About Omics Group

OMICS Group International through its Open Access Initiative is committed to make genuine and reliable contributions to the scientific community. OMICS Group hosts over 400 leading-edge peer reviewed Open Access Journals and organize over 300 International Conferences annually all over the world. OMICS Publishing Group journals have over 3 million readers and the fame and success of the same can be attributed to the strong editorial board which contains over 30000 eminent personalities that ensure a rapid, quality and quick review process.

About Omics Group conferences

- OMICS Group signed an agreement with more than 1000 International Societies to make healthcare information Open Access. OMICS Group Conferences make the perfect platform for global networking as it brings together renowned speakers and scientists across the globe to a most exciting and memorable scientific event filled with much enlightening interactive sessions, world class exhibitions and poster presentations
- Omics group has organised 500 conferences, workshops and national symposium across the major cities including SanFrancisco,Omaha,Orlado,Rayleigh,SantaClara,Chicago,Philadelphia,Unitedkingdom,Baltimore,SanAntanio,Dubai,Hyderabad,Bangaluru and Mumbai.

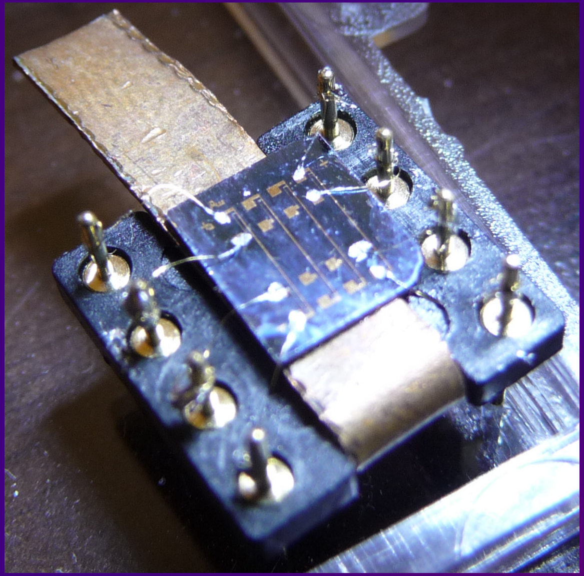
p▯▯ *n* - Transverse Thermoelectrics:
A new class of Materials with Possible Optoelectronic Applications

Matthew Grayson
m-grayson@northwestern.edu
EECS, Northwestern U.

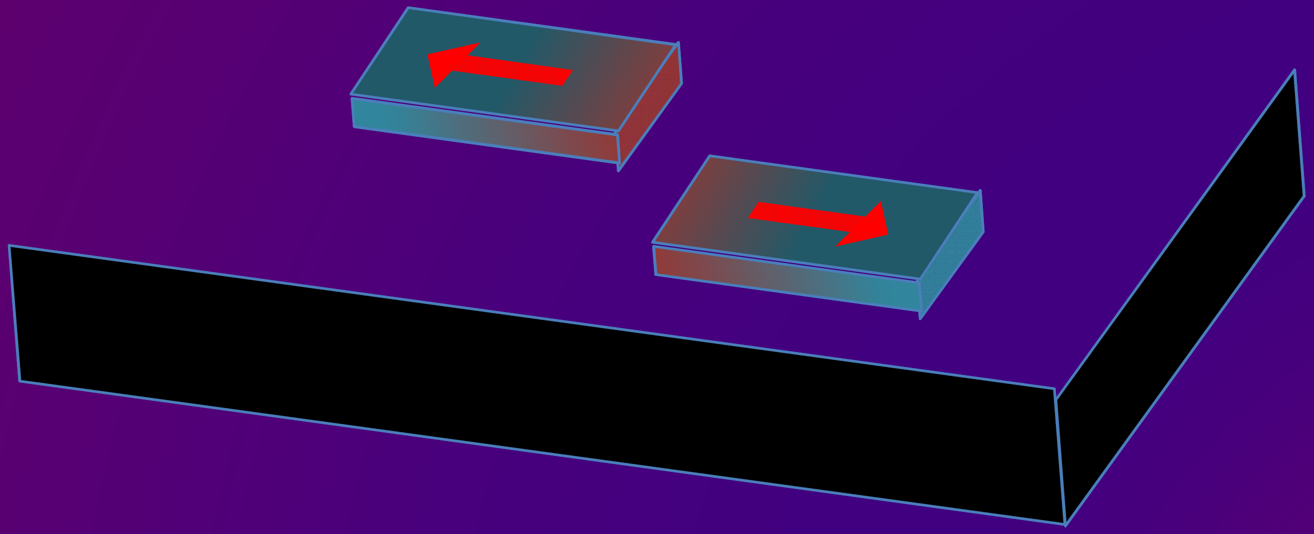
Chuanle Zhou (post-doc), Boya Cui, Yang Tang (PhD)
Stefan Birner (NextNano / TU Munich)
Karen Heinselman

Phys. Rev. Lett. 110, 227701 (2013)

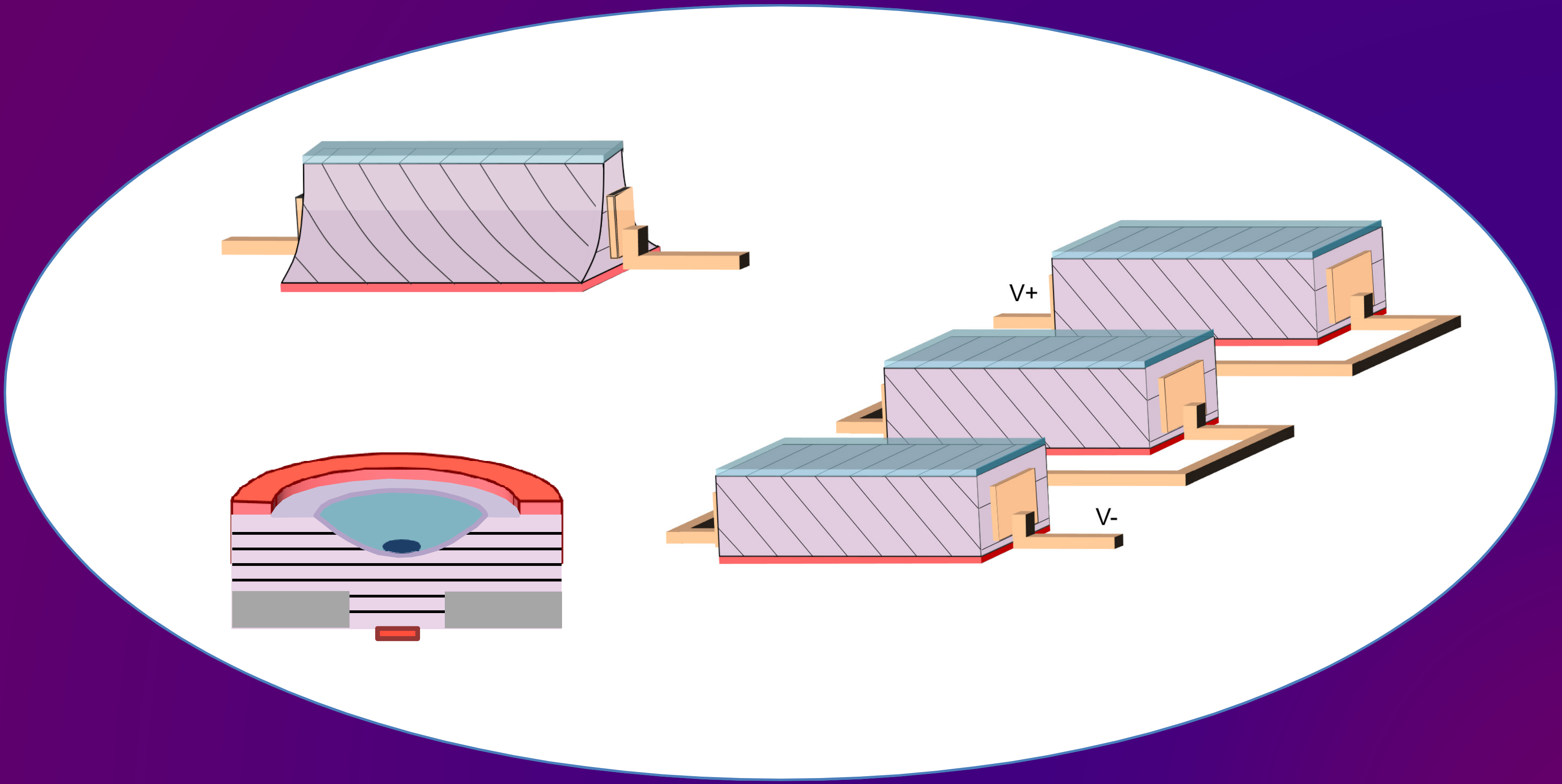
Motivation #1:
for *intrinsic* on-chip cryocooling



Motivation #2:
integrated thermal management



Motivation #3: overcome *ZT* limitations with geometric shaping



p x *n* Transverse Thermoelectrics:

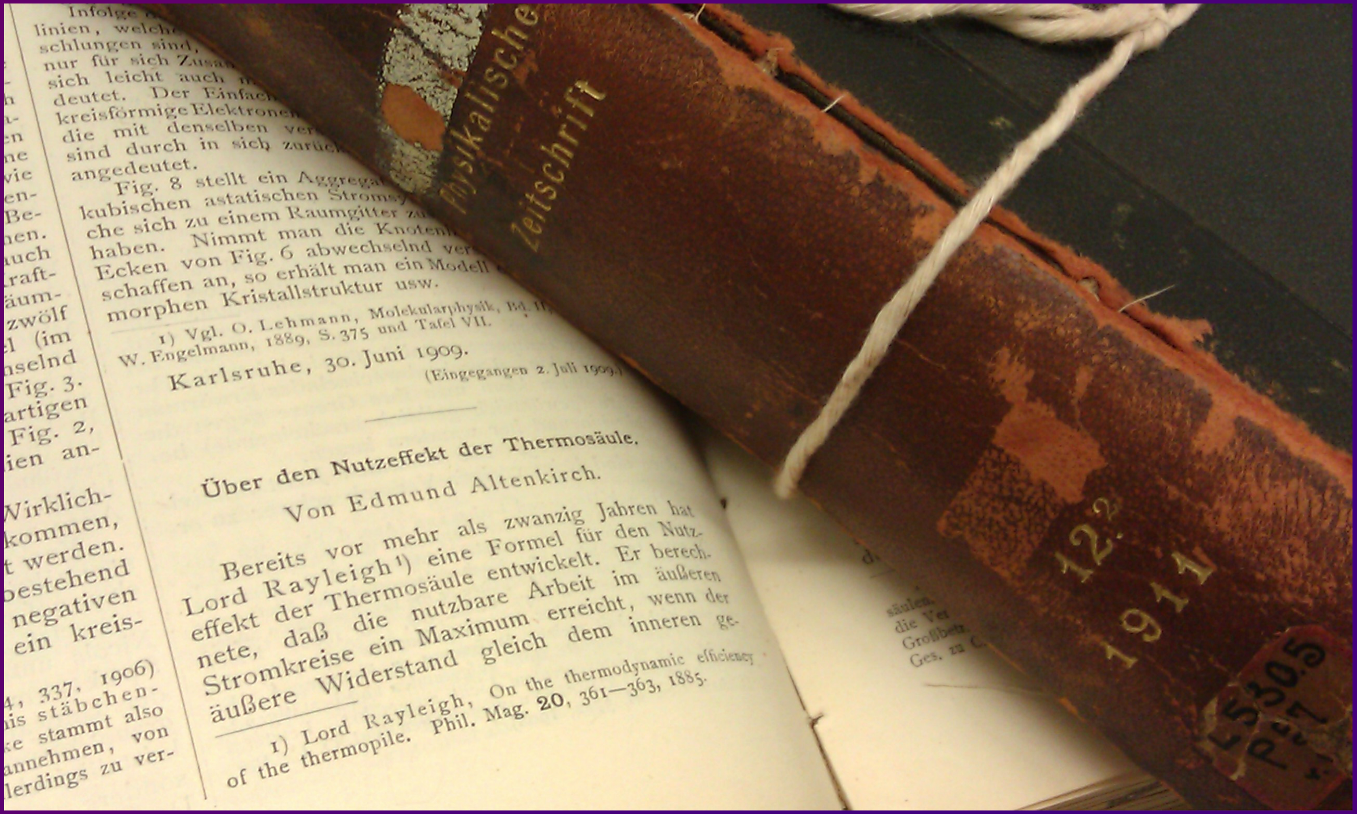
Outline:

I. Transverse Thermoelectricity

II. Type II broken-gap superlattices

The Dawn of Thermoelectricity

Edmund Altenkirch, Phys.Zeits. **10**, 560 (1909); **12**, 920 (1911).



