Nanostructured Thermoelectric Materials: From Basic Physics to Applications

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J.P. Fleurial
DOE, NSF, and Industry

Outline

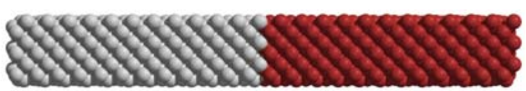
- Why nanocomposites?
- What we have achieved?
- What we do not understood?
- Application opportunities

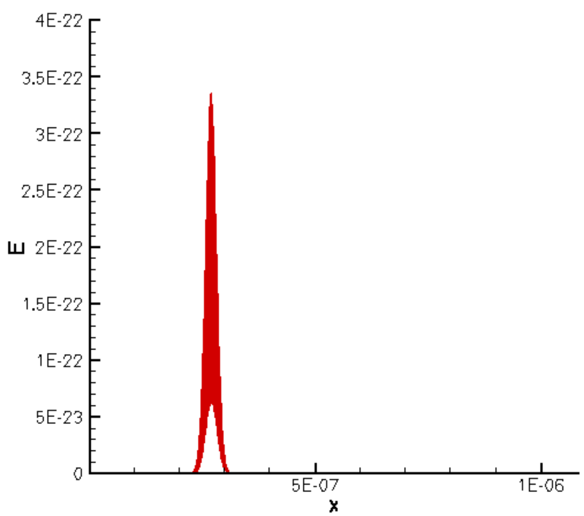
Nanoscale Effects for Thermoelectrics

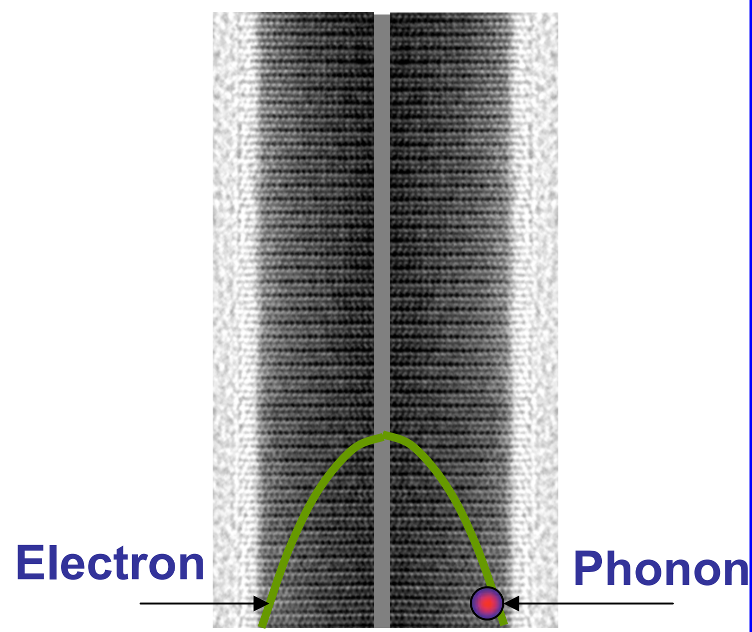
Interfaces that Scatter Phonons but not Electrons

