Nanoscale Opto Thermo Electric Energy Conversion Devices

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UCSC (Schmidt), **Berkeley** (Majumdar), **Harvard** (Narayanamurti), **MIT** (Ram), **ASU** (Nemanich), **NCSU** (Sitar), **Purdue** (Sands), **UCSB** (Bowers, Gossard, Stemmer)

Acknowledgement: ONR MURI

(Dr. Mihal Gross)

Purdue University; 9 May 2008

Outline

Introduction/ Motivation

- Mutual interaction of heat, light and electricity in nanoscale devices

Micro Refrigerators on a Chip

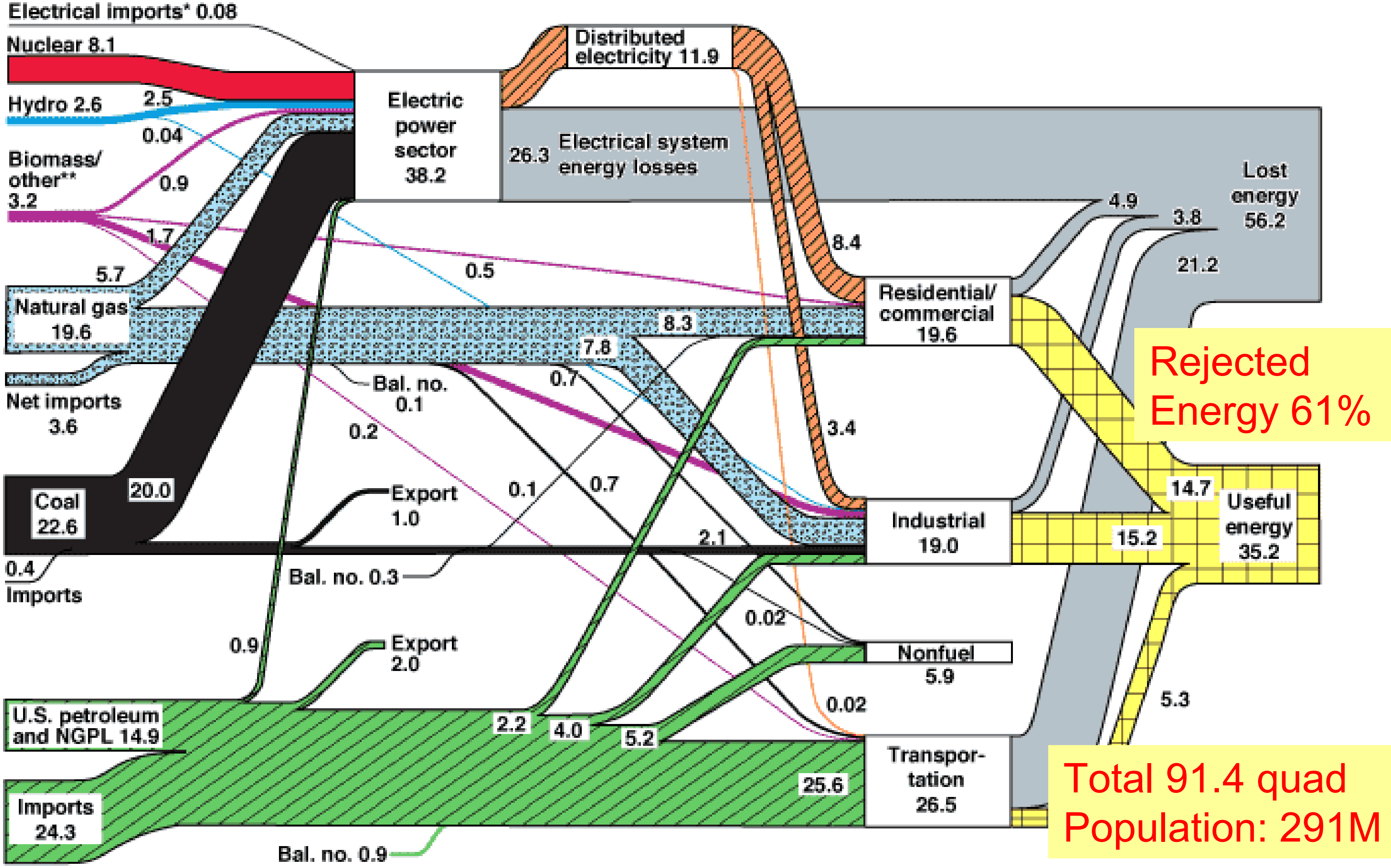
Thermoreflectance Imaging

Thermal Runaway in Electroabsorption Modulators

Thermionic Energy Conversion Center

Internally Cooled Devices

U.S. Energy Flow Trends – 2002
Net Primary Resource Consumption ~97 Quads



Source: Production and end-use data from Energy Information Administration, *Annual Energy Review 2002*.
*Net fossil-fuel electrical imports.
**Biomass/other includes wood, waste, alcohol, geothermal, solar, and wind.

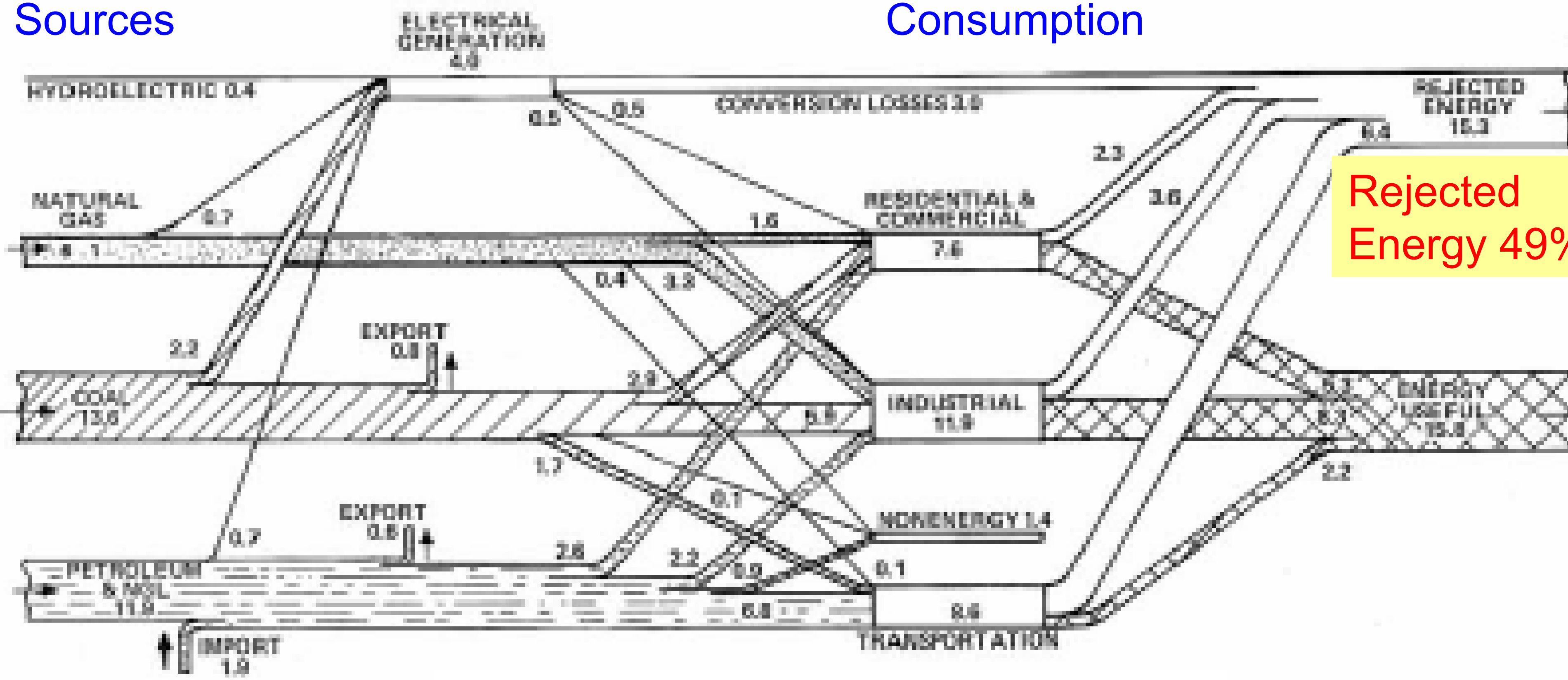
June 2004
Lawrence Livermore
National Laboratory
http://eed.llnl.gov/flow

US Energy Flow 1950

AS 4/28/2008

Energy Sources

Energy Consumption



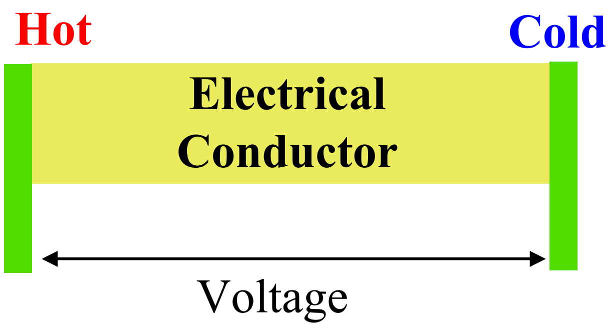
Rejected Energy 49%

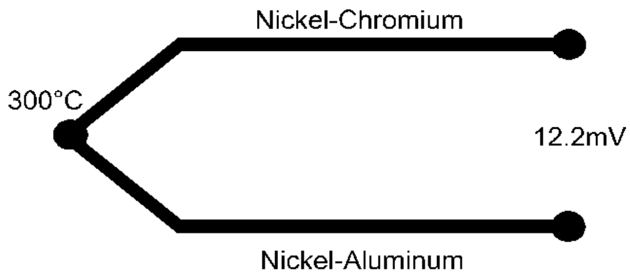
LLNL

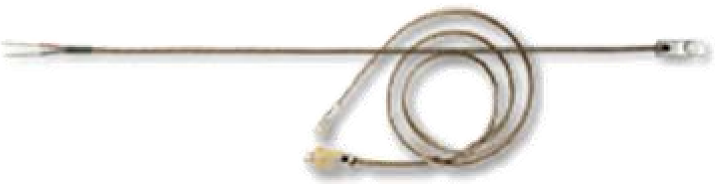
Total 31.8 Quad
Population: 161M

Seebeck Effect (1821)

Seebeck: $S = \frac{\Delta V}{\Delta T}$



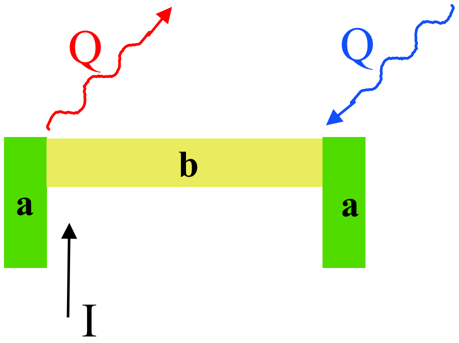


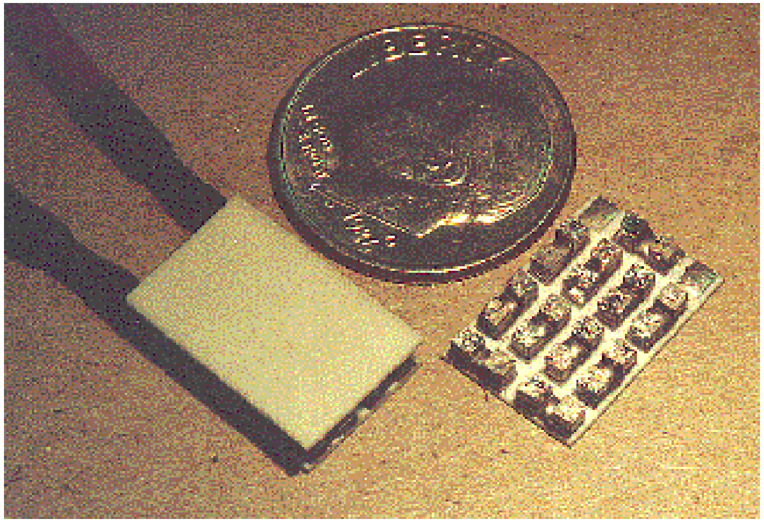


Temperature difference between two junctions can produce a voltage

Peltier Effect (1834)

Peltier: $$\pi_{ab} = \pi_a - \pi_b = \frac{Q}{I}$$





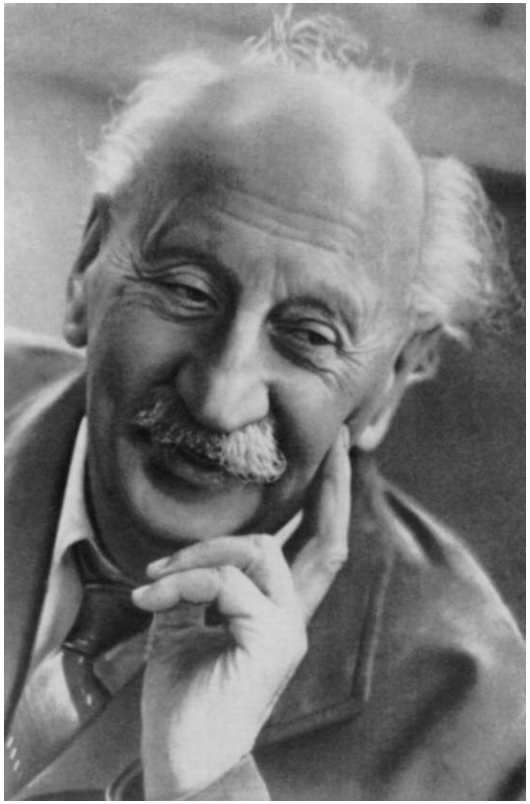
Commercial TE Module

- ΔT=72C (no heat load)
- Cooling density <10W/cm^2
- Efficiency 6-8% of Carnot

When the current flows from material (a) into material (b) and then back to material (a), it heats the first junction and cools the second one (or vice versa). Thus, heat is transferred from one junction to the other one.

Early Thermoelectricity

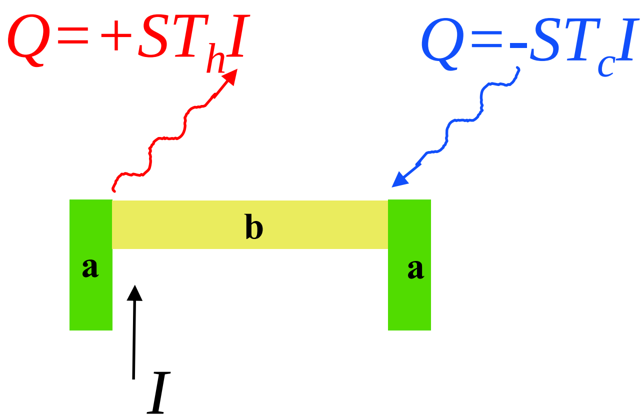
- First practical devices USSR during WWII
  - Tens of thousands built, to power radios from any available heat source.
- In the 1950s-60s many in the US & USSR felt semiconductor thermoelectrics could replace mechanical engines, much as semiconductor electronics were replacing vacuum tube technology.
  - Hint: it didn't happen!



Abram F. Ioffe 1880-1960

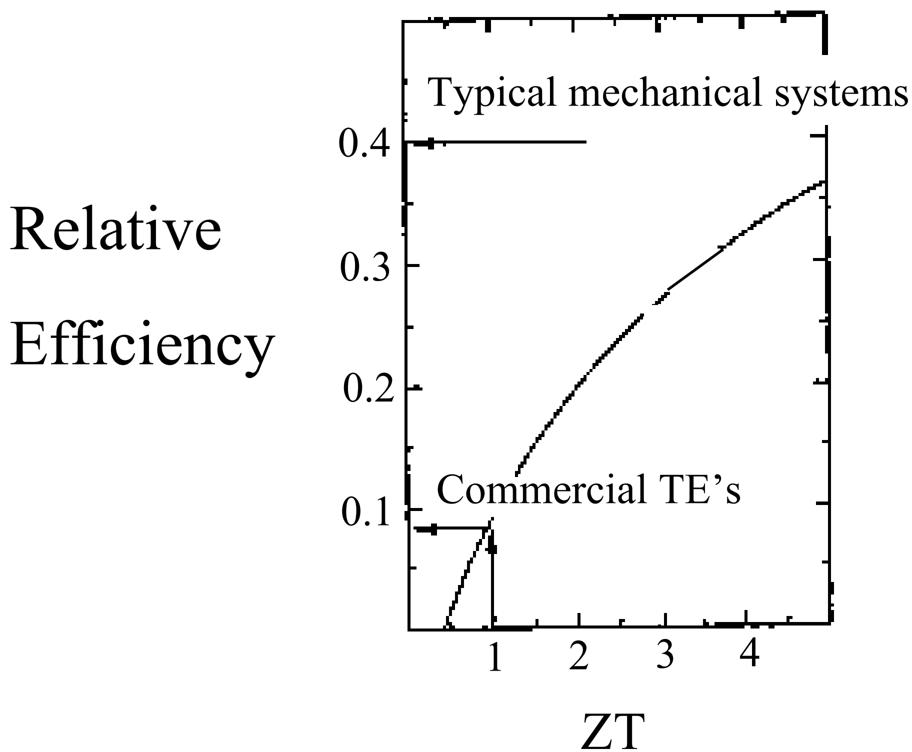
Ioffe, A. F. (1957). Semiconductor Thermoelements and Thermoelectric Cooling. London, Infosearch Limited.

Efficiency of Thermoelectric Devices



$$Z = \frac{S^2\sigma}{\beta}$$

$$Z = \frac{(Seebeck)^2 (electrical \quad conductivity)}{(thermal \quad conductivity)}$$



TEs for Telecom Cooling

- Melcor, Marlow and many other TE manufacturers provide coolers specifically designed for Telecom laser-cooling applications

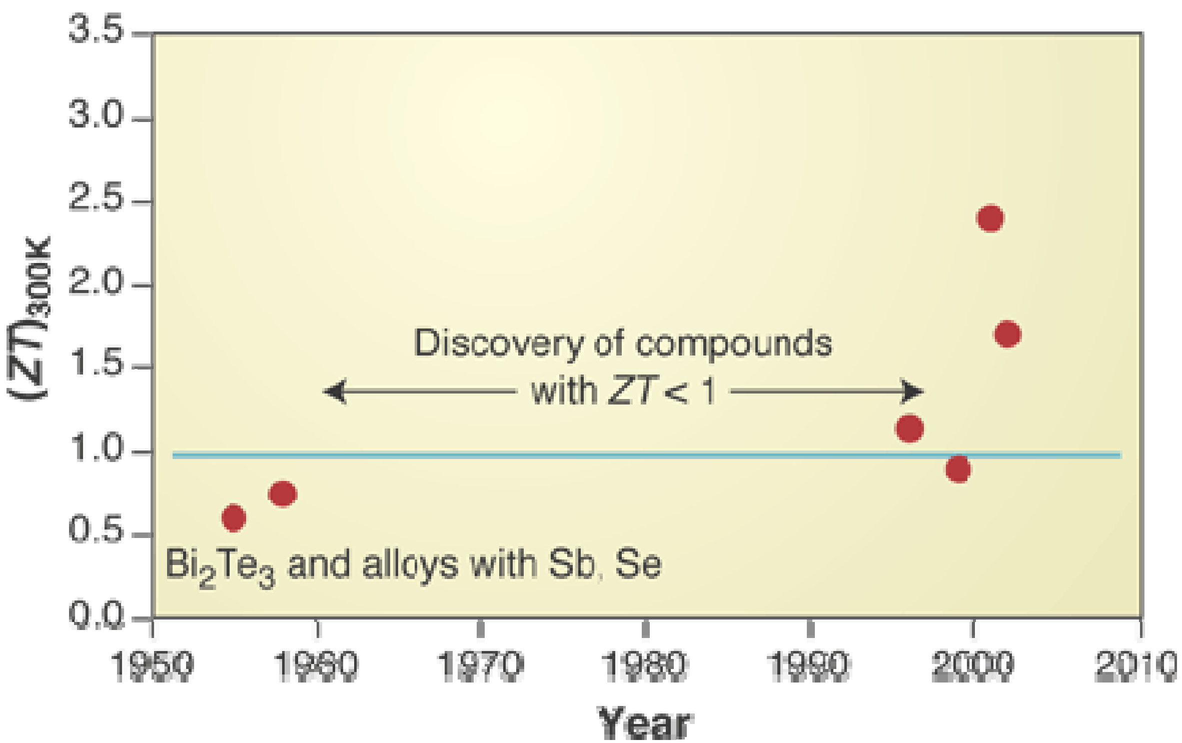
Typical Distributed Feedback Laser:

$\Delta\lambda/\Delta T$= <u>0.1 nm/^{o}C</u>

Heat generation <u>kW/cm^2</u>

Cronin Vining, ZT Services

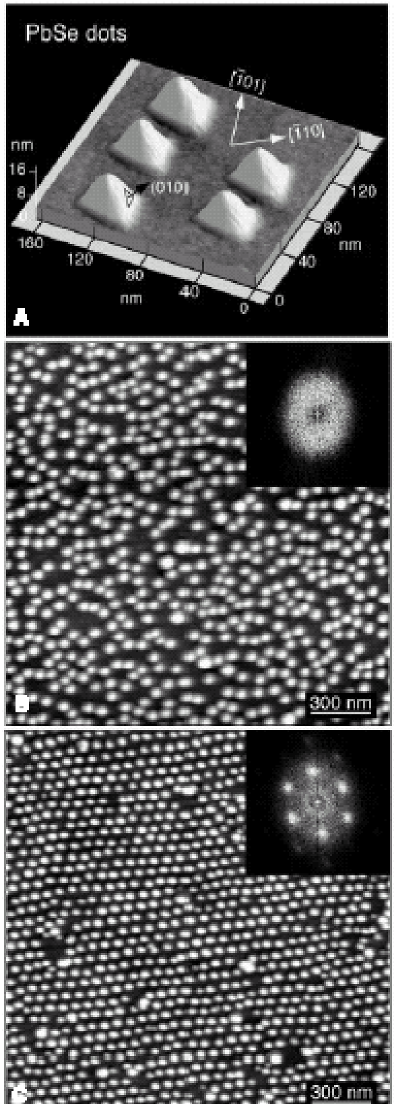
Recent Advances in Thermoelectrics



- Recent advances in nanostructured thermoelectric materials led to a sudden increase in $(ZT)_{300K} > 1$

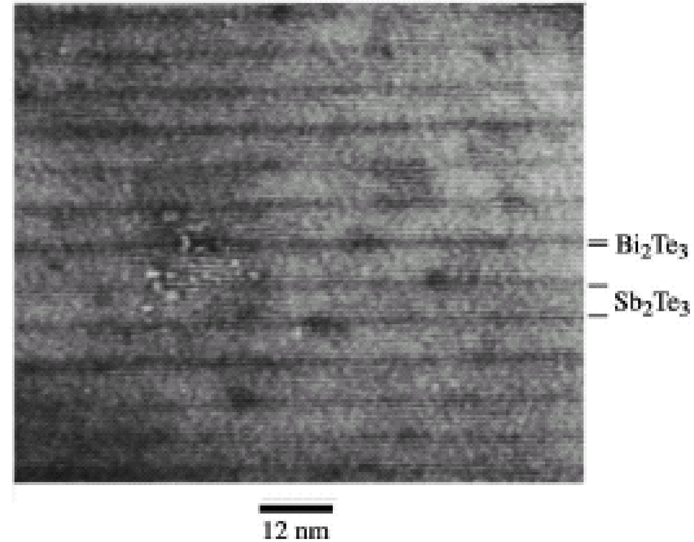
A. Majumdar, *Science* 303, 777 (2004)

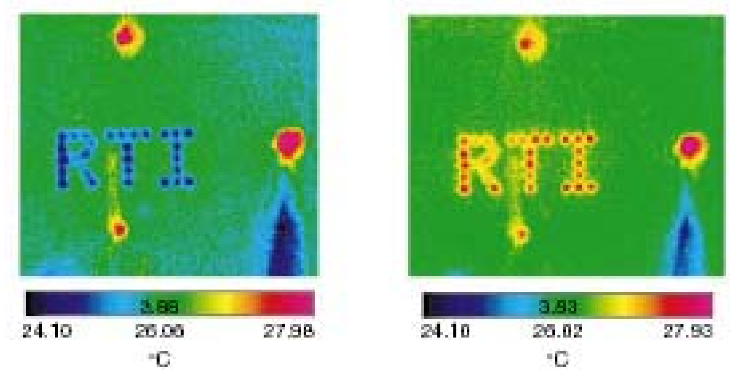
Superlattices/ Quantum Dot Thermoelectrics
Harman (2002) and Venkatasubramanian (2001)