Karlsruhe, 30. Juni 1909.

(Eingegangen 2. Juli 1909.)

Über den Nutzeffekt der Thermosäule.

Von Edmund Altenkirch.

Bereits vor mehr als zwanzig Jahren hat Lord Rayleigh1) eine Formel für den Nutzeffekt der Thermosäule entwickelt. Er berechnete, daß die nutzbare Arbeit im äußeren Stromkreise ein Maximum erreicht, wenn der äußere Widerstand gleich dem inneren ge-

1) Lord Rayleigh, On the thermodynamic efficiency of the thermopile. Phil. Mag. **20**, 361—363, 1885.

Figure of Merit

$$ZT = \frac{S^2}{\rho\,\kappa}\,T$$

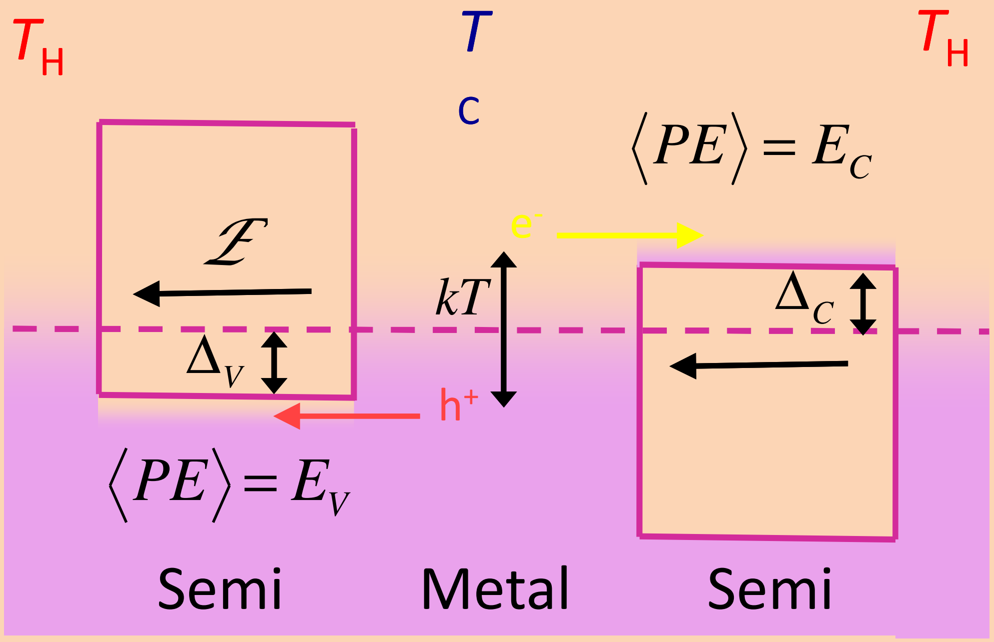
INTENSIVE PARAMETERS

S – Seebeck coefficent
ρ – Electrical resistivity
κ – Thermal conductivity

Longitudinal thermoelectric figure of merit:

$$Z_{\parallel} T = \frac{S_{xx}^{2}}{\rho_{xx} \kappa_{xx}} T$$

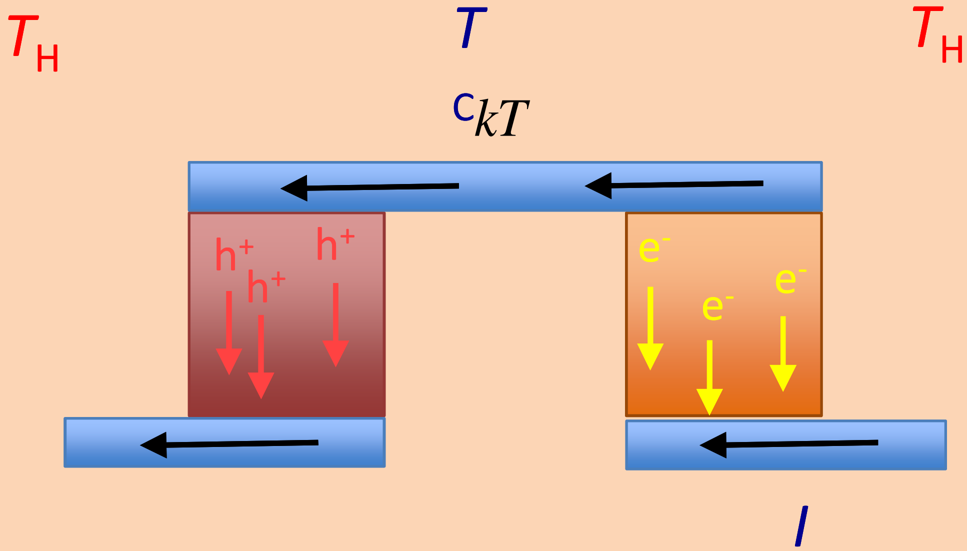
Longitudinal Thermoelectric:



$$\Delta \langle PE \rangle = (\Delta_V + \Delta_C)$$

Longitudinal Thermoelectric:

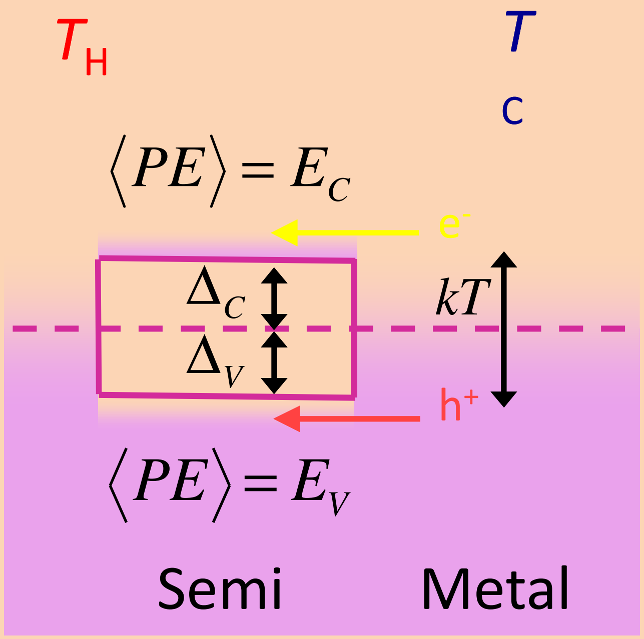
Double-leg



Transverse thermoelectric figure of merit:

$$Z_\perp T = \frac{S_{xz}^2}{\rho_{xx}\kappa_{zz}} T$$

Transverse Thermoelectric:



T_H

T_C

$\langle PE \rangle = E_C$

e^-

Δ_C

kT

Δ_V

h^+

$\langle PE \rangle = E_V$

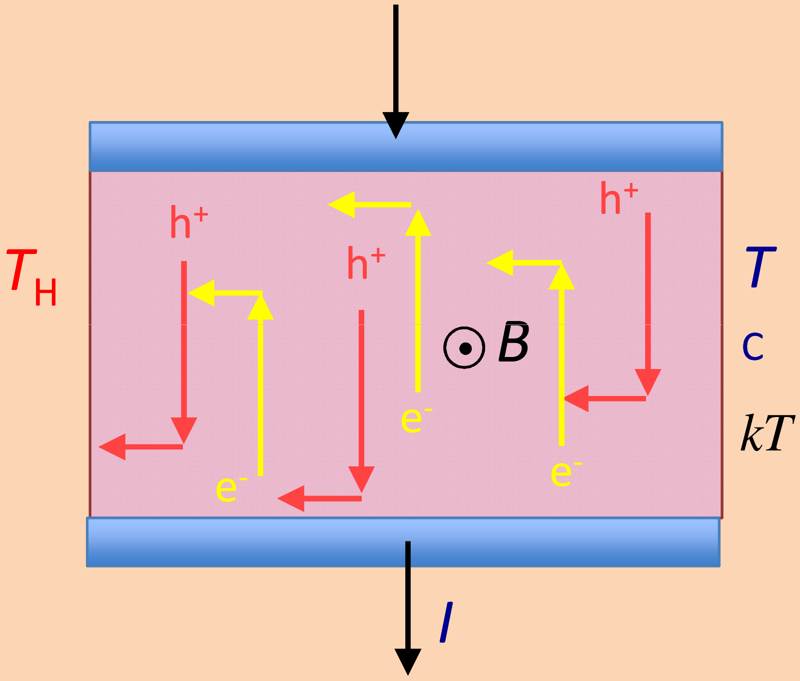
Semi

Metal

$$\Delta \langle PE \rangle = (\Delta_V + \Delta_C) = E_G$$

Transverse Thermoelectric:

Nernst-Ettingshausen effect
Single-leg



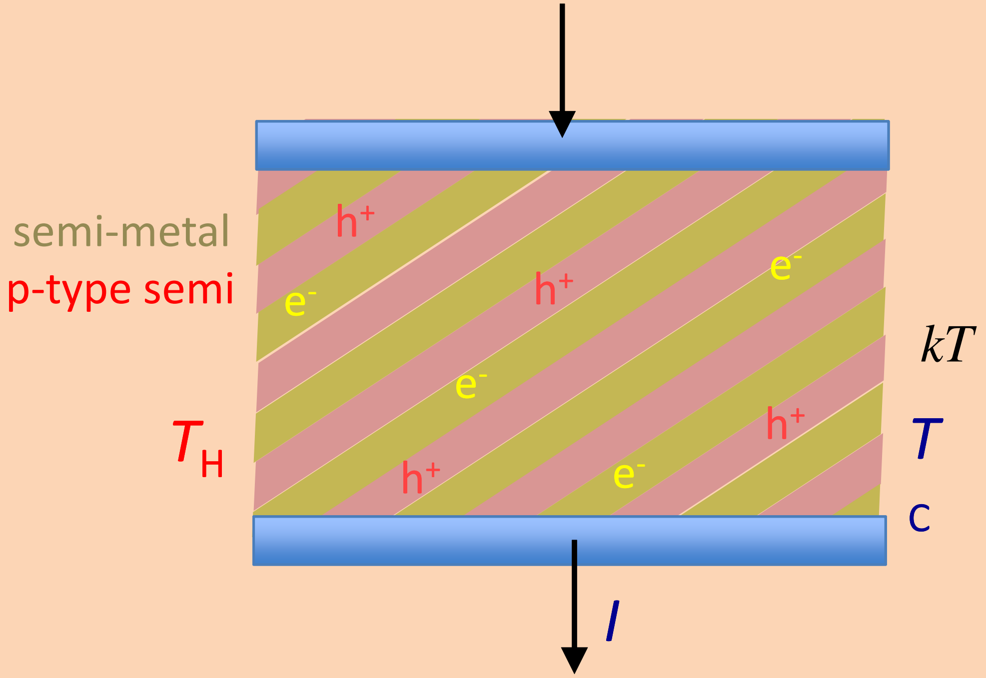
Symmetry broken by *B*-field

DISADVANTAGE: REQUIRES LARGE B-field (1.5 T)

K.F. Cuff, Appl. Phys. Lett. 2, 145 (1963); C.F. Kooi, J. Appl. Phys. 34, 1735 (1963)

Transverse Thermoelectric:

Stacked synthetic composites
Single-leg

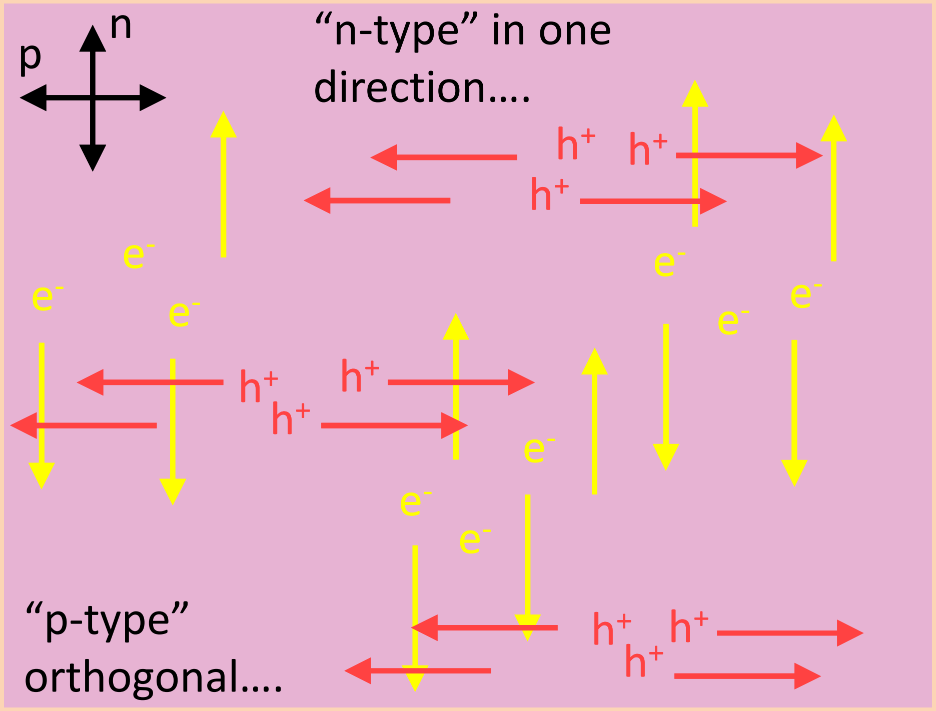


Symmetry broken by *structure*

DISADVANTAGE: Thick (~mm) layers cannot be scaled down
Labor intensive fabrication

V.P. Babin, Sov. Phys. Semicond. 8, 478 (1974); Reitmaier, Appl. Phys. A 99, 717 (2010)

p x n Transverse Thermoelectrics

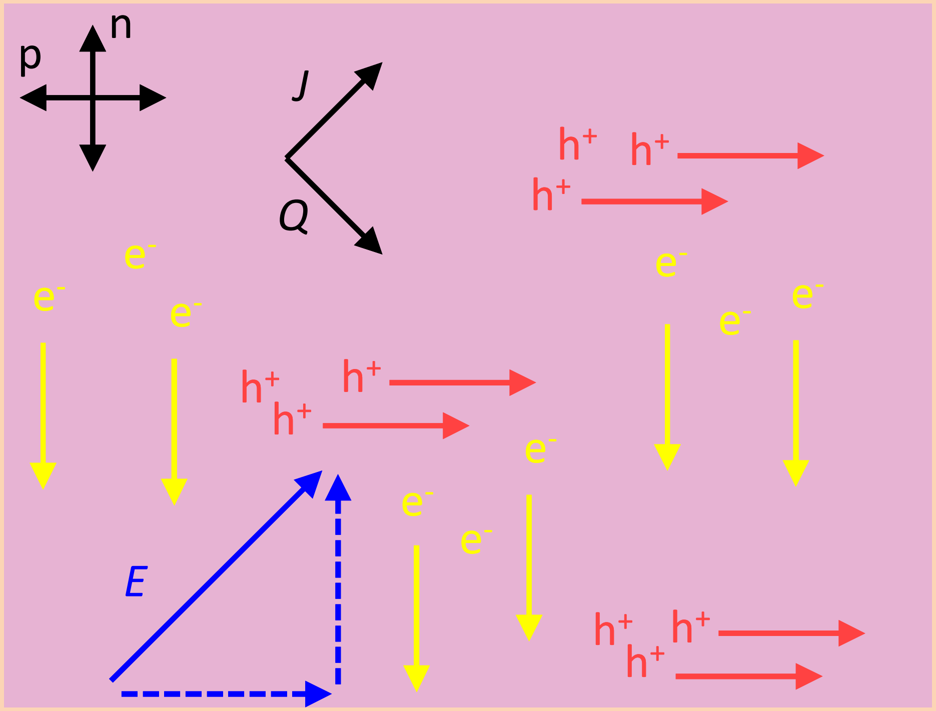


“n-type” in one direction….

“p-type” orthogonal….

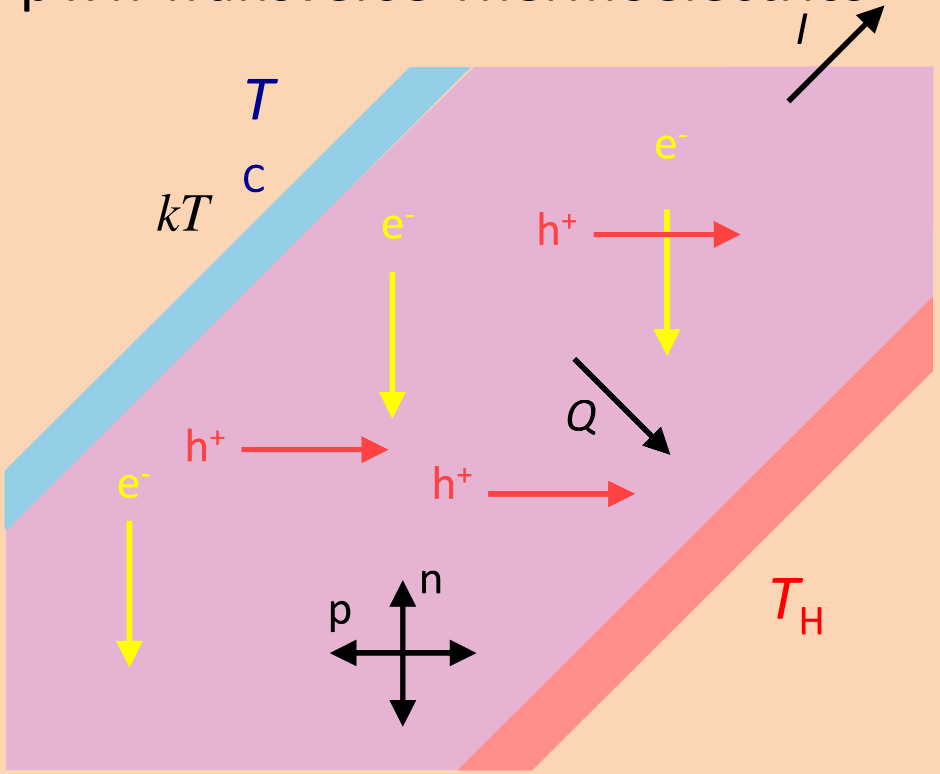
Symmetry broken by *band structure anisotropy*