Electrons
Λ=10-100 nm
λ=10-50 nm

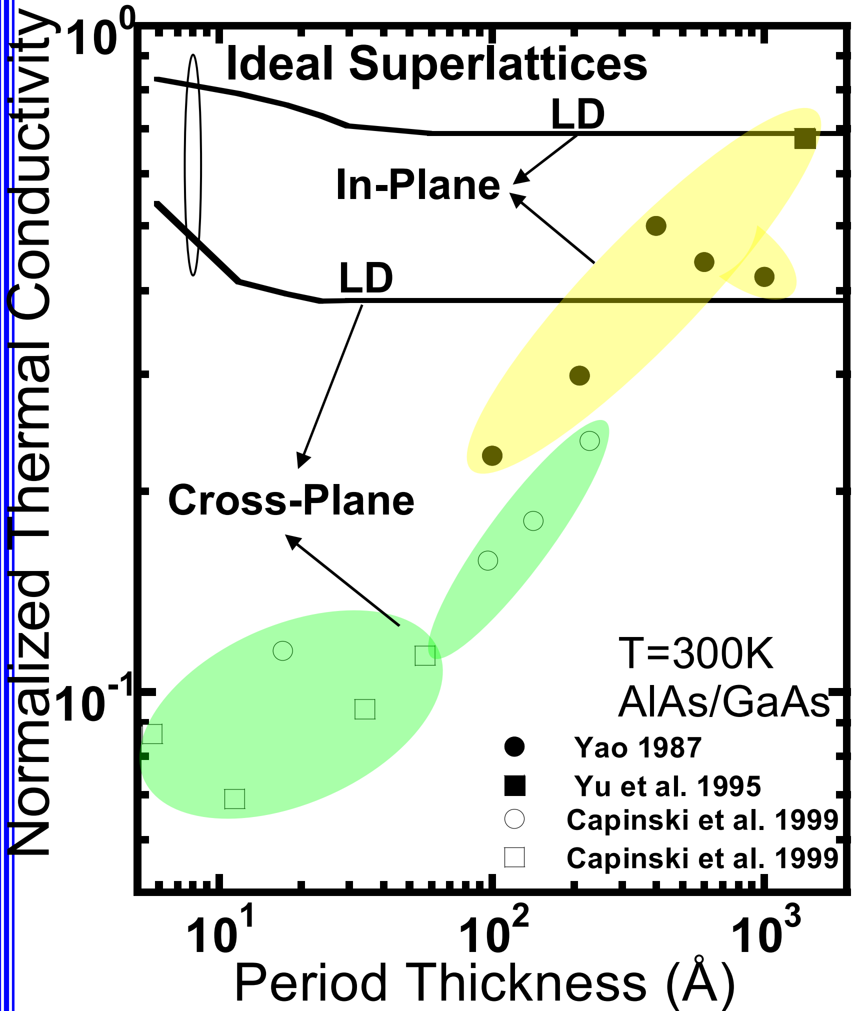
Phonons
Λ=10-100 nm
λ=1 nm

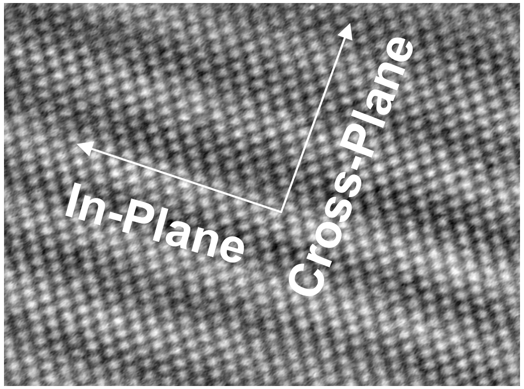






Heat Conduction Mechanisms in Superlattices



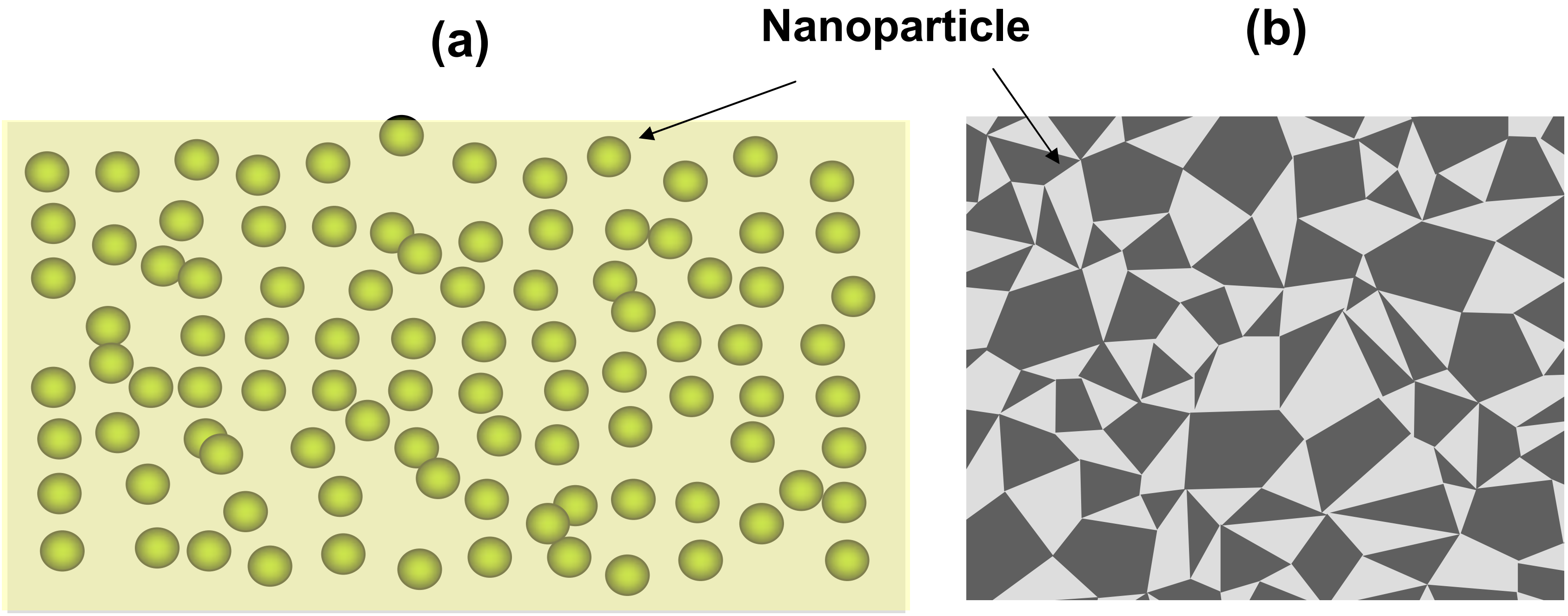


Major Conclusions:

- Ideal superlattices do not cut off all phonons due to pass-bands
- Individual interface reflection is more effective
- Diffuse phonon interface scattering is crucial

Periodic Structures Are Not Necessary, Nor Optimal!

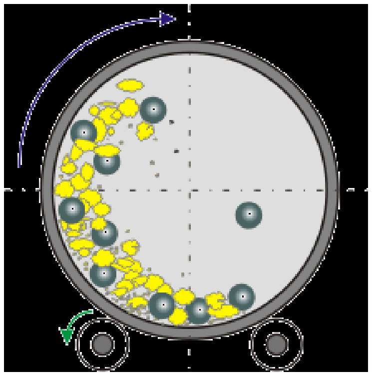
Nanocomposites Approach

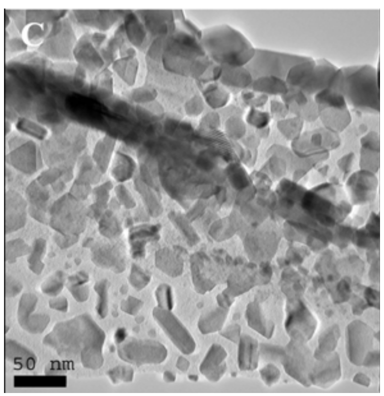


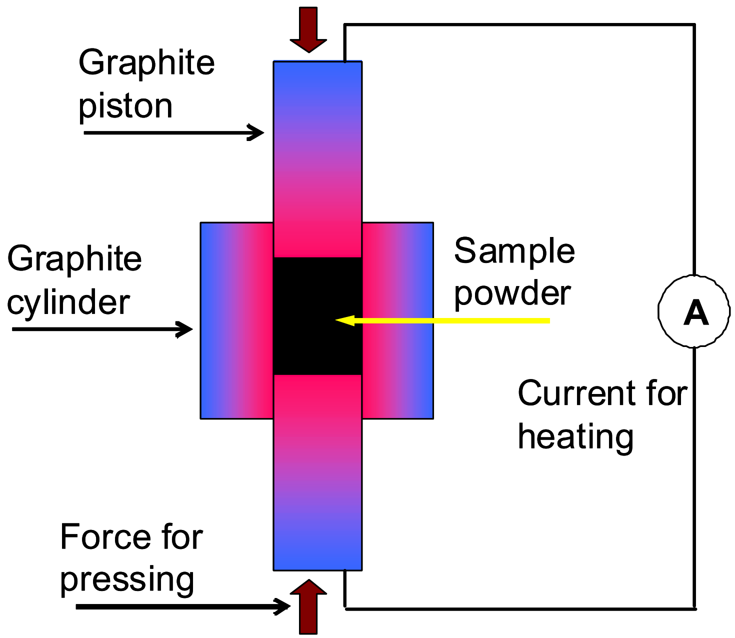
– Increase interfacial scattering by mixing nano-sized particles.