PbTe/PbTeSe Quantum Dot Superlattices

ZT=2
T.C. Harman, Science, 2002



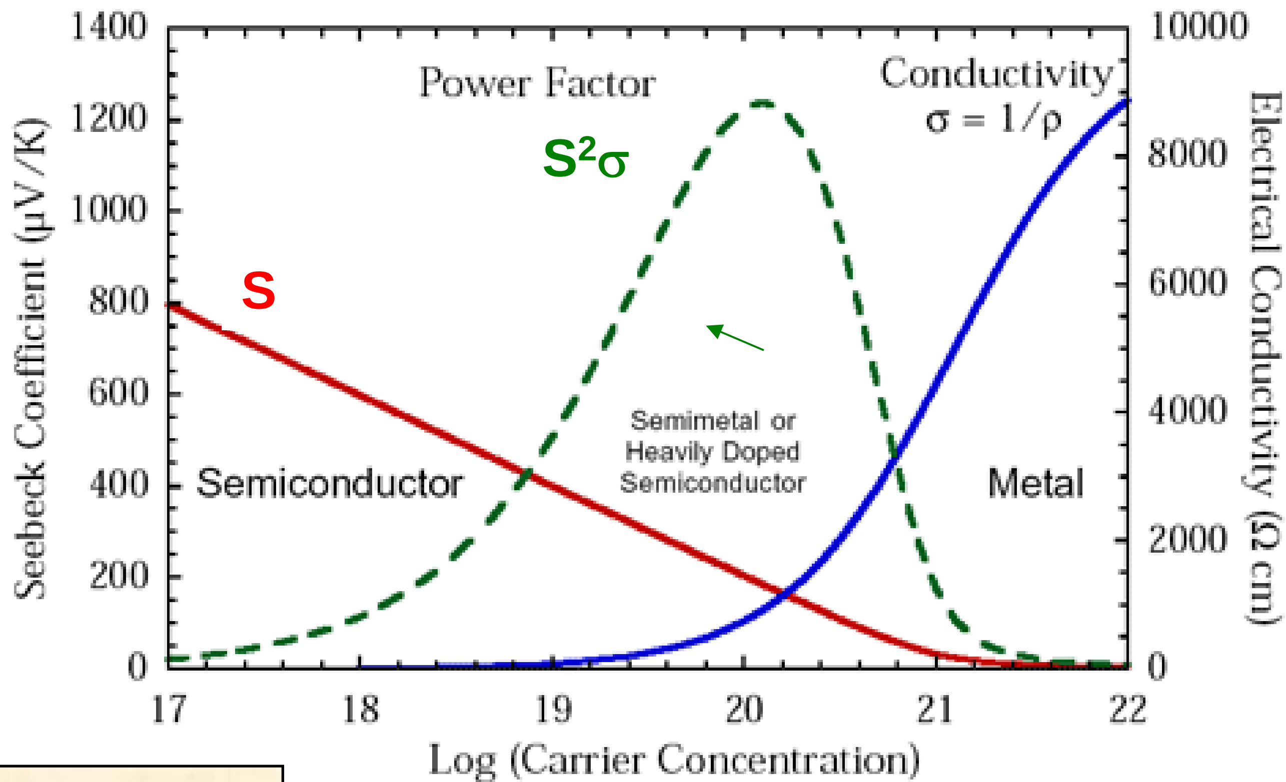


ΔT=32.2 K, ZT ~2-2.4
R. Venkatasubramanian, Nature, 2001

(From M. S. Dresselhaus, Rohsenow Symposium, 2003)

Best thermoelectrics Materials

AS 4/28/2008



$$Z = \frac{S^2 \sigma}{k}$$

$$Z = \frac{(Seebeck)^2 (electrical \quad conductivity)}{(thermal \quad conductivity)}$$

J. Snyder (2003)
http://www.its.caltech.edu/~jsnyder/thermoelectrics/science_page.htm

For almost all materials, if doping is increased, electrical conductivity increases but Seebeck coefficient is reduced. Similarly $\sigma \leftrightarrow \kappa$

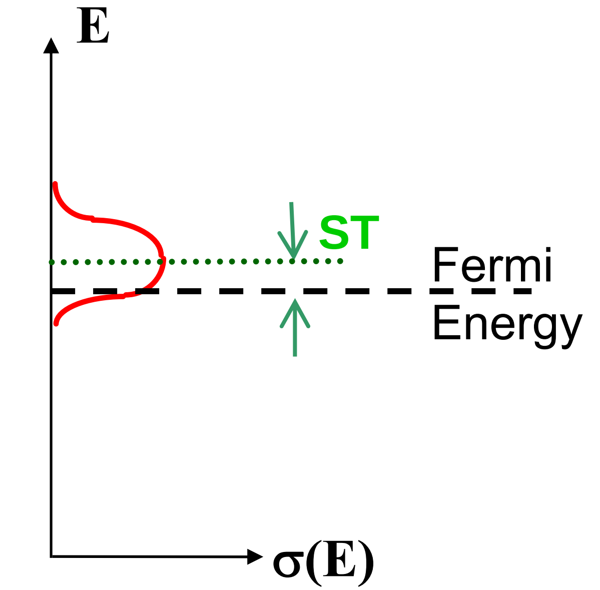
Differential Conductivity

Figure-of-Merit

$$Z = \frac{S^2 \sigma}{k_e + k_L}$$

$$Z = \frac{(Seebeck)^2 (electrical \quad conductivity)}{(thermal \quad conductivity)}$$

$$\begin{cases} \sigma = \int \sigma(E) dE \\ S = \dfrac{1}{eT} \dfrac{\int \sigma(E)(E - E_F) dE}{\int \sigma(E) dE} \propto \langle (E - E_f) \rangle \\ k_e = function\, of \; \langle (E - E_f)^2 \rangle \end{cases}$$

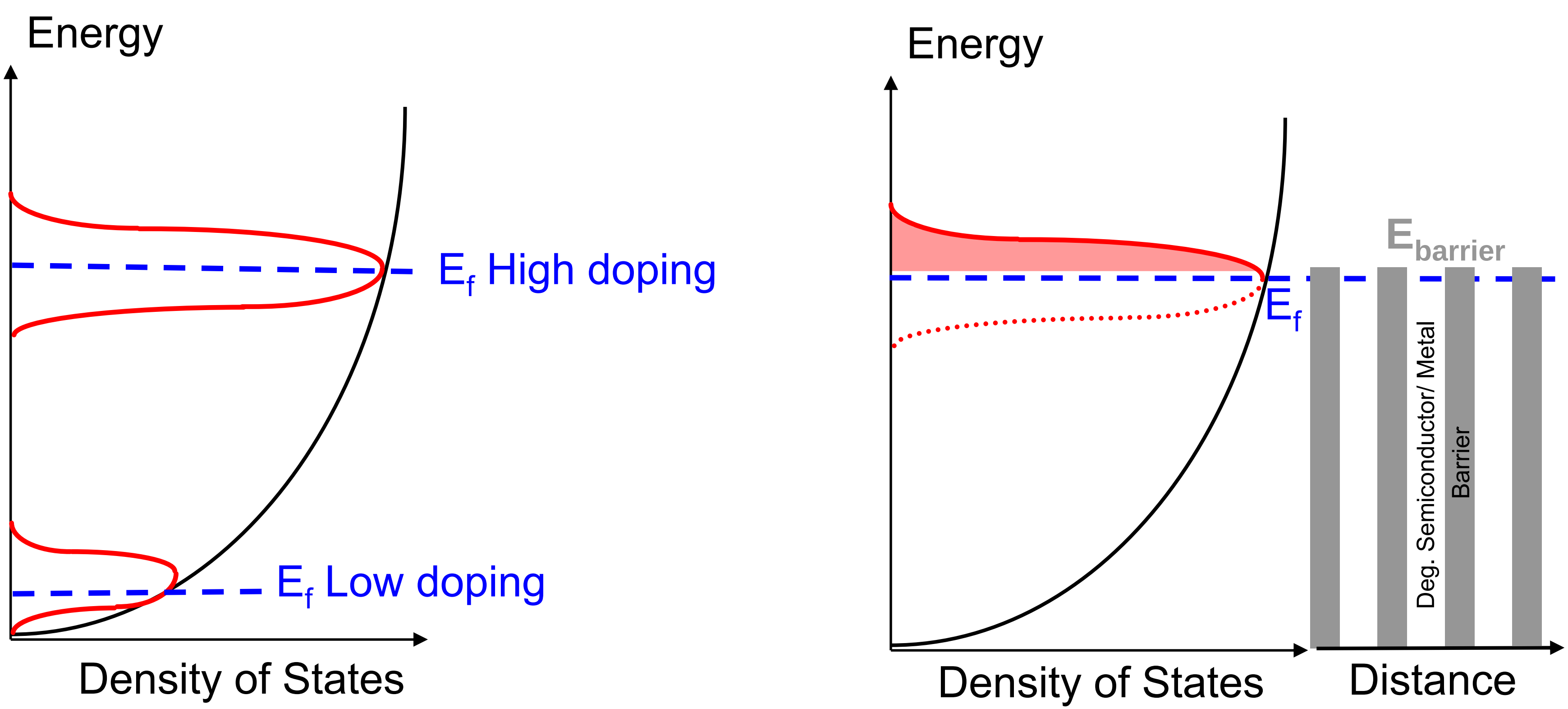


$$\sigma(E) \simeq e^2 \, \tau(E) \, \bar{v}_x^{\,2}(E) \, \bar{n}(E) \left(-\frac{\partial f_{eq}}{\partial E}\right)$$

Differential Conductivity is a function of relaxation time, group velocity and density-of-states

A. Shakouri, "Thermoelectric, thermionic and thermophotovoltaic energy conversion", ICT 2005

Seebeck –Conductivity Trade off



Doped Bulk Semiconductor

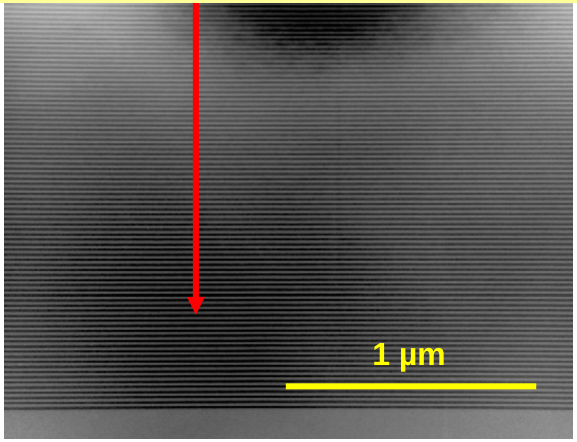
Deg. Semiconductor/Metal + Energy Filter (barriers)

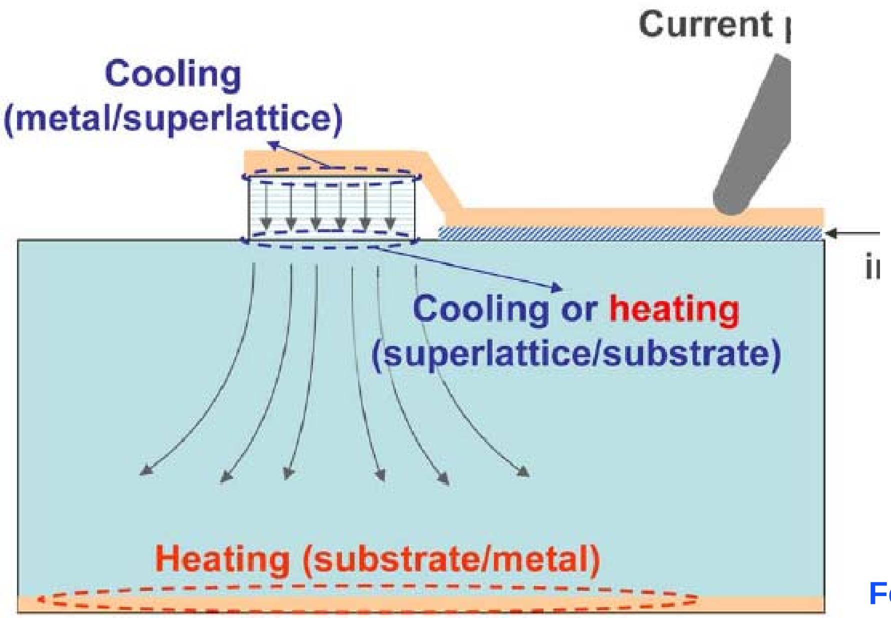
Symmetry of DOS near Fermi energy is the main factor determining Seebeck coefficient.

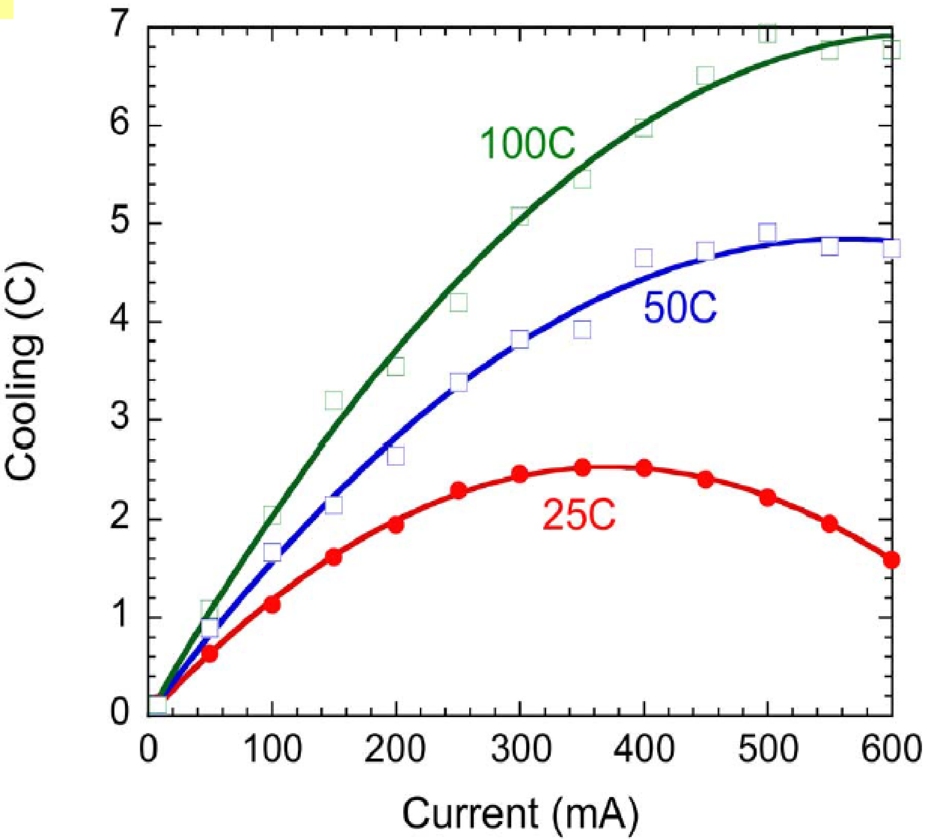
A. Shakouri, "Thermoelectric, thermionic and thermophotovoltaic energy conversion", ICT 2005

Microrefrigerators on a chip

- Monolithic integration on silicon
- ΔT_{max}~4C at room temp. (7C at 100C)







Nanoscale heat transport and microrefrigerators on a chip; A. Shakouri, **Proceedings of IEEE**, July 2006

Featured in Nature Science Update, Physics Today, AIP April 2001

Micro Refrigerator Integrated with Thin Film Heater

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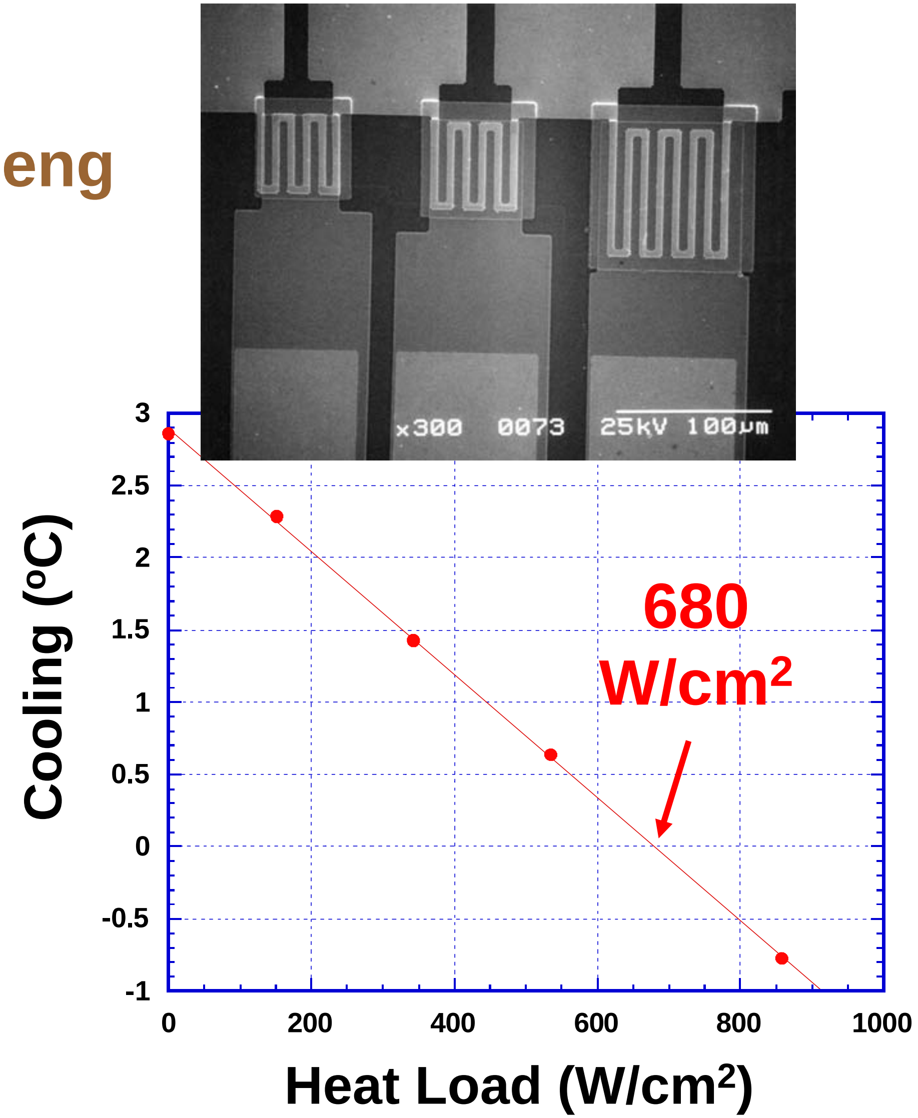
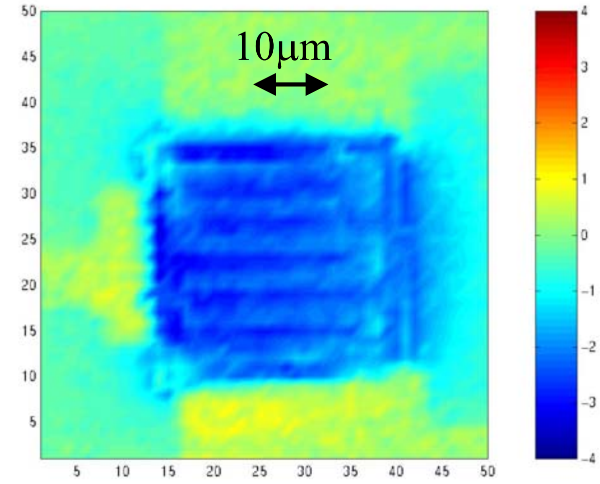
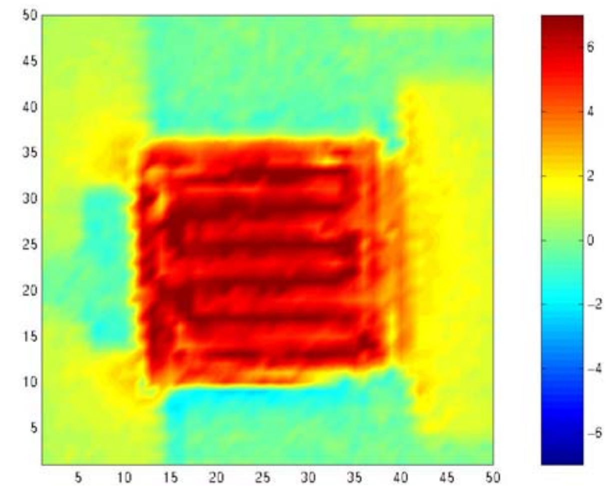
G. Zeng

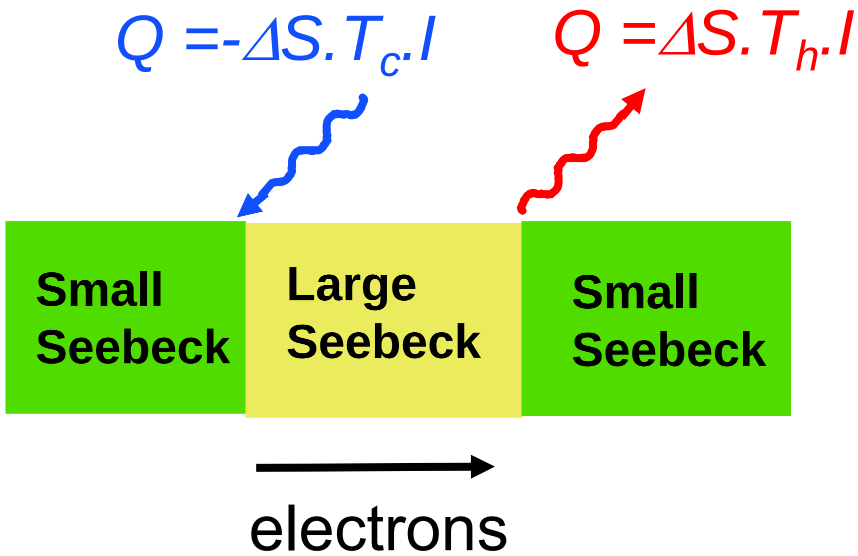


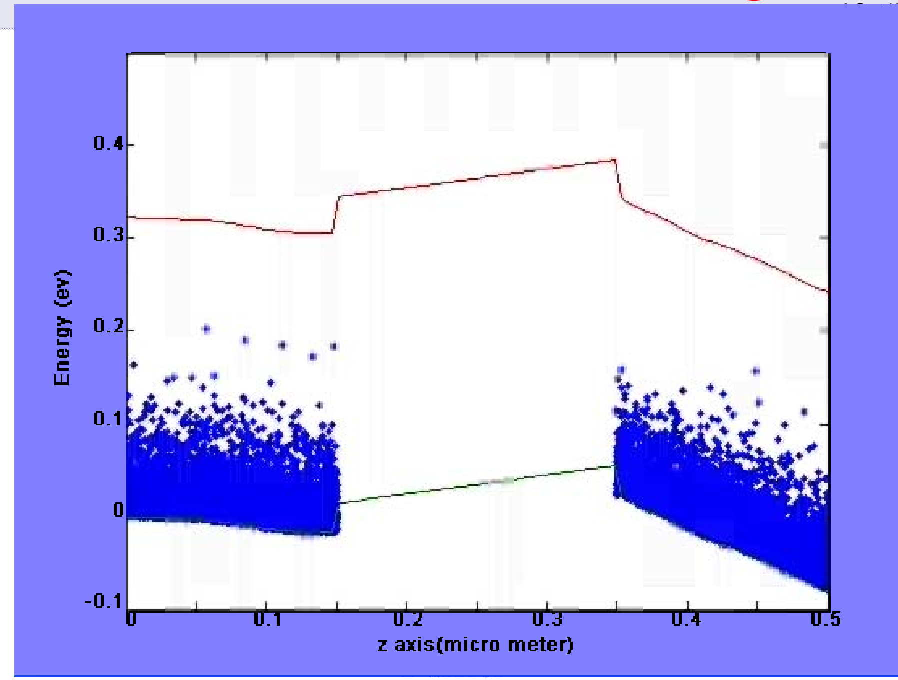


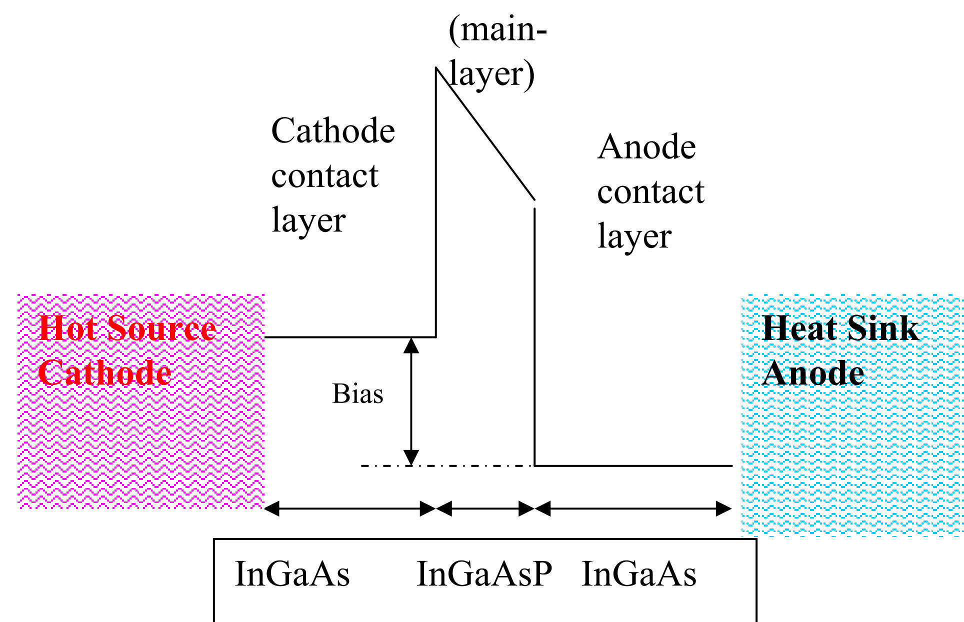


G. Zeng, X. Fan, C. LaBounty, J.E. Bowers, E.Croke, J. Christofferson, D. Vashaee, A. Shakouri, “**Direct Measurement of Cooling Power Density for Thin Film Suplerlattice Micro Coolers**,” MRS Fall 2003.

