Characterization, Devices, and Modeling

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OUTLINE

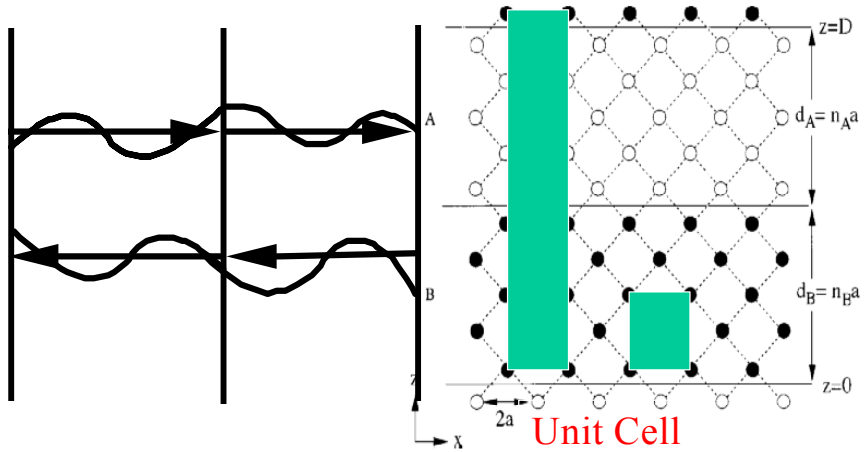
- **Summary of Major Results**

  Thermal Conductivity Reduction Mechanisms
  Anisotropic Thermal Conductivity Measurements
  Seebeck/Electrical Conductivity Measurements
  Broader Nanoscale Transport Modeling

- **Research in the Fifth Year**

  Seebeck Coefficient Measurements
  Quantum Dots Thermal Properties
  Nanowire Thermal Properties
  CVD-Based Device Fabrication
  Modeling on Thermoelectric Transport

Phonon Heat Conduction in Superlattices



Two Wave Pictures:

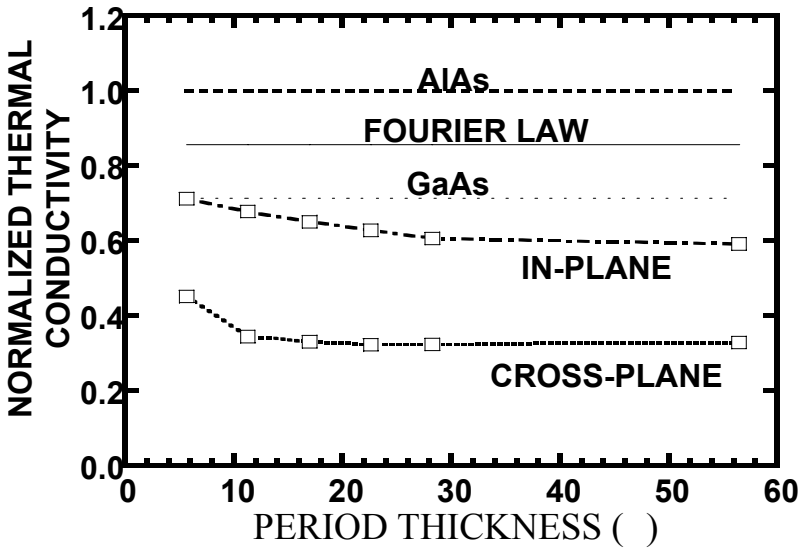
(a) Inhomogeneous Multilayer With Coherent Phonons: Interference Stop Bands, and Tunneling, Extended Wave Through Superlattices

(b) Homogeneous Material with Super Unit Cell: Group Velocity Reduction

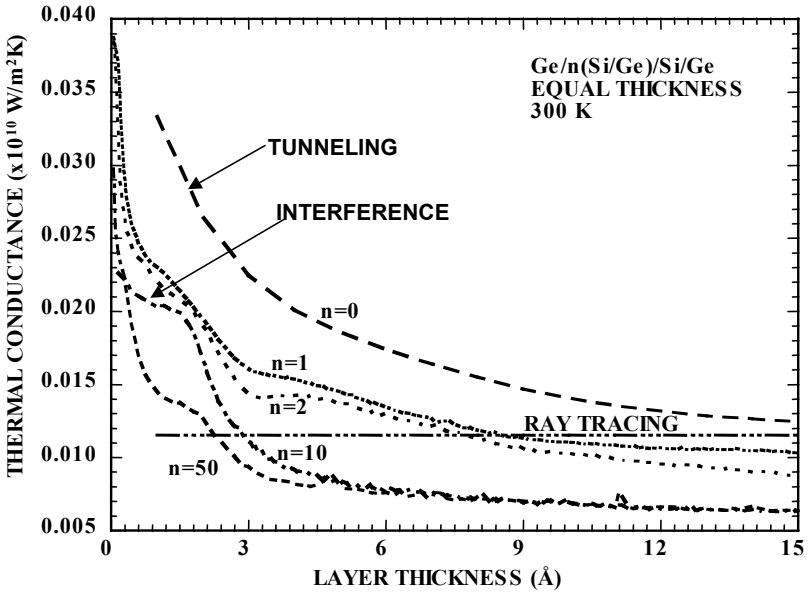
Conclusion:

Two Methods Equivalent in Physics

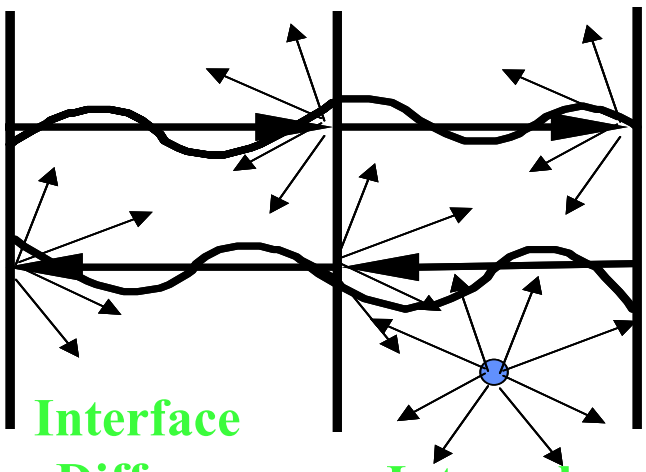
Neither Explains Majority Data



Lattice Dynamics



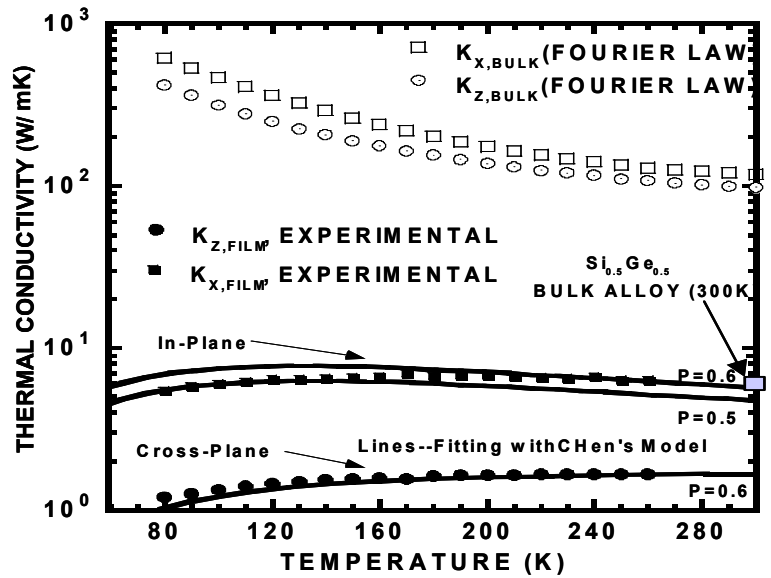
Incoherent Models

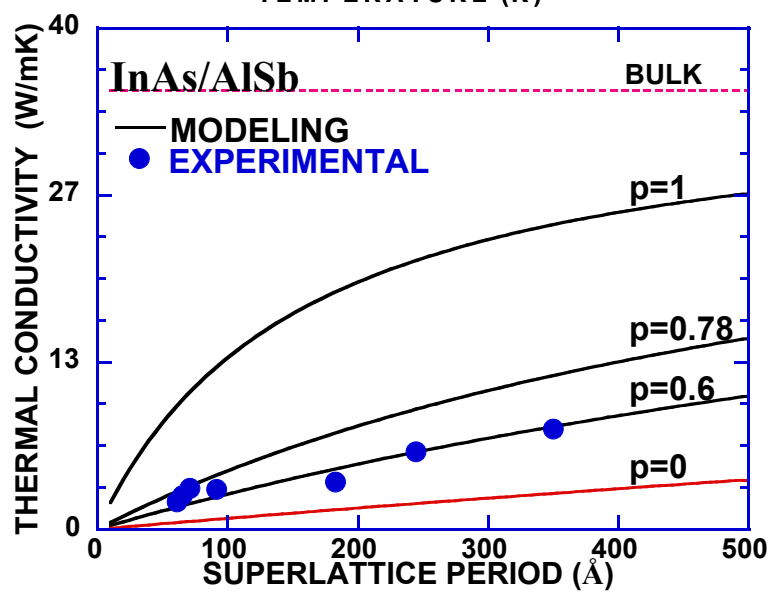


Interface Diffuse Scattering

Internal Scattering

Physical Processes





Major Conclusions:

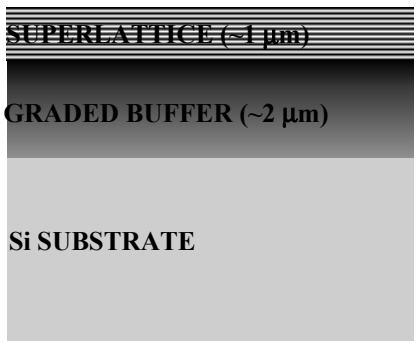
(1) Single Interface Scattering Dominant

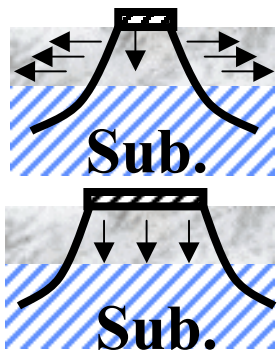
(2) In-Plane Reduction due to Diffuse Interface Scattering.

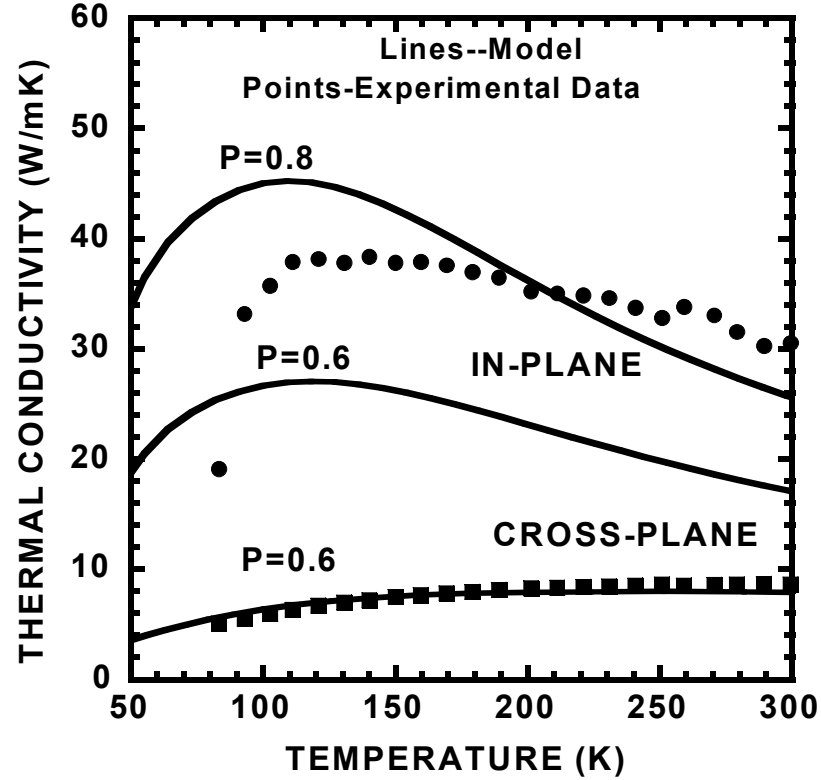
(3) Both Specular and Diffuse Reflection Reduce Cross-Plane Conductivity.

(4) Recovery of Thermal Conductivity at Very Thin Film Limit due to Tunneling or Alloying Effects.

THERMAL CONDUCTIVITY MEASUREMENTS







Major Challenges:

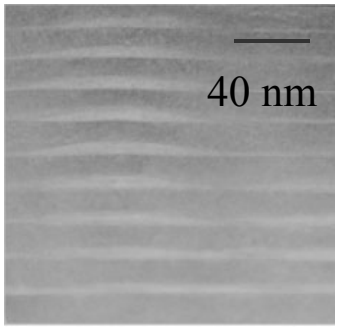
Buffer Properties Unknown
Semiconducting Films
Unknown Insulator Property
Anisotropic Thermal Conductivity

Solutions:

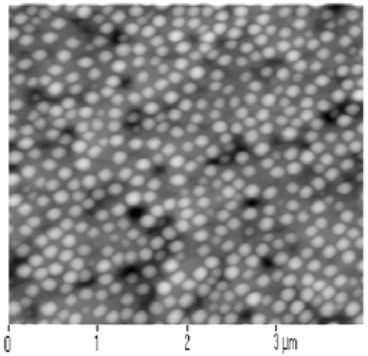
2-Wire 3ω Method
Reference Substraction
Modeling to Extract Anisotropy

Samples Studied:

Si/Ge, Si/SiGe, Si/Ge Dots
$CoSb_3/IrSb_3$, Bi/Sb, B_4C/B_9C
GaAs/AlAs, InAs/AlSb
Nanoporous Bismuth