– Enable batch fabrication for large scale application.

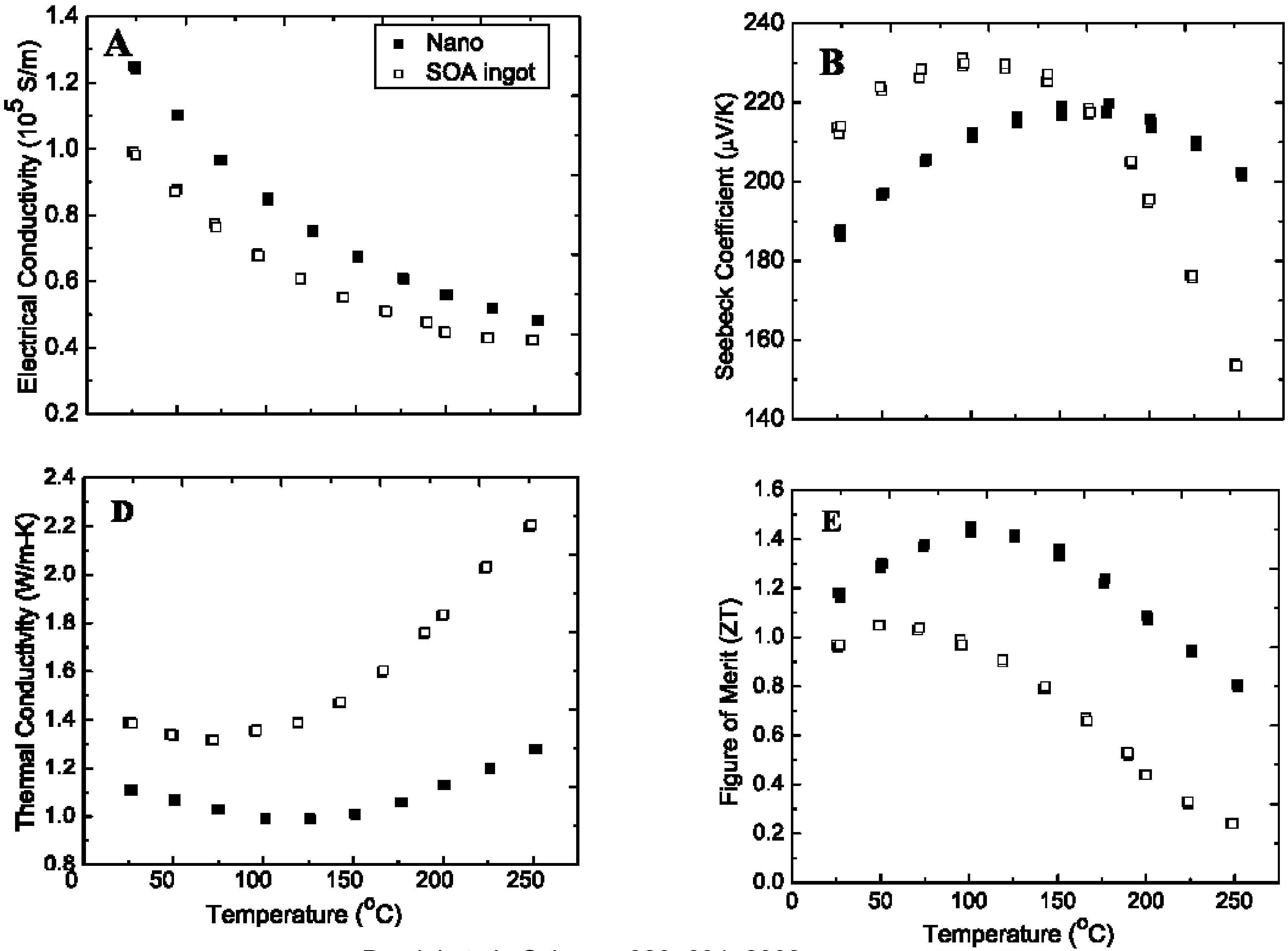
Low-Cost Synthesis





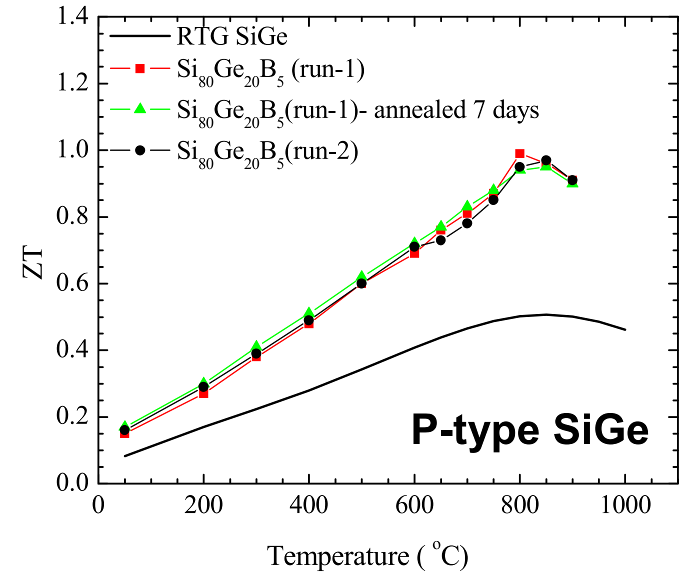


Thermoelectric Properties: Bi_2Te_3

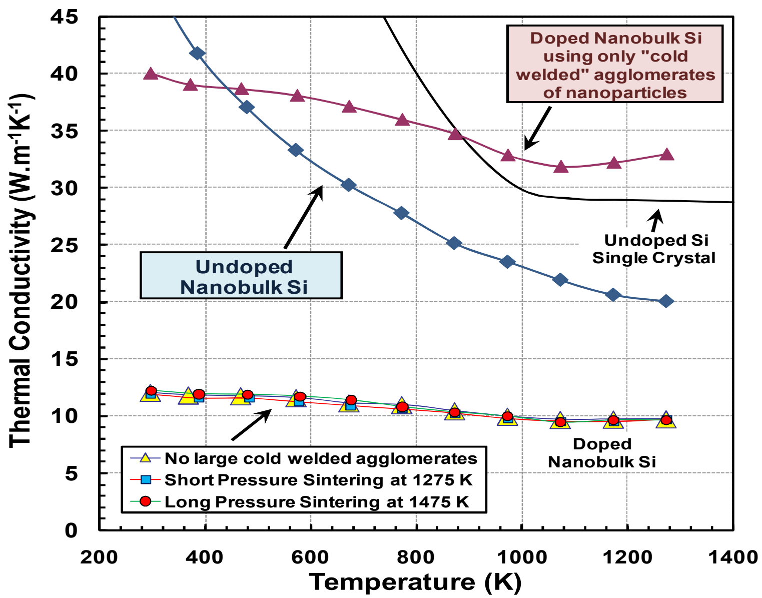


Poudel et al., Science, 320, 634, 2008

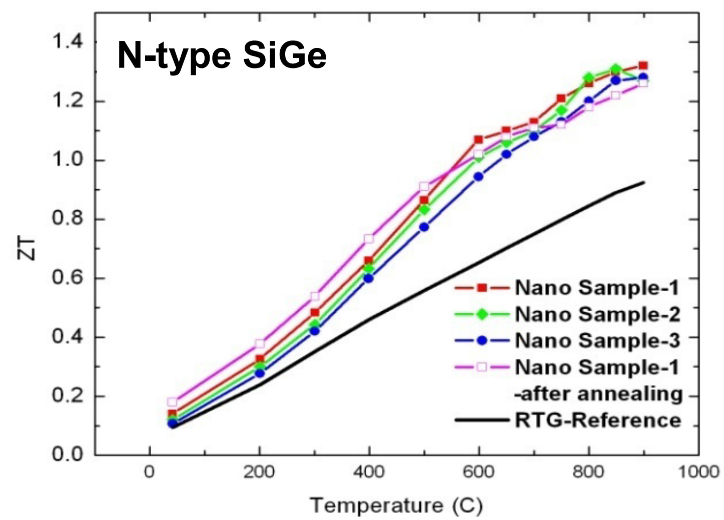