Monte Carlo simulation of TE/TI cooling







Mona Zebarjadi, Keivan Esfarjani, Ali Shakouri (PRB 2006)

Monte Carlo simulation of TE/TI cooling

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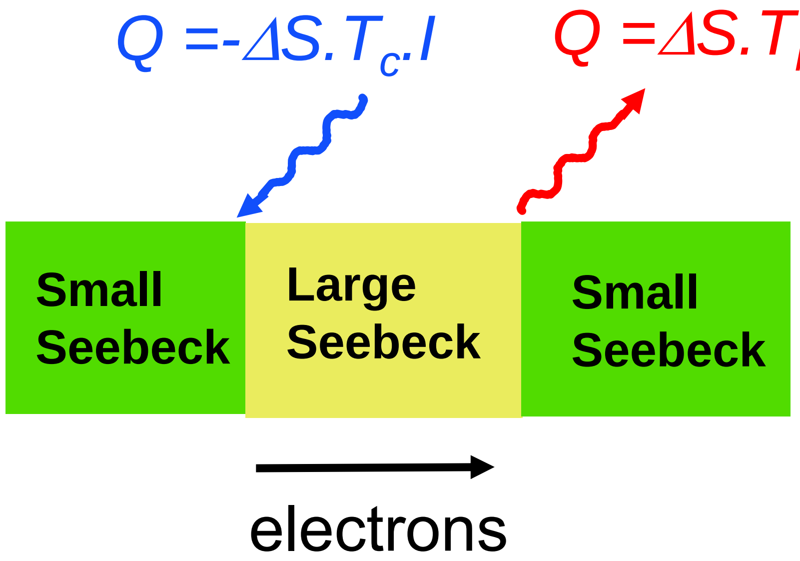

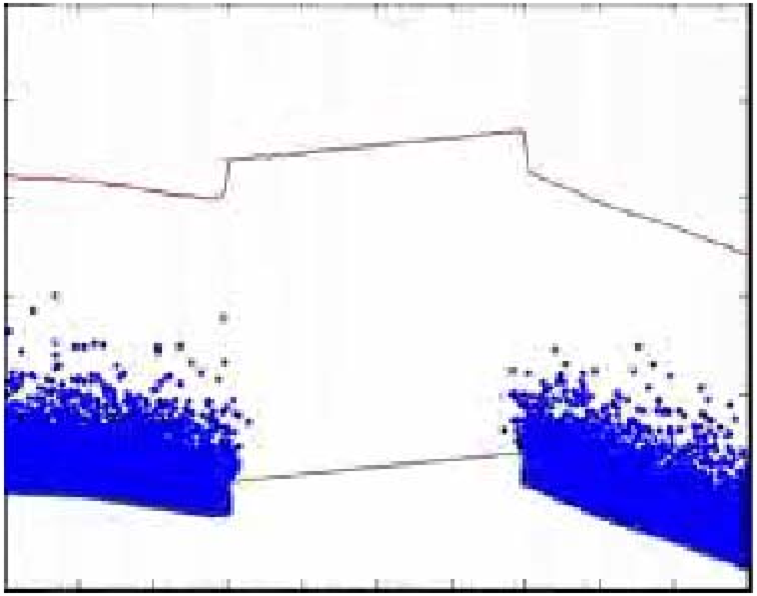

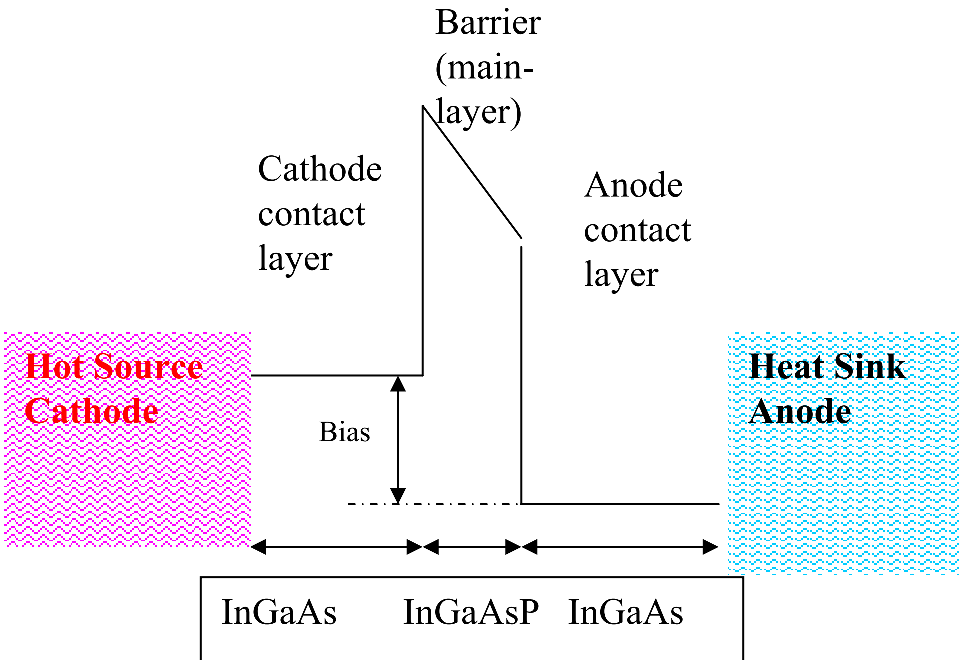

Mona Zebarjadi, Keivan Esfarjani, Ali Shakouri (PRB 2006)

Effective Seebeck Coefficient vs. Barrier Thickness

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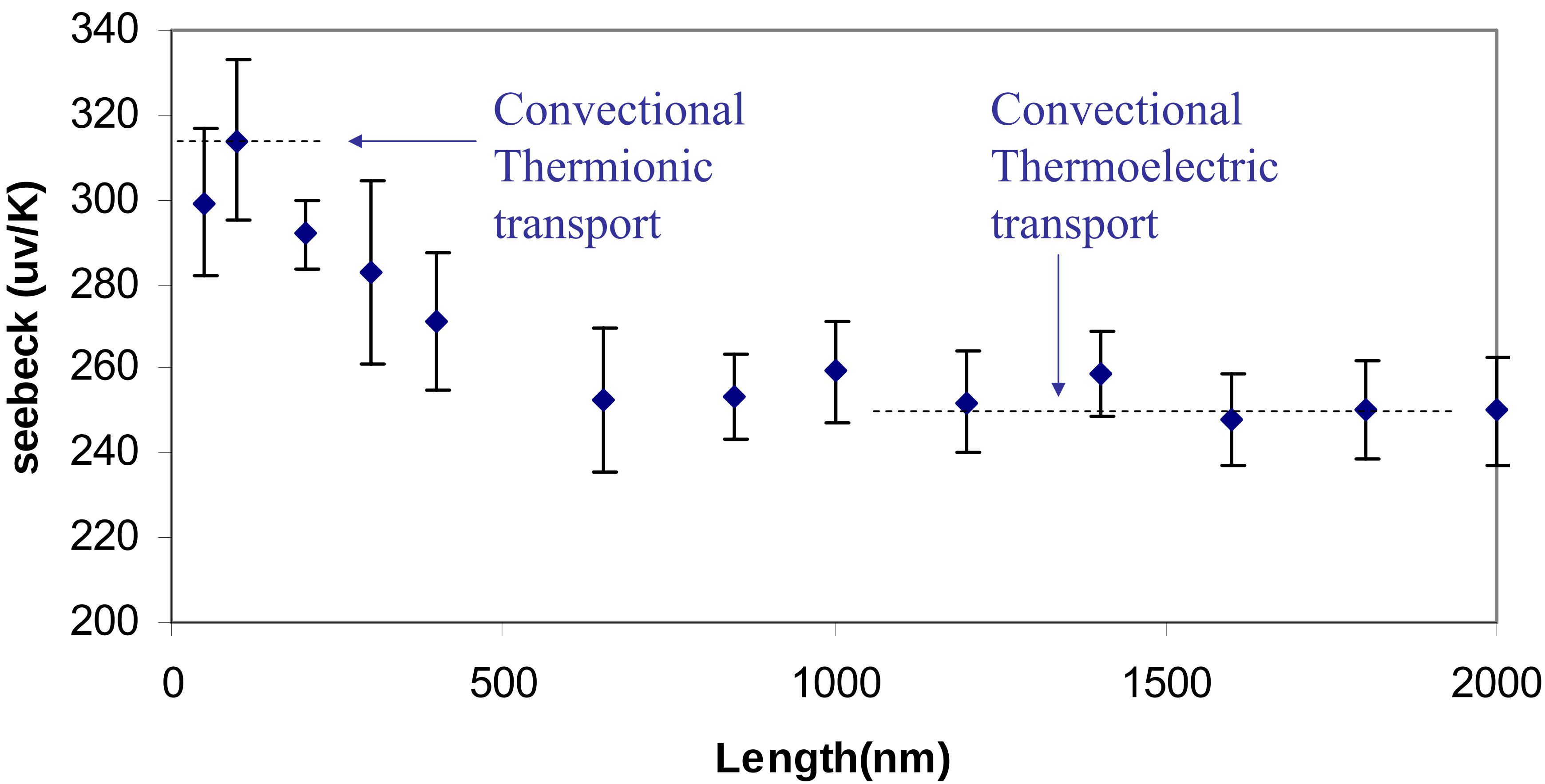
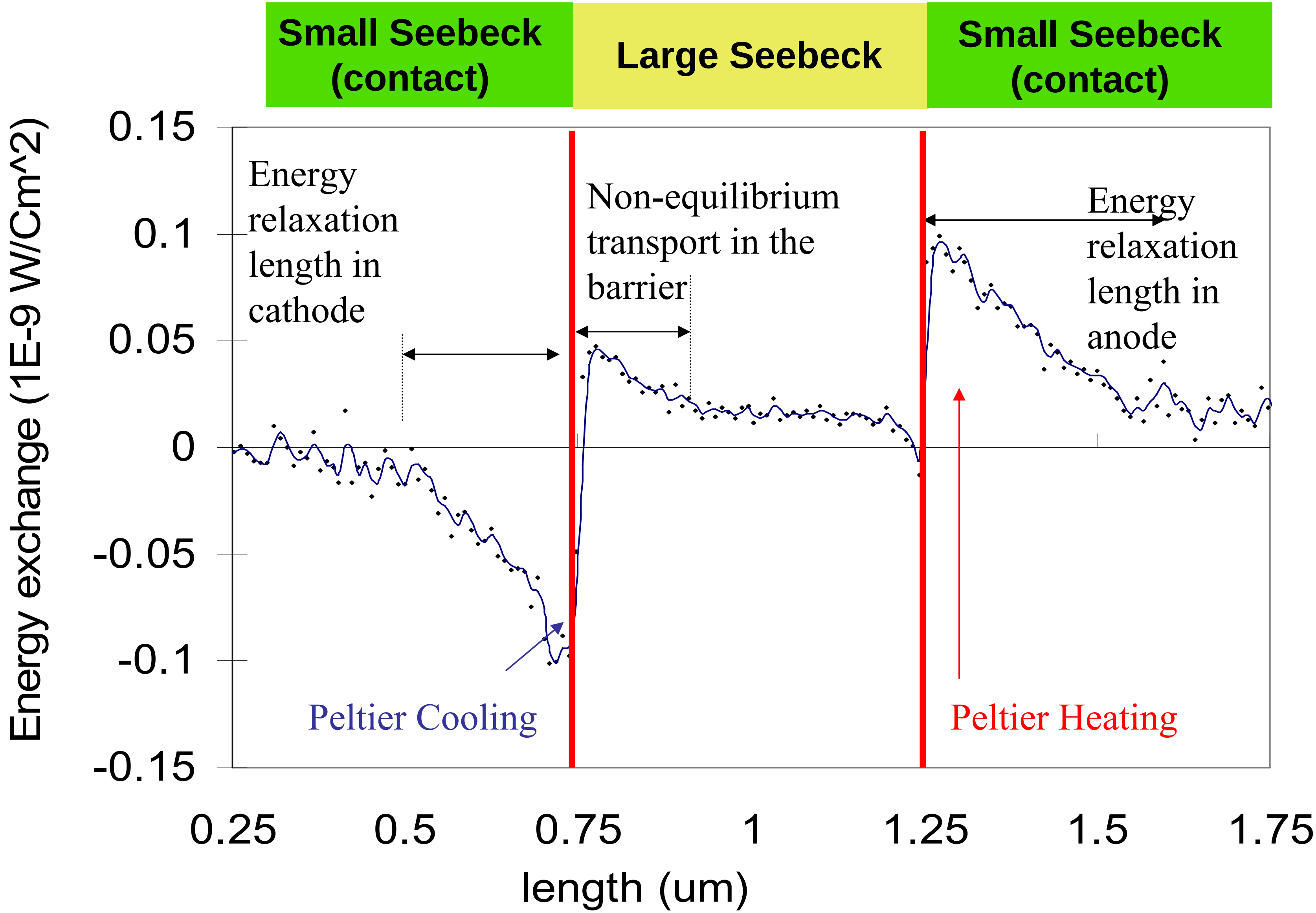


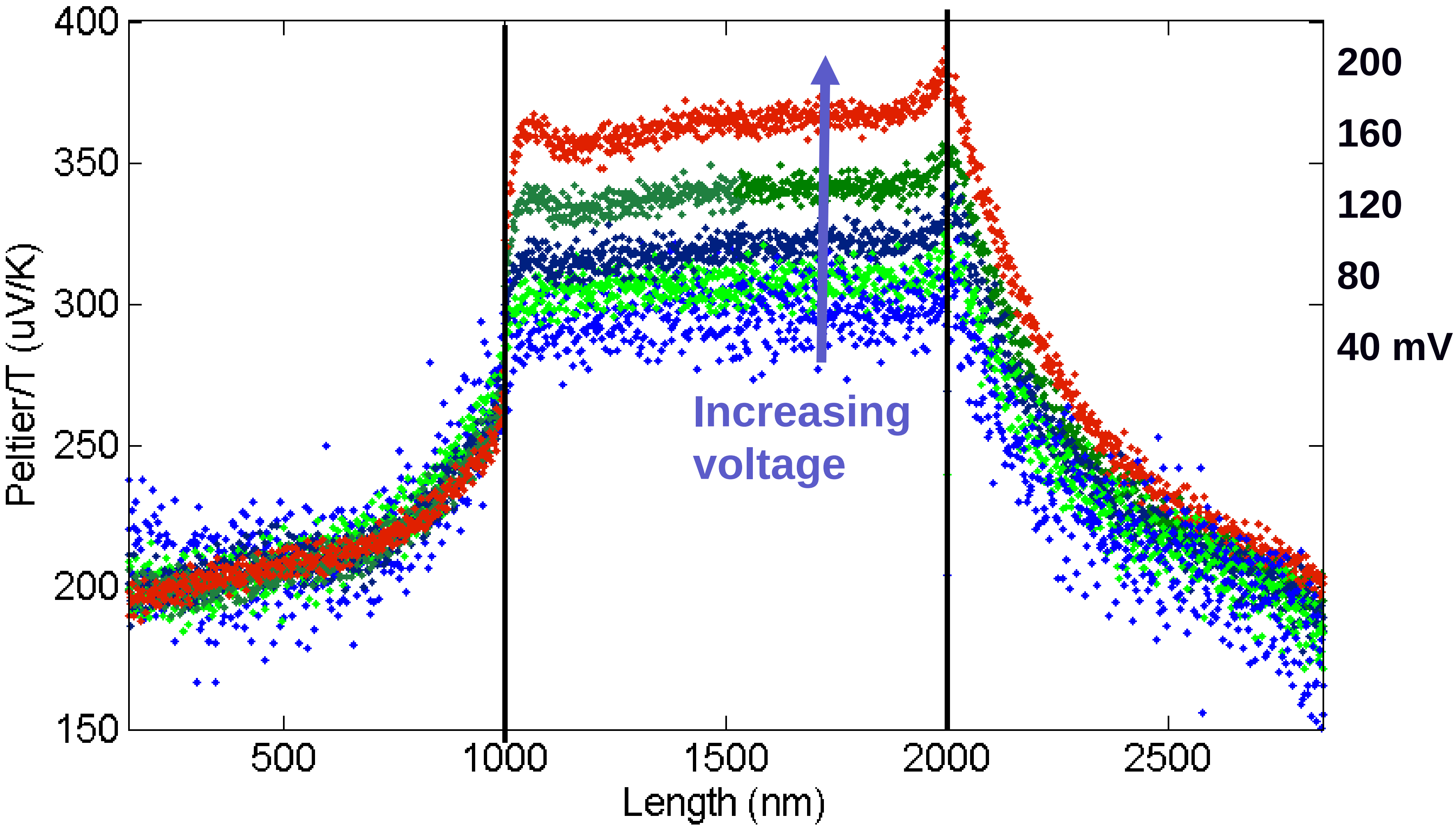
Mona Zebarjadi, Keivan Esfarjani, Ali Shakouri Phys. Rev. B 74, 195331 (2006)

Electron-phonon energy exchange



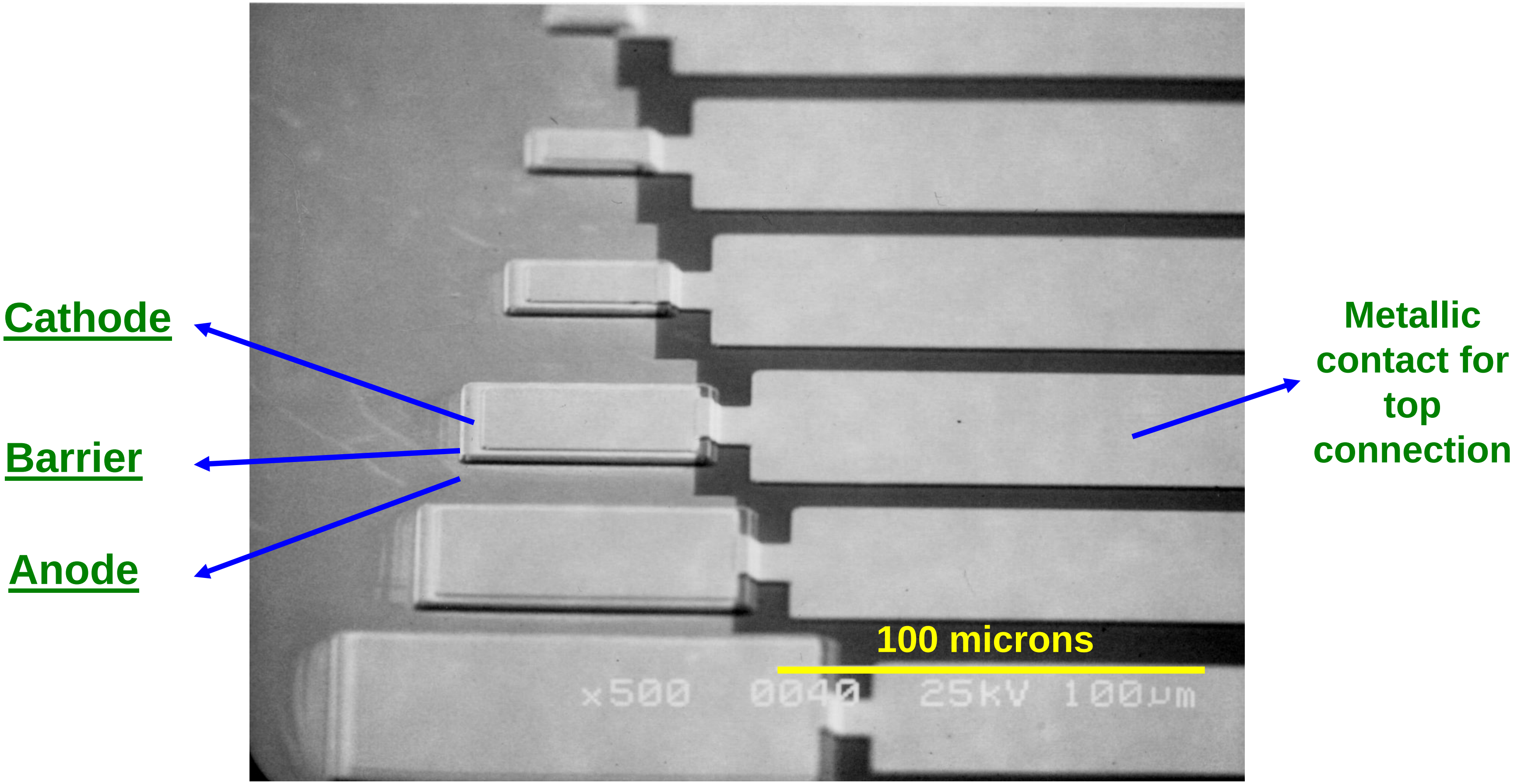
Mona Zebarjadi, K. Esfarjani, A. Shakouri, Phys. Rev. B, 74, 195331 (2006)