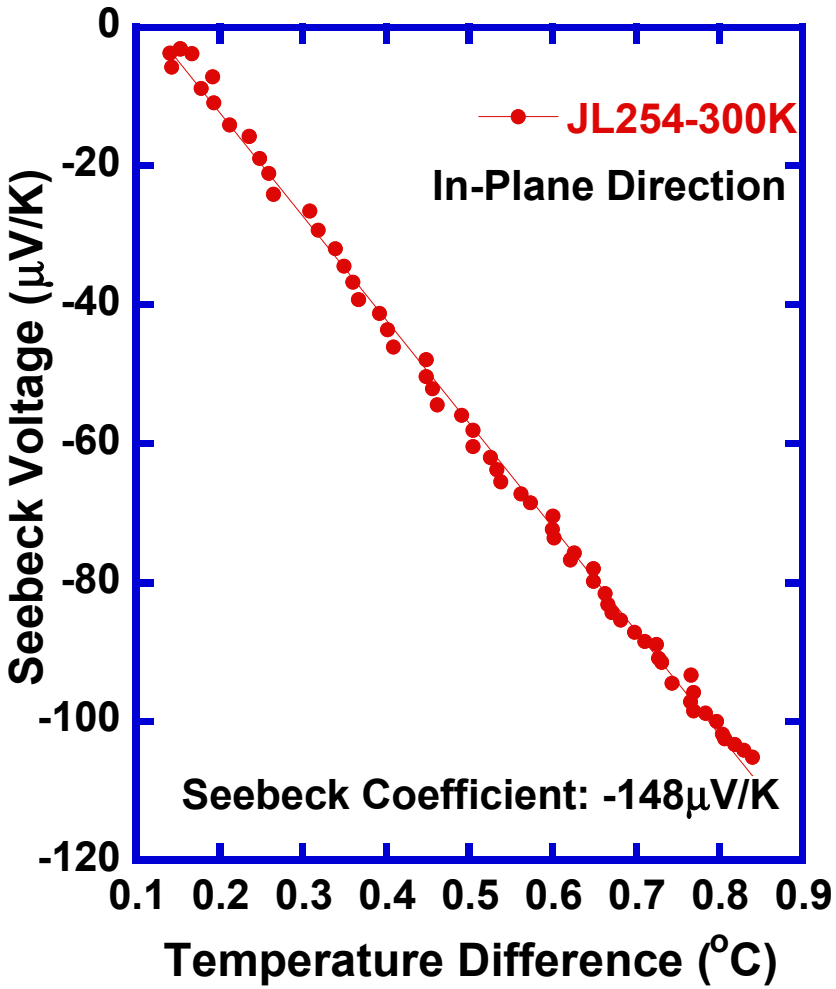


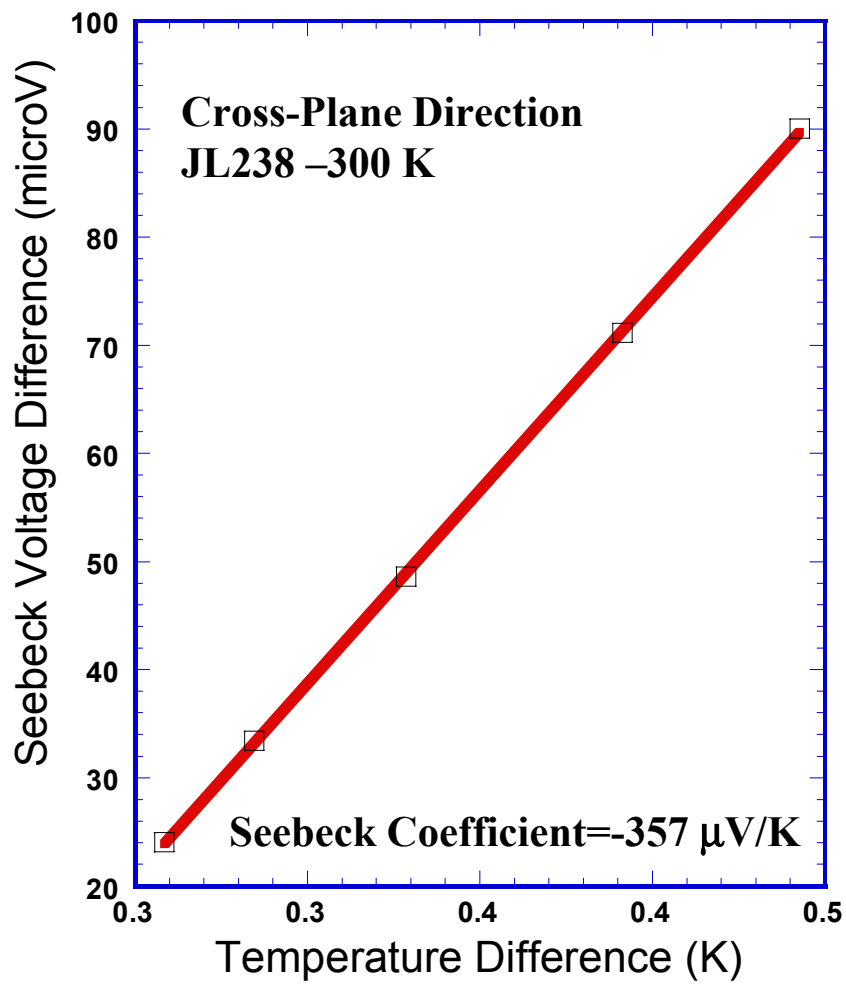
(a)



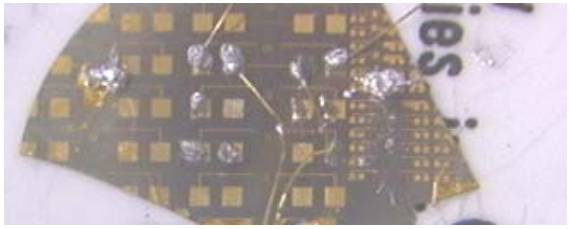
(b)

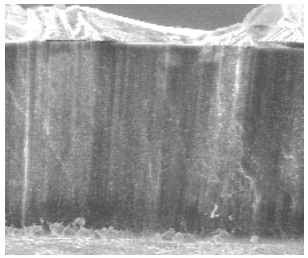
THERMOELECTRIC PROPERTIES

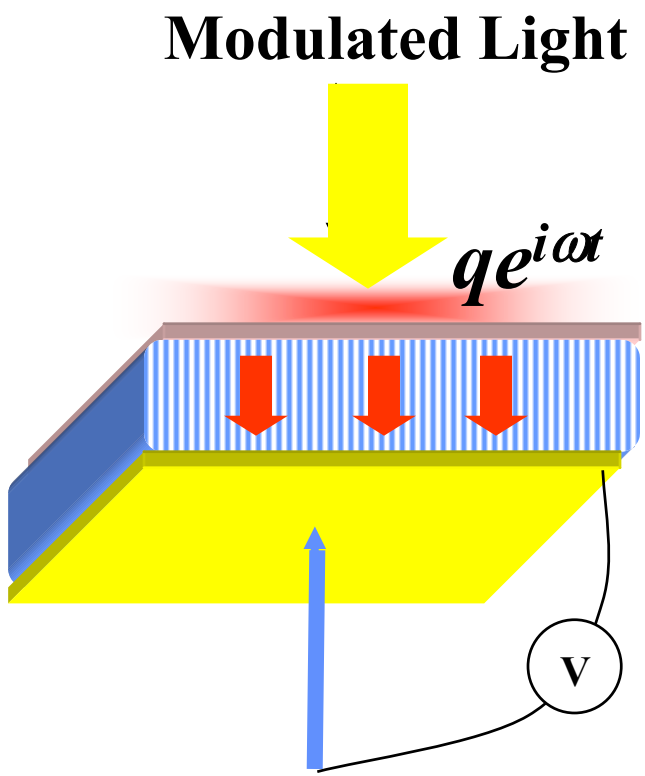


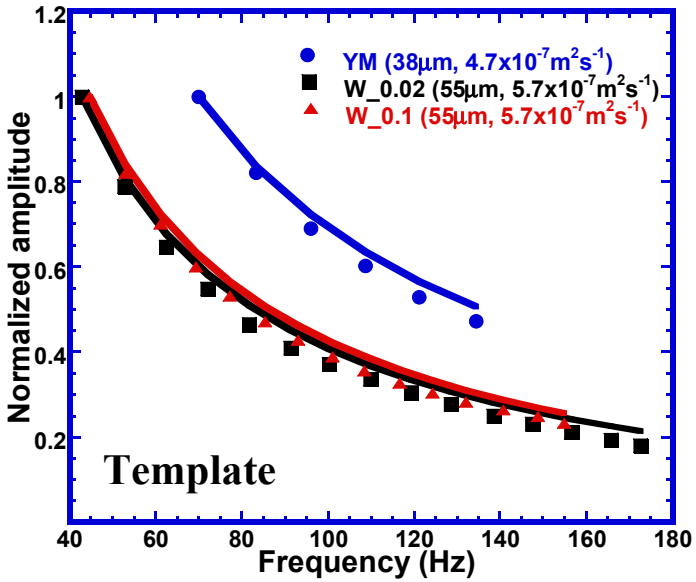


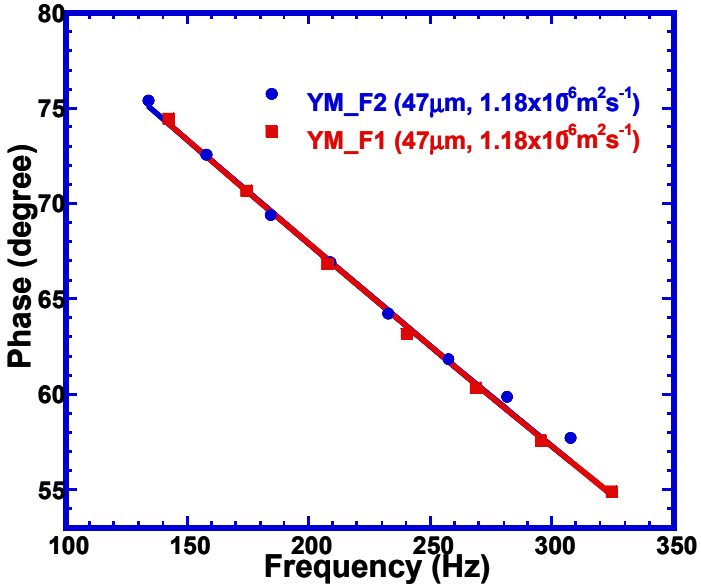
NANOWIRE THERMAL MEASUREMENTS



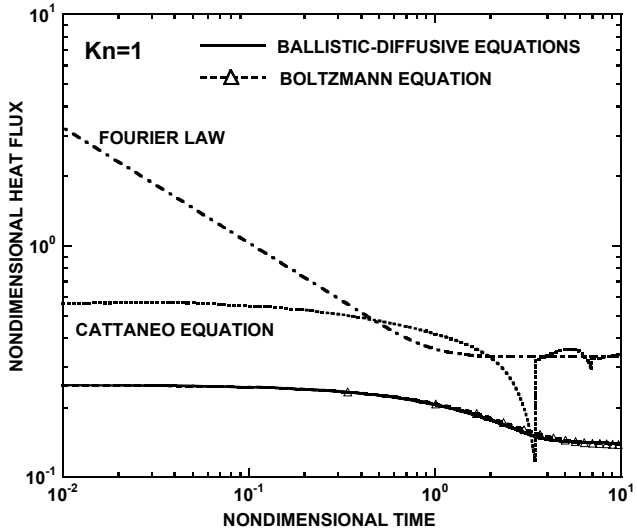








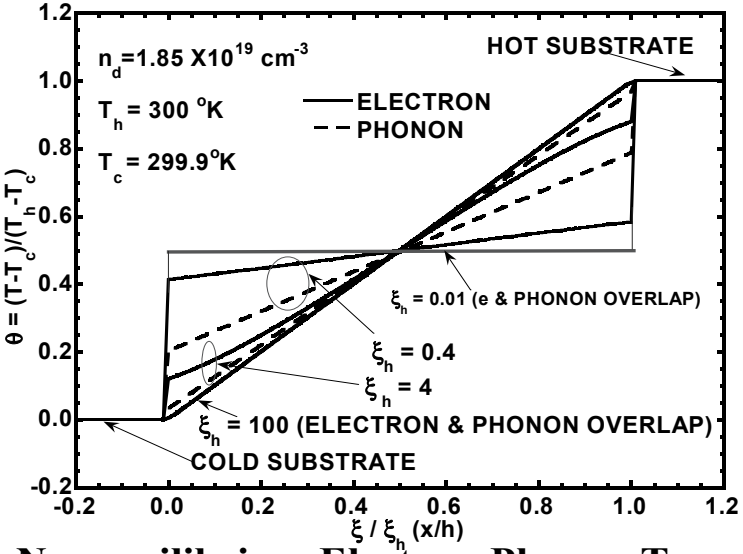
BASIC TRANSPORT THEORY



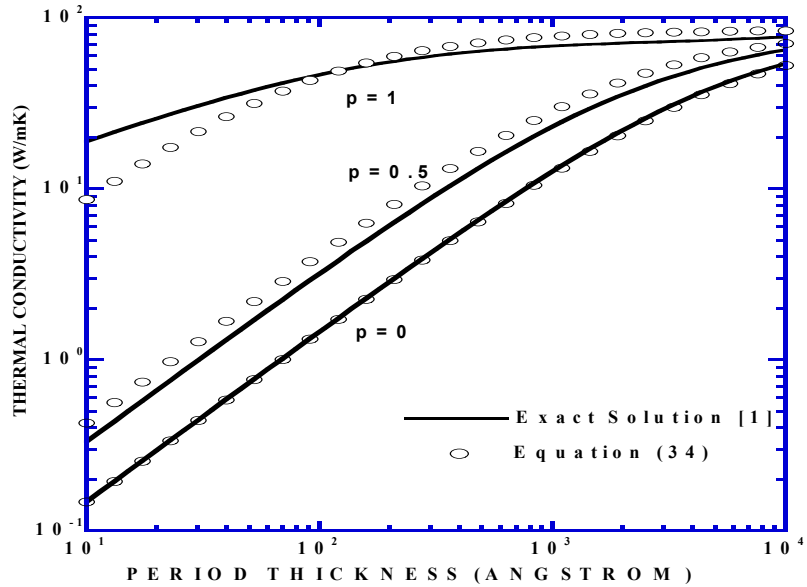
Ballistic-diffusive equations

Major Results

- Established ballistic-diffusive heat conduction for phonon transport in nanostructures.
- First model treating nonequilibrium electron, nonequilibrium phonon, and nonequilibrium electron phonon interactions.
- Diffusion-transmission boundary condition: (1) a new thermionic emission formula covering arbitrary barrier heights; (2) extension of diffusion theory right to the interface.



Nonequilibrium Electron-Phonon Transport



Diffusion-Transmission Boundary Condition

TEAM WORK AND COLLABORATION

Dresselhaus: Superlattice Modeling and Combined Electrical and Thermal Modeling
Nanowire Thermal Conductivity Measurements, Modeling, …
Dunn: Nanoporous Bismuth Measurement.
Ehrlich: Measurement Techniques (including Browning and Fulla-Mora)
Elsner/Ghamaty: B_4C/B_7C Measurements.
Fleurial: Nanowires, Device Fabrication, Cooling Applications.
Goorsky: Interface Characterization and Thickness Measurement.
Gronsky: Si/Ge Characterization for Explaining Superlattice Results.
Kim: Device Fabrication and MEMS Techniques.
Lyon: Learning in Applications.
Reinecke: Bismuth Mean Free Path Estimation.
Sands: Skutterudites Thermal Conductivity Measurements.
Wang: Si/Ge Superlattice Samples, Quantum Dots Samples, Phonon Modeling.
Venkatasubramanian: Round-Robin.