Si_xGe_{1-x} System



Joshi *et al.*, *Nano Letters* 8, 4670 (2008)

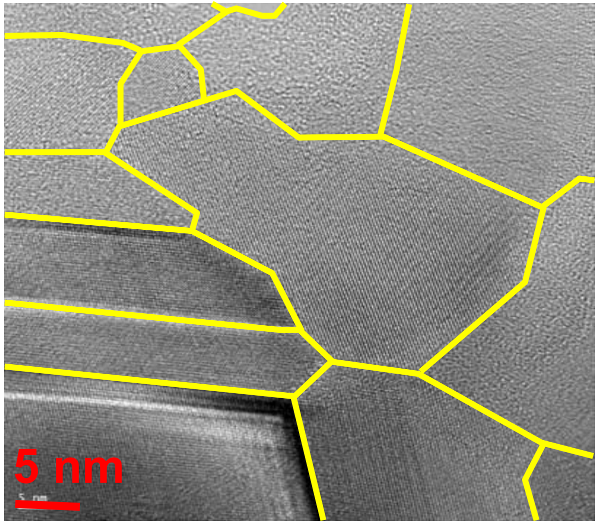


Bux et al., Adv. Func. Mat., 2009



Wang, *et al.* Appl. Phy. Lett. 93, 193121 (2008)

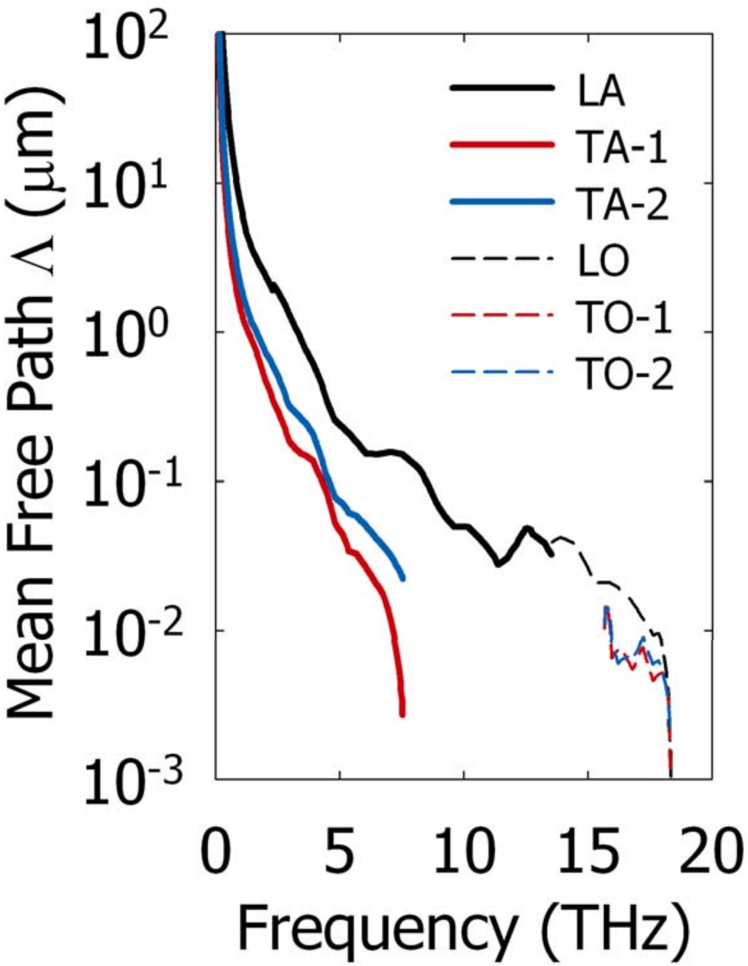
Understanding Electron and Phonon Transport in Random Nanostructures