Nonlinear Peltier Coefficient



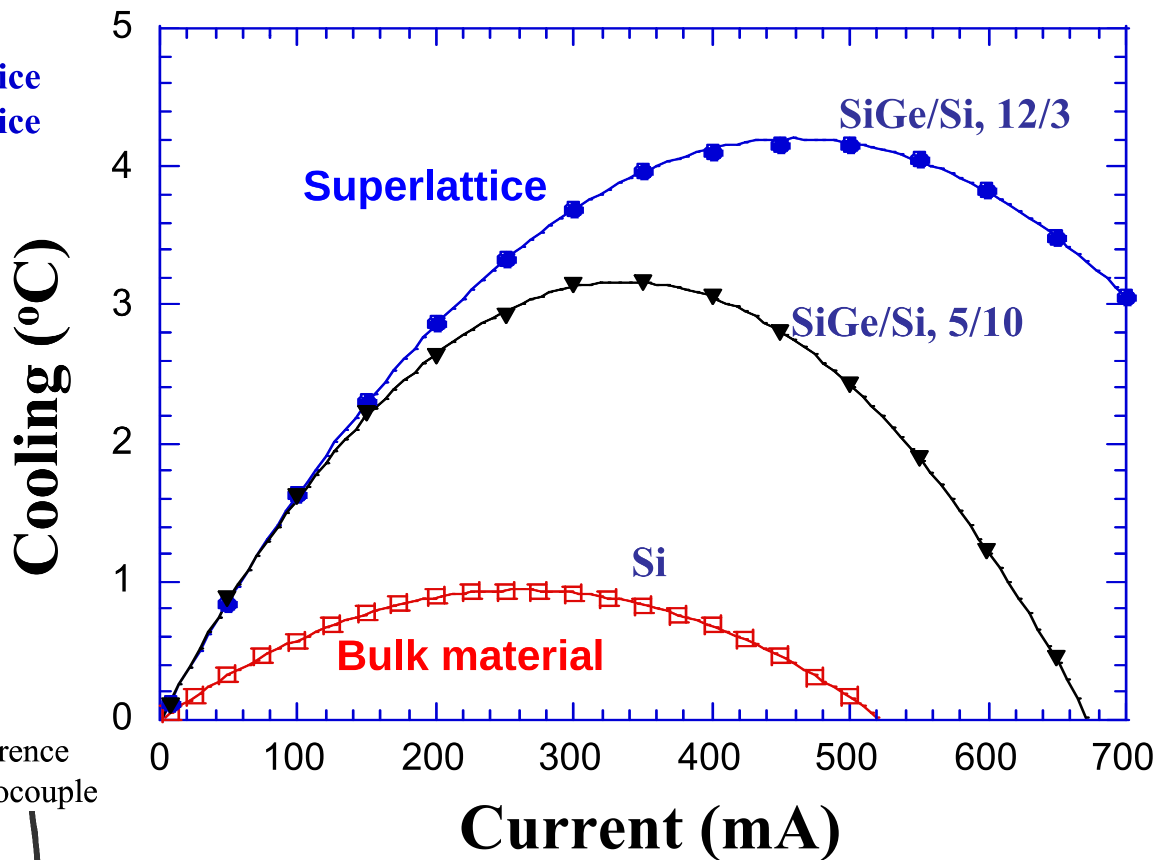
Mona Zebarjadi, Keivan Esfarjani, A. Shakouri –Applied Physics Letter 2007

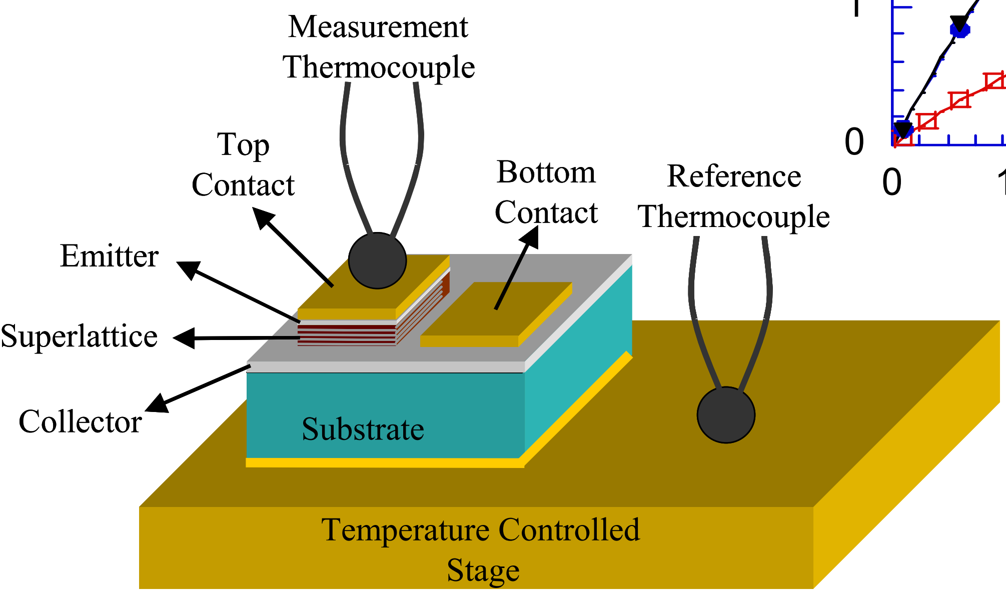
Scanning Electron Micrograph of Thin Film Cooler



Experimental Cooling vs. Current

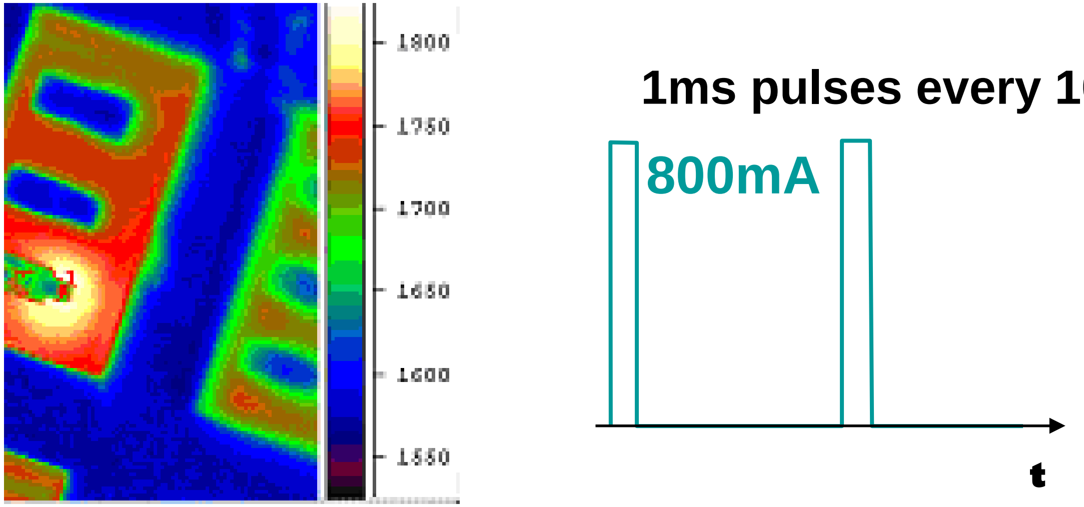
3µm 200x(12nm $Si_{0.75}Ge_{0.25}$/3nm Si) superlattice
3µm 200x(5nm $Si_{0.75}Ge_{0.25}$/10nm Si) superlattice
p+ Si substrate (60x60 µm^2)

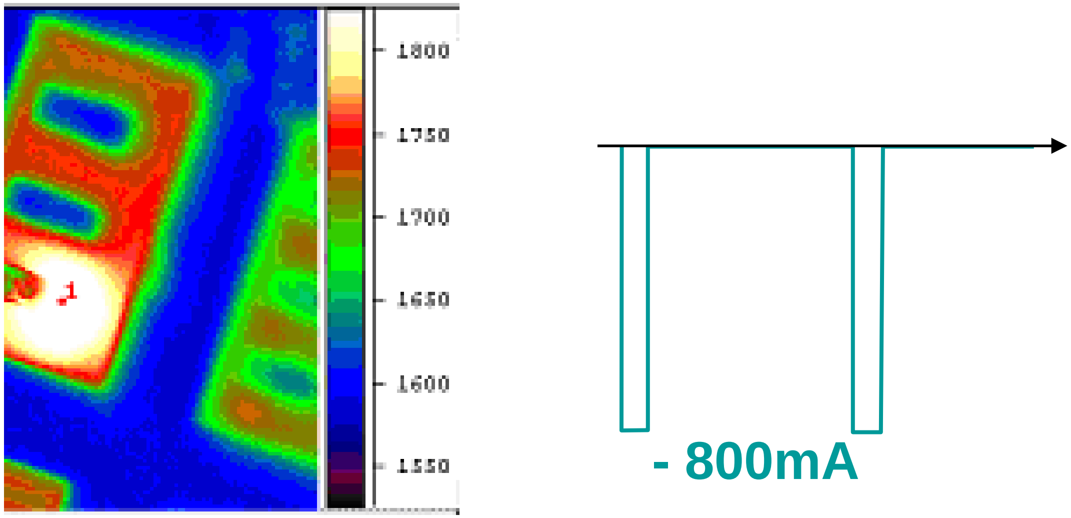




X. Fan, E. Croke, A. Shakouri, J. E. Bowers, … "**SiGe/Si Superlattice Coolers**," Phys. Low-Dim. Struct., 5/6 (2000) pp. 1-10.

IR Imaging of SiGe Superlattice Coolers

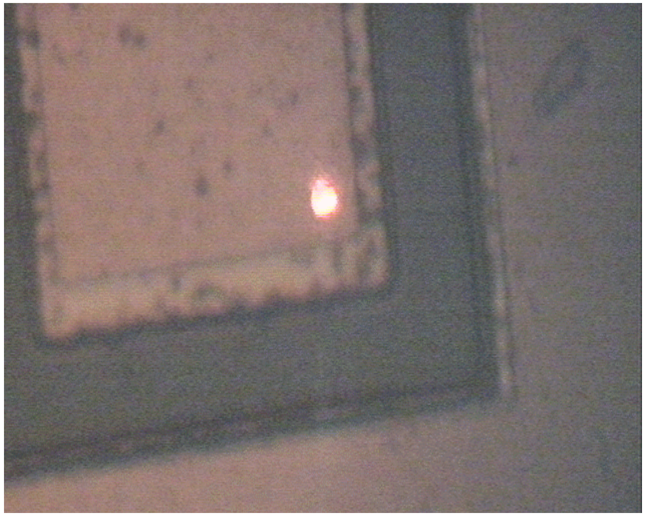




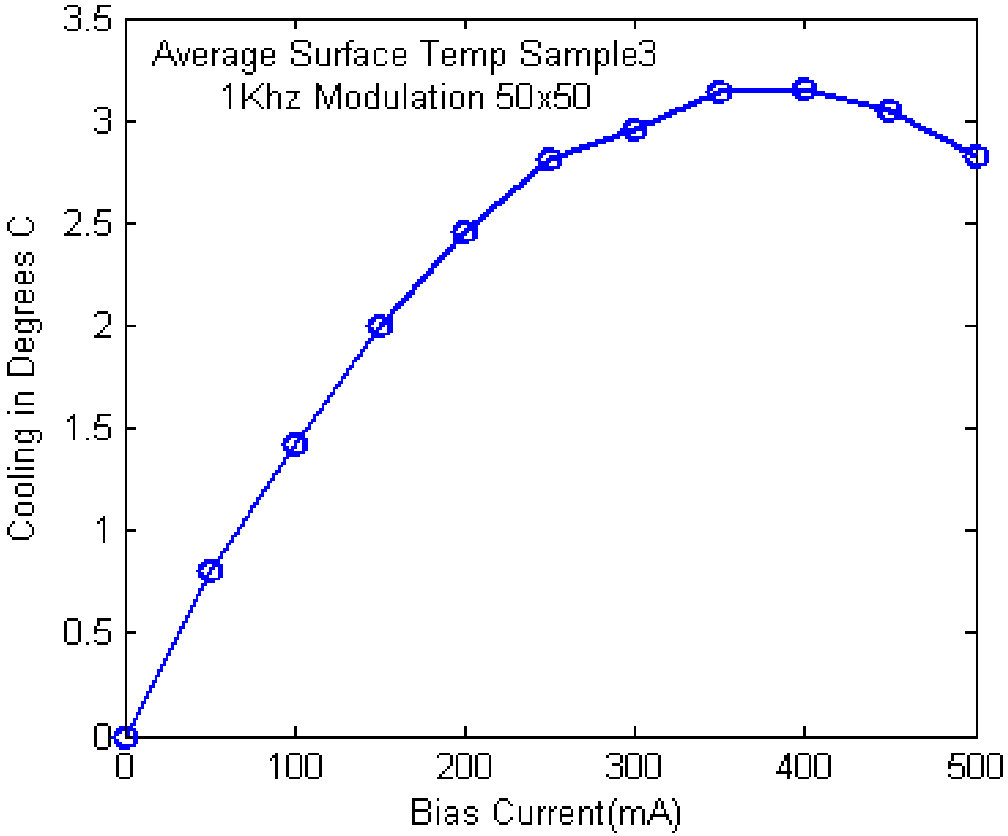
In collaboration with Hsin Wang, Oak Ridge National Lab

Laser measurement of localized temperature

J. Christofferson et al., SEMITHERM XVII , San Jose, Ca, March 2001.



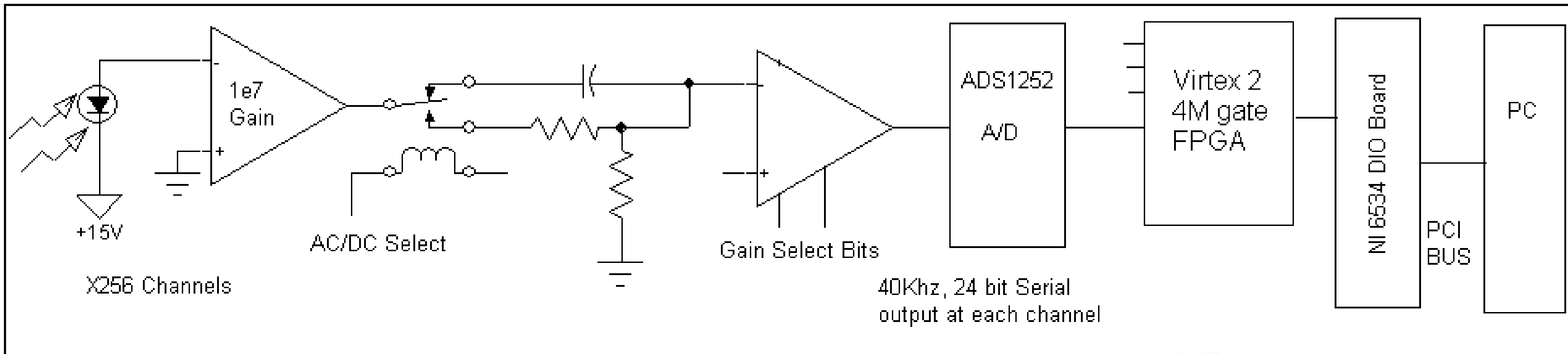
Laser Probe on a micro cooler, lock-in detection at 1KHz



By modulating the device temperature, and by lock-in detection a small change in surface reflectivity due to temperature variation is detected.

Lock-in imaging camera

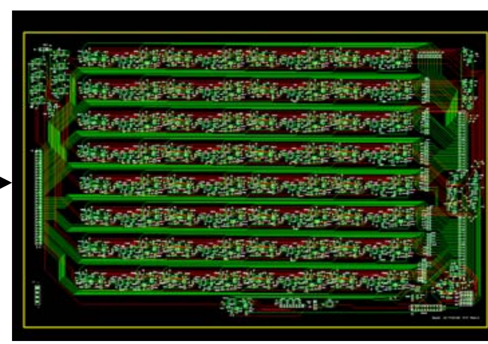
- AC/DC coupled, dedicated ADC per channel
- FPGA to offload processing



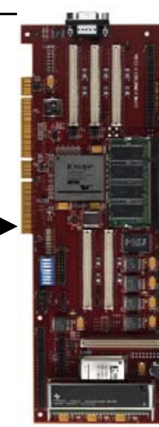
256 Analog

Hamamatsu C4675 16x16 pixel photodiode array

256 serial



Four 64 channel in-house designed signal conditioning, A/D boards



Avnet Development Kit, Virtex2, 128Mb RAM

PCI interface

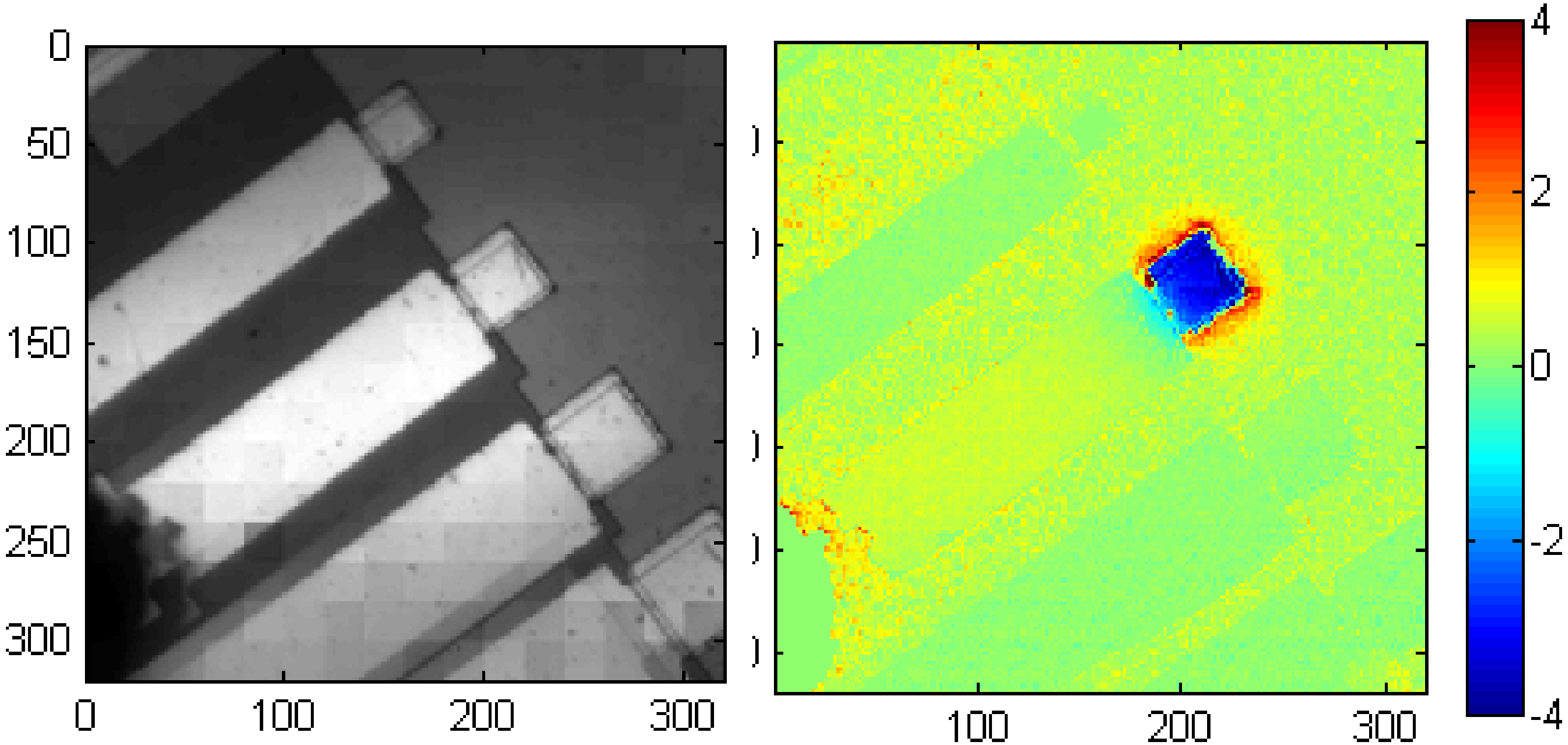
PC running LabVIEW

J. Christofferson, A. Shakouri *Review of Scientific Instruments* Feb 2005.

Ultra high resolution thermal imaging

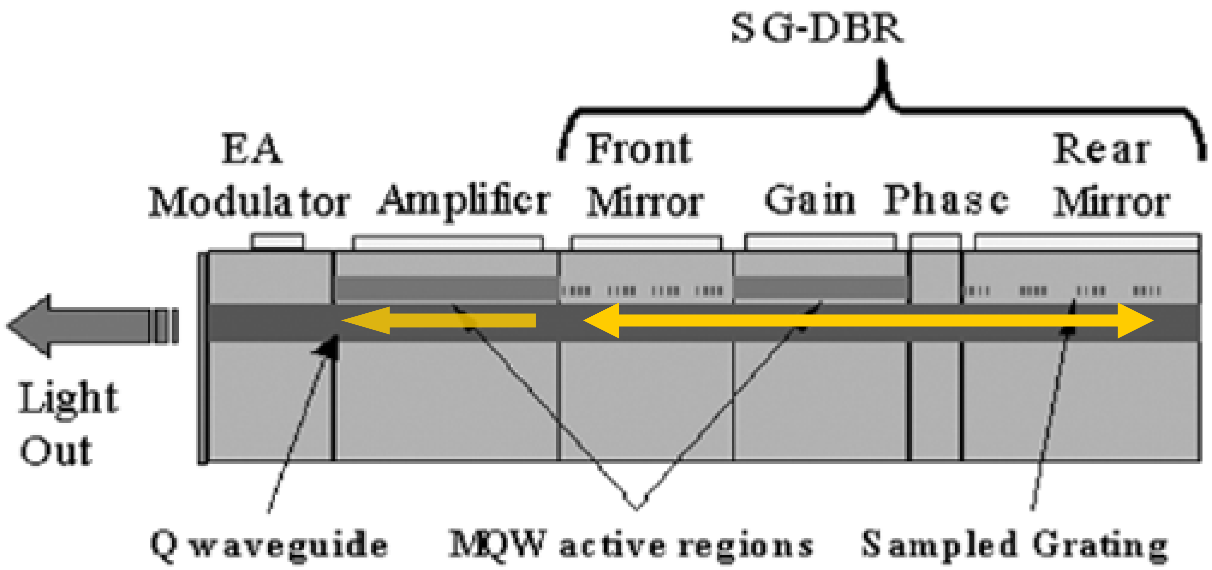
Acquisition time: seconds-minutes

- Temperature resolution: 0.006°C
- Spatial resolution: submicron



Thermal Issues in Electroabsorption Modulator (EAM)

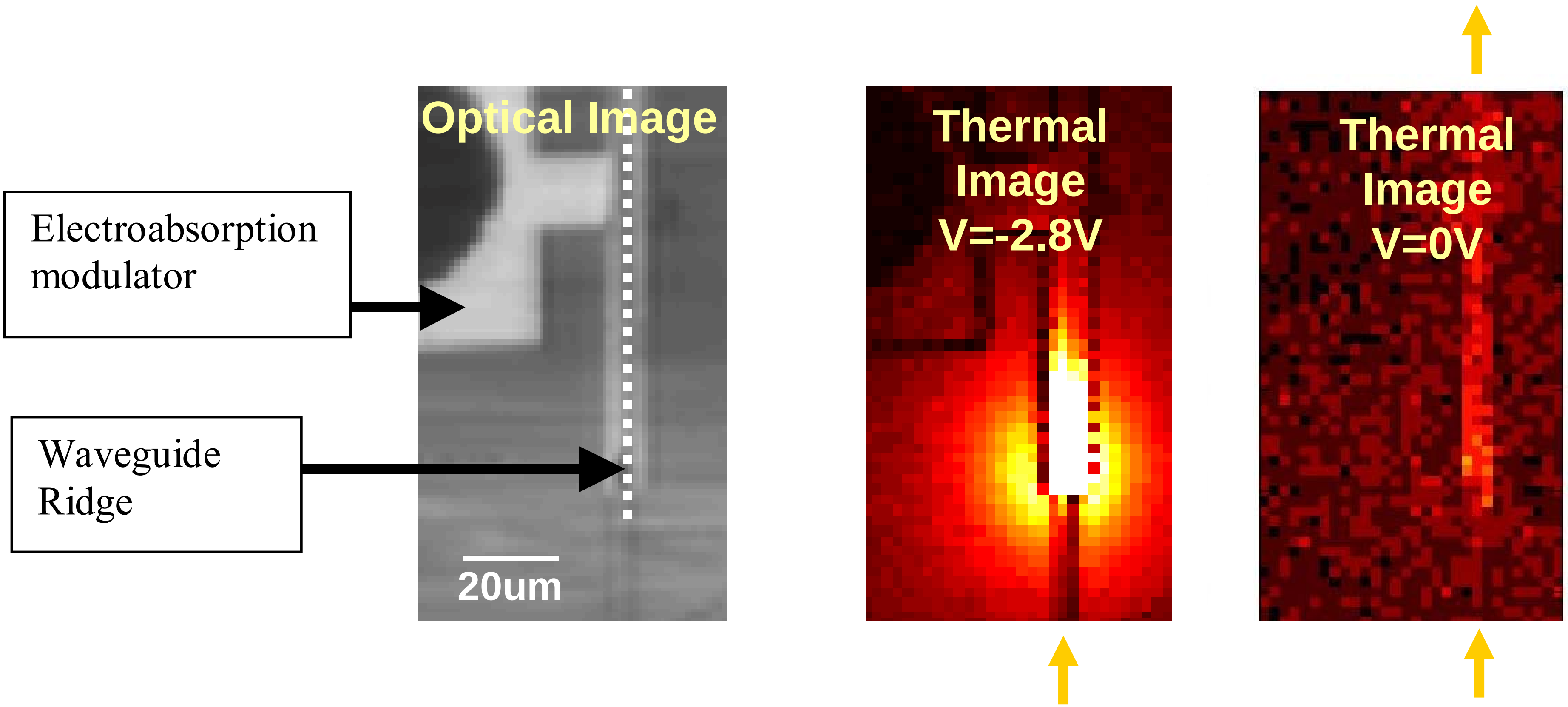
- EAM can be easily integrated into tunable lasers to offer high bandwidth (>10Gb/s), low chirp, low drive voltage and high extinction ratio