STUDENTS TRAINING AND PUBLICATIONS

Post-Docs:

Dr. Sebastian Volz (25%)
Now Associate Professor at Ecole Centrale de Paris
Dr. Taofang Zeng (50%)
Now Assistant Professor at North Carolina State University

Ph.D. Students:

Dr. T. Borca-Tasciuc (2001)
Now Assistant Professor at Ressenlaer Polytechnic Institute
Dr. D.-J. Yao (2001) (co-Advised with Kim)
Mr. Weili Liu (Ph.D. Expected 2002)
Mr. David Song (Ph.D. Expected 2002)
Mr. Bao Yang (75%, Ph.D. Expected 2002)
Ms. D. Borca-Tasciuc (50%, MS 2001)

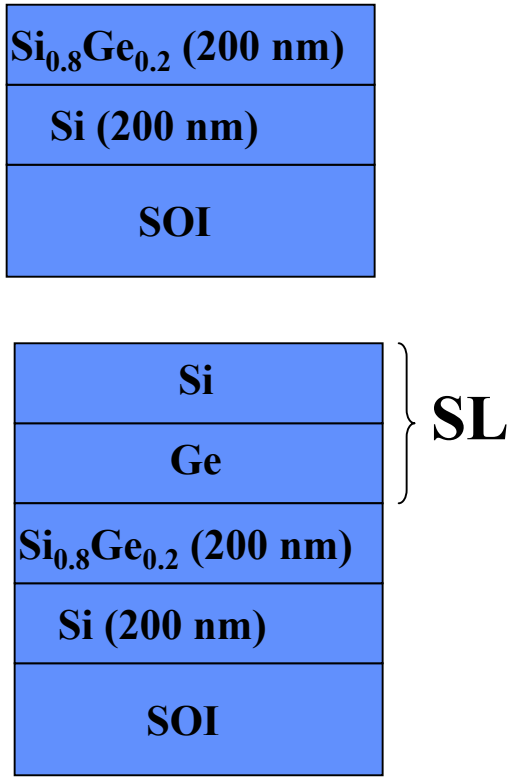
Publications:

2 Book Chapters; 1 Book (Target to Finish 2002);
? Invited Papers ? Journal Papers;
? Invited Conference Presentations; ? Conference Papers

ANISOTROPIC THERMOELECTRIC PROPERTIES OF SUPERLATTICES

Targeted Properties

- **Anisotropic Thermal Conductivity**
- **Anisotropic Seebeck Coefficient**
- **Anisotropic Electrical Conductivity**
- **Thickness Dependency of Properties**

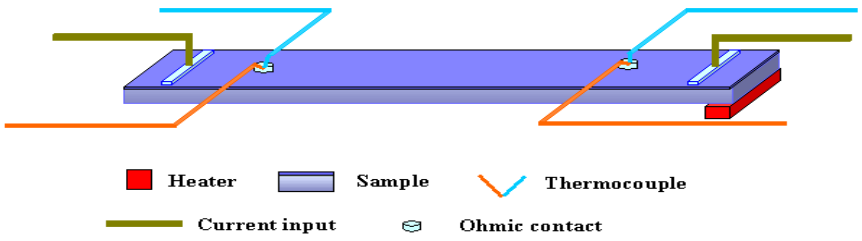


Sample	period	Si (A)	Ge (A)
JL254	91	88	22
JL255	133	60	15
JL256	250	32	8

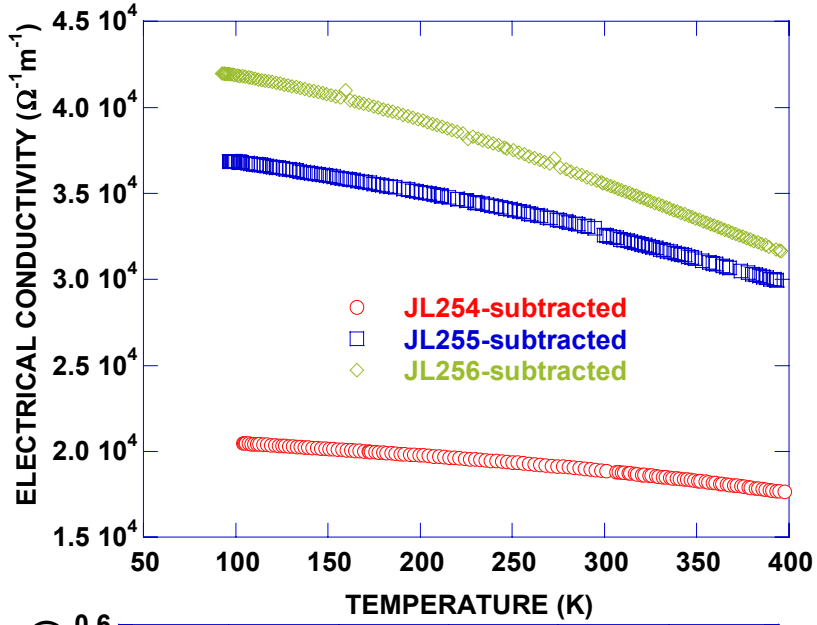
Buffer doping: n-type doping ~2×10^{18} cm^{-3}

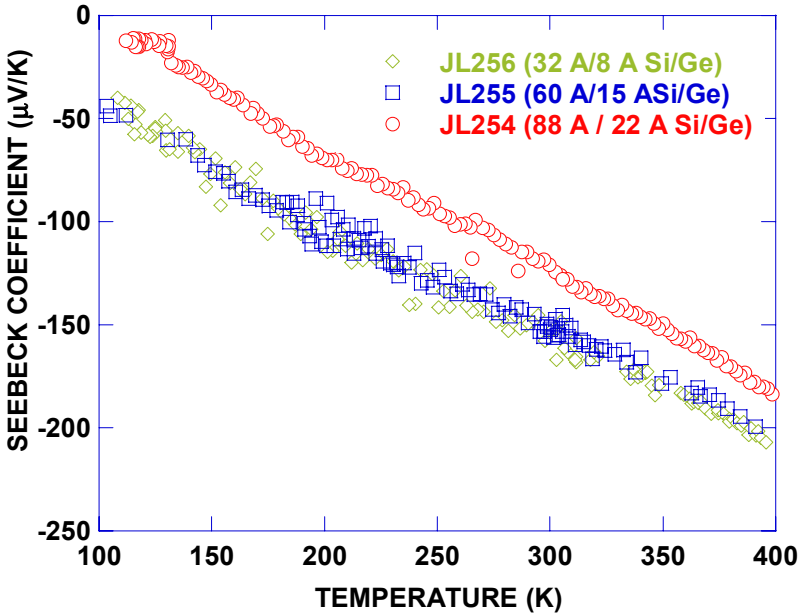
SL doping: n-type doping ~1×10^{19} cm^{-3}

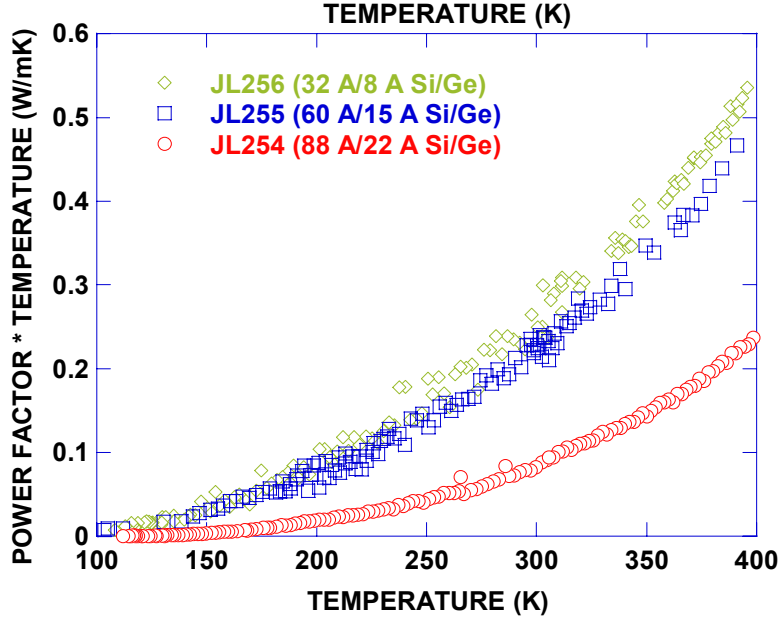
IN-PLANE POWER FACTOR MEASUREMENTS



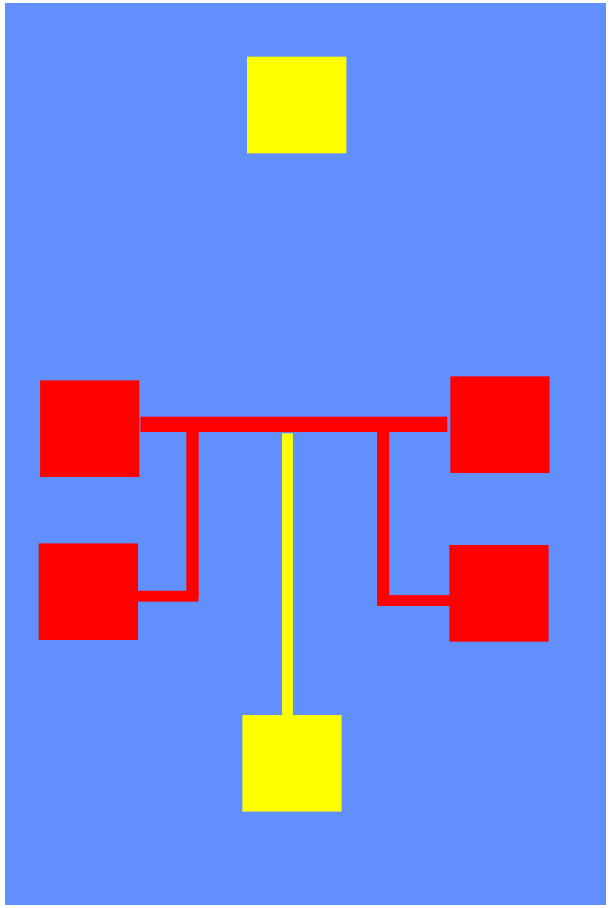
Seebeck and Electrical Conductivity Measurements Buffer Effects Subtracted



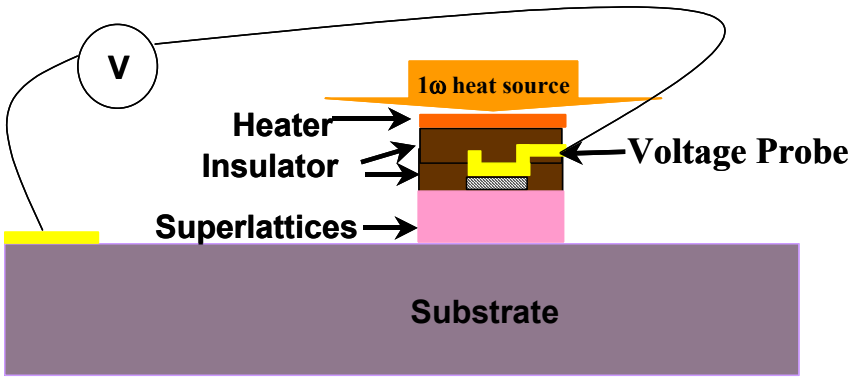




CROSS-PLANE SEEBECK MEASUREMENT



SUPERLATTICES SAMPLE



Differential Method:

SL Sample: Thick SL Layer

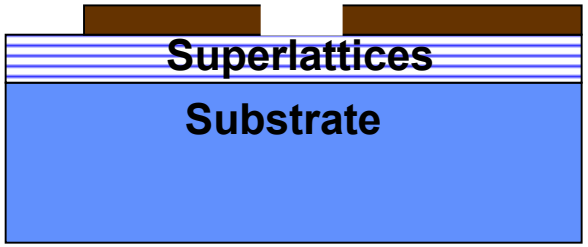
Reference Sample: Thin SL layer

Seebeck= $(V_{SL} - V_{Ref})/(T_{SL} - T_{1Ref})$

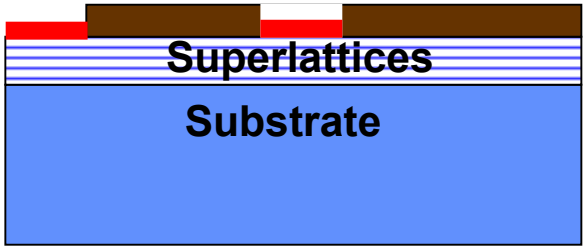
Differential 3ω for $T_{SL} - T_{Ref}$

Directly measure $V_{SL} - V_{Ref}$

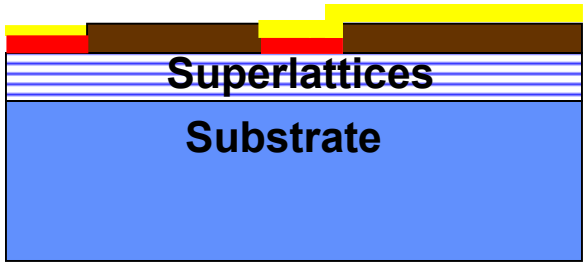
FABRICATION PROCESS



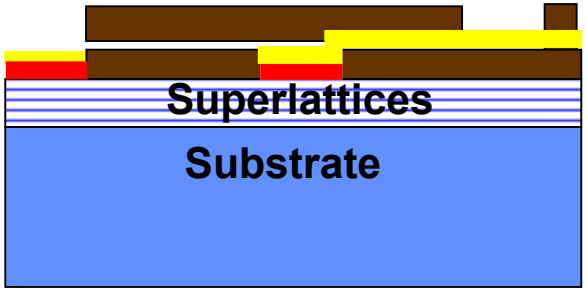
PECVD SiO_2 & OPEN CONTACT WINDOW



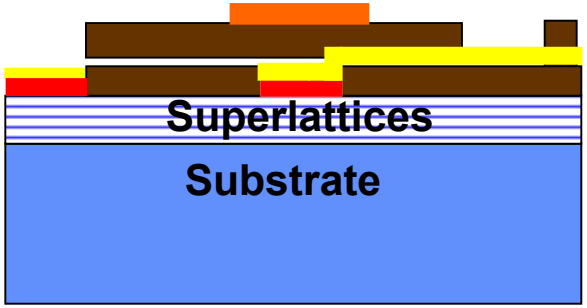
DEPOSIT Ti



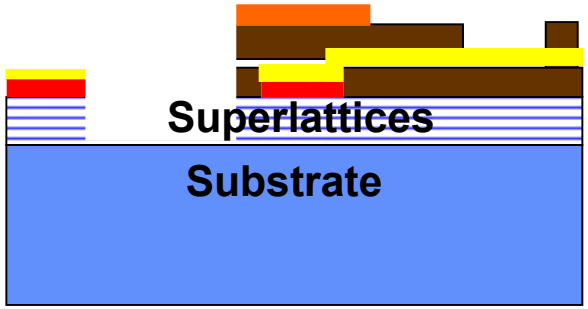
DEPOSIT Ti/Au LEAD



PECVD SiO_2, OPEN CONTACT PADS

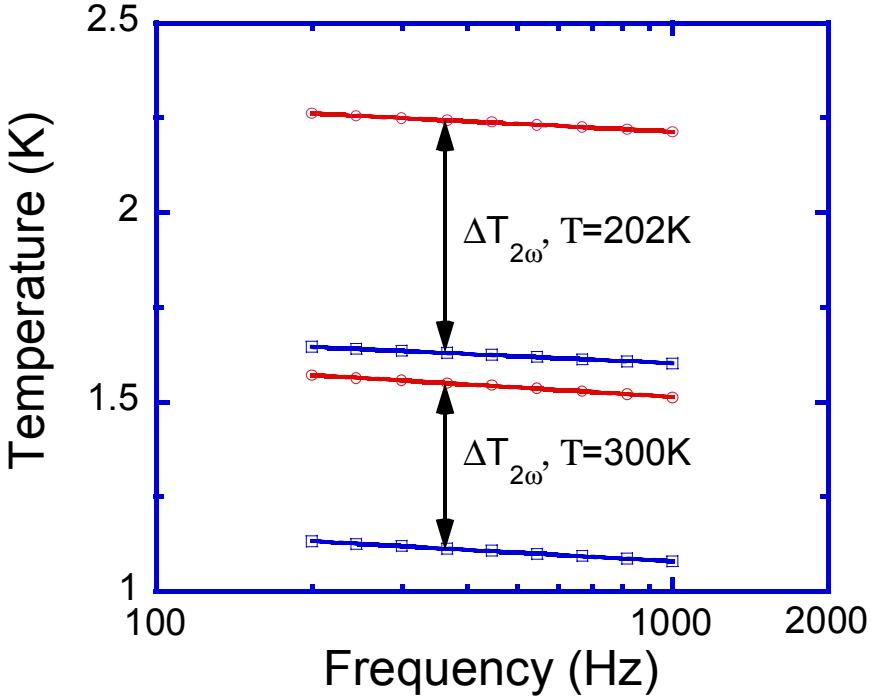


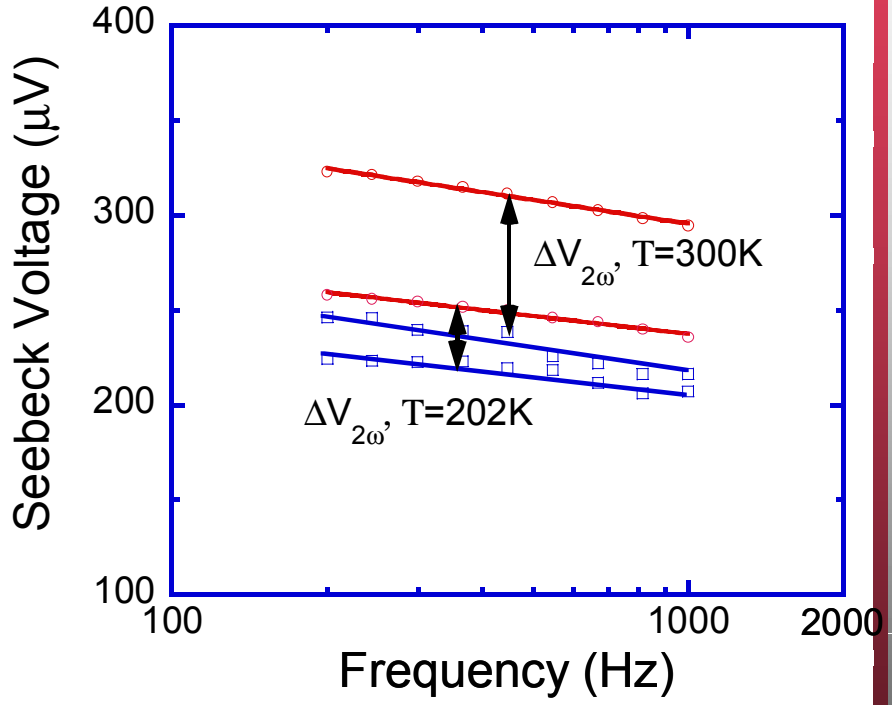
DEPOSIT Au/Cr HEATER



RIE etch mesa structure

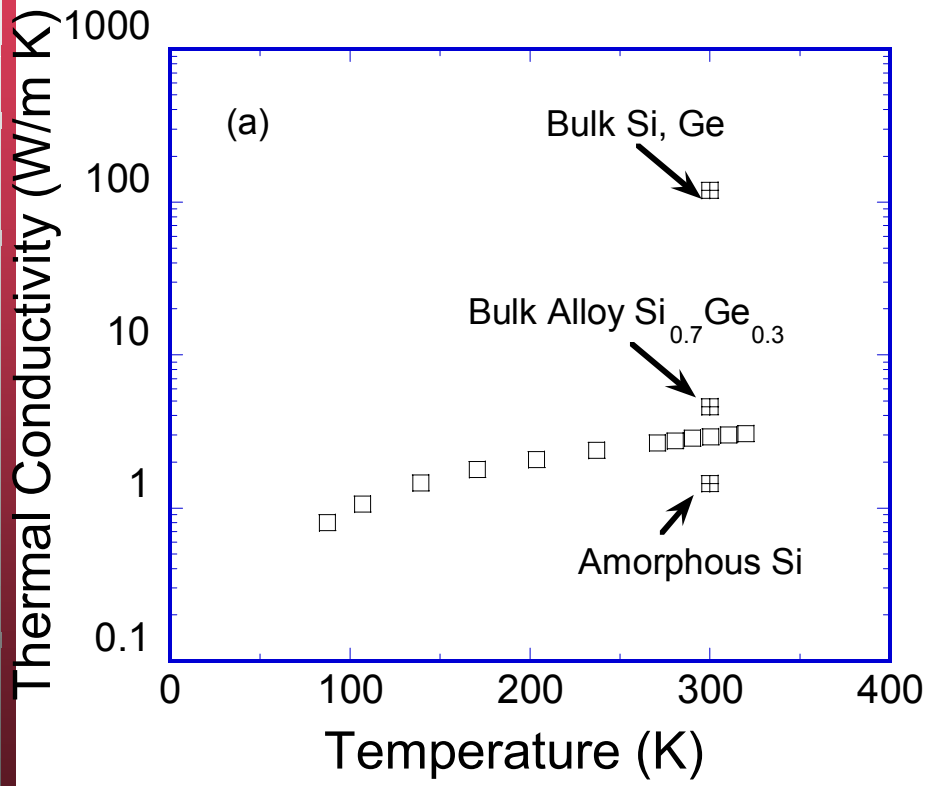
TEMPERATURE & VOLTAGE DATA

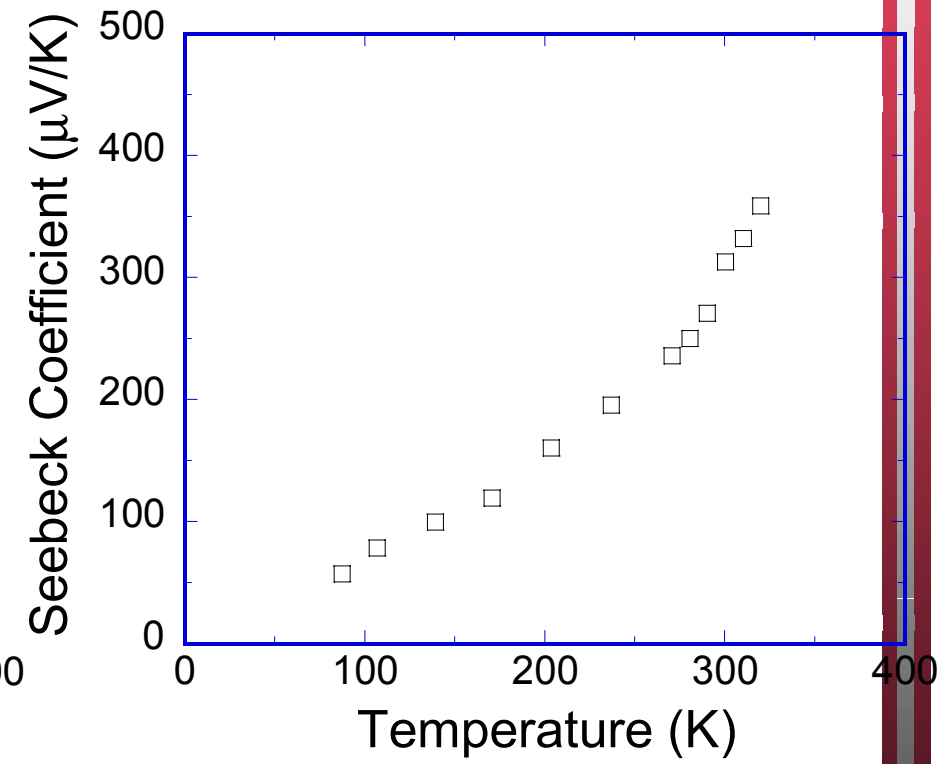




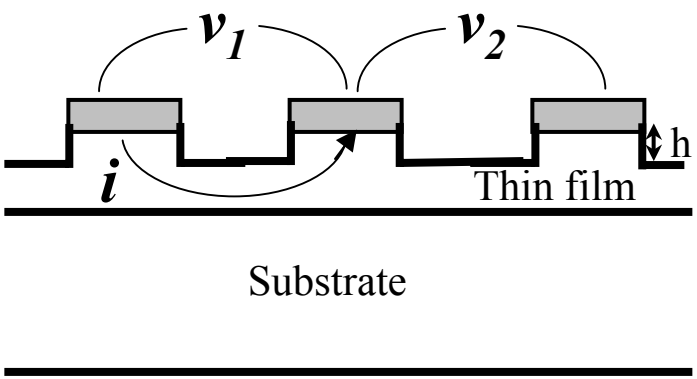
Seebeck Coefficient = Slope of ($\Delta V/\Delta T$)

CROSS PLANE *K* and *S*





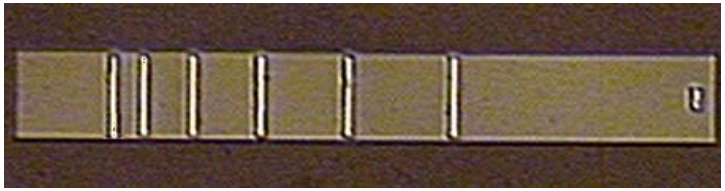
CROSS PLANE ELECTRICAL CONDUCTIVITY



End Contact Resistance:

$$R_e = \frac{\sqrt{\rho_c^* R_s}}{w \cdot Sinh\left(\sqrt{\frac{R_s}{\rho_c^*}} d\right)}$$

Cross-plane Resistivity:

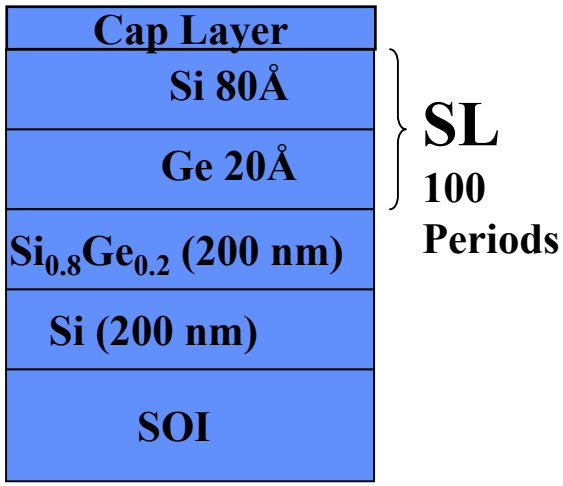


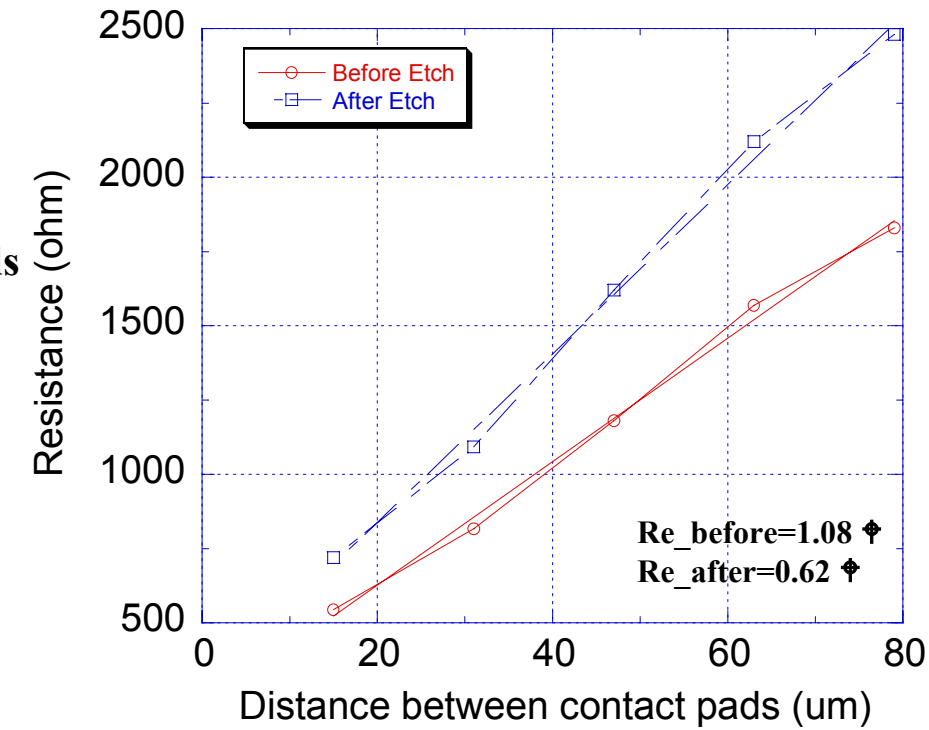
Solution:

TLM + Mesa Structure

$$\rho_c^* = \rho_c + \rho_{cross-plane} \cdot h$$

ANISOTROPIC ELECTRICAL CONDUCTIVITY

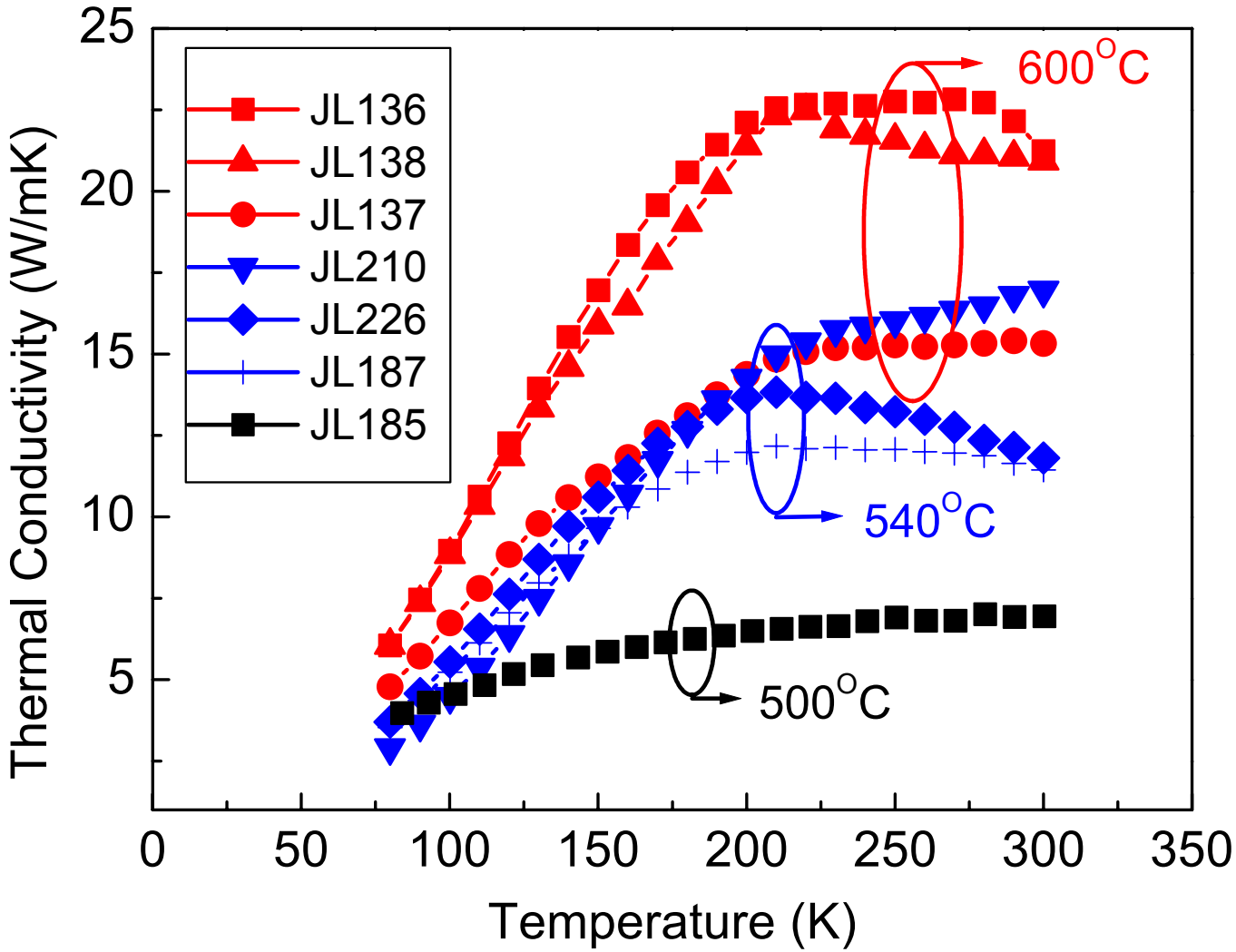




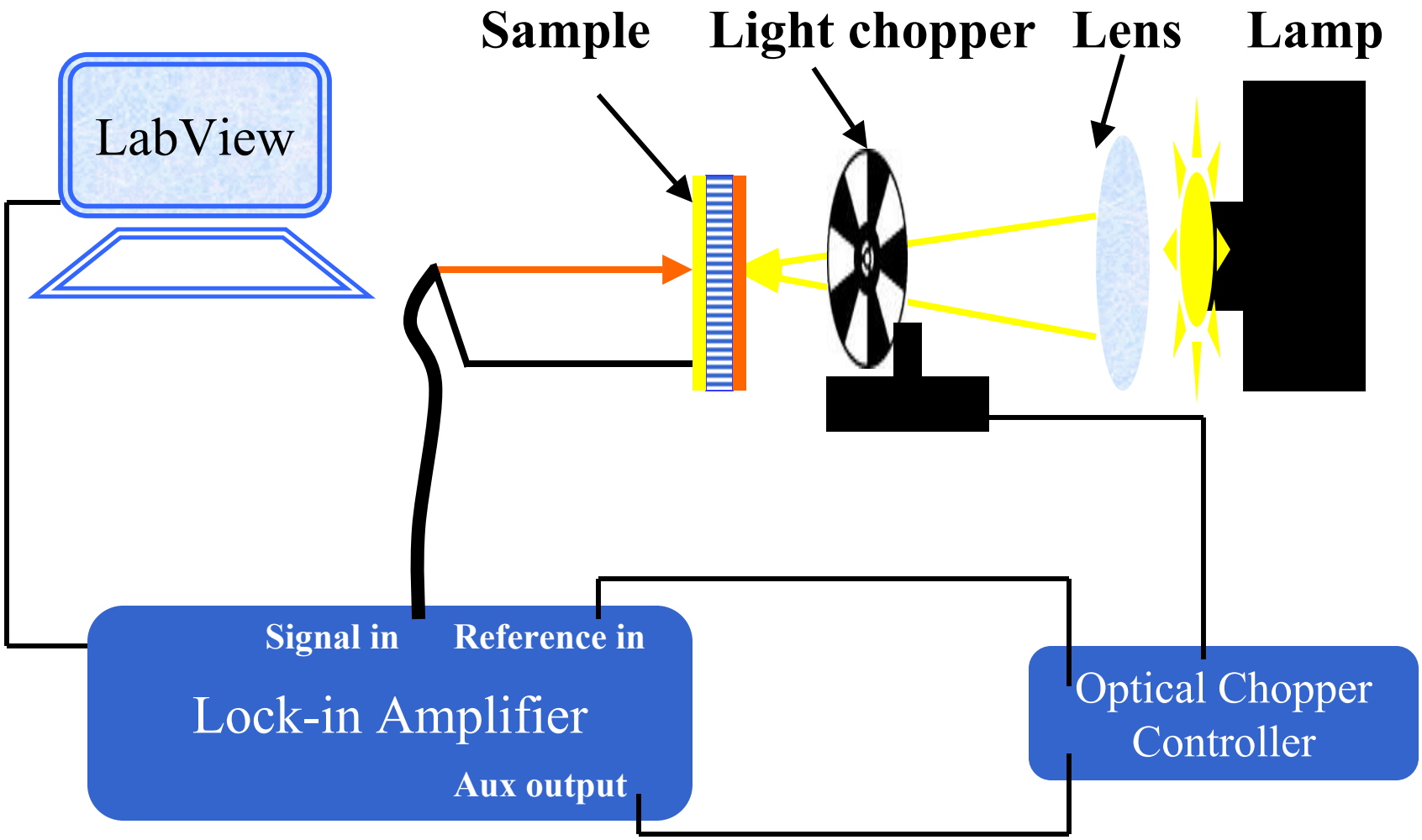
$\rho_{in\text{-}plane}$=0.17 Φcm

$\rho_{cross\text{-}plane}$=0.86 Φcm

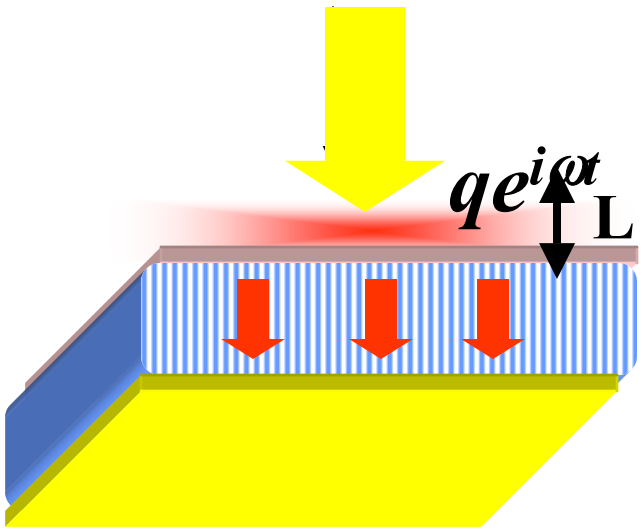
QUANTUM DOT SUPERLATTICES



MEASUREMENT TECHNIQUE



MODELING



Assumptions:

- **one-dimensional heat conduction.**
- **adiabatic boundary condition.**

Temperature at the back side:

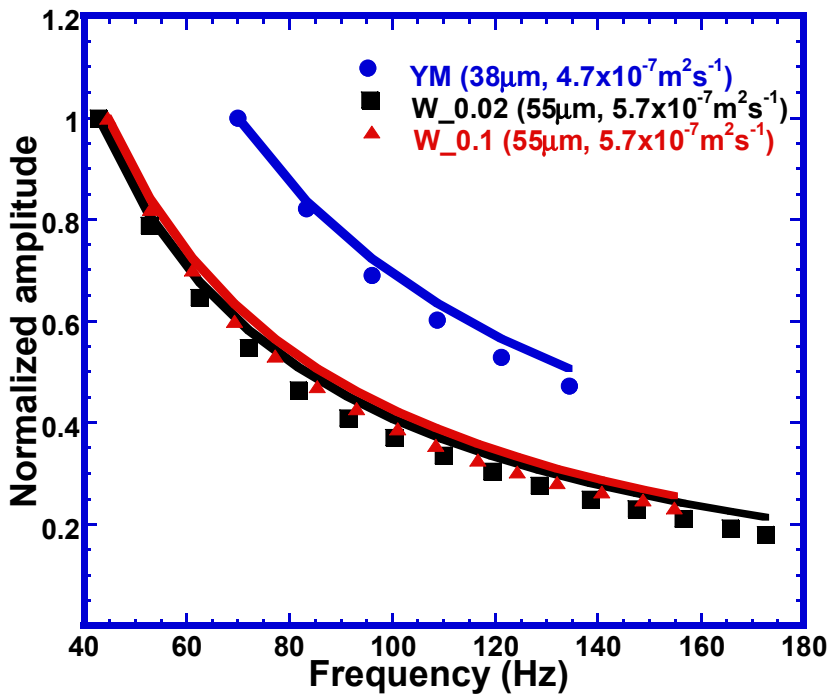
$$T(L) = \frac{2Pe^{mL}}{Akm(1-e^{2mL})} \qquad m = \sqrt{i\frac{2\pi f}{\alpha}}$$

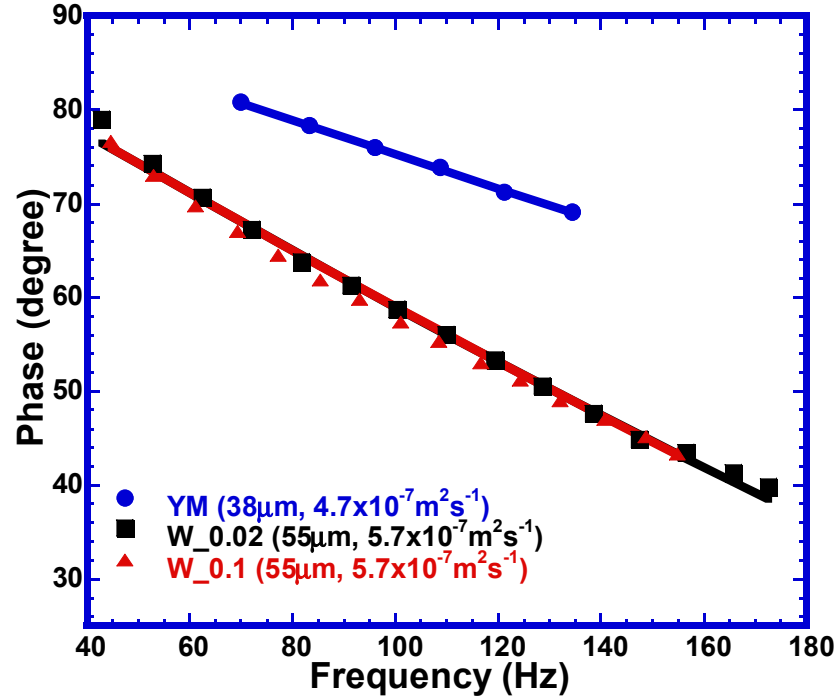
P –power k-thermal conductivity
A- area f-frequency
α-thermal difussivity

Fitting procedure

Guess thermal diffusivity and compare calculated normalized amplitude and phase with experimental signal.

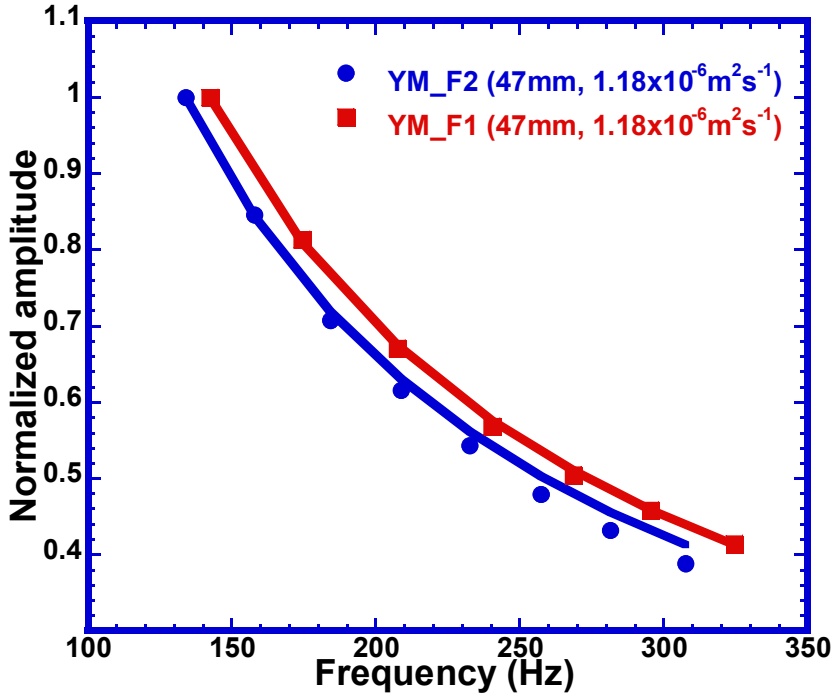
MATRIX THERMAL DIFFUSIVITY

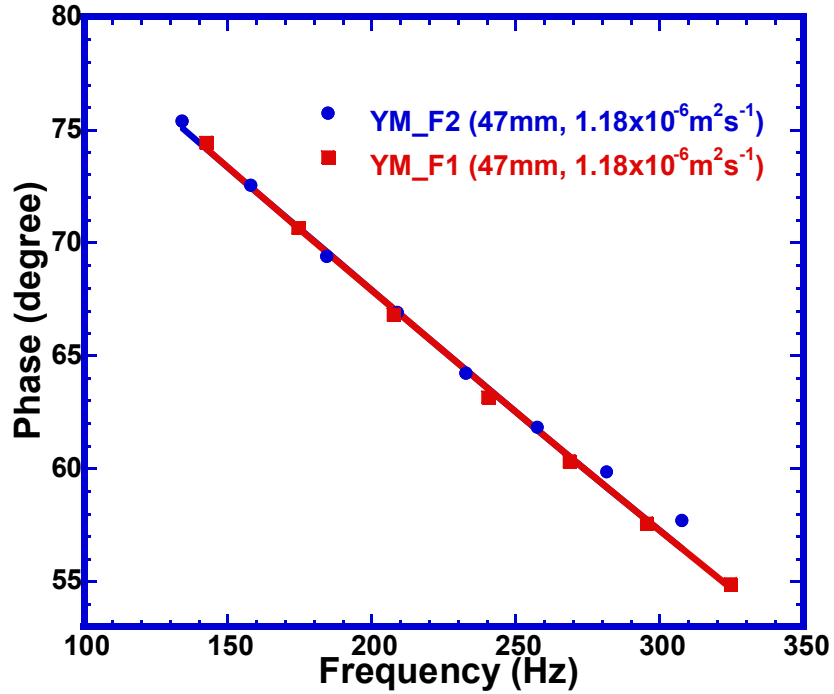




YM: template fabricated by MIT group 0.04μm pore size& 15% porosity.
W_0.02: Whatman template 0.02μm pore opening& 36% average porosity.
W_0.1: Whatman template 0.1μm pore opening& 50% average porosity.