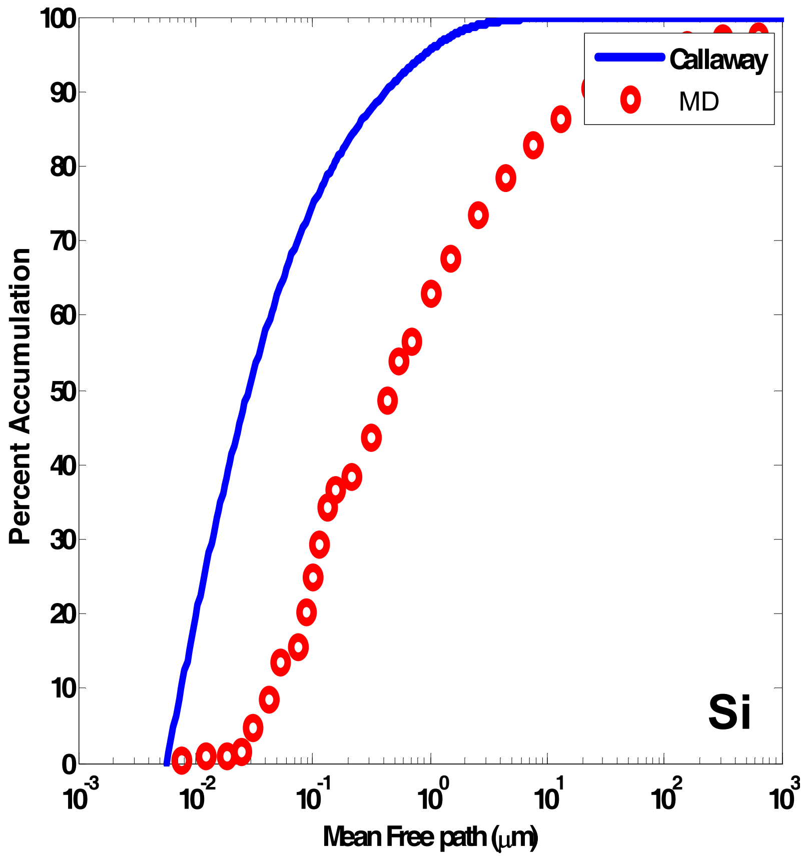


Phonons:

- What is the mean free path in bulk materials
  - ❑ Phonon-phonon
  - ❑ Dopants
  - ❑ Alloy
  - ❑ Electron scattering
  - ❑ Defects
- How phonons are scattered at an interfaces
  - ❑ Interface roughness
  - ❑ Crystallographic directions
  - ❑ Anharmonic effect

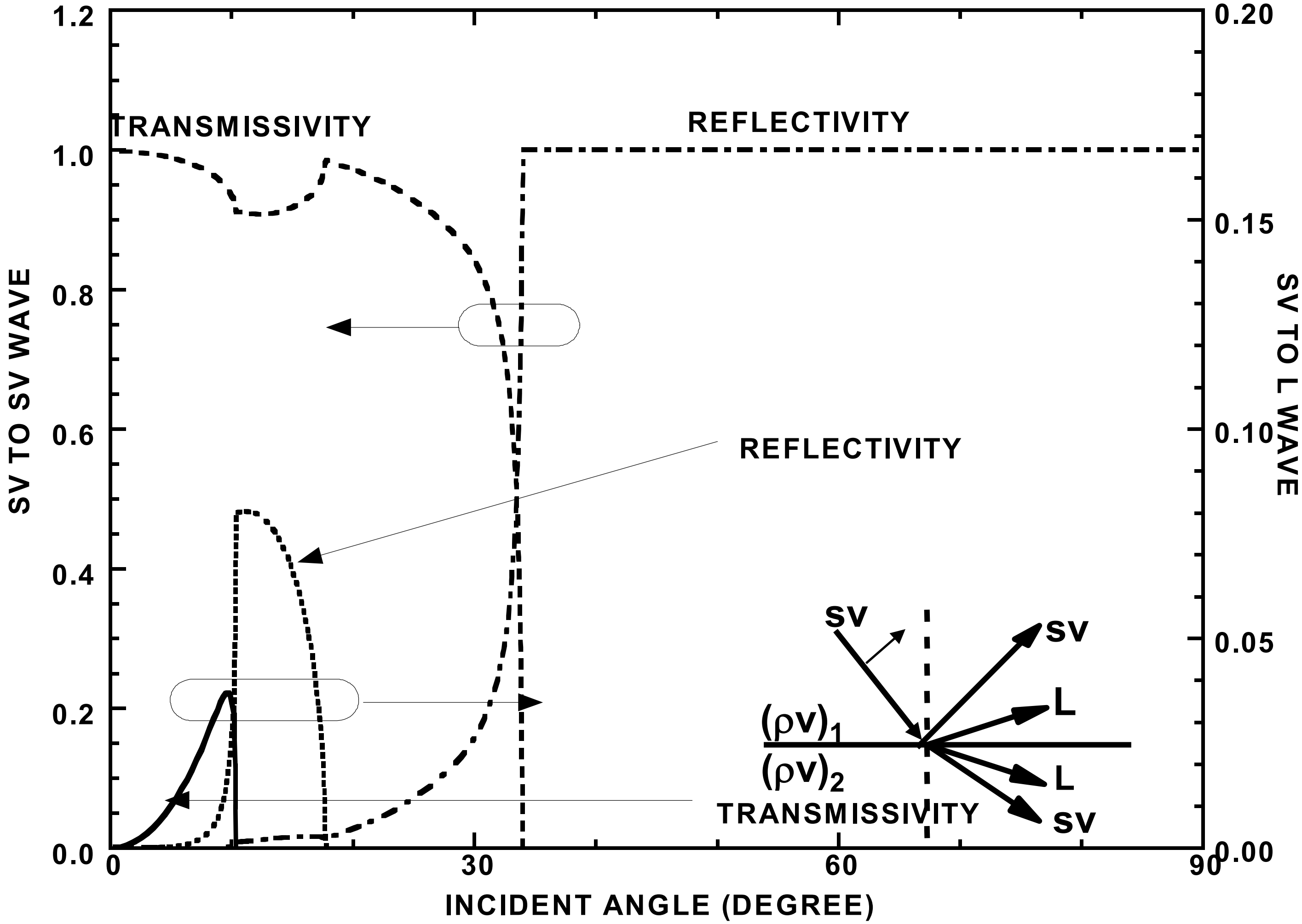
Molecular Dynamics Simulation of Phonon Mean Free Path