Peter Kozodoy, et al., IEEE Trans. on Components and Packaging Techn., 28 pp. 651, 2005

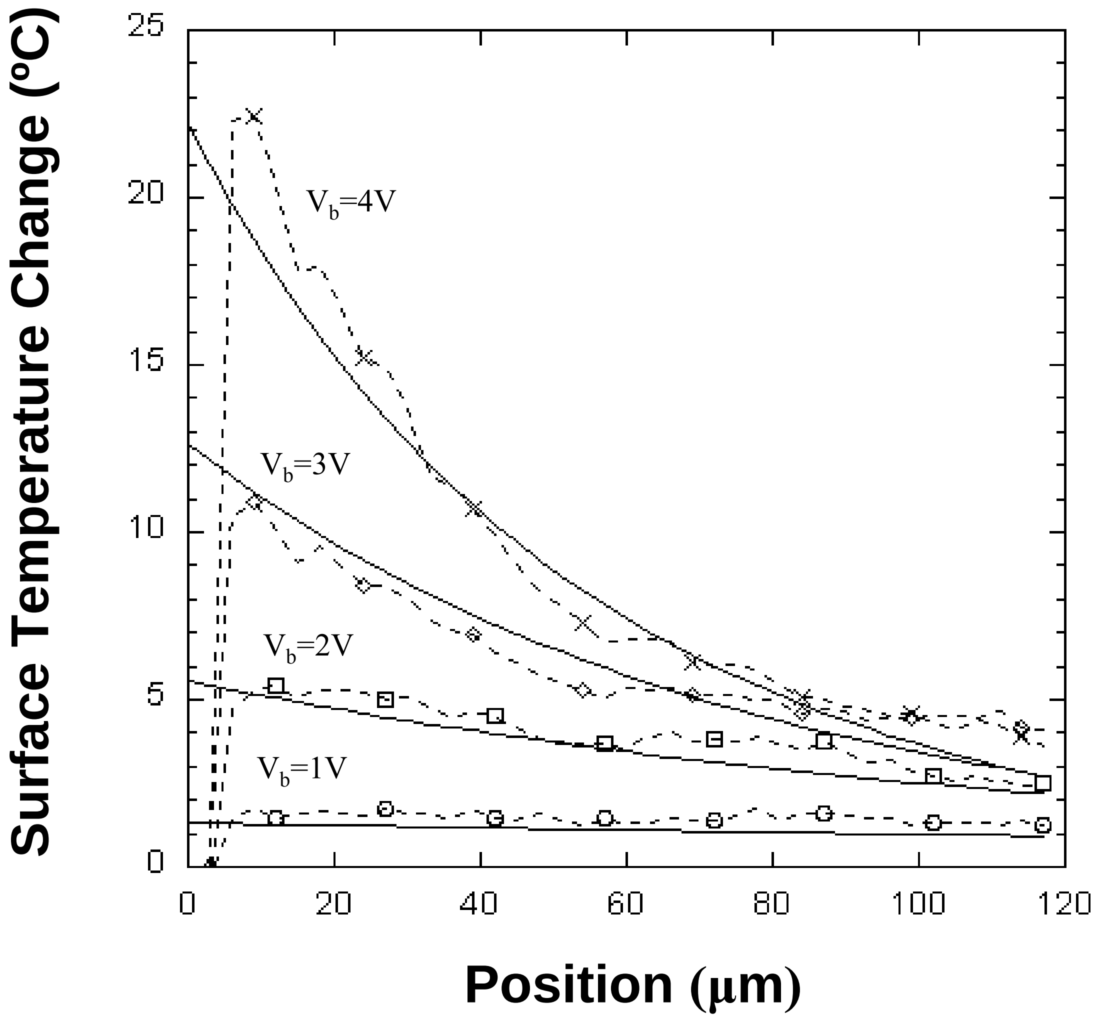
Collaborators: P. Kozodoy, P. Abraham (Agility Communications)

Thermal Imaging of Integrated Electroabsorption Modulator



A. Shakouri, J. Christofferson, Z. Bian, and P. Kozodoy, "High Spatial Resolution Thermal Imaging of Multiple Section Semiconductor Lasers," (invited talk) Proceeding of Photonic Devices and System Packaging Symposium (PhoPack 2002), pp22-25, July 2002, Stanford CA.

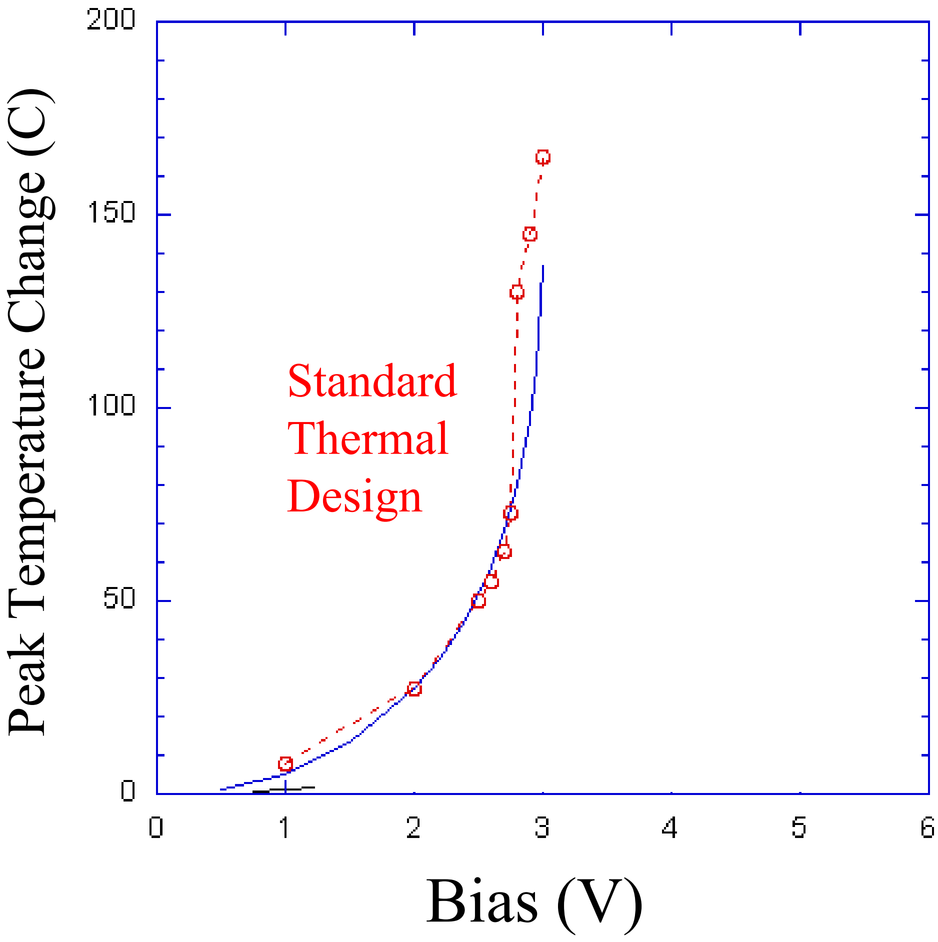
Temperature Profile along Modulator at Low Power Operation



Input power 6mW

Z. Bian, J. Christofferson, P. Kozodoy, A. Shakouri, Applied Physics Letters 2003

Peak Surface Temperature at High Input Power



measurement (points)

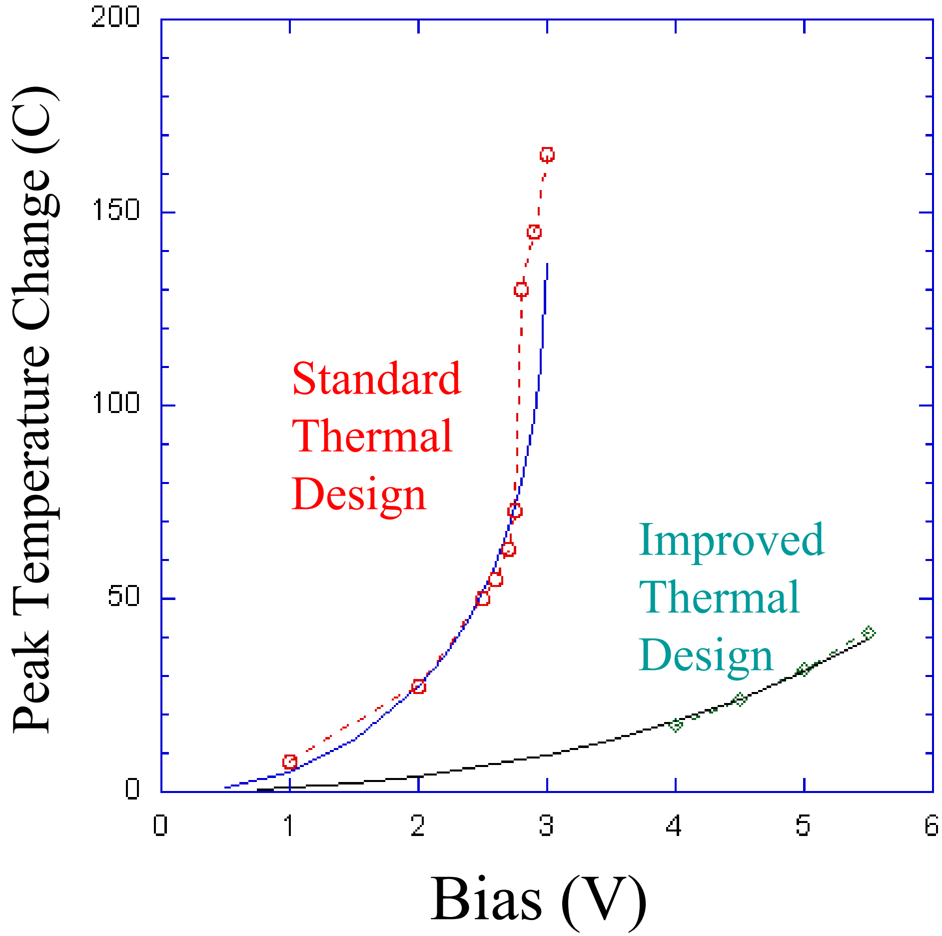
theory (line)

Input power ~ 35 mW
Wavelength ~1.55 μm.

There is thermal runaway with standard device design

Z. Bian, J. Christofferson, P. Kozodoy, A. Shakouri, Applied Physics Letters 2003

Peak Surface Temperature at High Input Power



measurement (points)

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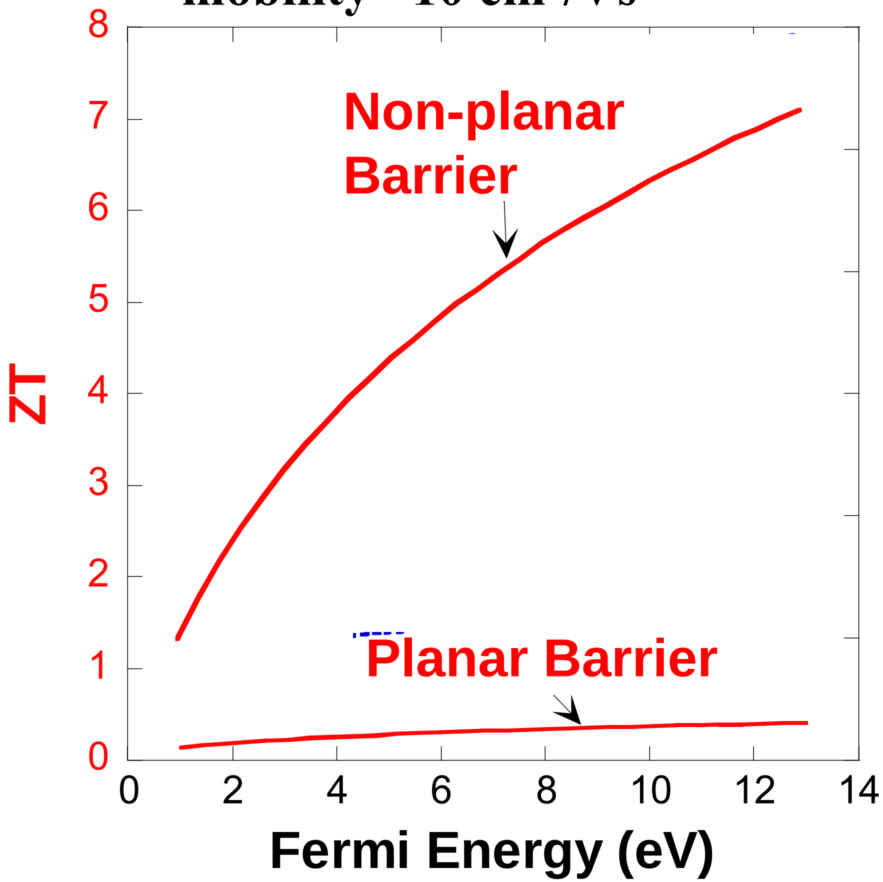
Z. Bian, J. Christofferson, P. Kozodoy, A. Shakouri, Applied Physics Letters 2003

ZT for metallic superlattices

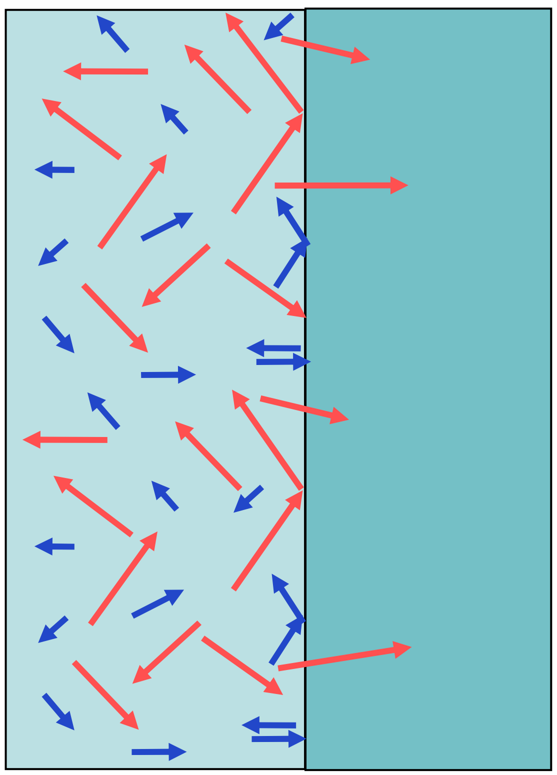
UCSC
Berkeley
Harvard
MIT
NCSU
Purdue
UCSB

Assume: $\beta_{lattice}$=1W/mK, mobility ~10 cm^2/Vs



Hot and cold electrons in equilibrium

Hot electron filter

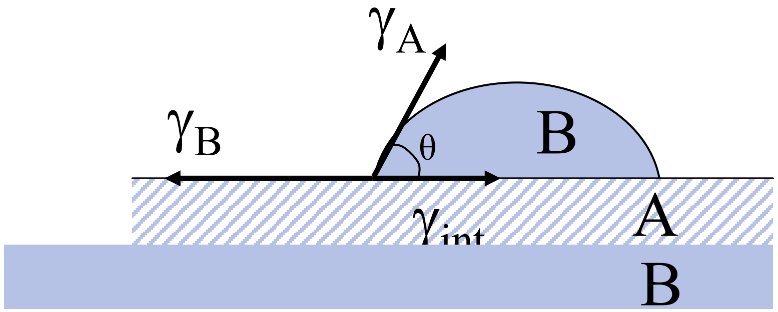


D. Vashaee, A. Shakouri, Physical Review Letters, March 12, 2004

Even with modest low $k_{lattice}$ and mobility of typical metals, ZT>5 is possible with hot electron filters and non-planar barrier.

Can metal/semiconductor multilayers be grown?

Challenge: *No prior examples of metal/semiconductor multilayers or superlattices with nanoscale periods*



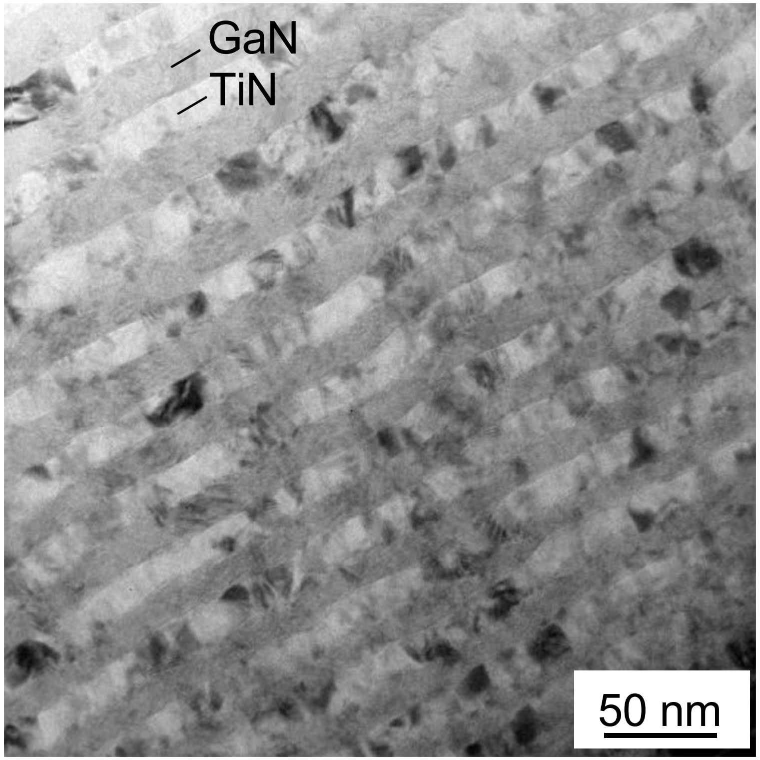
- Minimization of surface energy: If A wets B, B will not wet A.
- Different crystal structures: high defect density; multilayer will not be stable
- Lattice mismatch effect: strain may lead to island growth

Late 80's: High speed metal base transistors → Not successful

Tim Sands (Purdue)

TiN/GaN multilayers for high-T operation

- **Good metals (e.g., TiN with ρ = 20 $\mu\Omega$-cm)**
- **Semiconducting (hp-GaN [1.7 eV] and ScN [2.15 eV]) and insulating (hp-AlN) rocksalt nitrides**
- **High melting points (e.g., 3290ºC for TiN); negligible sublimation**
- **Excellent corrosion resistance, mechanical hardness and toughness**
- ***But high bulk thermal conductivities (e.g. 130 W/m-K for GaN)***



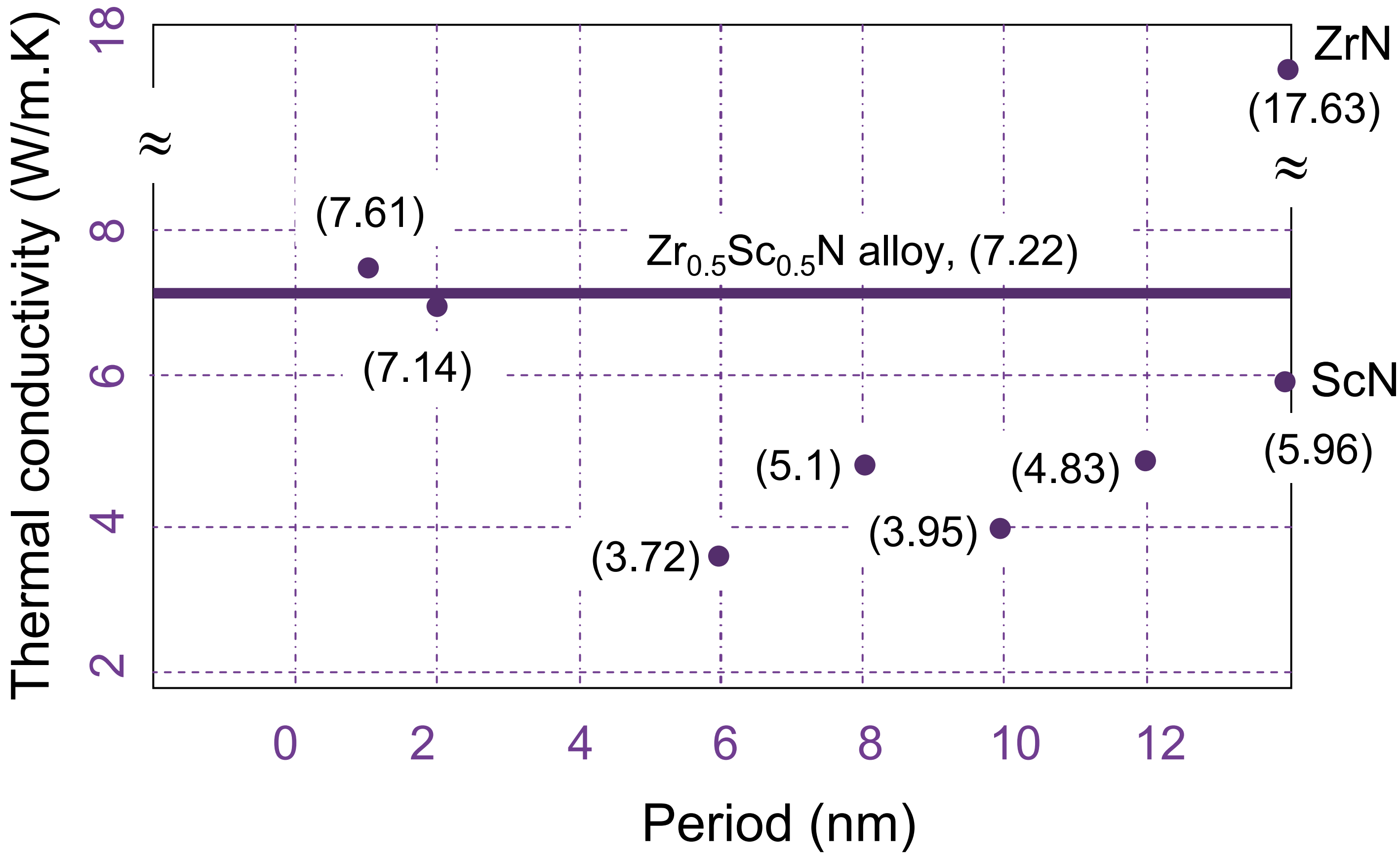
20 nm TiN/variable GaN on (100) MgO

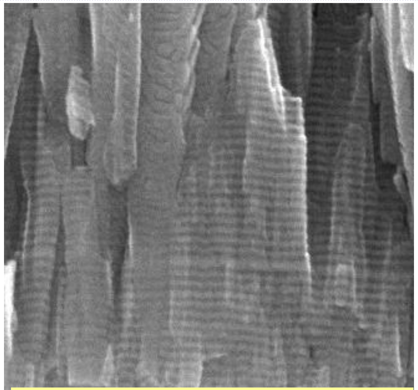
GaN and TiN layers are uniform and pinhole free down to a few nm in thickness

V. Rawat, Tim Sands (Purdue)

Thermal conductivity of metal/ semiconductor multi layers

Room temperature thermal conductivity as a function of multilayer period (3ω) -
$k_{multilayer} < k_{alloy}$

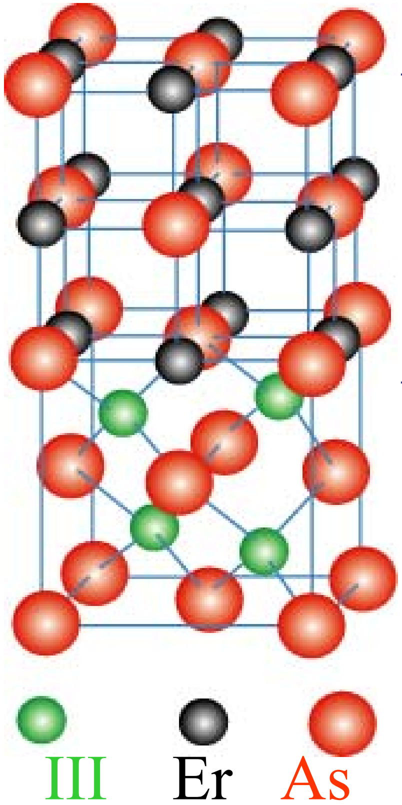




1.16 μm thick ZrN(6nm)/ScN(6nm) multilayer grown on MgO substrate

Rawat, Sands (Purdue), Singer, Majumdar (Berkeley)