THERMAL DIFFUSIVITY OF Bi FILLED TEMPLATE

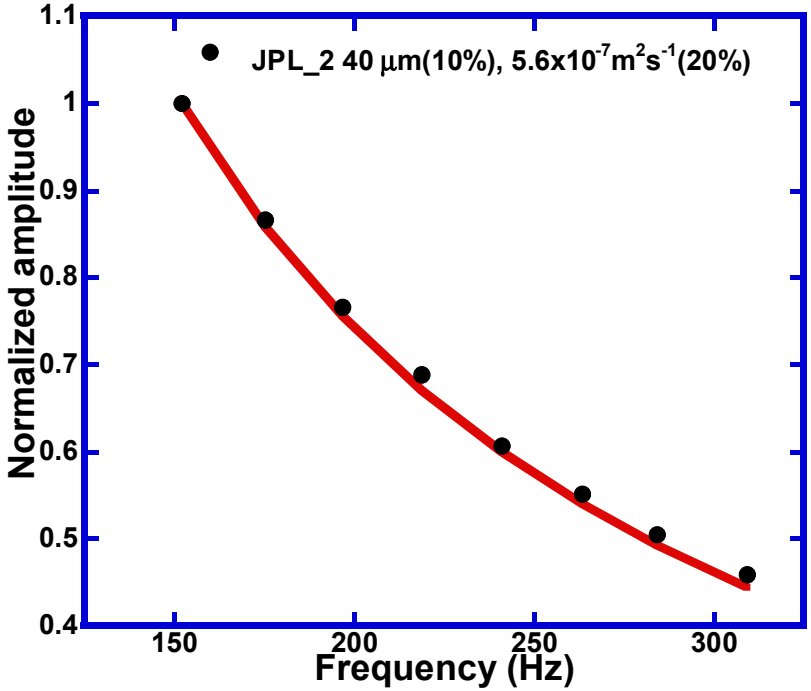


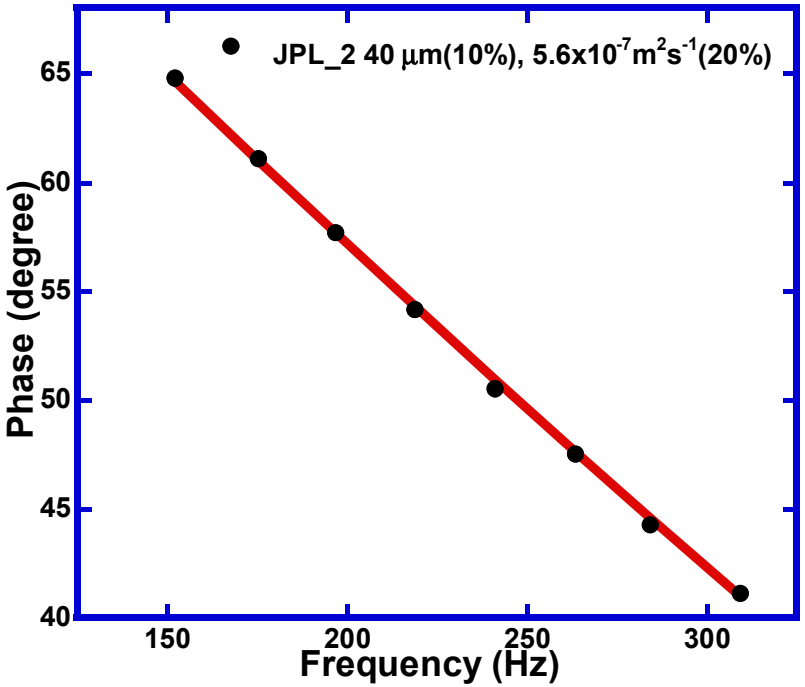


YM: pressure injection filled templates of 0.04μm pore size.

$\alpha_{composite}$=1.32x10^{-7}m^{2}s^{-1}

THERMAL DIFFUSIVITY OF Bi_2Te_3 FILLED TEMPLATE

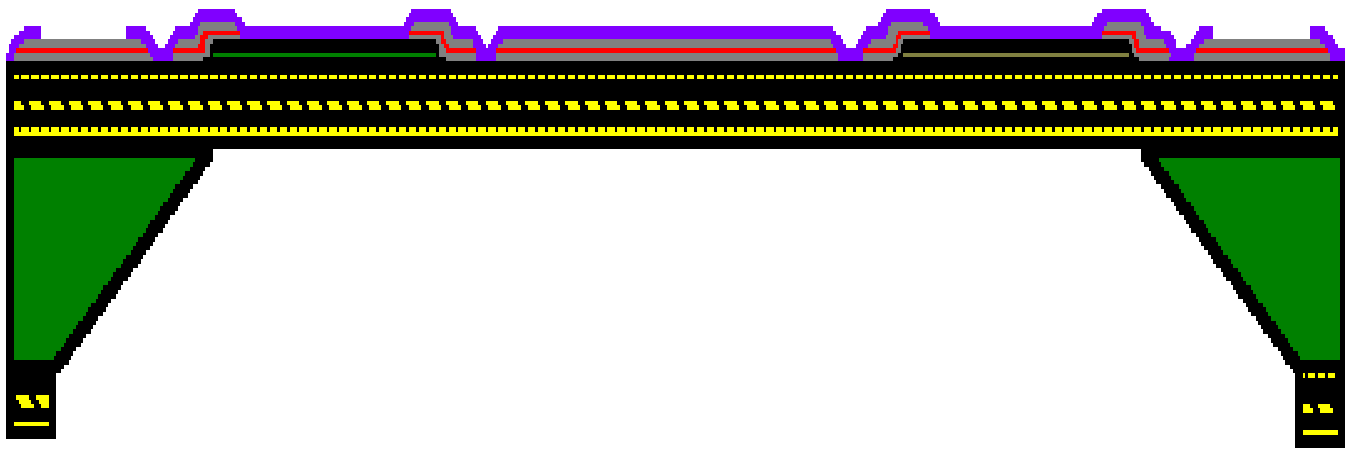




JPL_2: filled Whatman template (0.1μm) -electrochemical deposition of doped Bi_2Te_3. $\alpha_{composite}=5.6x10^{-7}m^2s^{-1}$

CVD BASED DEVICE FABRICATION

Objectives:
(1) Low-Grain Si/Ge Reduces Thermal Conductivity
(2) Developing Integrated Fabrication Processes
(3) Integration with Alpha Particle Heat Source for Space System-on-a-Chip Power Source



Silicon frame

Cr/Au/Cr heater/connecting lines

PECVD SiN_x caping layer

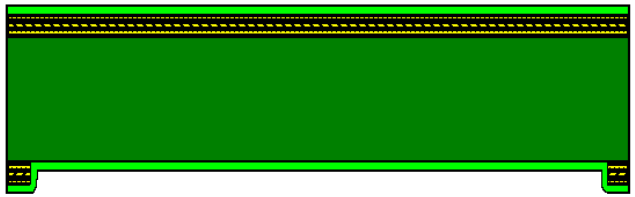
Low σ LPCVD SiN_x/LTO SiO_2/SiNx

p type Poly-SiGe

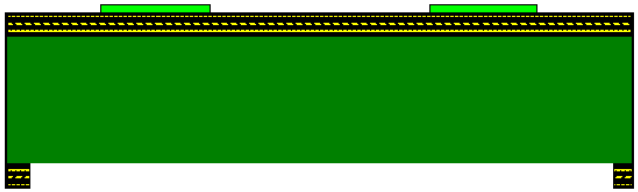
n type Poly-SiGe

MAJOR PROCESSING STEPS

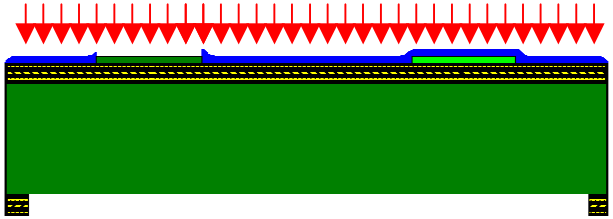
(1) Low-Stress $SiN_x/SiO_2/SiN_x$ Deposition & Etch Window Opening.



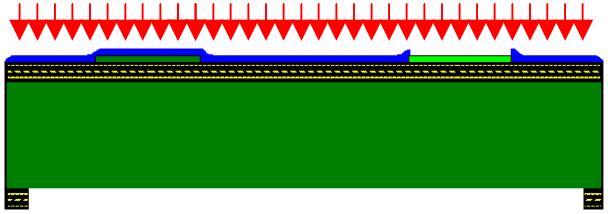
(2) Poly-Si (eventually Poly-SiGe) Deposition.



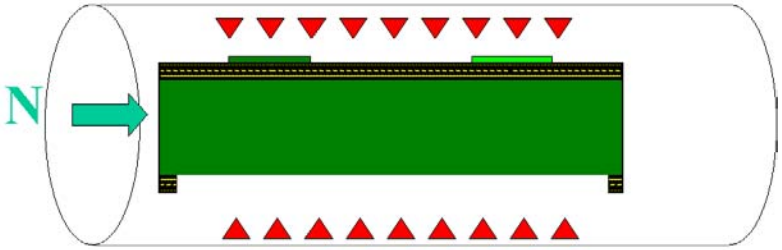
(3) Patterning of Thermoelectric Legs.



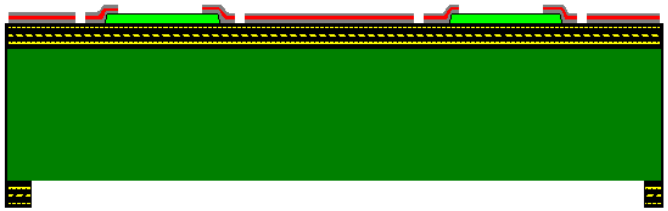
(4) PECVD Oxide Mask+Ion-Implantation.



(5) Repeat for n-type Dopant Implatantion.



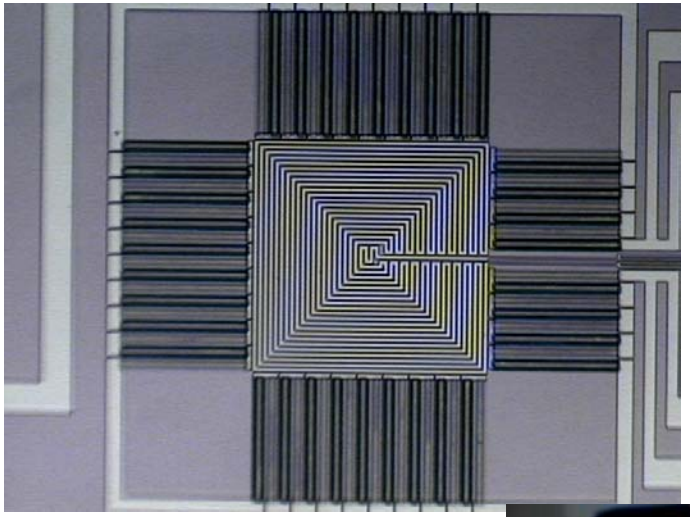
(6) Annealing for Dopant Activation.

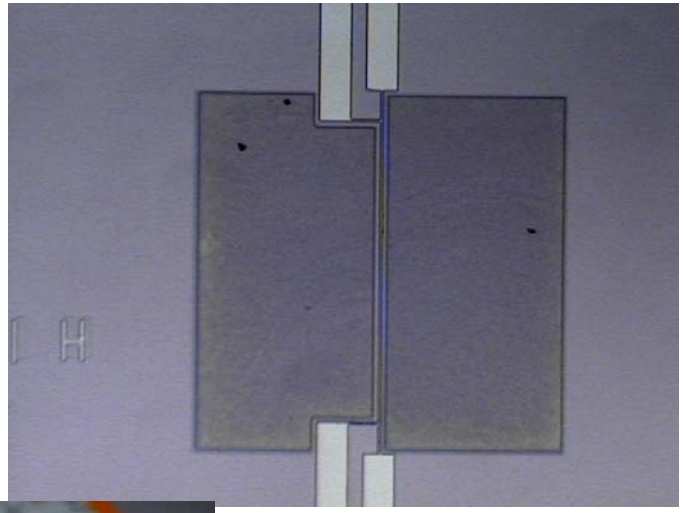


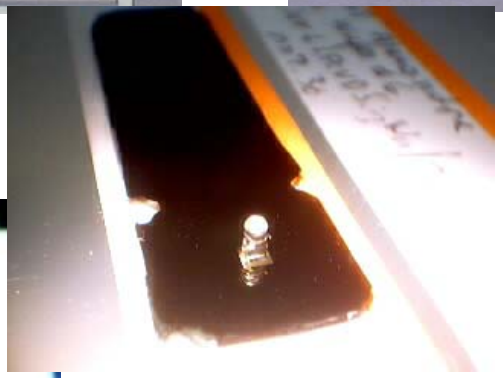
(7) Pattern Heater and Open Contacts

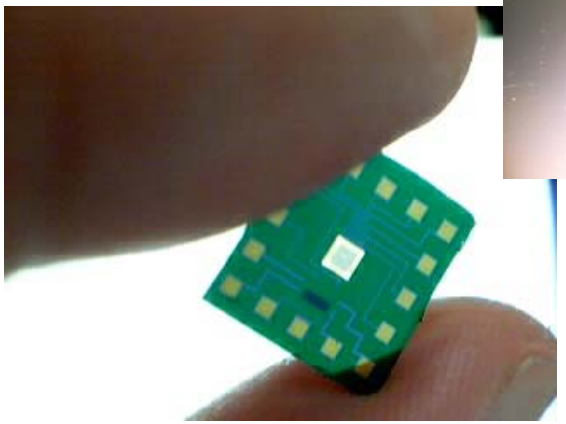
(8) Remove Substrate by KOH.