p x n Transverse Thermoelectrics



Symmetry broken by *band structure anisotropy*

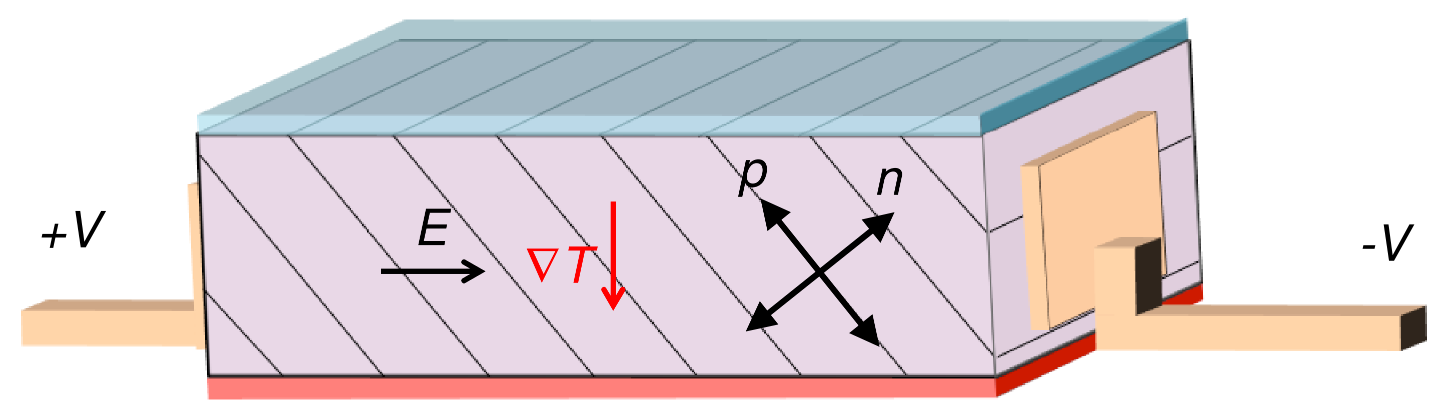
p x n Transverse Thermoelectrics



Symmetry broken by *band structure anisotropy*

ADVANTAGE: Scalable to cm or μm
No external B-field

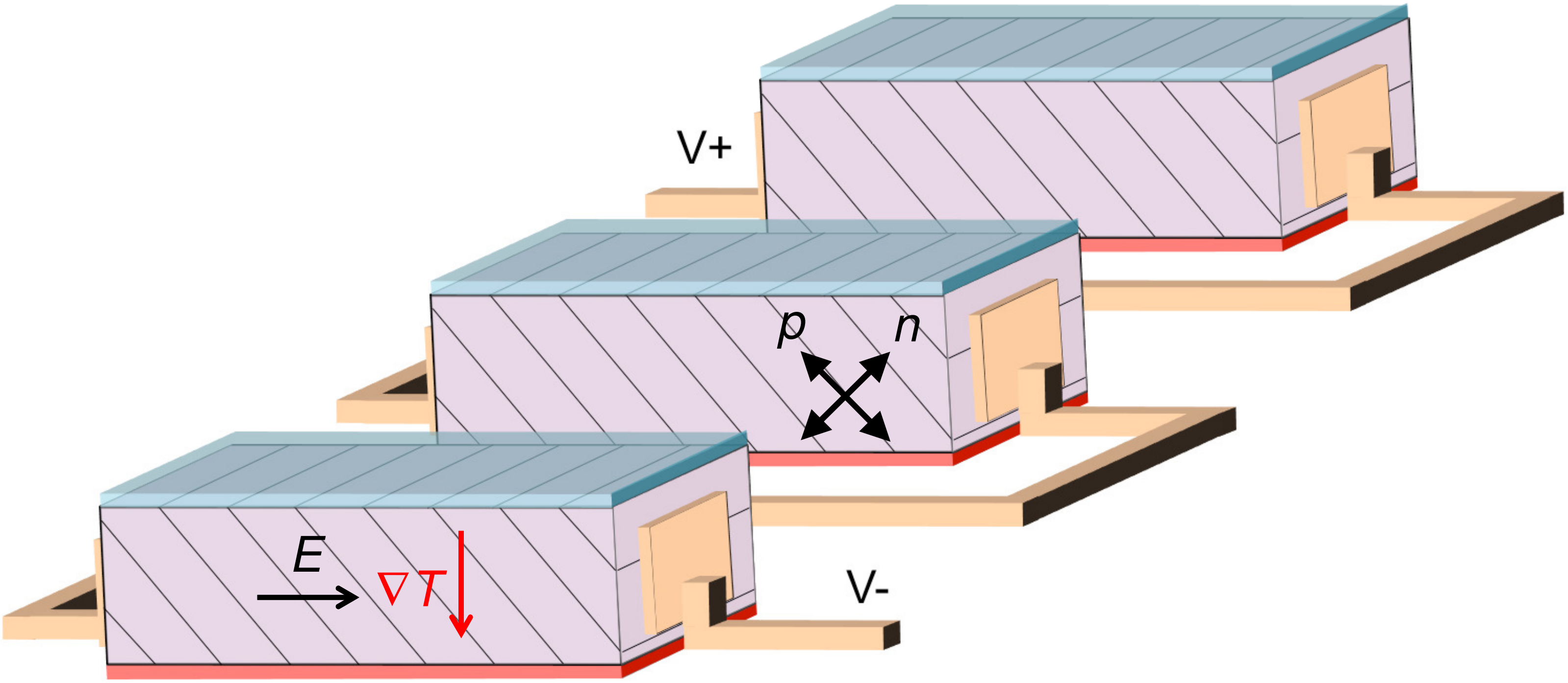
Transverse Seebeck voltage generator



Transverse Seebeck voltage generator

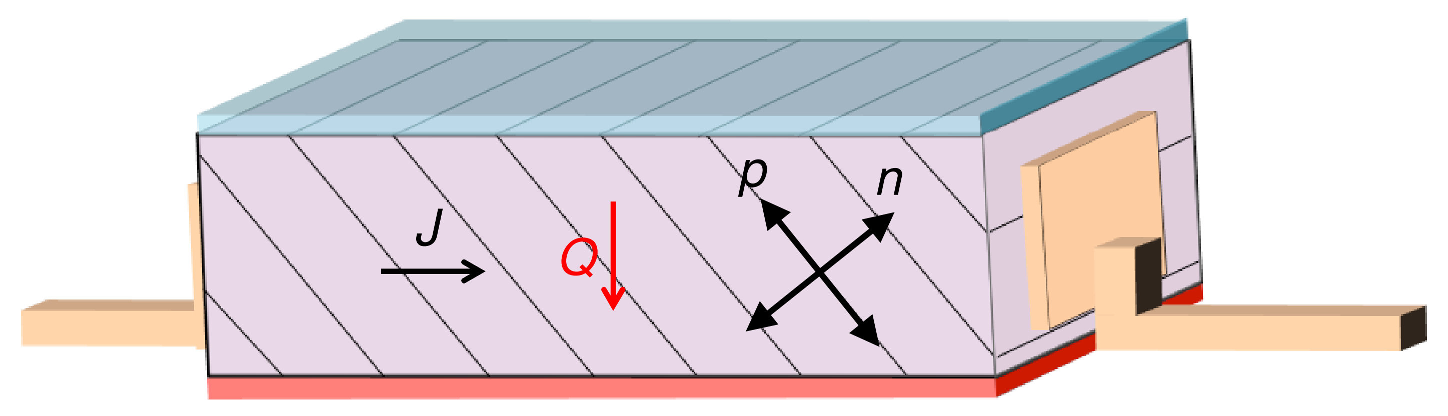
Meander structure:

Arbitrarily large Seebeck voltages *V* with small ΔT



H. J. Goldsmid, J. Elec. Mat.,40 5, 1254 (2010).

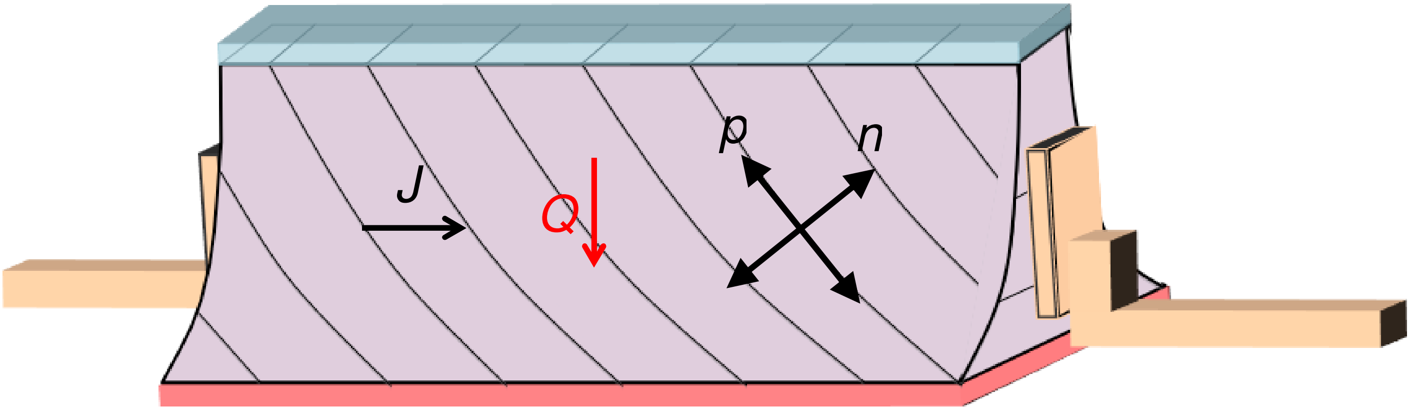
Transverse Peltier cooler



Transverse Peltier cooler

Exponential Taper:

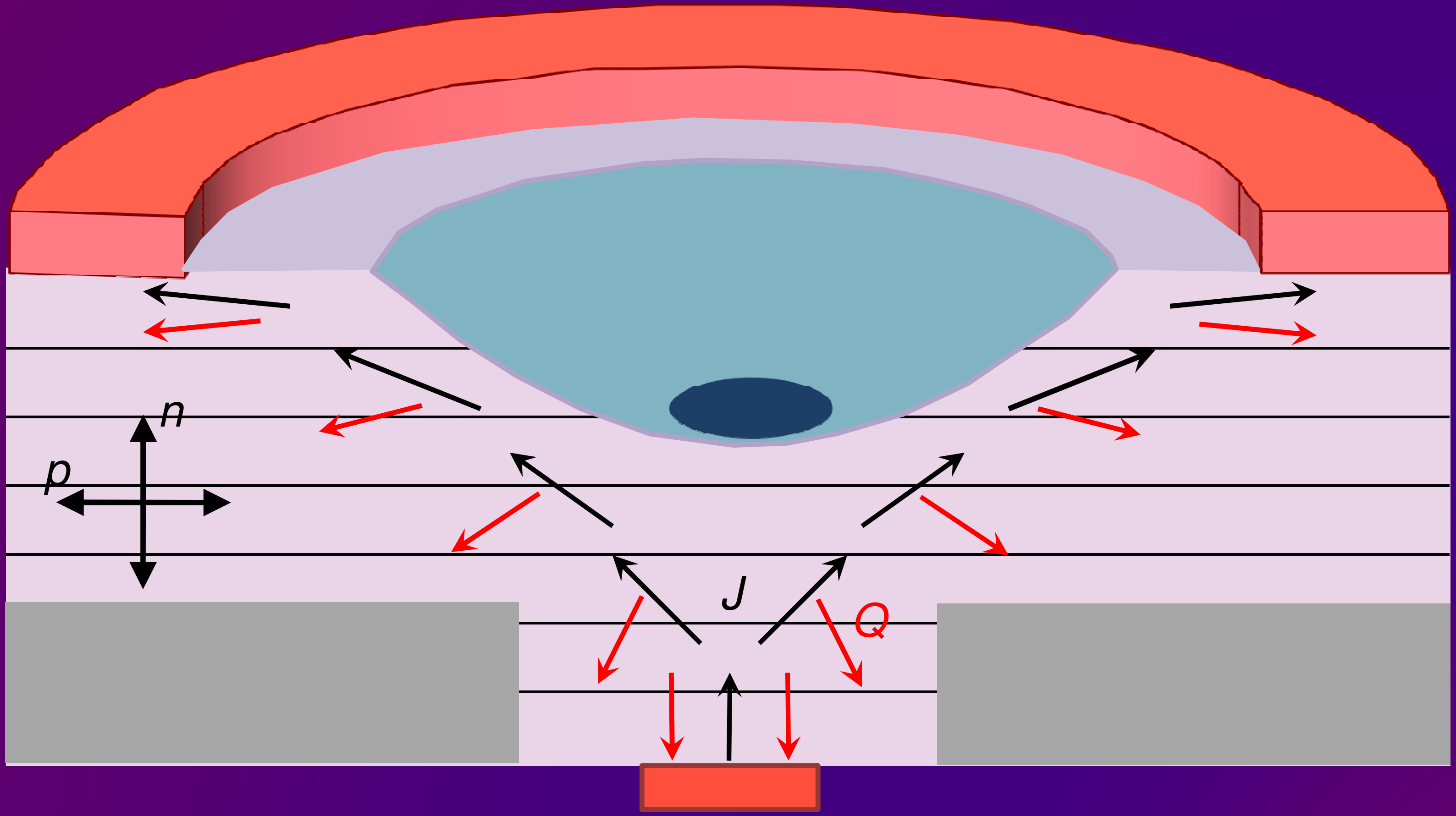
Arbitrarily large ΔT with finite current J



