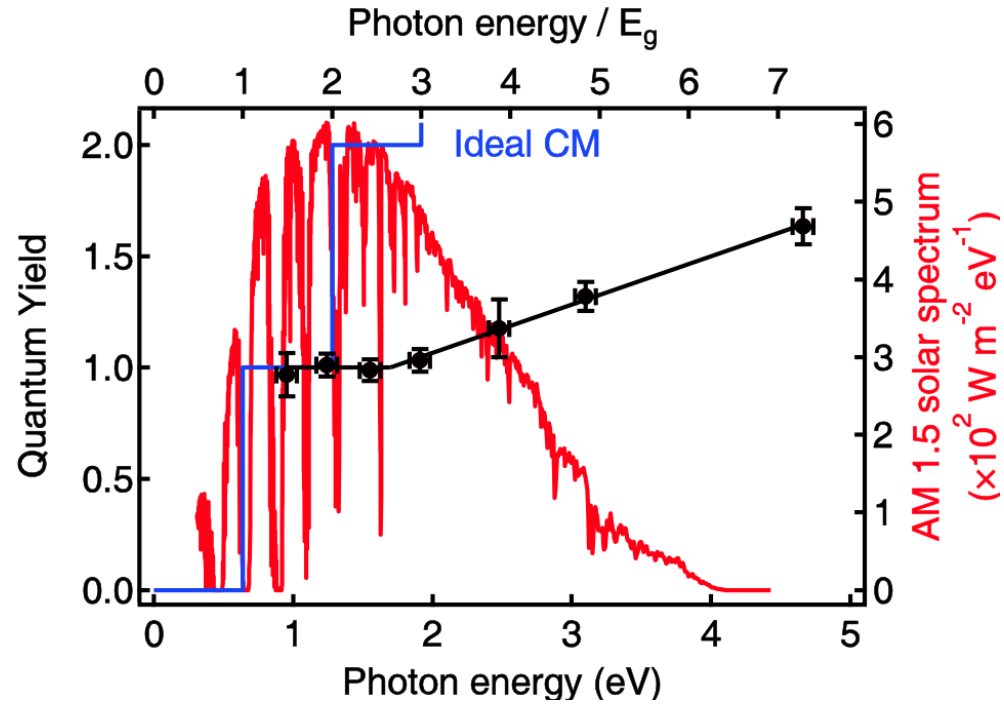
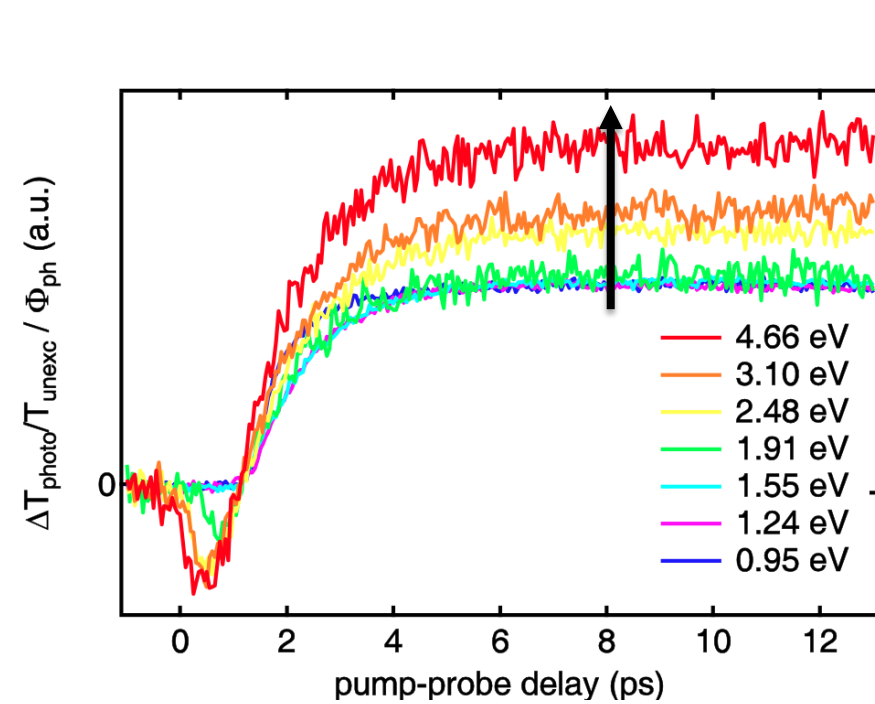


Brown & Wu. Laser & Photon Rev. 3, 394 (2009)

Impact Ionization seen in InSb, Si, PbS, and PbSe, and now InN!



InN: multi-exciton generation



$$S(\omega) = N \cdot e \cdot m(\omega) = N \cdot \frac{e^2 t_s}{m^*} \cdot \frac{1}{1 - i\omega t_s}$$

Jensen, Sellers, Bonn et al, APL **101**, 222113 2012



Summary and Acknowledgements

- While the performance and cost of solar cells has improved considerably TW implementation require further improvements and *all* and *new* technologies
- Stable high efficiency single junction solar cells in excess of 30% likely require III-Vs!
- Hot carrier solar cells have potential to exceed the single gap limit but innovation and cost-effective approaches are required
- The phonons in InN suggest it has the potential to inhibit thermalization – *much more work needed!*



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<http://okpvri.okstate.edu/>

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