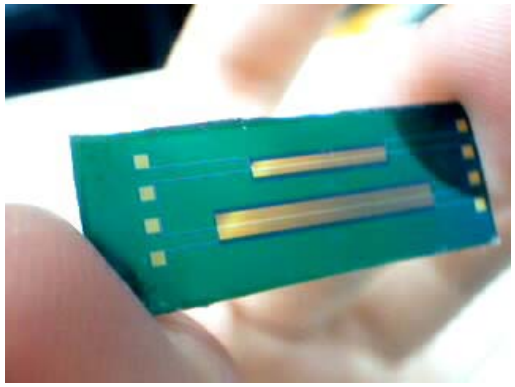
FABRICATED DEVICE AND TESTING STRUCTURES



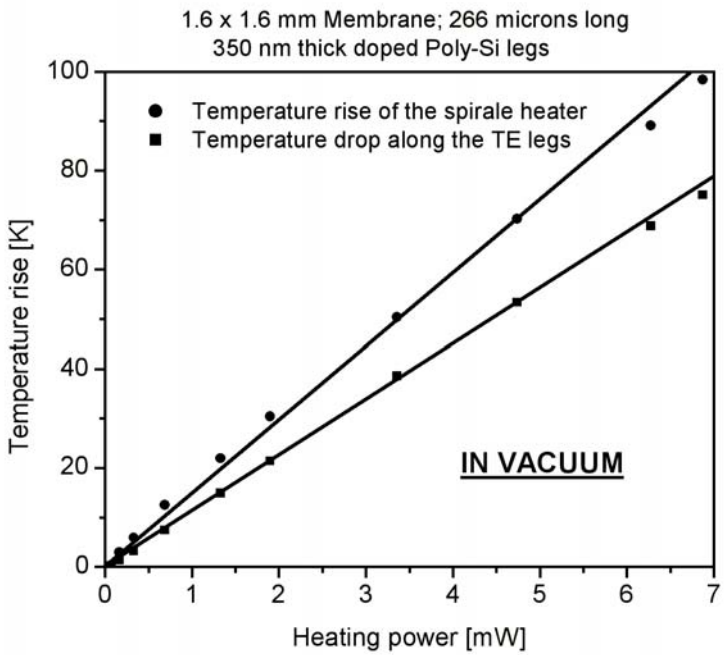


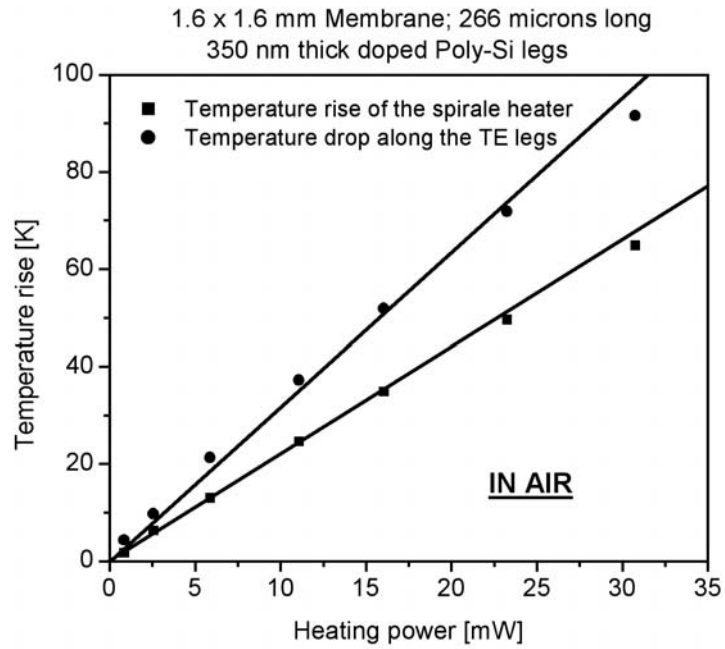






POWER INPUT VS. TEMPERATURE RISE

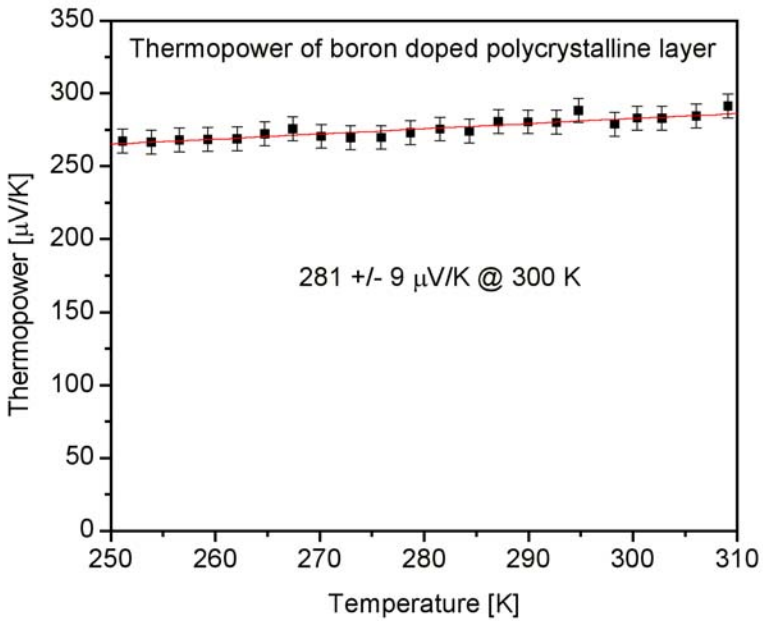


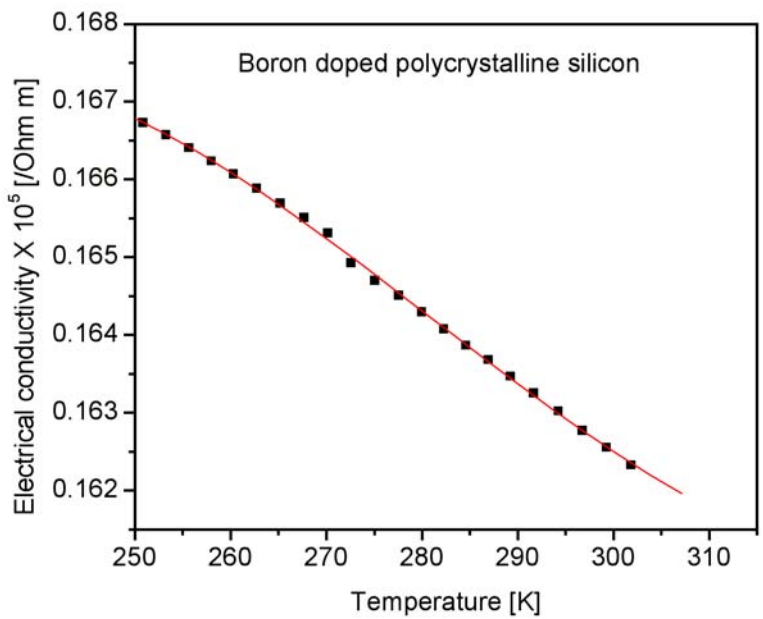


PROPERTIES OF MEMBRANES

Materials	Results	
	Thermal conductivity ($W.m^{-1}.K^{-1}$)	Emissivity
200 nm low σ LPCVD SiN_x / 400 nm low temperature LPCVD oxide / 200 nm low σ LPCVD SiN_x	2.6	0.18
20 nm Cr/ 100 nm Au / 20 nm Cr	140	< 0.1
Undoped polycrystalline silicon deposited at 600 ° C by LPCVD	12.8 (poly Si)	0.55 (membrane)
350 nm thick Phosphorous ion implanted LPCVD polycrystalline silicon deposited at 600°C and annealed at 900°C during 30 min ($n \sim 5 \times 10^{20}$ cm^{-3}) on a $SiN_x/SiO_2/SiN_x$ multilayer	14.8 (poly Si)	0.55 (dielectric multilayer+Poly Si)
350 nm thick Boron ion implanted LPCVD polycrystalline silicon deposited at 600°C and annealed at 900°C during 30 min ($n \sim 8.6 \times 10^{19}$ cm^{-3}) on a $SiN_x/SiO_2/SiN_x$ multilayer	14.2	0.58 (dielectric multilayer+poly Si)

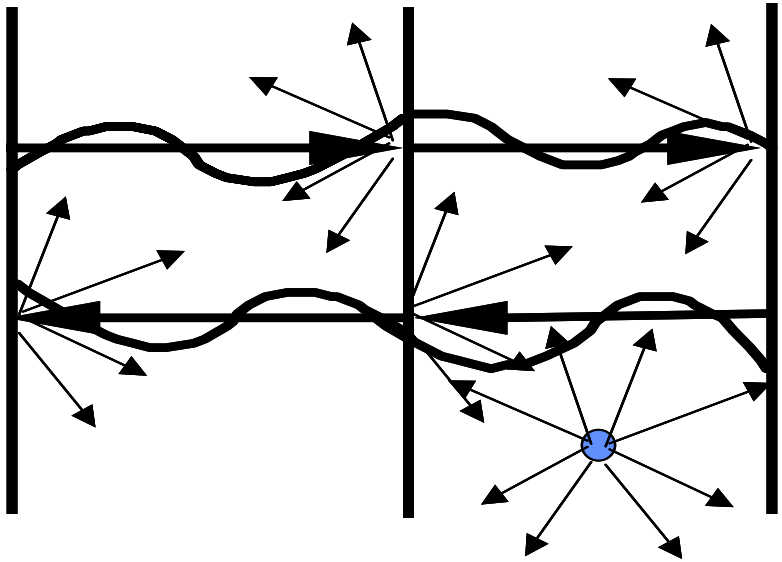
ELECTRONIC PROPERTIES

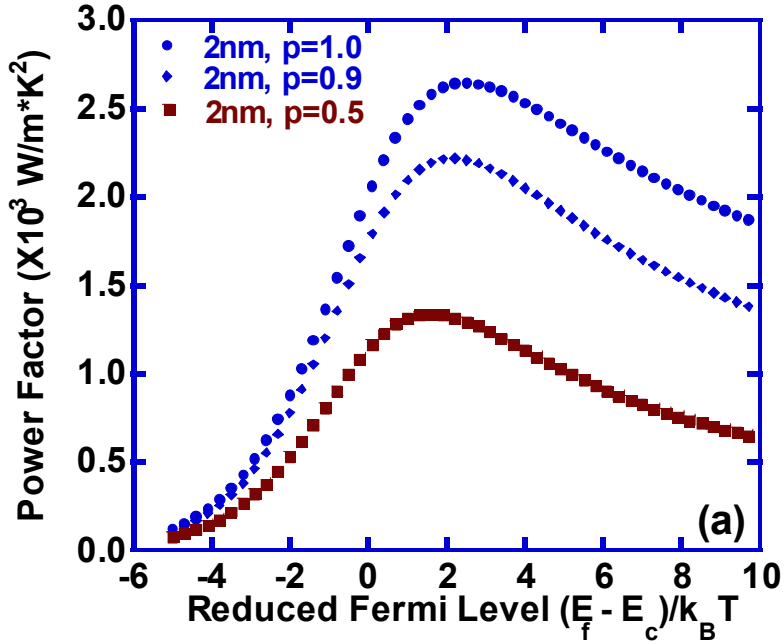




Next Step: Use Smaller Grains and Also SiGe Films

CLASSICAL SIZE EFFECTS

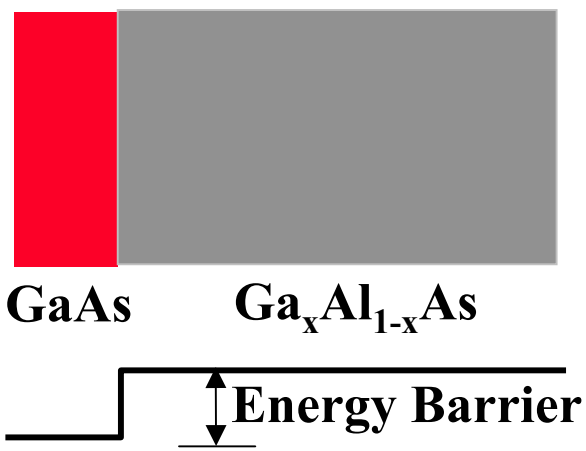


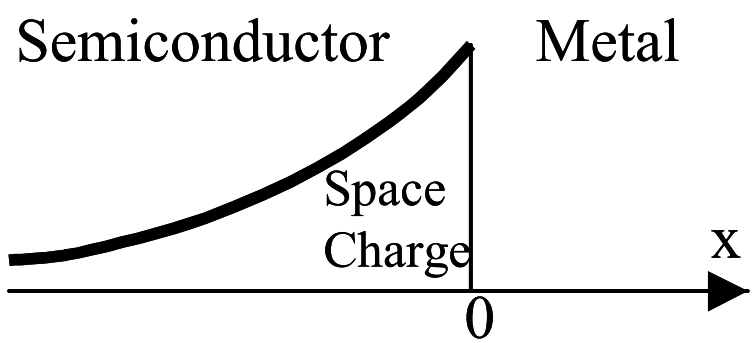


Classical Size Effects

Current Effort: Combine Classical and Quantum Size Effects for Both Electrons and Phonons

INTERFACE CONDITIONS



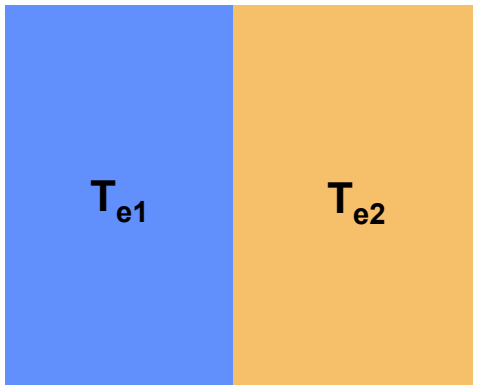


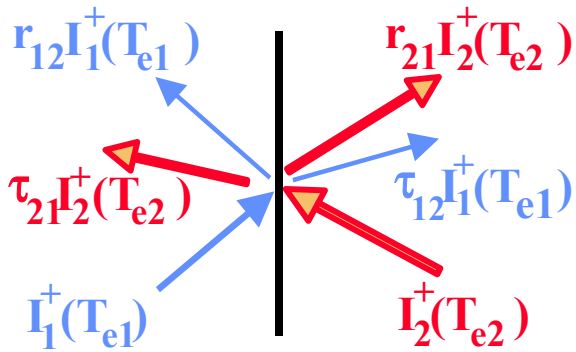
Metal-Semiconductor Interface

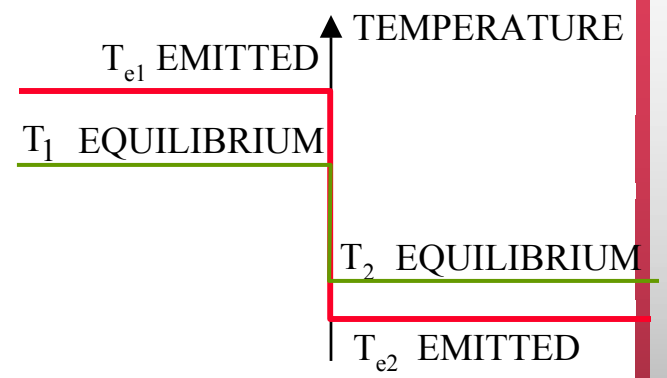
THERMIONIC EMISSION THEORIES REQUIRE BARRIER>>Kt (Bethe Theory, Schottky Theory, Crowell-Sze Theory)