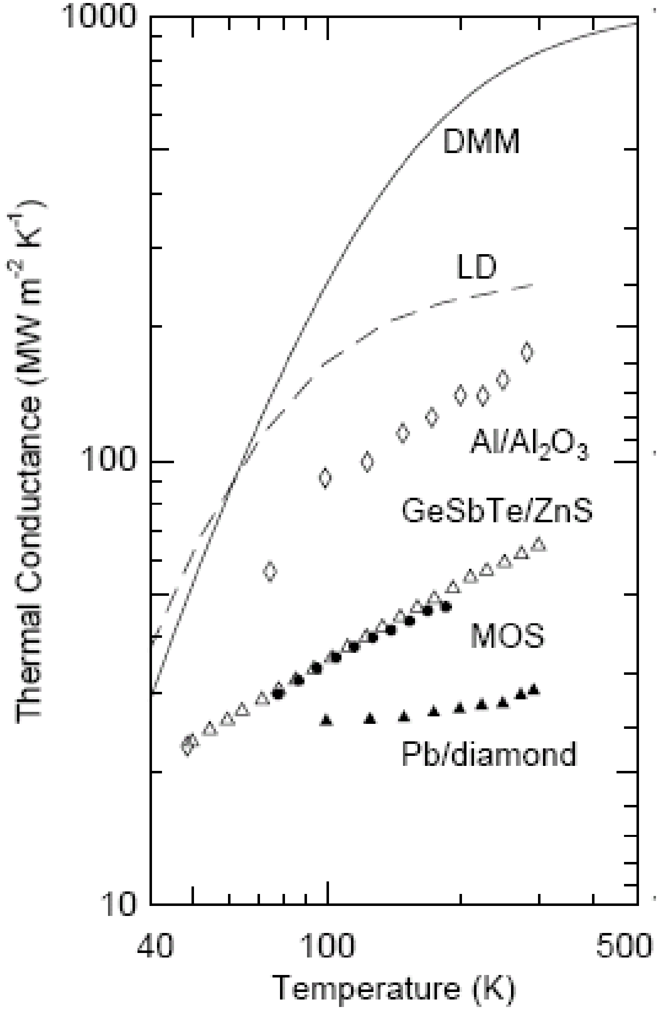
Henry and Chen, J. Comp. Theo. Nanosci., 5, 141 (2008).

Interface Reflectivity and Transmissivity



We know how to do it only in the continuum limit, with perfect interfaces!

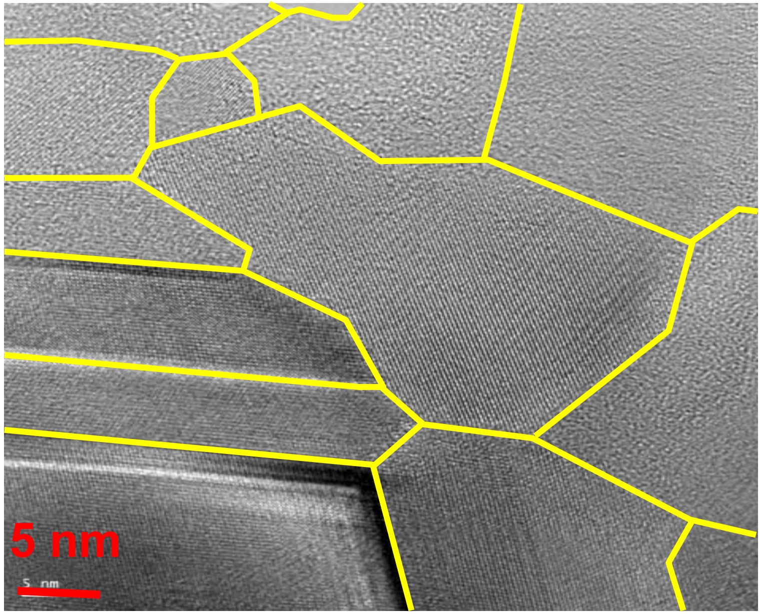
Thermal Interface Resistance Between Perfectly Contact Solids



Cahill et al., JAP, 2003

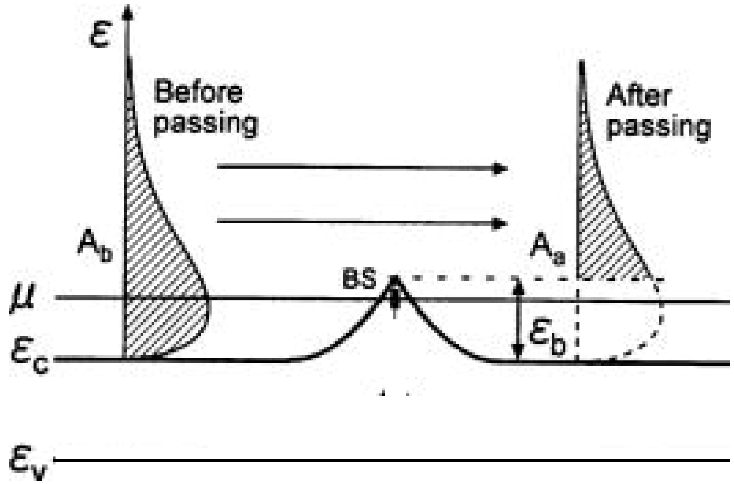
- No model can predict interface thermal conductance except at very low temperatures.
- Phonon transmissivity and reflectivity at interfaces are crucial parameters to model heat conduction in thermoelectric materials.