C. F. Kooi *et al.*, Appl. Phys. 34, 1735 (1963)

Annular Peltier cooler

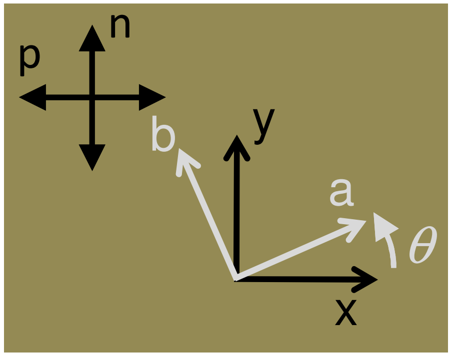
Every angle of current takes heat away from center



p x *n* Seebeck tensor

- Seebeck Tensor

$$\mathbf{s}_n = \begin{bmatrix} s_n & 0 \\ 0 & s_n \end{bmatrix}, \mathbf{s}_p = \begin{bmatrix} s_p & 0 \\ 0 & s_p \end{bmatrix}$$



- Electrical conductivity Tensor

$$\boldsymbol{\sigma}_n = \begin{bmatrix} 0 & 0 \\ 0 & \sigma_{n,yy} \end{bmatrix}, \boldsymbol{\sigma}_p = \begin{bmatrix} \sigma_{p,xx} & 0 \\ 0 & 0 \end{bmatrix}$$

- Total Seebeck Tensor

$$\mathbf{S} = (\boldsymbol{\sigma}_p + \boldsymbol{\sigma}_n)^{-1}(\boldsymbol{\sigma}_p \mathbf{s}_p + \boldsymbol{\sigma}_n \mathbf{s}_n)$$

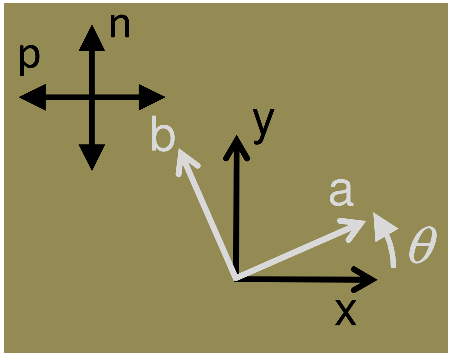
$$\boxed{\mathbf{S} = \begin{bmatrix} s_p & 0 \\ 0 & s_n \end{bmatrix}}, s_p > 0, s_n < 0$$

$$\mathbf{S}' = \mathbf{R}_\theta^{-1} \begin{bmatrix} s_p & 0 \\ 0 & s_n \end{bmatrix} \mathbf{R}_\theta = \begin{bmatrix} s_{aa} & \boxed{s_{ab}} \\ \boxed{s_{ba}} & s_{bb} \end{bmatrix}$$

Optimal transport coefficients

- Optimal angle

$$\cos^2\theta_\perp = \frac{1}{1+\sqrt{\dfrac{\kappa_{yy}/\kappa_{xx}}{\rho_{yy}/\rho_{xx}}}}$$



- Optimal transverse figure of merit

$$\boxed{Z_\perp T = Z_{ba}(\theta_\perp)T = \frac{(S_{p,xx}-S_{n,yy})^2 T}{\left(\sqrt{\rho_{xx}\kappa_{xx}}+\sqrt{\rho_{yy}\kappa_{yy}}\right)^2}}$$

p x *n* Transverse Thermoelectrics:

Outline:

I. Transverse Thermoelectricity

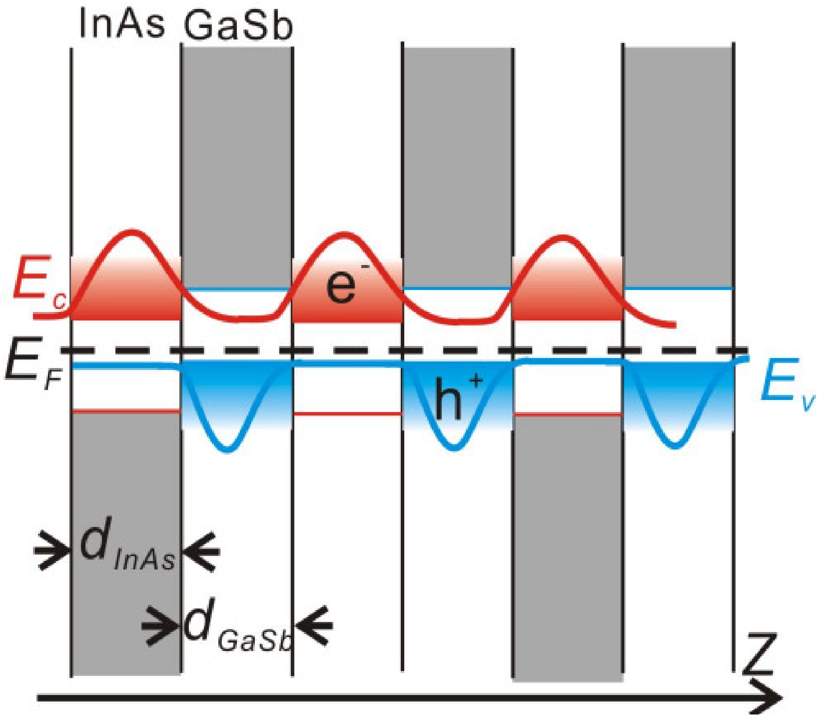
II. Type II broken-gap superlattices

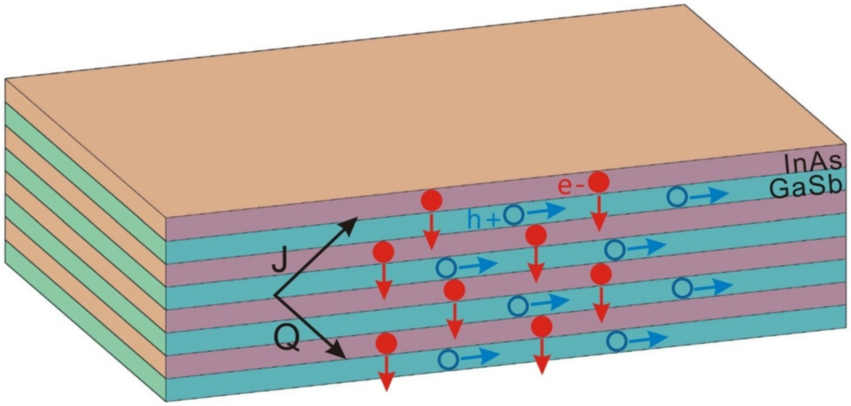
Transverse thermoelectric figure of merit:

$$Z_{\perp}T = \frac{S_{xz}^{2}}{\rho_{xx}\kappa_{zz}}T$$

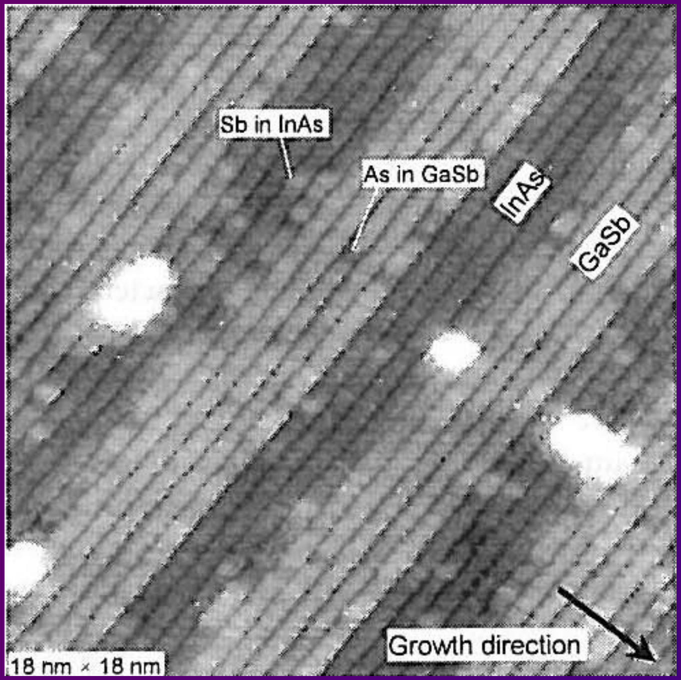
InAs/GaSb Type II superlattice

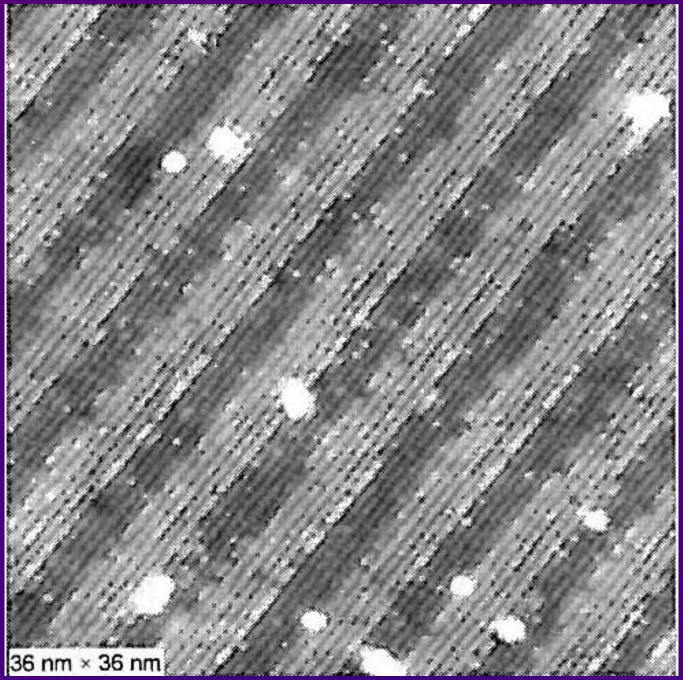
- InAs/GaSb type II broken-gap superlattice (T2SL)
  - Tunable bandgap
  - Anisotropic electron-hole transport
  - Fabrication challenge: strain, interface diffusion





Interface Quality:





Minimal Sb segregation

Up to 15 um superlattice growth with smooth morphology

M. Razeghi, Binh-Minh Nguyen, et al.
Proc. SPIE **6206,** 0277-786X/06 (2006)
Type II superlattice photodetectors for MWIR to VLWIR Focal Plane Arrays

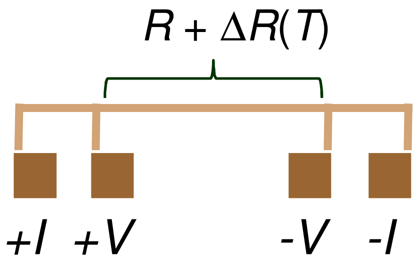
Thermal Conductivity: Experiment

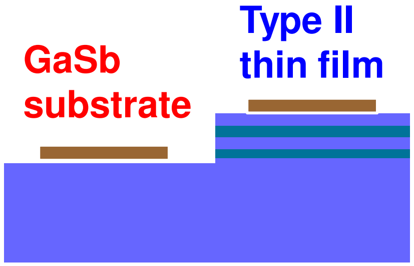
$$Z_\perp T = \frac{S_{xz}^2}{\rho_{xx}\boxed{\kappa_{zz}}} T$$