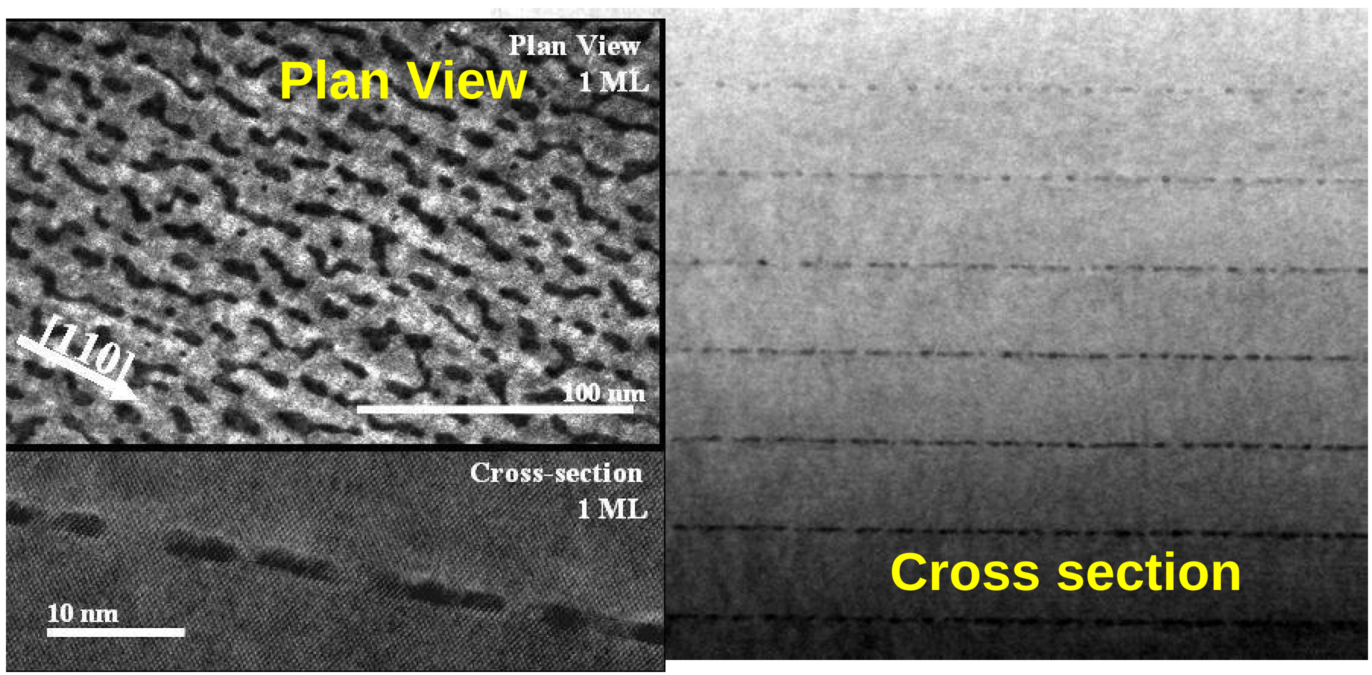
Semimetallic Nanoparticles: ErAs/III-V



Semimetal
ErAs (Rock-salt)
a=5.74 Å

Semiconductor
e.g. InGaAs (Zinc blende)
a=5.85 Å

- ErAs is a rocksalt semimetal with a fairly small lattice mismatch to several III-V semiconductors.
- It can be grown epitaxially on the semiconductor, and the arsenic has a continuous fcc sublattice.



Co-deposited ErAs Particles in InGaAs

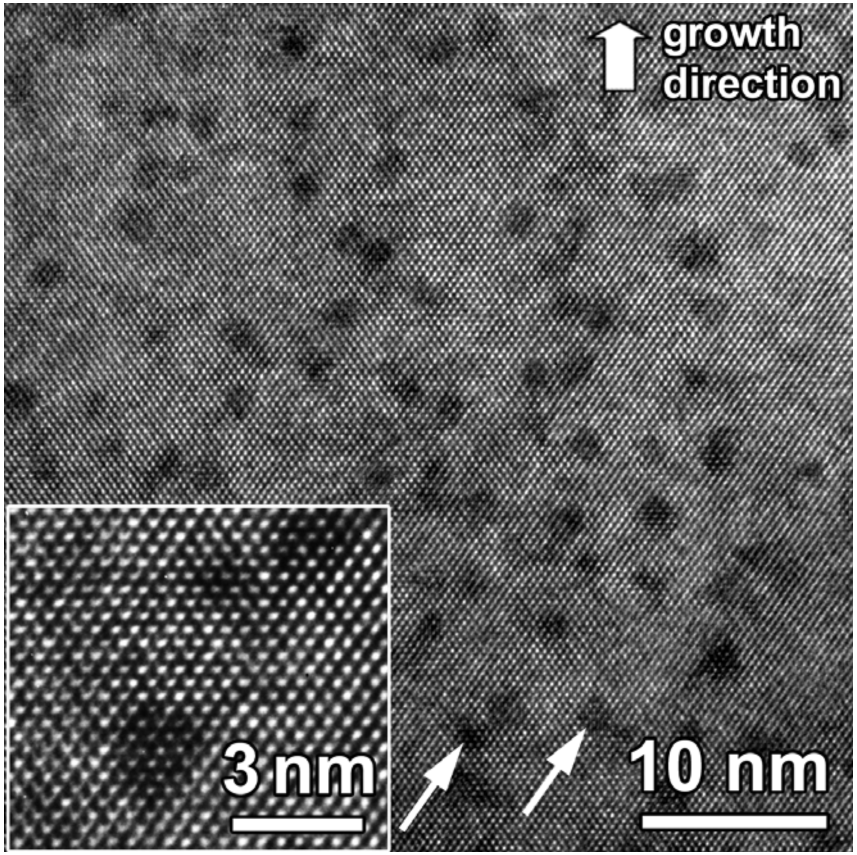
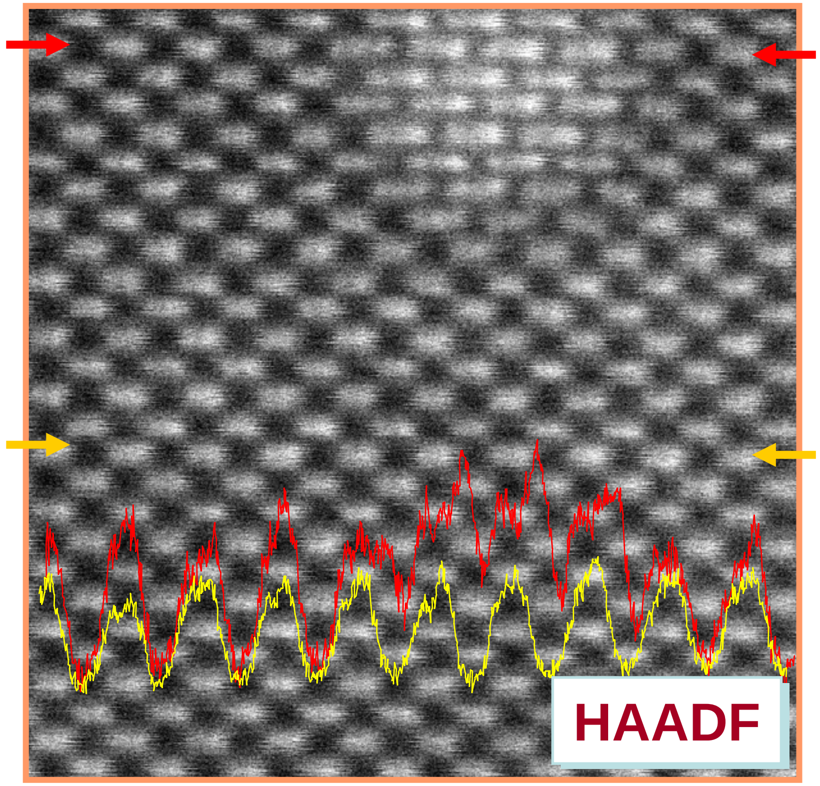
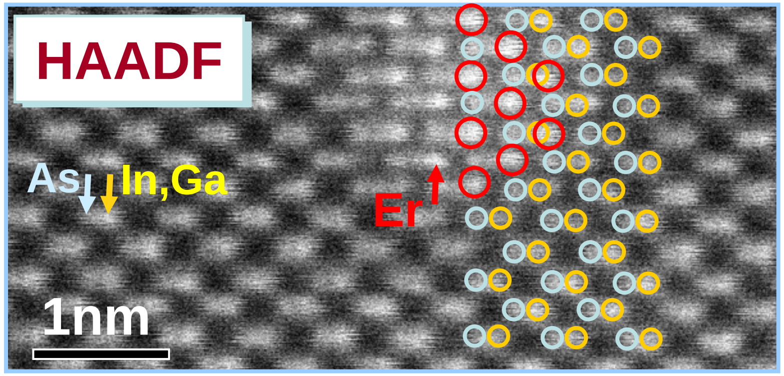


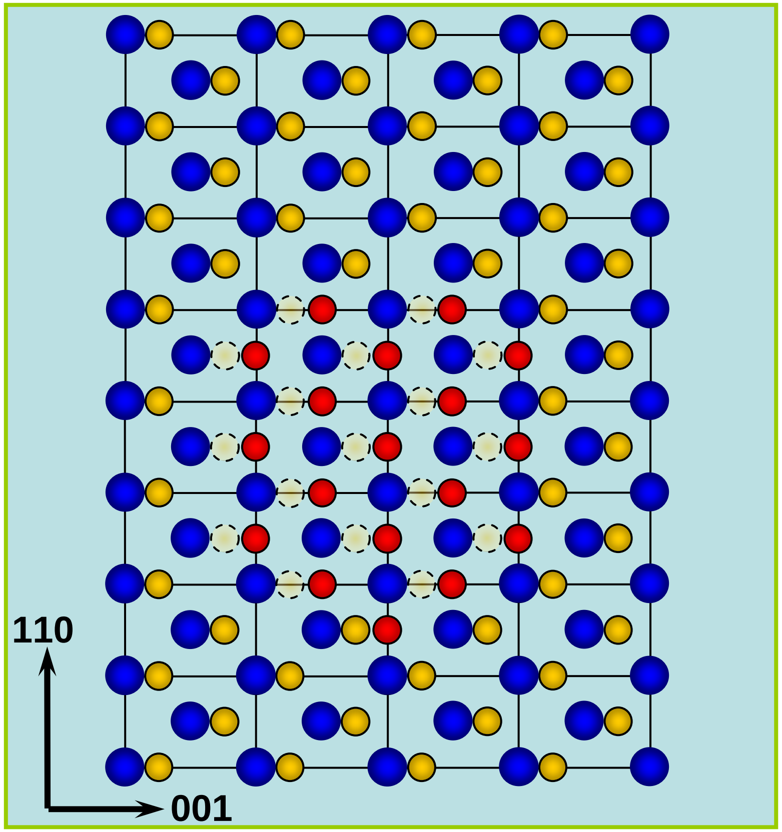
Image from D. Klenov
J.M. Zide, *et al.* Appl. Phys. Lett. **87,** 112103 (2005)

- Erbium is co-deposited at a growth rate which is a fixed fraction of the InGaAs growth rate.
- Solubility limit is exceeded → islands are formed.
- Size is similar to that of very small (0.05ML) depositions.

HAADF/STEM of ErAs Nanoparticles





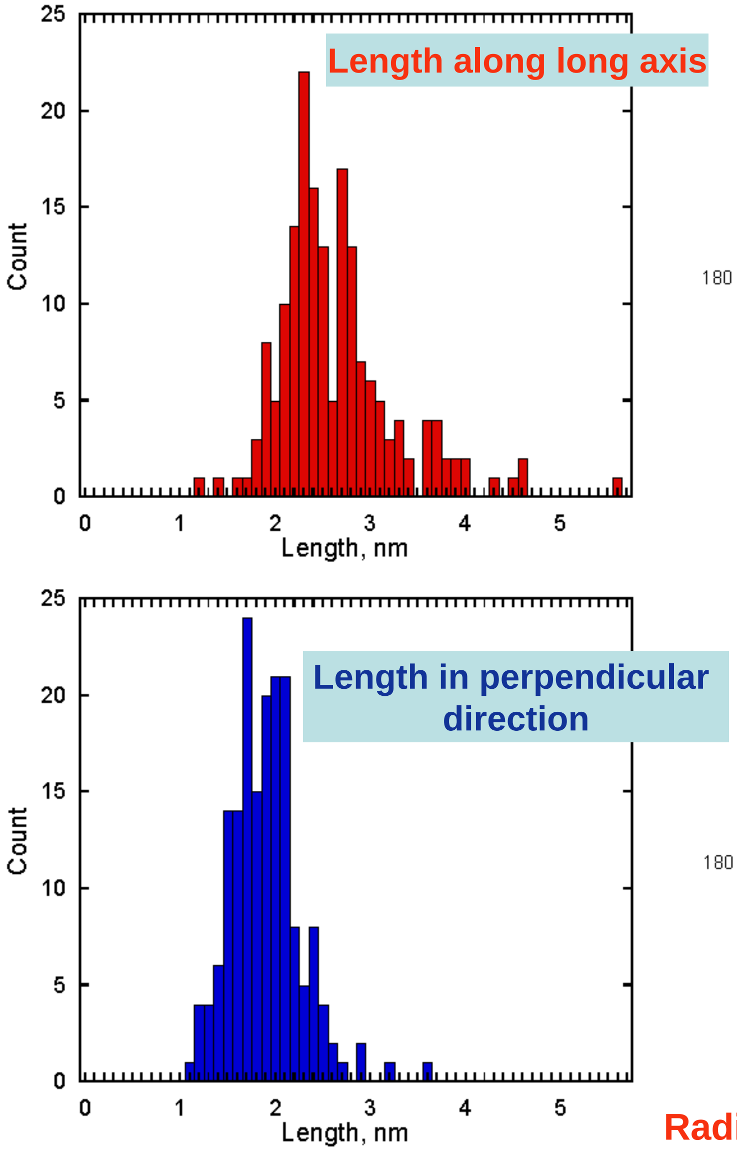


STEM images show that the ErAs particles have the rock salt structure. The As sublattice is continuous across the interface.

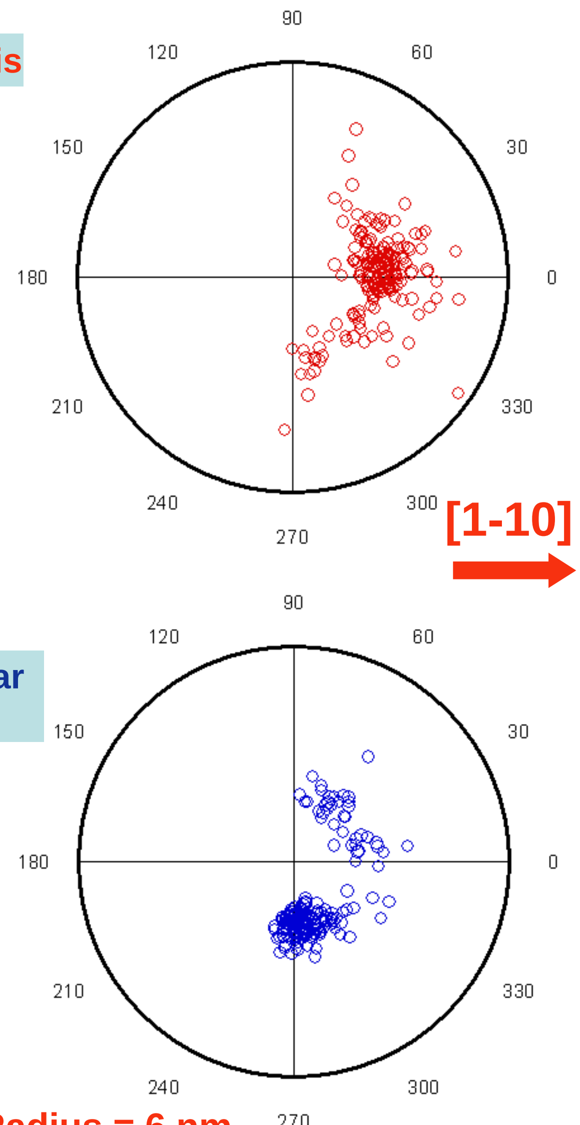
D. O. Klenov, D. C. Driscoll, A. C. Gossard, S. Stemmer, Appl. Phys. Lett. 86, 111912 (2005)

Particle sizes and shapes for 3% ErAs

Size



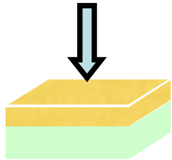
Orientation



Radius = 6 nm

- Particles are slightly elongated (~ 28%) along the fast [1-10] diffusion direction

Similar results as for superlattices.

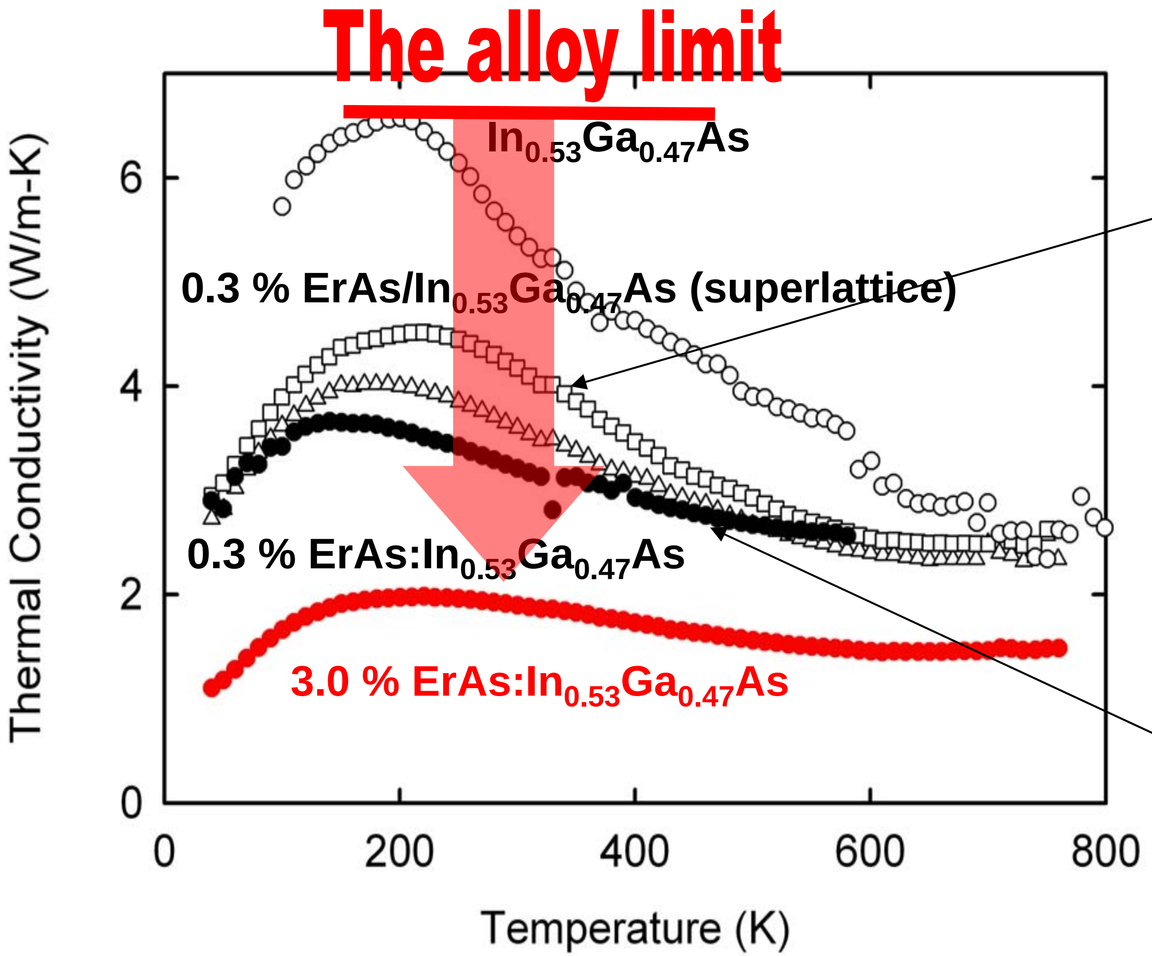


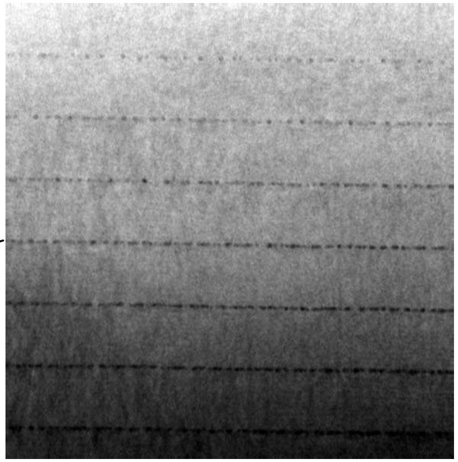
Plan-view

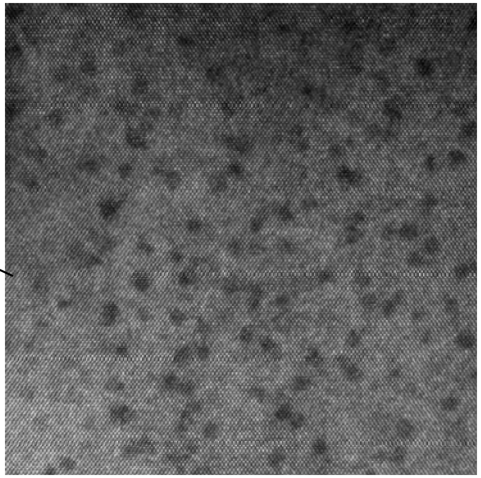
S. Stemmer et al.