FOR ENERGY CONVERSION APPLICATIONS: BARRIER ~ kT

PHONON THERMAL BOUNDARY RESISTANCE







$$R_e = \frac{T_{e1} - T_{e2}}{q_{12}} = \frac{1}{4Cv\tau_{12}''}$$

$$R = \frac{T_1 - T_2}{q} = \frac{4\left[1 - \left(\tau_{12}' + \tau_{21}'\right)/2\right]}{C_1 v_1 \tau_{12}''}$$

Dilemma:

When $\tau_{12}=1$, $R_e \neq 0$

(No Artificial Interface)

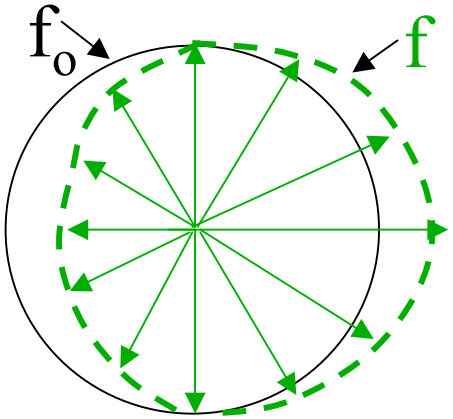
$$\tau_{12}' = \int_0^1 \tau_{12}(\mu)d\mu \quad \tau_{12}'' = \int_0^1 \tau_{12}(\mu_1)\mu_1 d\mu_1$$

When $\tau_{12}=\tau_{21}=1$, R=0

DIFFUSION APPROXIMATION

- **Diffusion Approximation**

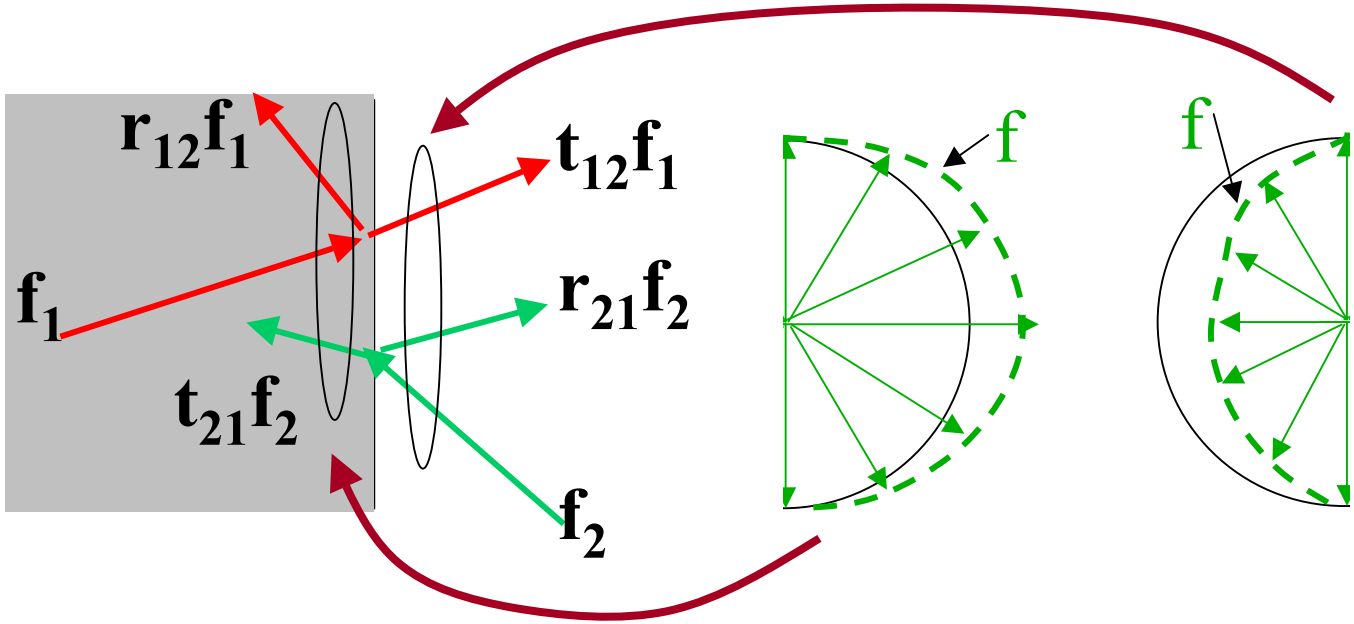
$$f = f_o - \tau \mathbf{v} \bullet \frac{df_o}{dx}$$



f_o Does not Contribution to Flux

→ **Fourier Law, Ohm's Law, Newton's Shear Stress Law**

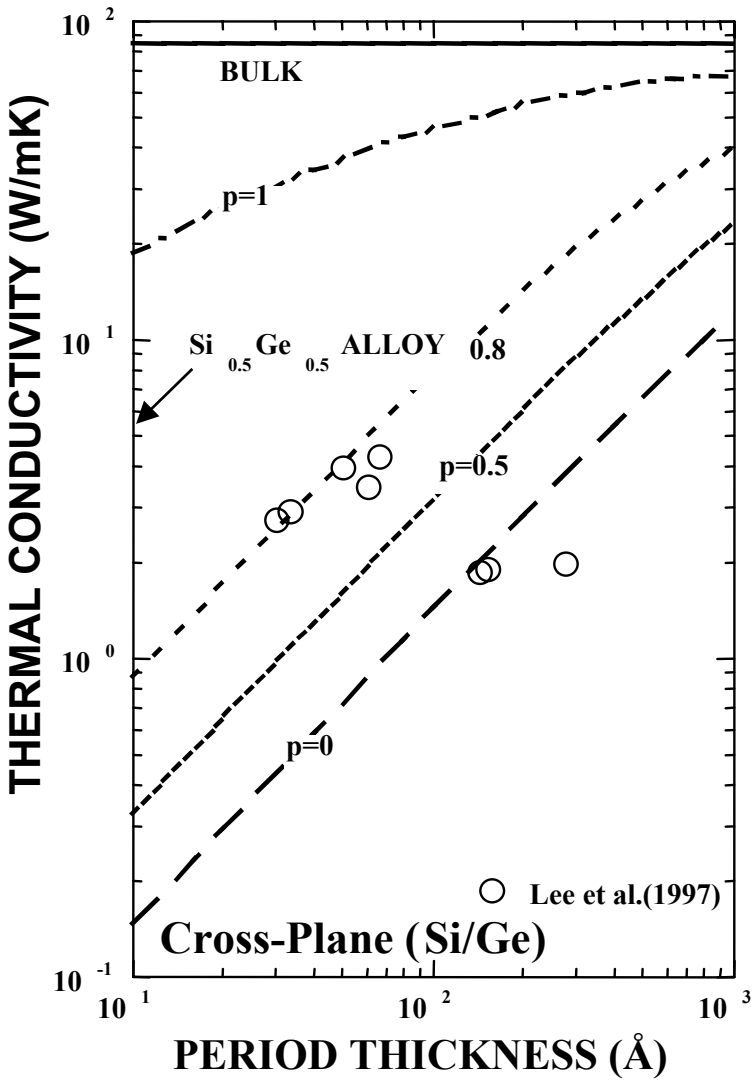
DIFFUSION-TRANSMISSION BOUNDARY/INTERFACE CONDITION

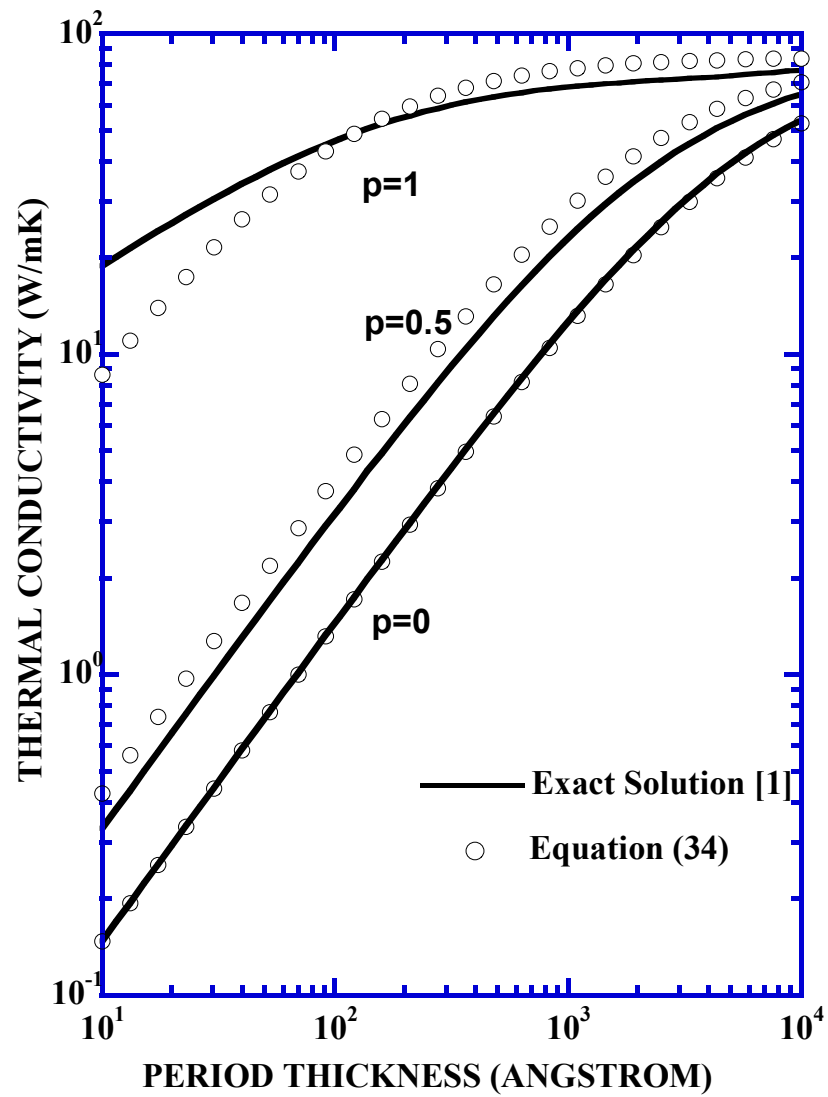


$$[1-(t_{12}''+t_{21}'')/2]J_b = \frac{t_{12}'}{(2\pi)^3}\int_{k_x>0} b\left[f_{o1}(E,T_1,E_{f1})-f_{o1}(E,T_2,E_{f2})\right]v_{x1}d^3\mathbf{k}_1$$

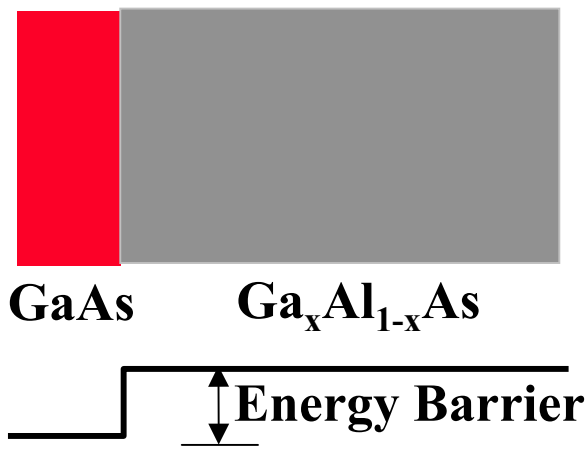
Transmissivity From Side 1 to 2 For Diffusion Flux	Flux of Microscopic Quantity b	Transmissivity From Side 1 to 2 For 0th Order Term	Equivalent Equilibrium Distribution	Velocity And Wavevector

COMPARISON FOR SUPERLATTICES

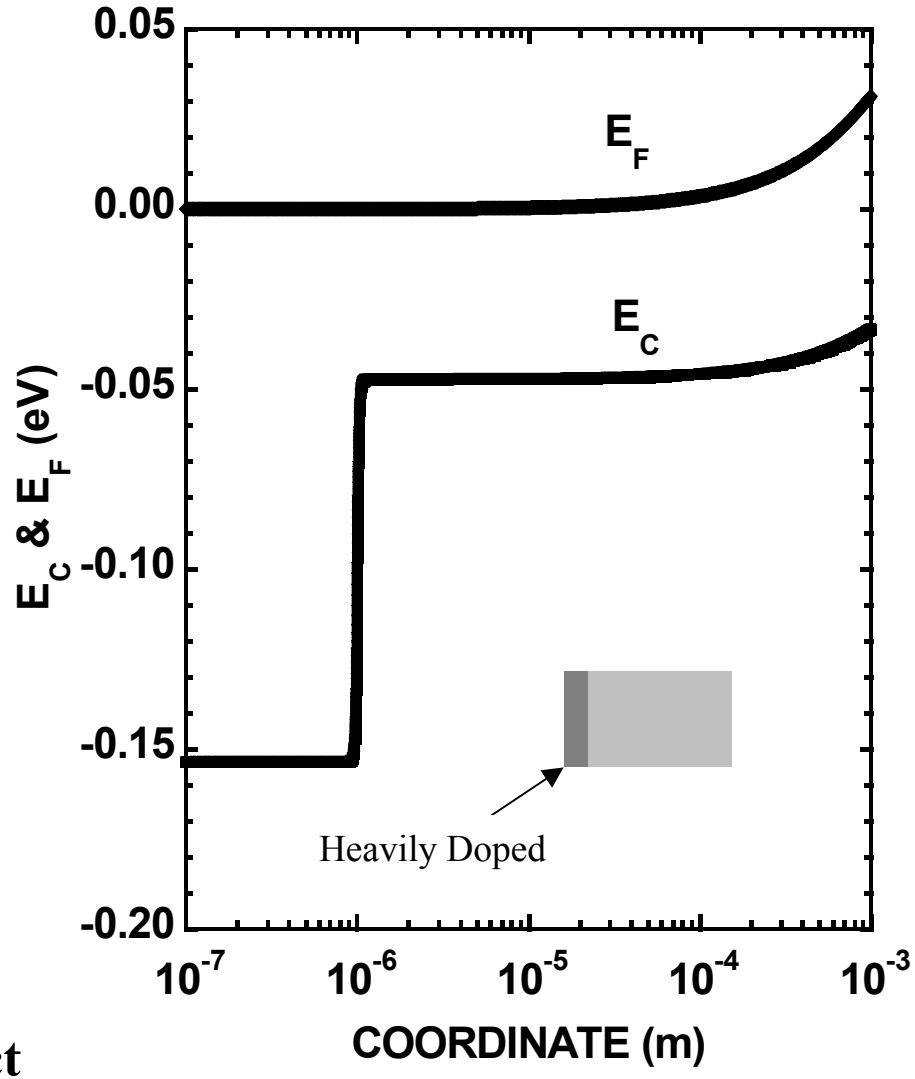




ELECTRON THERMIONIC EMISSION



Heterojunction



- **Developed**

  A New Thermionic Emission Formula Valid for Arbitrary Barrier Height.

- **Current**

  Extension to Hot Electron Effect