3ω Thermal Conductivity

- Vertical thermal conductivity

  proportional to 3rd harmonic





$$\kappa = \frac{V_{\omega}^{3} \ln\left|f_1/f_2\right|}{4\pi L R^{2}\left(V_{3\omega,1} - V_{3\omega,2}\right)} \frac{dR}{dT}$$

$$I \sim e^{i\omega t}$$

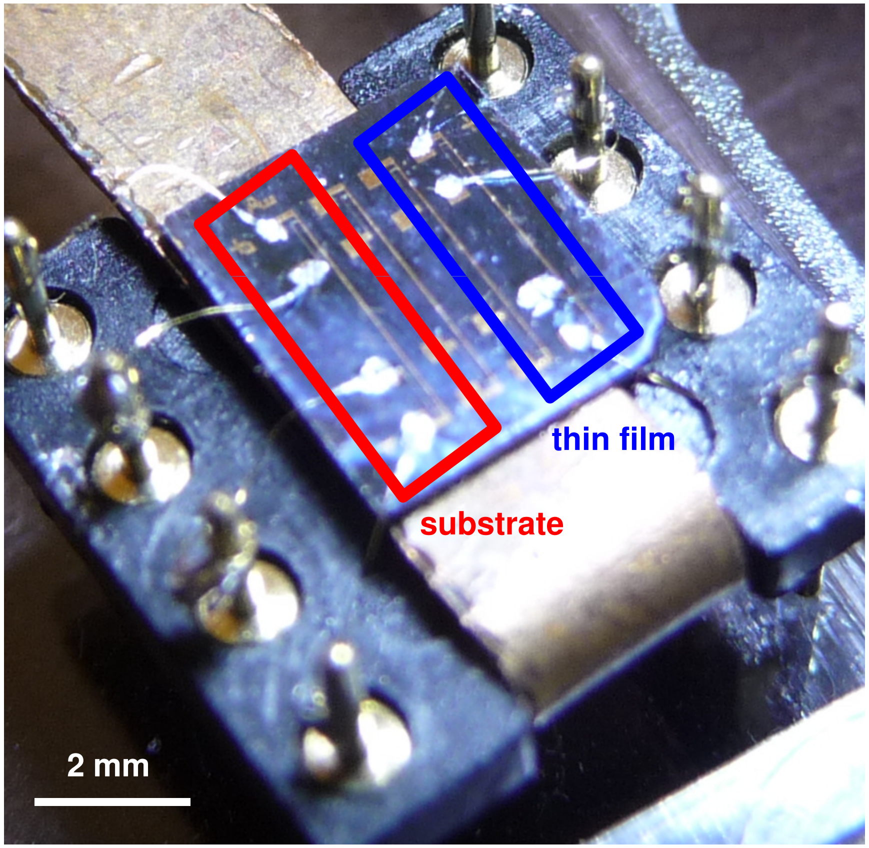
$$\Delta T \sim P = I^2 R \sim e^{i2\omega t}$$

$$\Delta R \sim (dR/dT)T \sim e^{i2\omega t}$$

$$\Delta V = I\Delta R \sim \boxed{e^{i3\omega t}}$$

D. G. Cahill, Rev. Sci. Instrum. 61(2) 802, (1990).

D. G. Cahill, Phys. Rev. B 50, 6077 (1994).

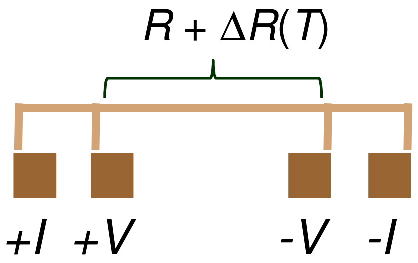


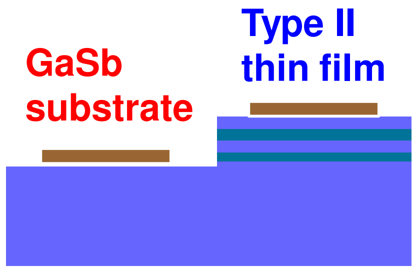
Chuanle Zhou, MG, et al. J. Elect. Mat. (2012)

3ω Thermal Conductivity

- Vertical thermal conductivity

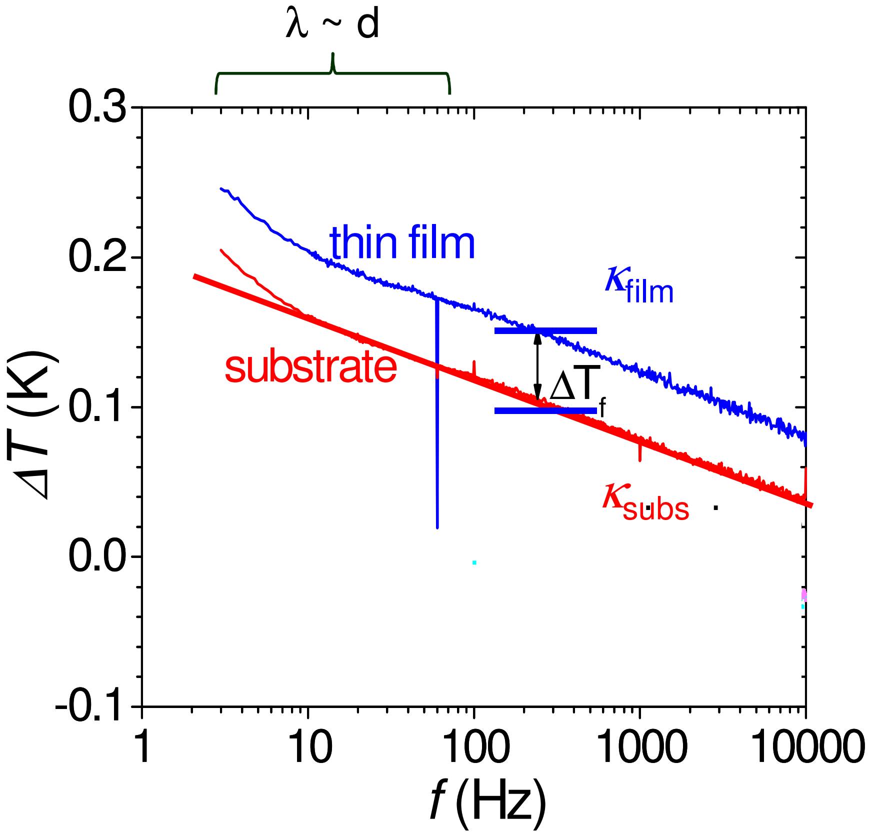
  proportional to 3rd harmonic





$$\kappa = \frac{V_\omega^3 \ln\left|f_1/f_2\right|}{4\pi L R^2 (V_{3\omega,1} - V_{3\omega,2})} \frac{dR}{dT}$$

$$\Delta V = I \Delta R \sim \boxed{e^{i3\omega t}}$$



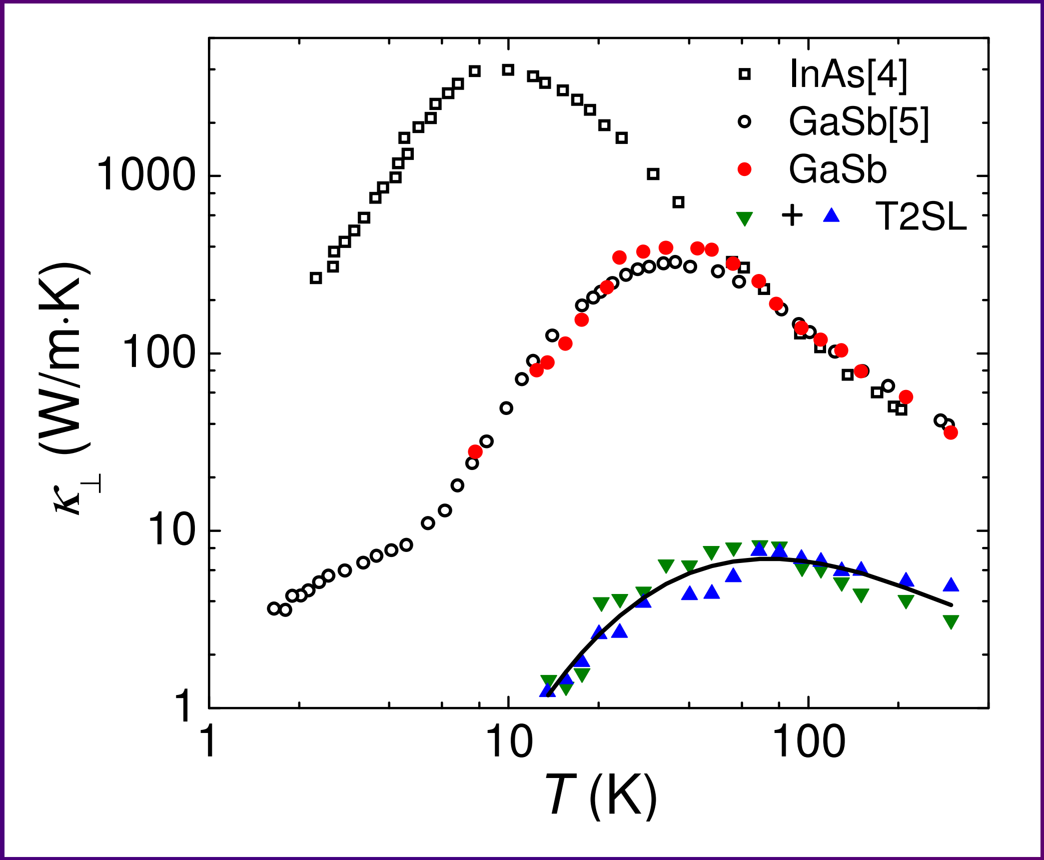
D. G. Cahill, Rev. Sci. Instrum. 61(2) 802, (1990).