Thermal Conductivity Below Alloy Limit

EXPERIMENT $ErAs:In_{0.53}Ga_{0.47}As$







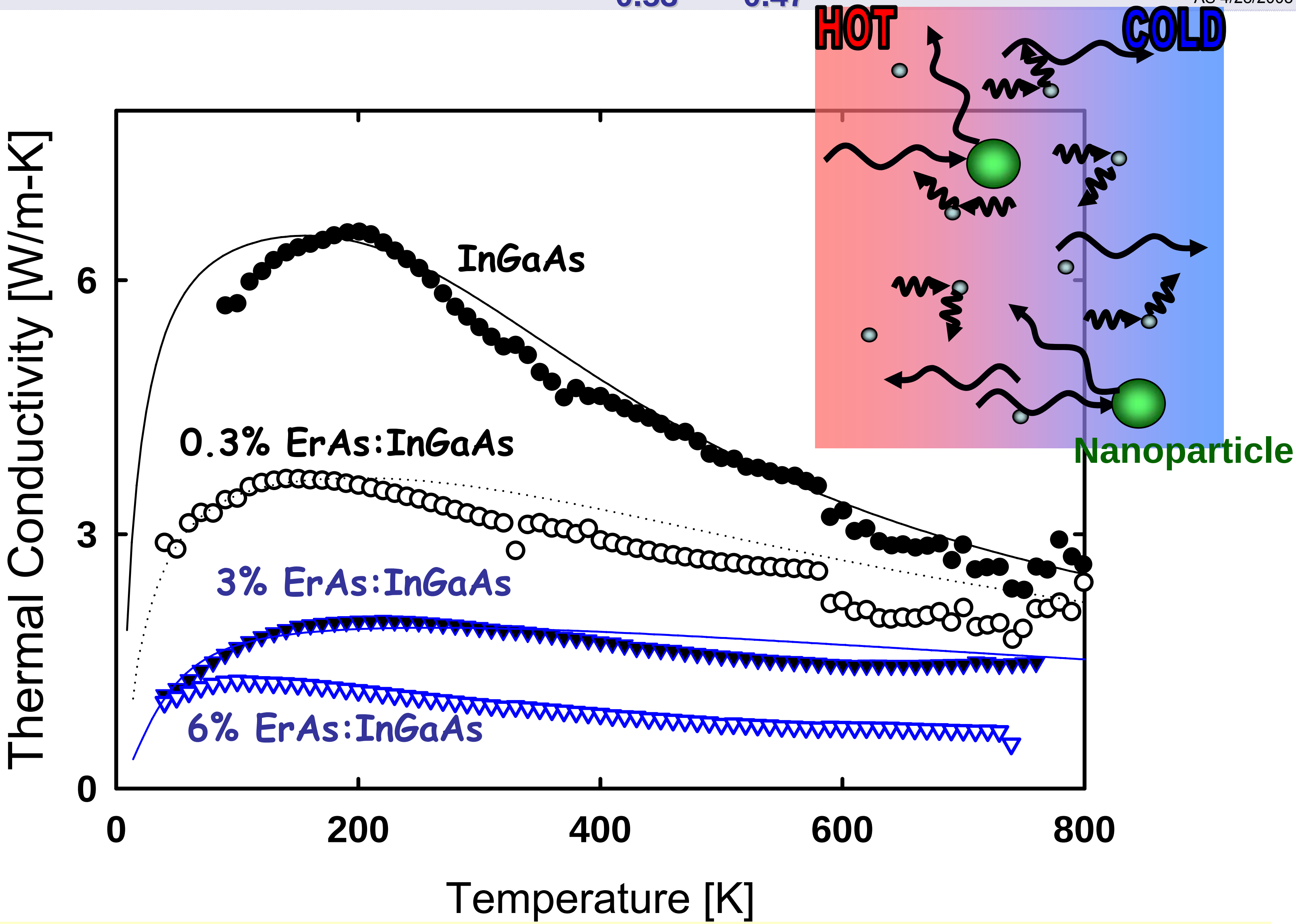
Superlattice to "Random" Nanoparticle Distribution

- Improved Performance (k lower)
- Faster Depositions (MBE grown 60μm films)

Thermal Conductivity Below Alloy Limit

THEORY $ErAs:In_{0.53}Ga_{0.47}As$

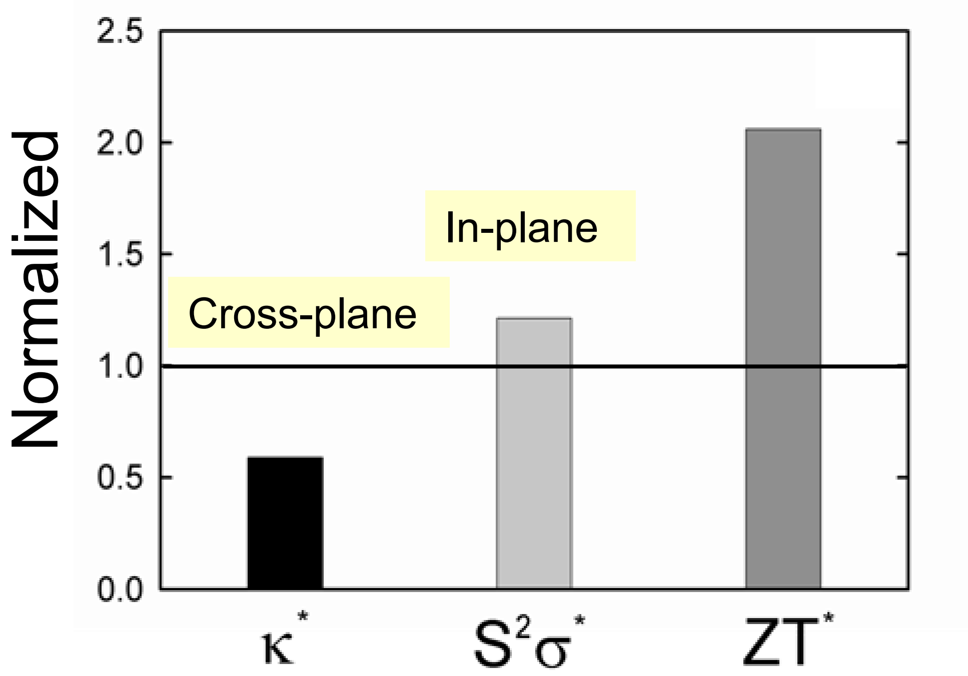
AS 4/28/2008

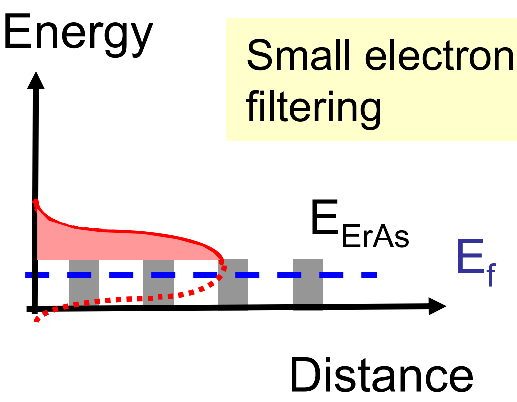


Long and Short Wavelength Phonon Scattering ➤ Thermal Conductivity Reduction

Electrical and Thermoelectric Properties of ErAs: InGaAs

Thermal conductivity, power factor, ZT of randomly distributed ErAs (0.3%) nanoparticles in InGaAs normalized to those of InGaAs

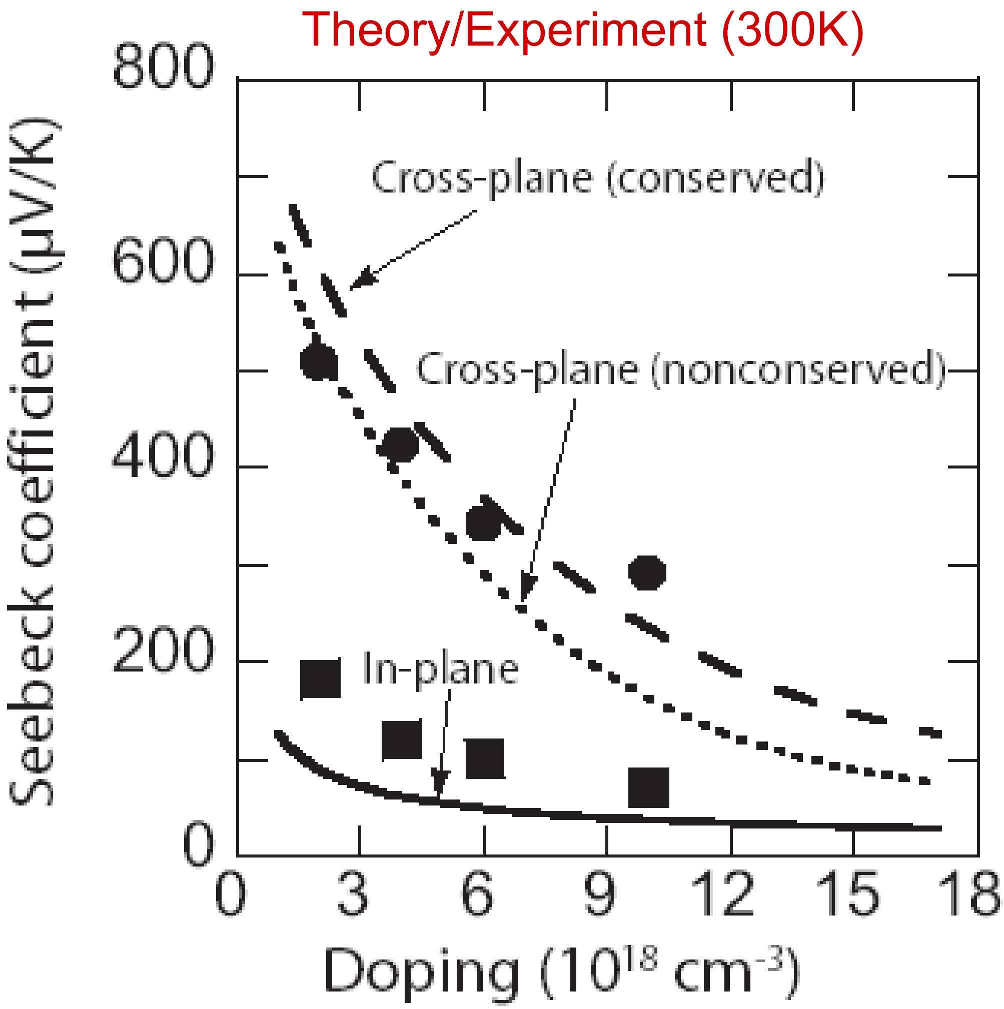


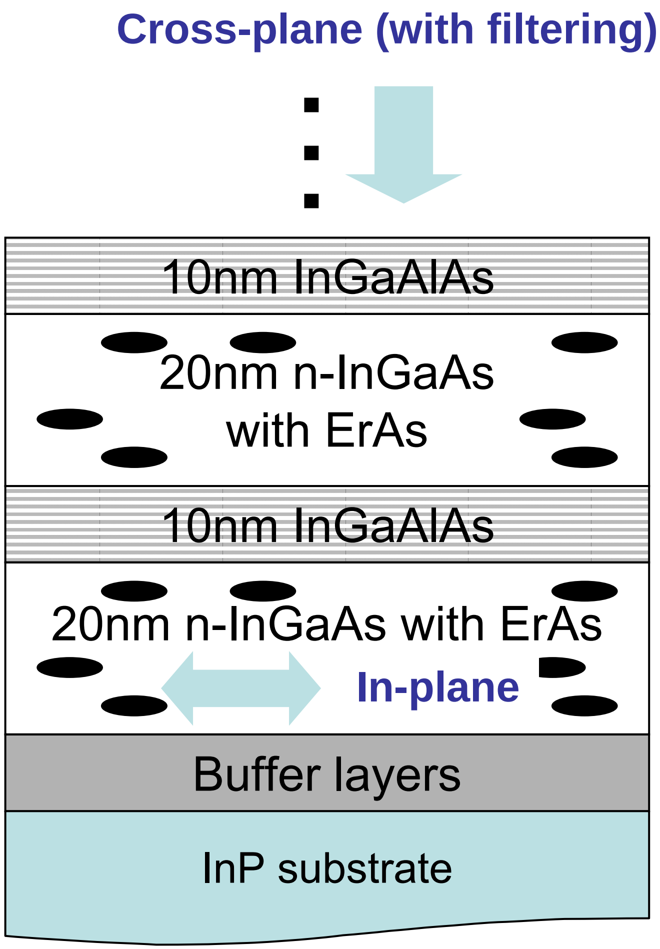


- Energy Filtering in ErAs:InGaAs is small => Small enhancement in Seebeck coefficient

Semi-metal Nanoparticles ➤ Reduce thermal conductivity while improving slightly electrical properties ➤ ZT x2

0.3% ErAs in InGaAs/InGaAlAs Superlattices





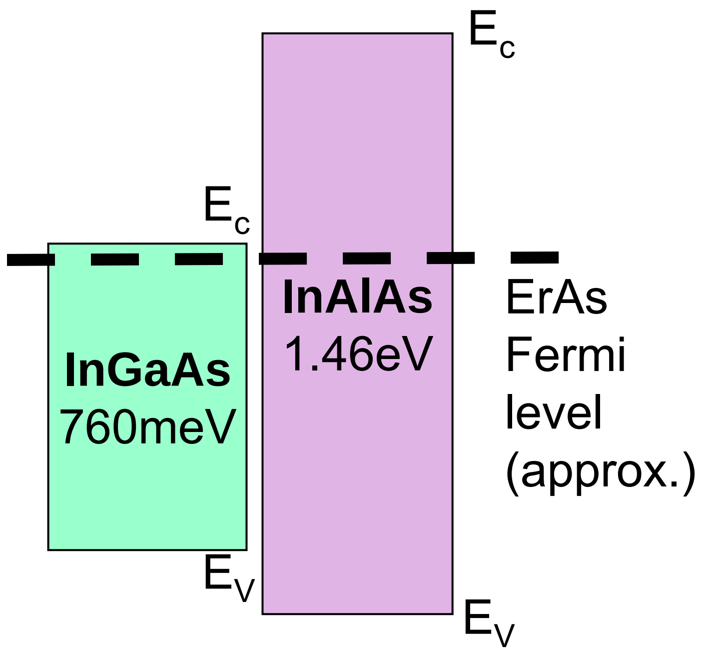
Energy filtering by inserting InGaAlAs layers inside ErAs:InGaAs can enhance cross-plane Seebeck by a factor of 3

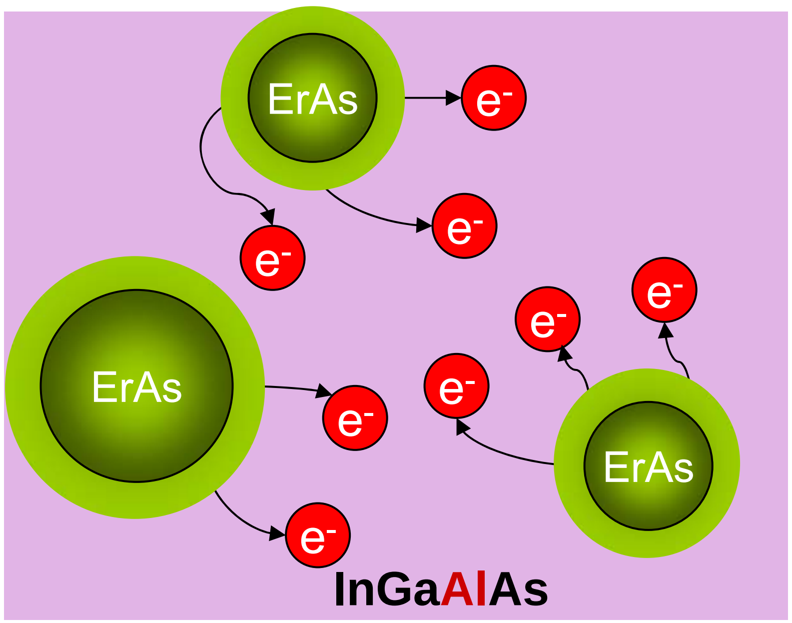
ErAs Semi-metal – InGaAlAs Semiconductor Nanoparticle Composites

Metal nanoparticles

- enhance electrical conductivity
- reduce thermal conductivity
- increase Seebeck coefficient

$$Z = \frac{(Seebeck)^2 (electrical\ \ conductivity)}{(thermal\ \ conductivity)}$$

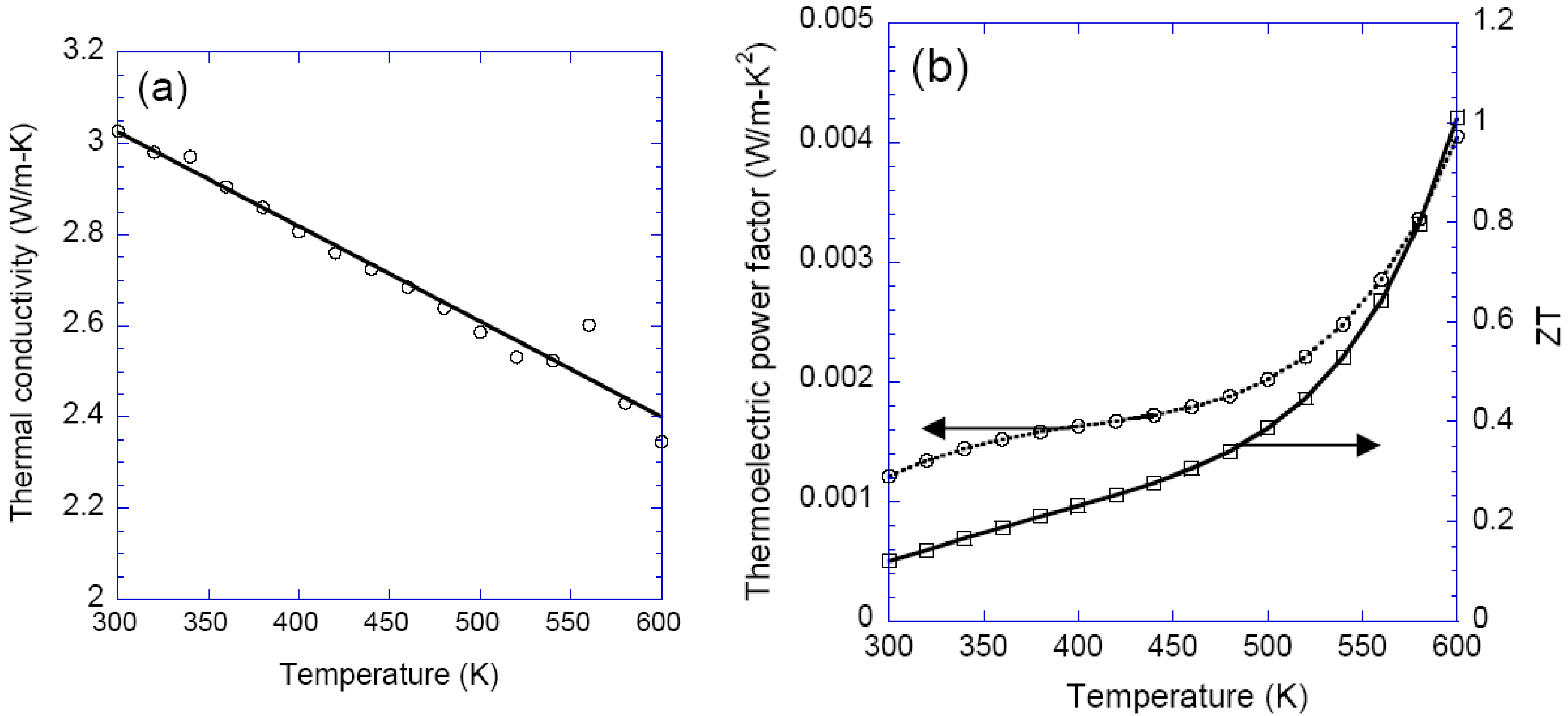




ErAs:InGaAlAs –High Temperature Results

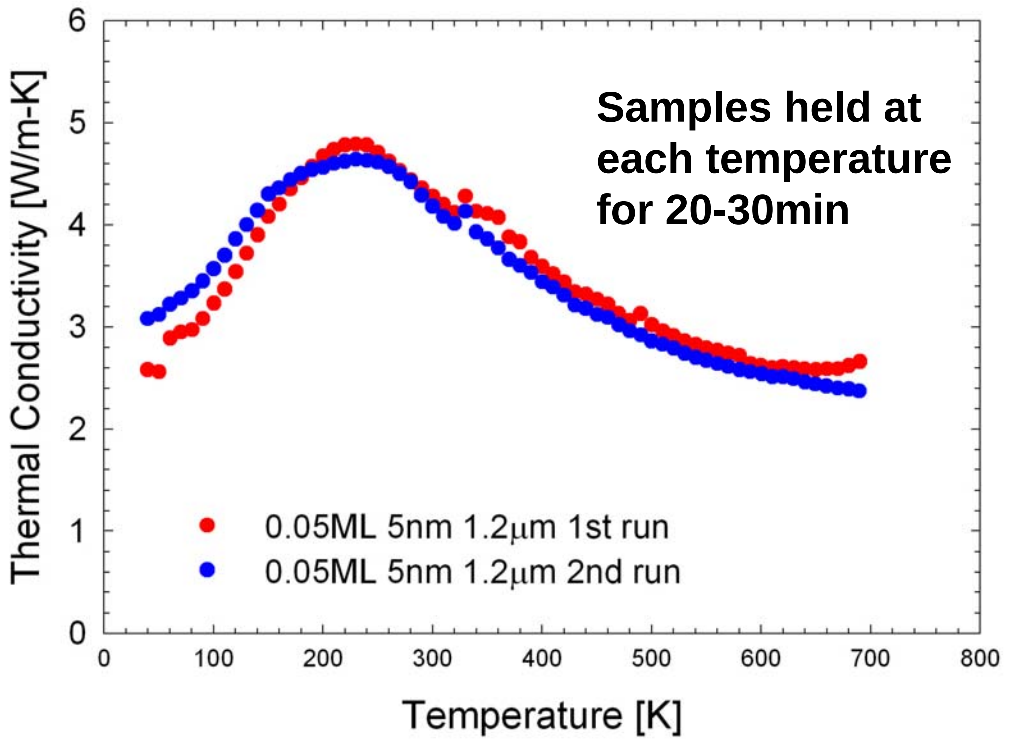
ErAs : InGaAlAs

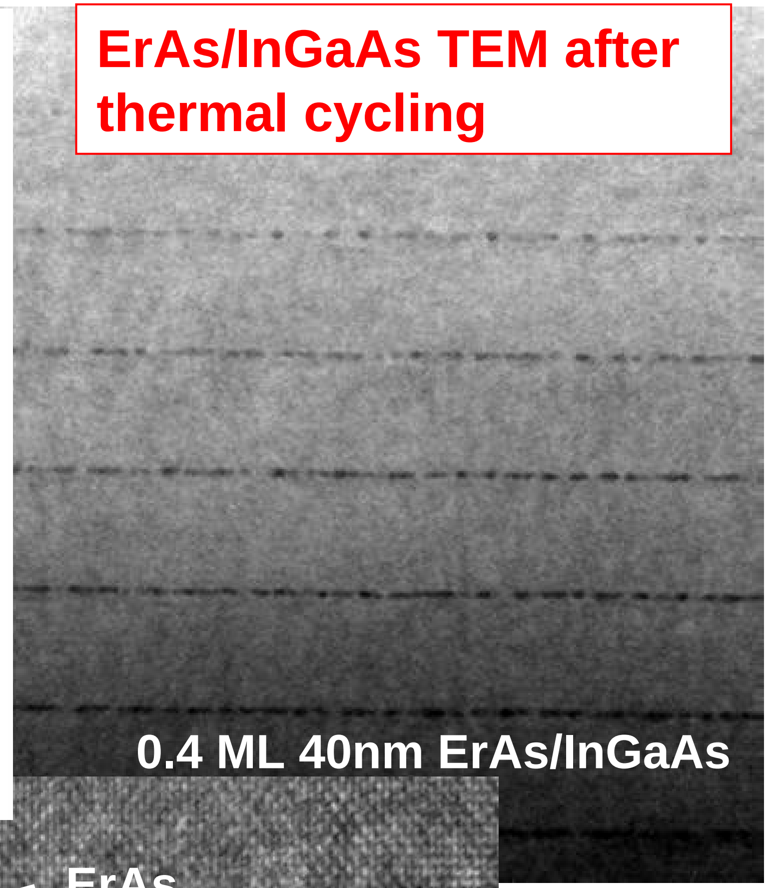
(0.3%) : (20% InAlAs)