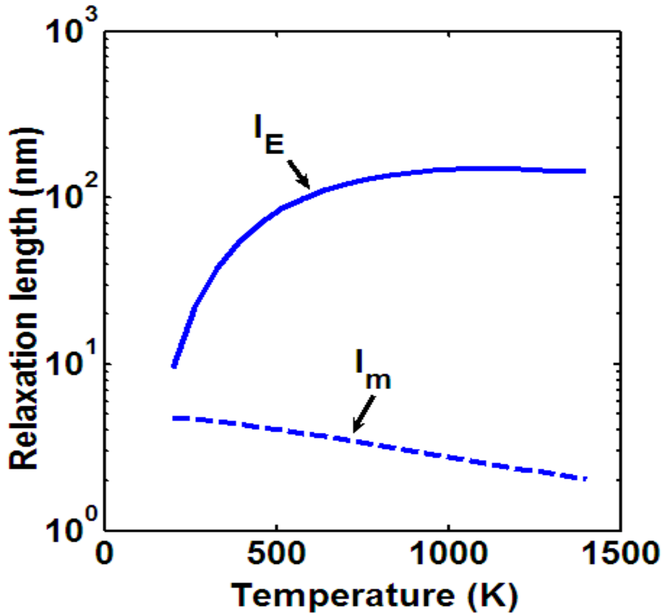
Electron Transport

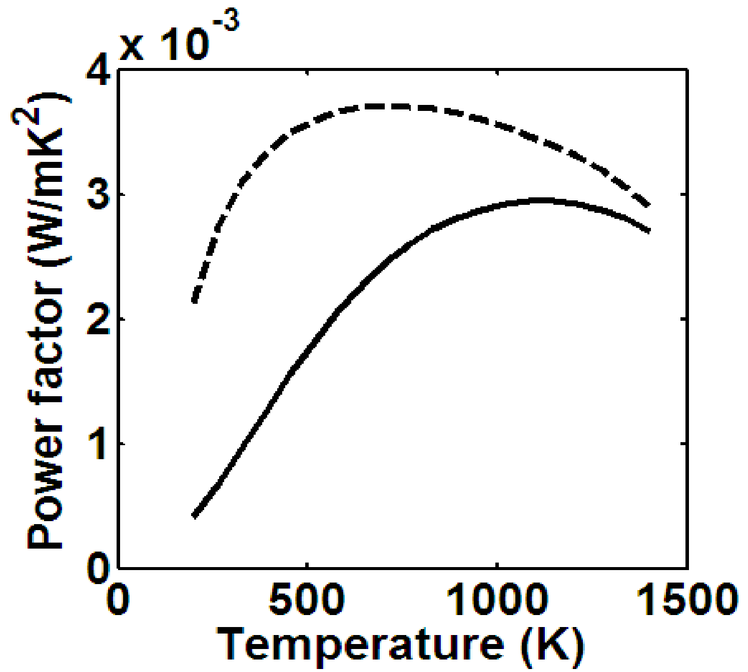


- **Where thermoelectric effect happens?**
- **Interfacial barrier height**
- **Momentum conservation at interfaces**
- **Scattering inside particles**
- **Energy dependency of scattering**