D. G. Cahill, Phys. Rev. B 50, 6077 (1994).

Chuanle Zhou, MG, et al. J. Elect. Mat. (2012)

Type II Superlattice Thermal Conductivity

Thermal conductivity suppressed up to 2 orders of magnitude from GaSb bulk value



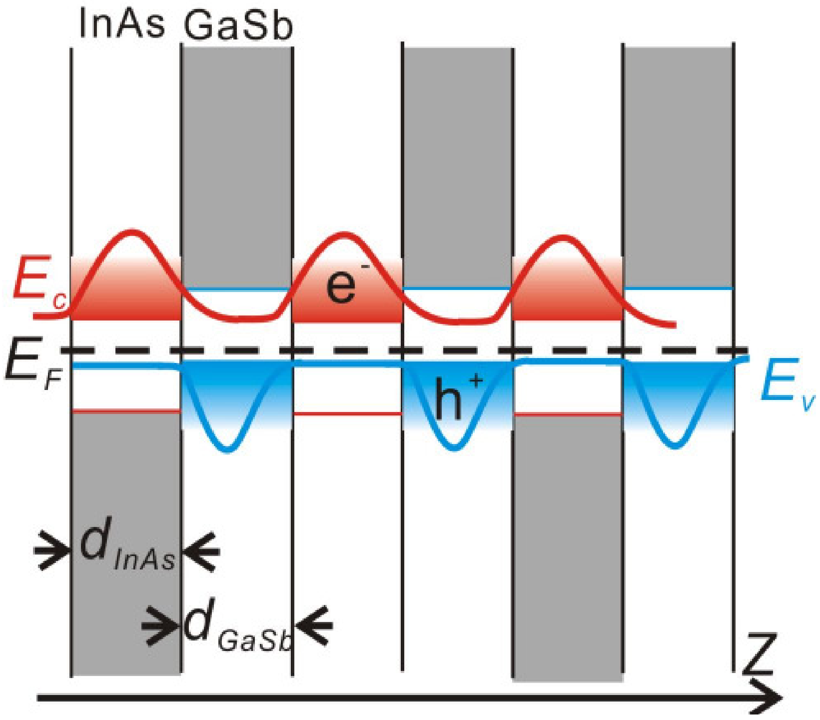
Chuanle Zhou, MG, et al unpublished

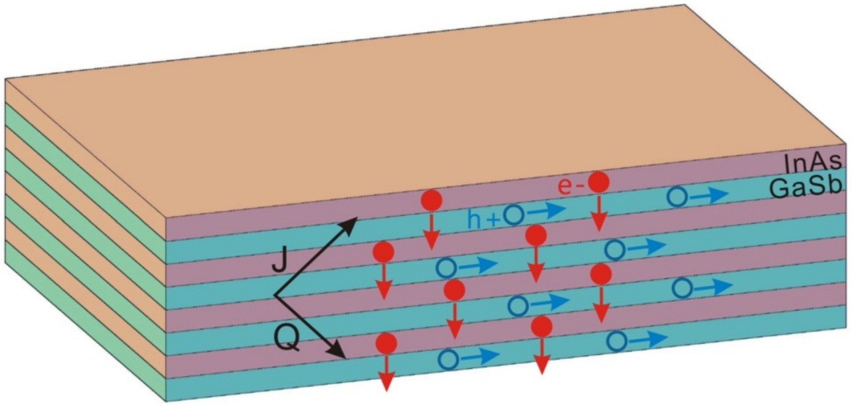
Power Factor: Theory

$$Z_\perp T = \frac{S_{xz}^2}{\rho_{xx}\kappa_{zz}} T$$

InAs/GaSb Type II superlattice

- InAs/GaSb type II broken-gap superlattice (T2SL)
  - Tunable bandgap
  - Anisotropic electron-hole transport
  - Fabrication challenge: strain, interface diffusion



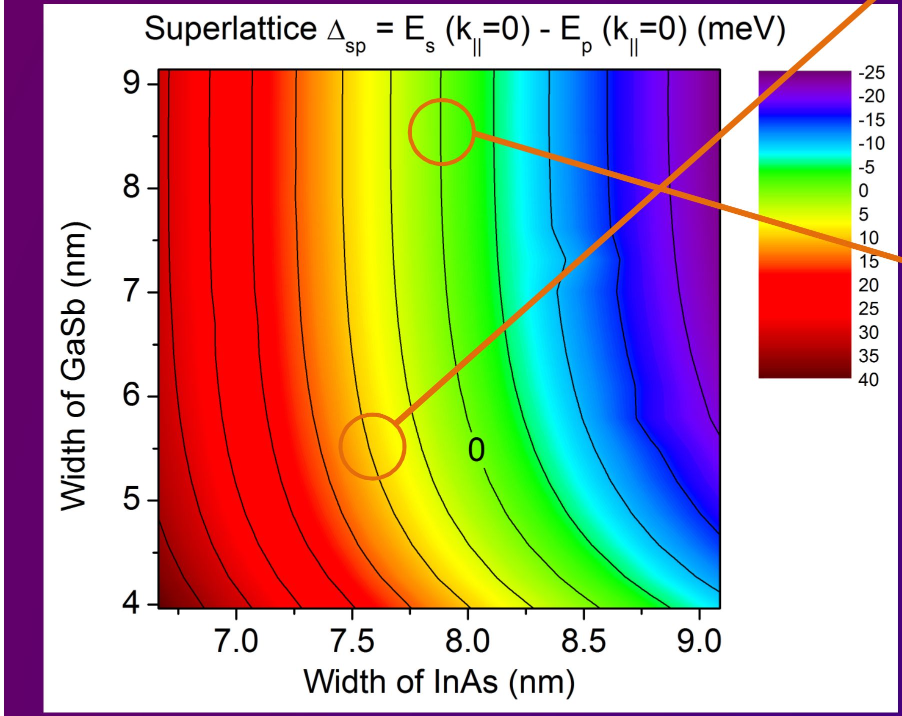


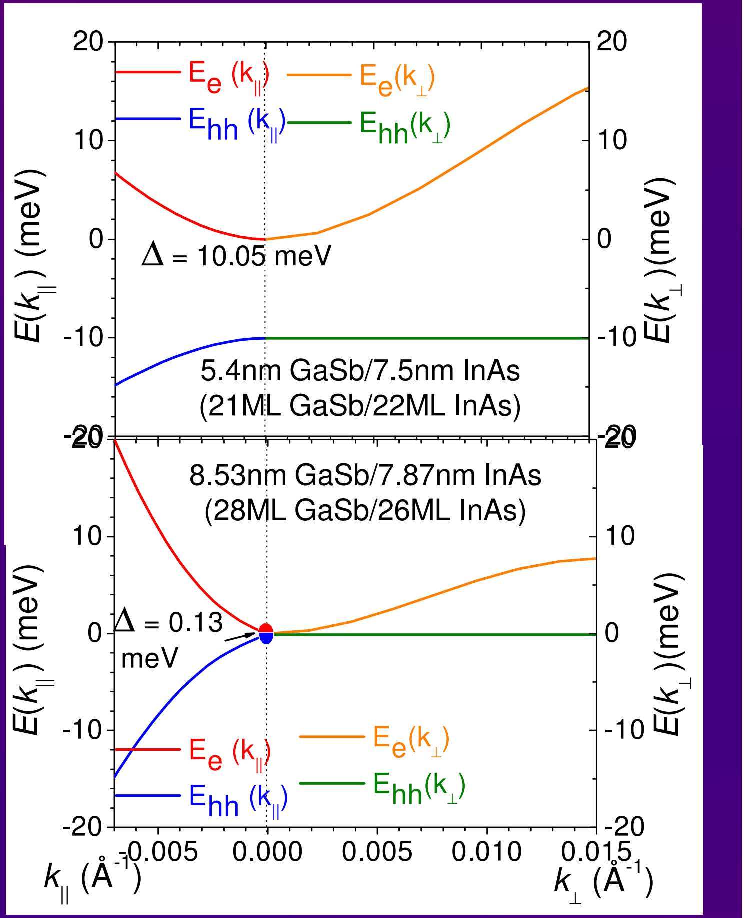
Type II Superlattice

NextNANO^3: Full-band envelope-function simulation InAs/GaSb superlattice dispersion

Positive gap: Semiconductor

Zero gap





NORTHWESTERN
UNIVERSITY

Deduce Conductivity & Seebeck Tensor

From band structure => $m_{n,x}, m_{n,y}, m_{p,y}, E_g \; (m_{p,y} = \infty)$

For *n*-conductivity & Seebeck:
anisotropic 3D dispersion

$$\sigma_{n,xx} = \frac{2\sqrt{2}e^2\gamma}{3\pi^2\hbar^3}\sqrt{m_{n,y}}(k_BT)^{s+3/2}\Gamma(s+\frac{3}{2})F_{3/2+s}\left(\frac{\mu-E_g}{k_BT}\right),$$

$$\sigma_{n,yy} = \frac{2\sqrt{2}e^2\gamma}{3\pi^2\hbar^3}\sqrt{\frac{m_{n,x}^2}{m_{n,y}}}(k_BT)^{s+3/2}\Gamma(s+\frac{3}{2})F_{3/2+s}\left(\frac{\mu-E_g}{k_BT}\right)$$

$$s_n = \frac{-k_B}{e}\left[\frac{(s+5/2)F_{s+\frac{3}{2}}\left(\frac{\mu-E_g}{k_BT}\right)}{(s+3/2)F_{s+\frac{1}{2}}\left(\frac{\mu-E_g}{k_BT}\right)} - \frac{\mu-E_g}{k_BT}\right]$$

For *p*-conductivity & Seebeck:
2D dispersion

$$\sigma_{p,xx} = \frac{e^2\gamma}{\pi d\hbar^2}(k_BT)^{s+1}\Gamma(s+2)F_{1+s}\left(\frac{-\mu}{k_BT}\right)$$

$$\sigma_{p,yy} = 0$$

$$s_p = \frac{k_B}{e}\left[\frac{(s+2)F_{s+1}\left(\frac{-\mu}{k_BT}\right)}{(s+1)F_s\left(\frac{-\mu}{k_BT}\right)} + \frac{\mu}{k_BT}\right]$$

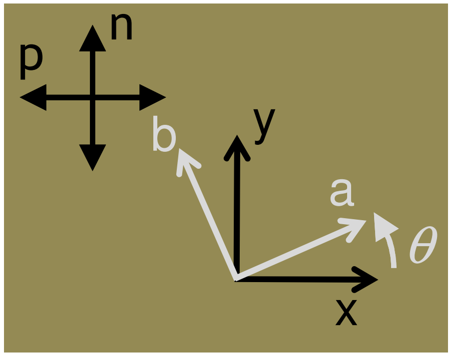
(Power-law scattering, $\tau = \gamma E^s$, where *s* = 0 observed for T2SL at 300 K)

Optimize transverse power factor $S^2\sigma$ => deduce optimal chemical potential μ

Chuanle Zhou, MG, submitted to PRL

INAS/GASB TYPE II SUPERLATTICE

- Optimal T2SL
  - $d_{\mathrm{GaSb}} = 3.96$ nm, $d_{\mathrm{InAs}} = 7.88$ nm
  - $E_g = 28.3$ meV, $\mu = 2.43$ meV
  - $\theta_\perp = 32°$
  - $\kappa = 4$ W/m·K (measured[1])
  - $\boxed{Z_\perp T = 0.025}$ at $T = 300$ K



[1] C. Zhou *et al.*, J. Elec. Mat. (2012)