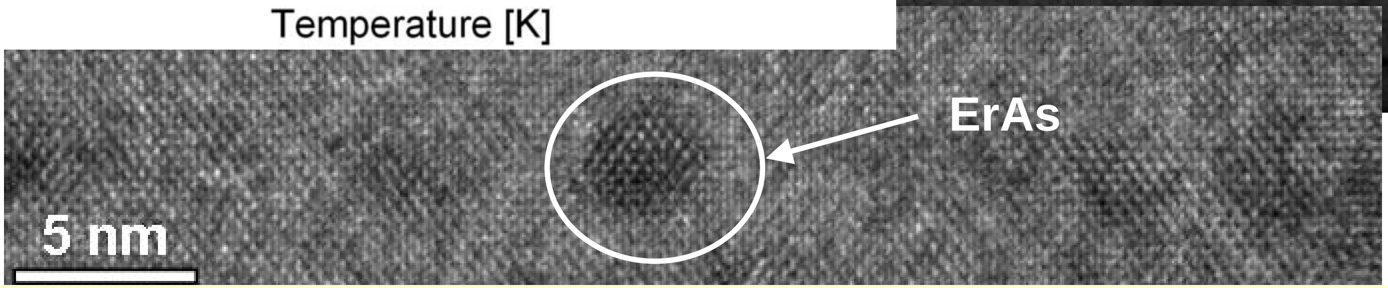


J. Zide, J-H. Bahk, R. Singh, Z. Bian et al. APL 2007

High Temperature Stability of Nanostructures



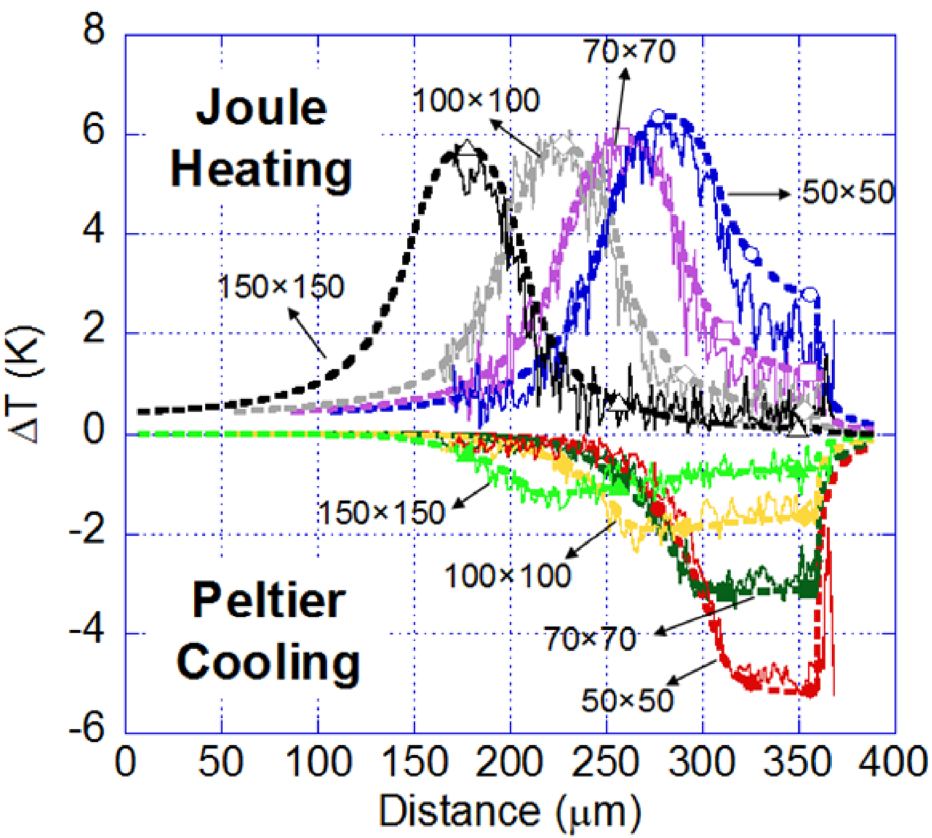


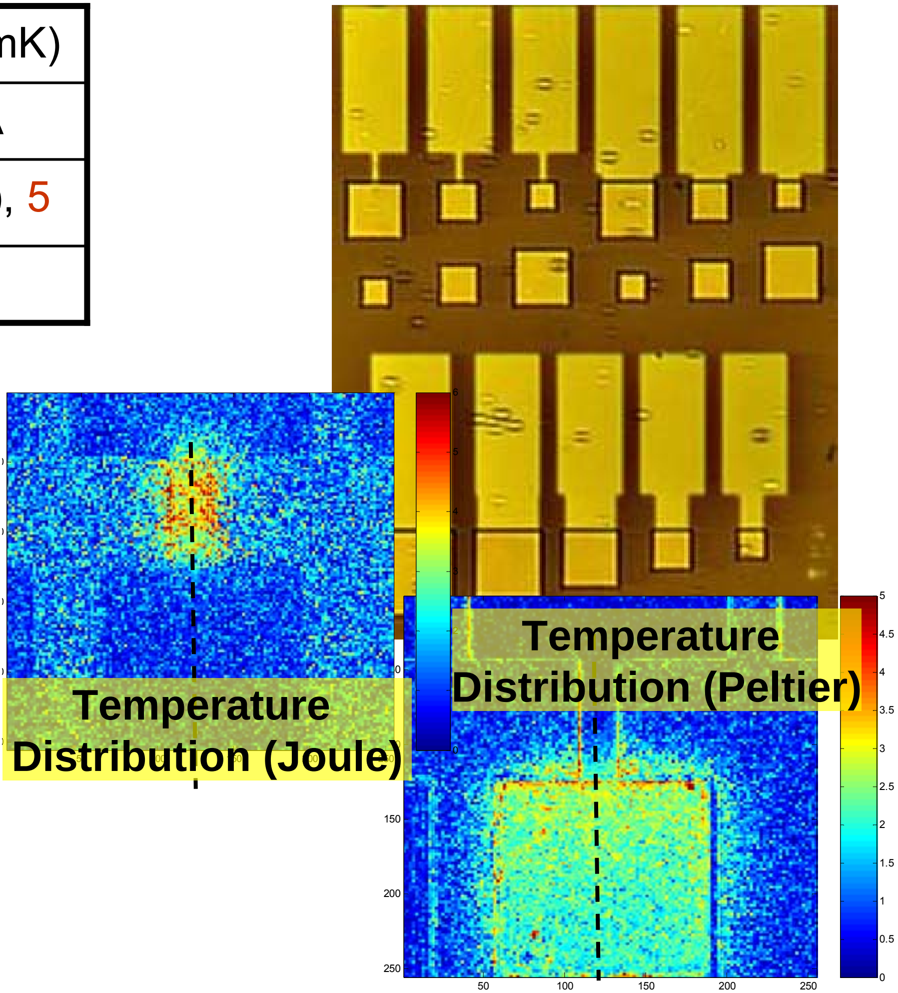


ErAs nanoparticles still visible in TEM after two cycles to 700K. No change in thermal conductivity

Extraction of Thin-film ZT

	S(μV/K)	σ(/Ωcm)	K (W/mK)
In-plane data	-224	348	N/A
Cross-plane	-233	347	3 (3ω), 5
Finite Element	-220	330	5

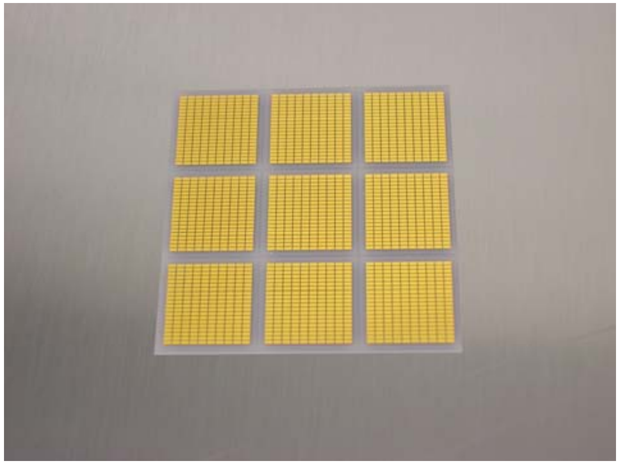


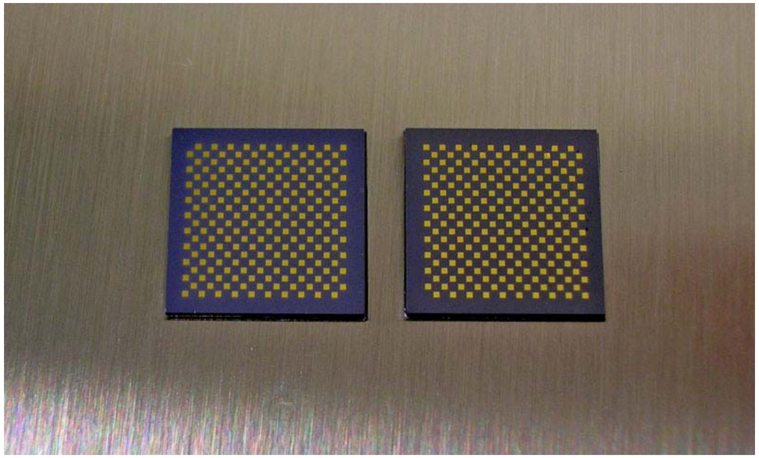


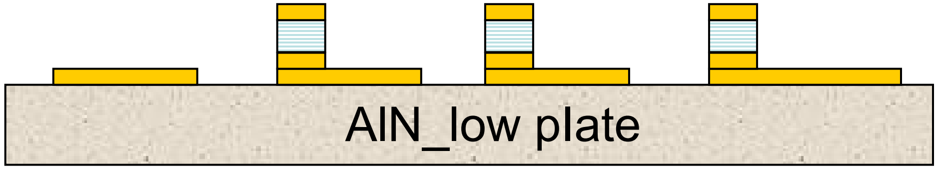
Single element microrefrigerator used to extract all thermoelectric properties of 20μm films

Wafer scale module fabrication

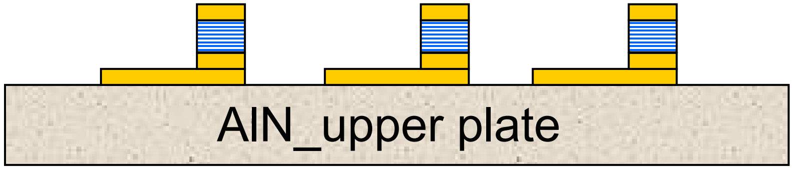
AS 4/28/2008



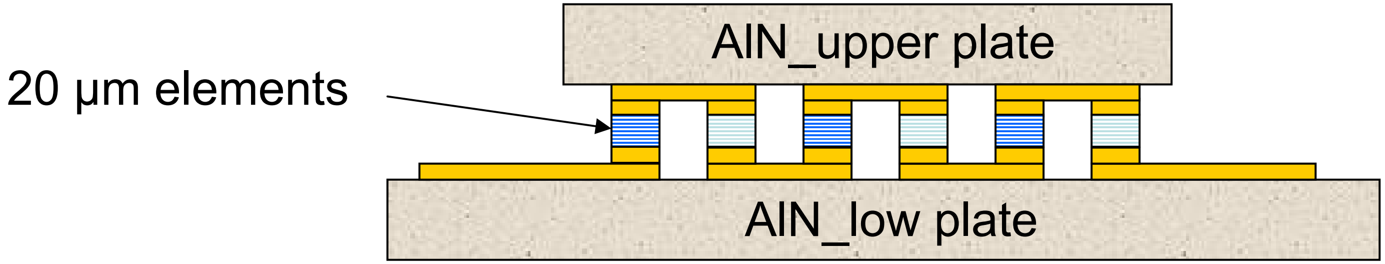




200 elements of p-ErAs array



200 elements of n-ErAs array



400 element generator

Gehong Zeng, John Bowers (UCSB)

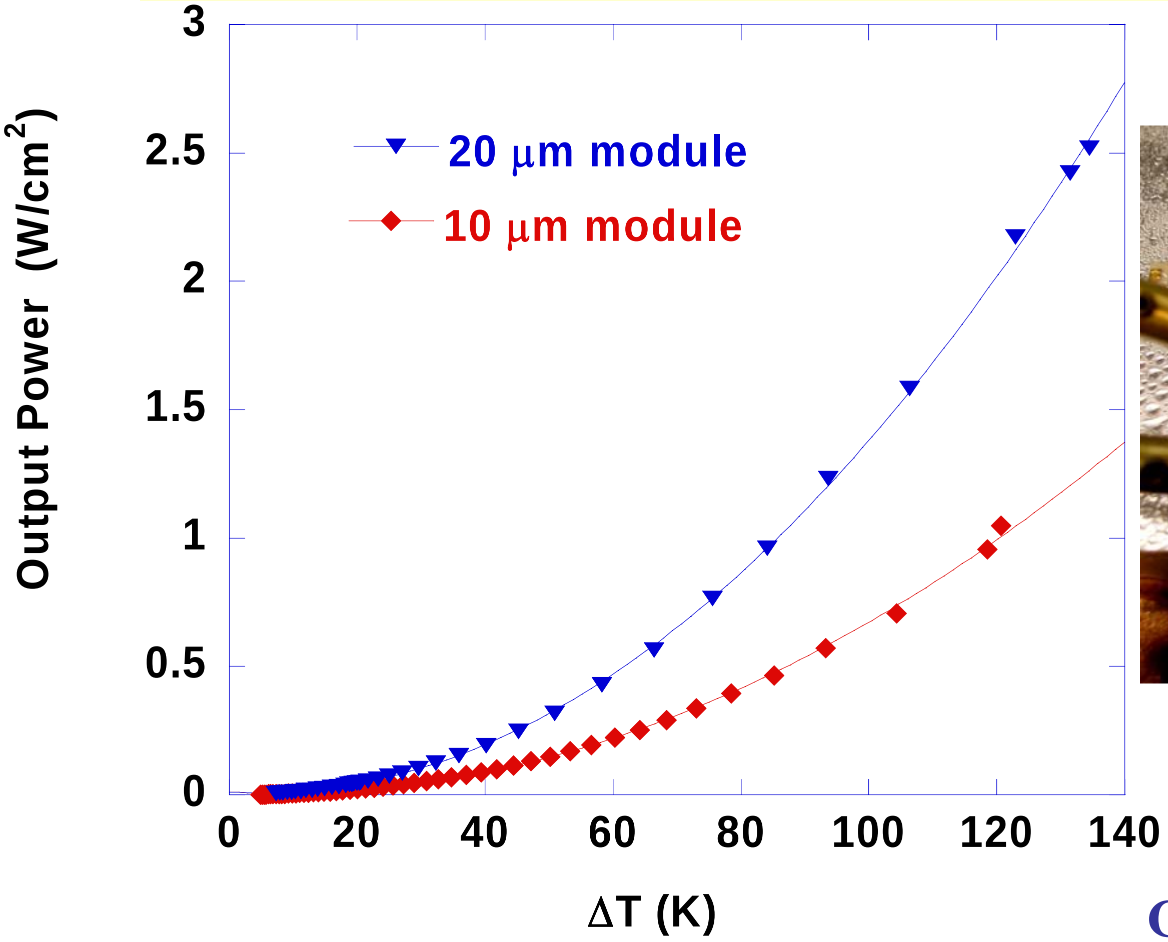
Module Fabrication

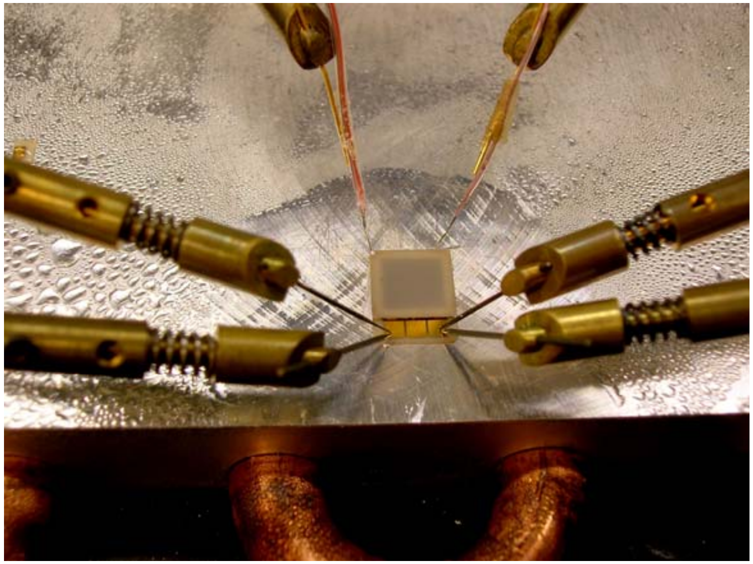
400 element ErAs:InGaAlAs thin film generator

Gehong Zeng, John Bowers (UCSB)

Module Power generation results

400 elements (10-20 microns ErAs:InGaAlAs thin films, 120x120μm^2)

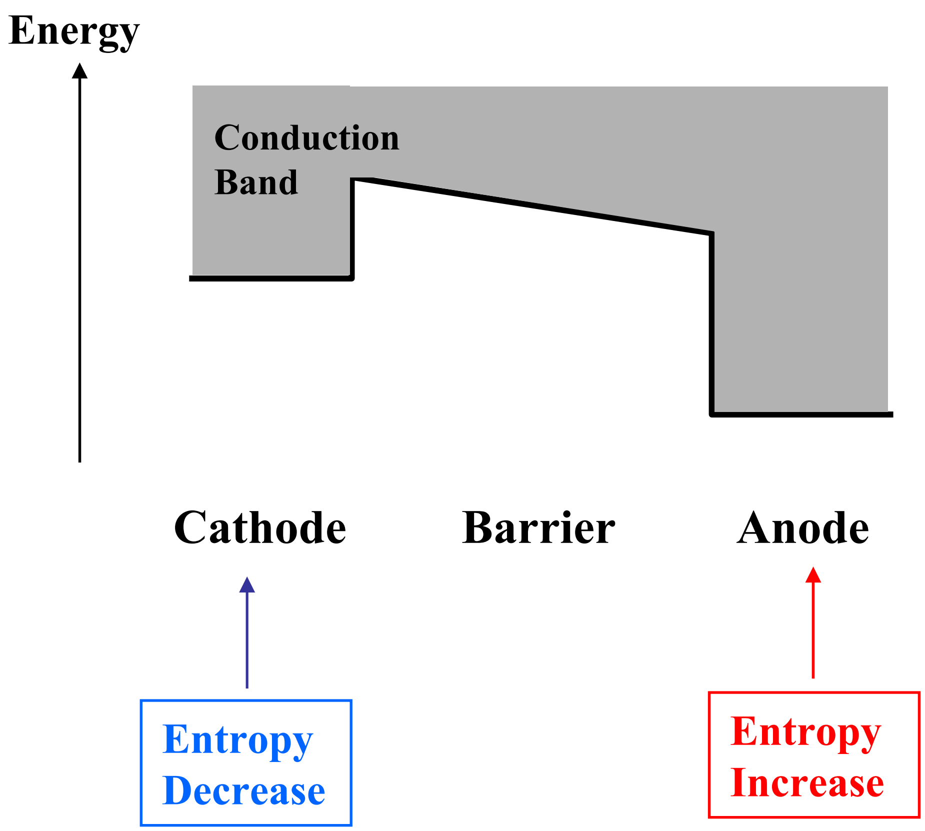




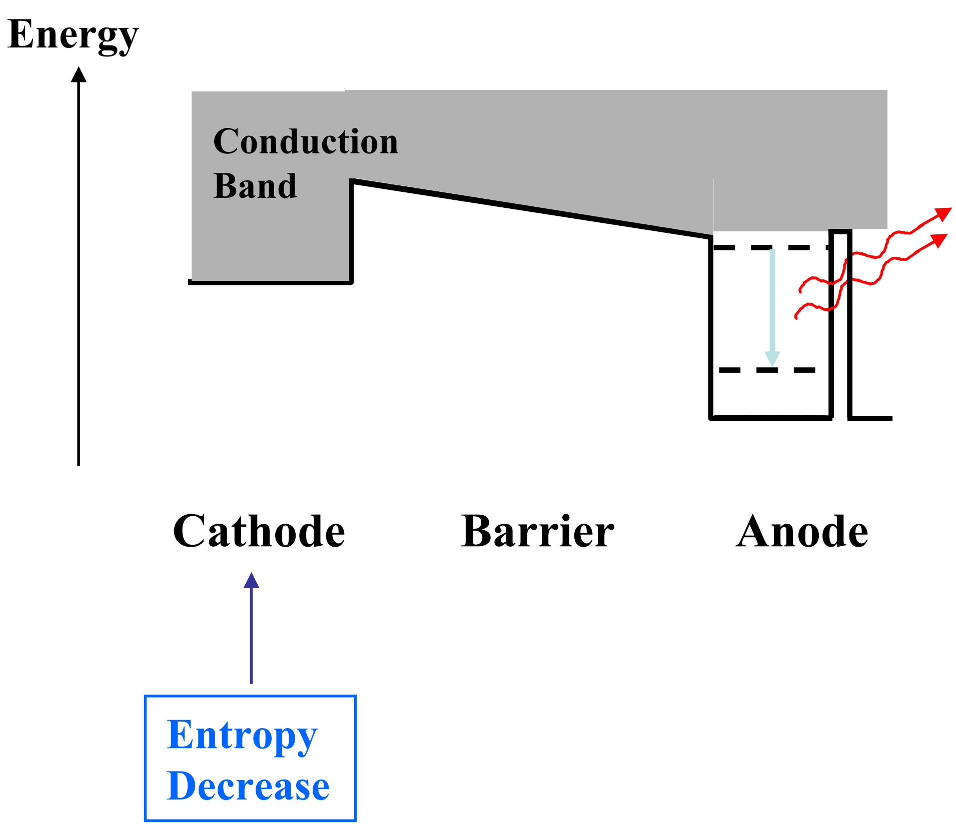
140 μm/140 μm AlN

G. Zeng, J. Bowers, et al. (UCSB, UCSC) Appl. Physics Letters 2006

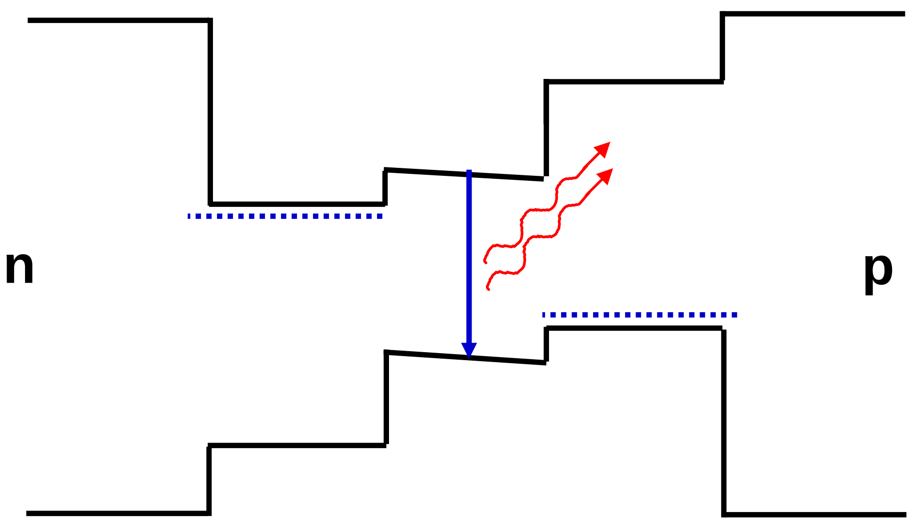
Miniature Refrigerator



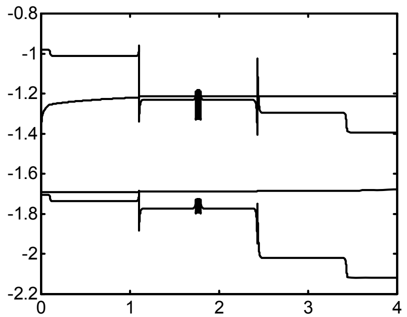
Second Law of Thermodynamics?

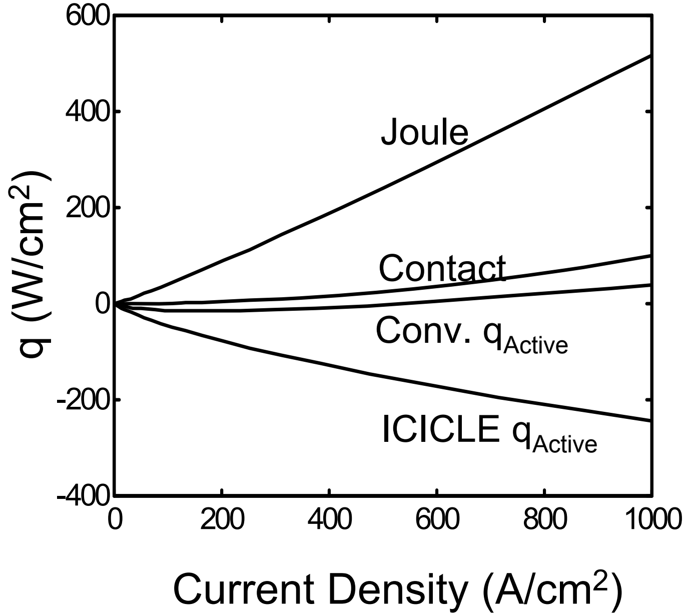


Injection Current Internally Cooled Light Emitter



GaSb/GaInAsSb.





Electrically pumped "optical refrigeration"

Kevin Pipe, Rajeev Ram and Ali Shakouri, Photonic Techn. Lett., Apr. 2002

Summary

- Micro Refrigerators on a Chip (Si, III-V)
  - Localized cooling 10 –150μm, Cooling power density > 500 W/cm^2
- Thermoreflectance Imaging
  – Visible, near IR (sub microns, 0.006K, 1μs)
- Thermal Runaway in Electro absorption Modulators
- Direct Thermal to Electric Energy Conversion
  - Metal/semiconductor nanocomposites for improved solid-state thermionic energy conversion.
- Opto Thermo Electronic Optimization Devices
  - Internal cooling of semiconductor lasers

Acknowledgement: ONR MURI, DARPA Heretic, Packard Foundation, NSF

Question & Answer