Differential Transport Equations

- Transverse Thermoelectrics

$$0=\left(\frac{E_a}{S_{ba}}-\frac{dT}{db}\right)^2+\frac{(1+Z_{ba}T)}{Z_{ba}}\frac{d^2T}{db^2}$$

$$\boxed{S_{ba}=S_{ab}}$$

- Longitudinal thermoelectrics

$$0=\left(\frac{E_a}{S_{ba}}\right)^2+\frac{1}{Z}\frac{d^2T}{db^2}$$

$$\boxed{S_{ba}=S_{ab}=0}$$

- Ettingshausen effect

$$0=\left(\frac{E_a}{S_{ba}}\right)^2-\left(\frac{dT}{db}\right)^2+\frac{(1-Z_{ba}T)}{Z_{ba}}\frac{d^2T}{db^2}$$

$$\boxed{S_{ba}=-S_{ab}}$$

Thermal distribution

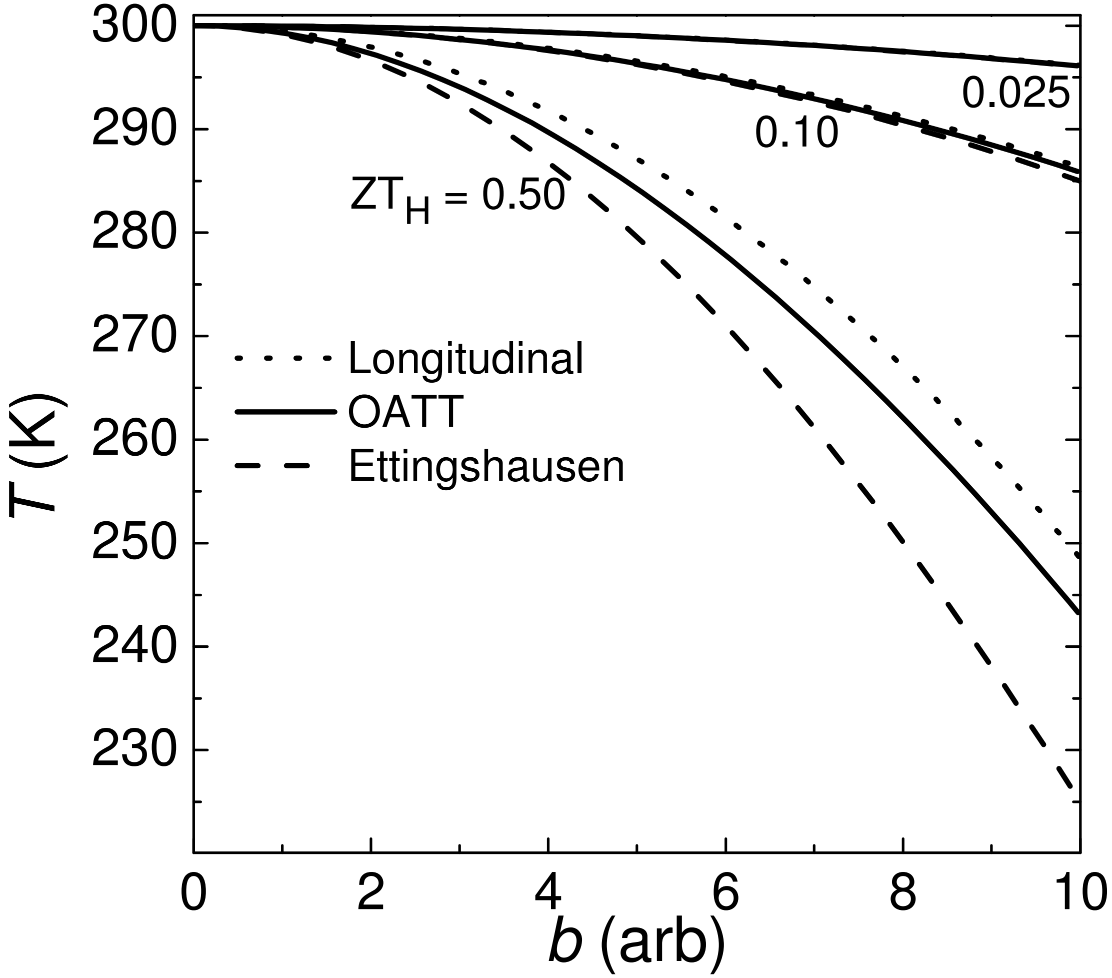
- Different from longitudinal and Ettingshausen cooling

- $\Delta T = 4$ K (ZT = 0.026)

$T_H = 300$ K, $b = 10$ µm

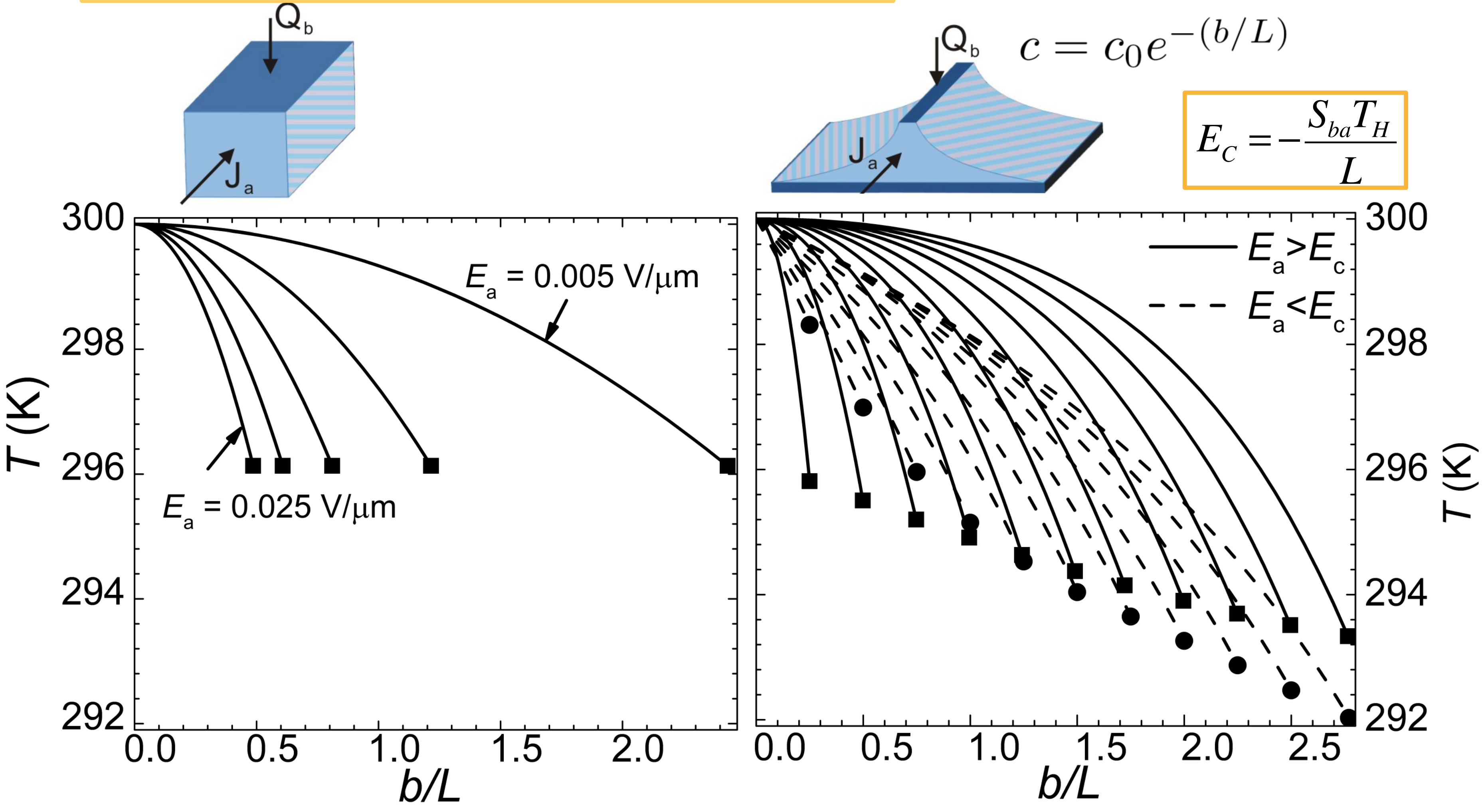
ΔT=14 K (ZT = 0.1)

ΔT=56 K (ZT = 0.5)



Exponentially tapering

- A competitive ΔT = 8 K (b/L=2.77)



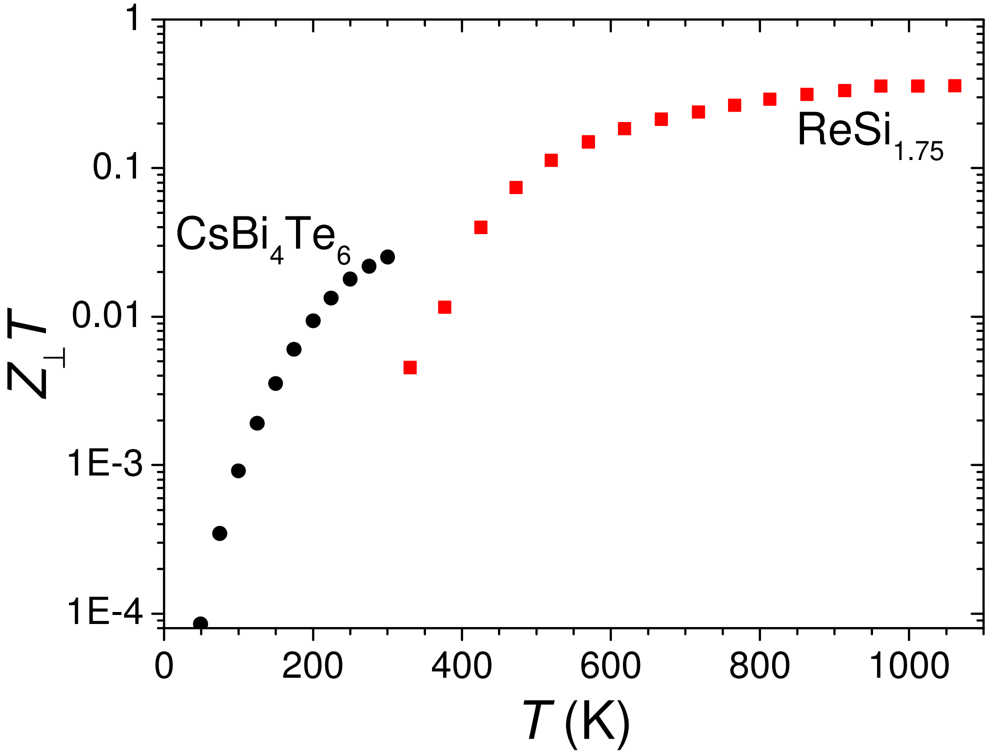
$$c = c_0 e^{-(b/L)}$$

$$E_C = -\frac{S_{ba} T_H}{L}$$

$p \times n$ Type material

- Bulk materials (monoclinic)[1,2]: $CsBi_4Te_6$, $ReGe_xSi_{1.75-x}$

  p-type in *a*-direction and *n*-type in *c*-direction



- Bulk material, geometric shaping
- Low $Z_\perp T$ at low temperature

[1] Gu, Zhang, PRB 71, 113201 (2005)
[2] Chyung, Mahanti, Kanatzidis, MRS Proc 793 (2004)

p x *n* Transverse Thermoelectrics:

Outline:

I. Transverse Thermoelectricity

II. Type II broken-gap superlattices

Let Us Meet Again

We welcome all to our future group conferences of Omics group international

Please visit:

www.omicsgroup.com

www.Conferenceseries.com

http://optics.conferenceseries.com/