Thermionic emission at grain boundaries







SiGe nanocomposite,

E_b=0.2eV, N_D=4x10^{20} cm^{-3}

Need: $\ell_m \ll \ell \ll \ell_E$

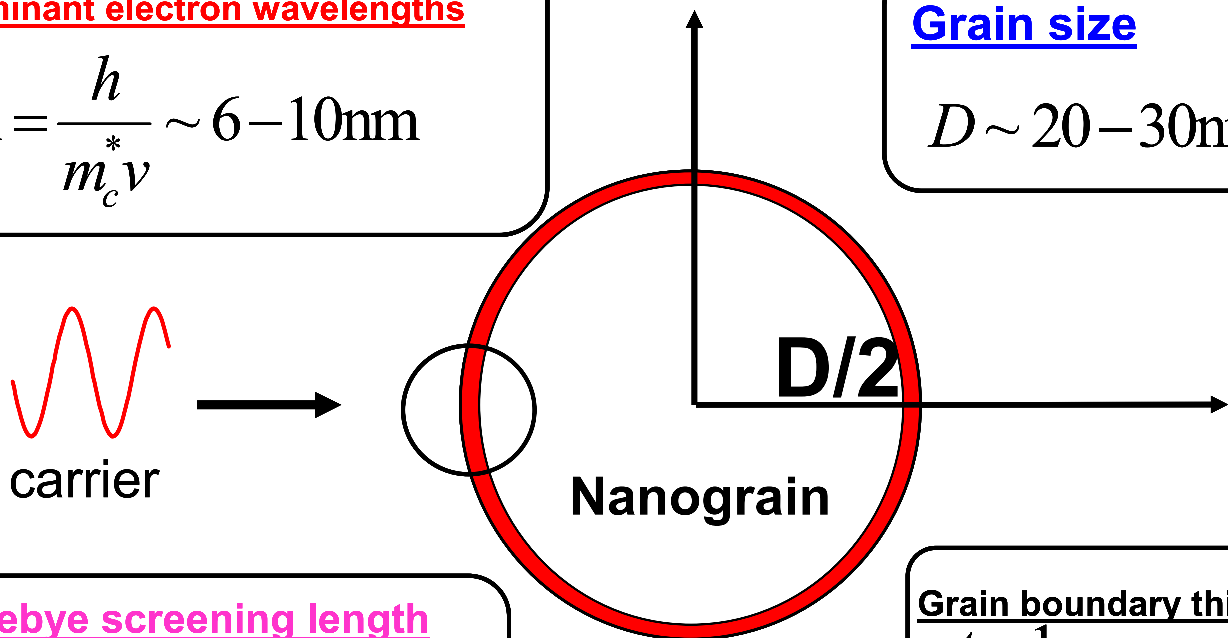
Nanoparticle/Nanograin Scattering

Dominant electron wavelengths

$$\Lambda = \frac{h}{m_c^* v} \sim 6-10\text{nm}$$

Grain size

$$D \sim 20-30\text{nm}$$



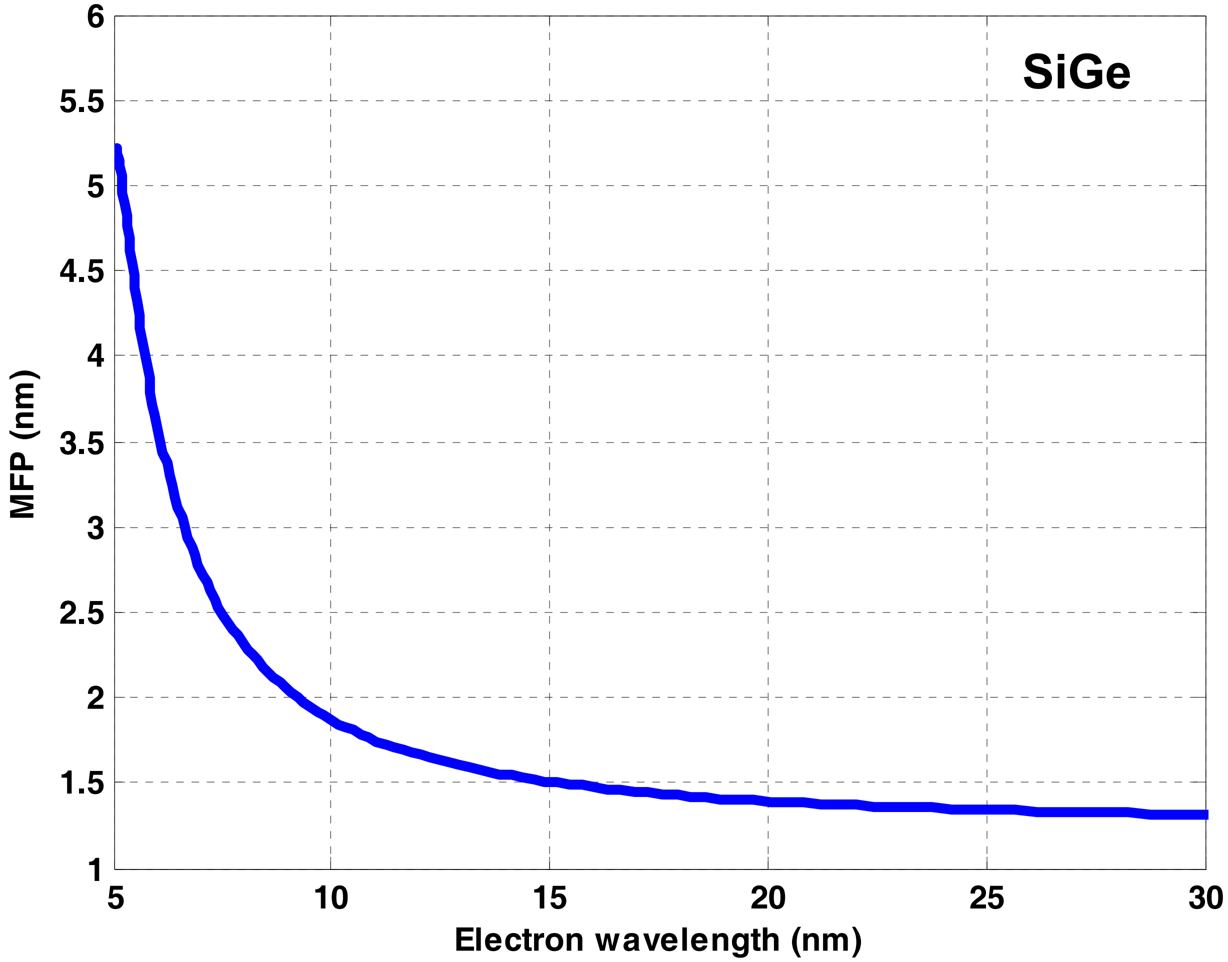
Debye screening length

$$L_D = \left(\frac{\varepsilon k T}{e^2 N} \right)^{1/2} \sim 0.5-1\text{ nm}$$

Grain boundary thickness

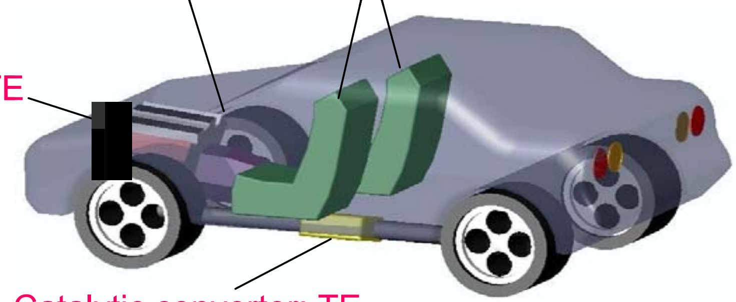
$$t \sim 1\text{ nm}$$

Electrons: MFP vs λ



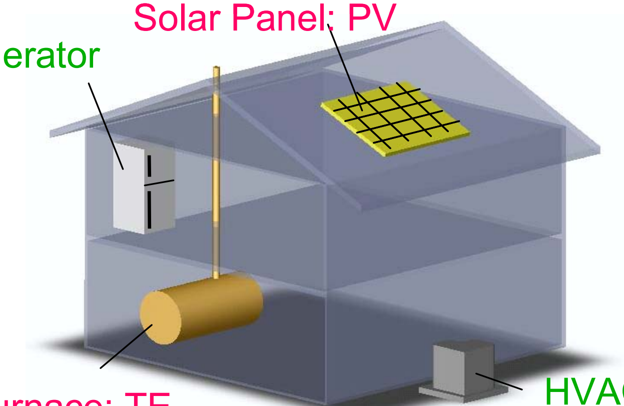
Minnich et al., Energy & Env. Sci., 2009.

Potential Applications

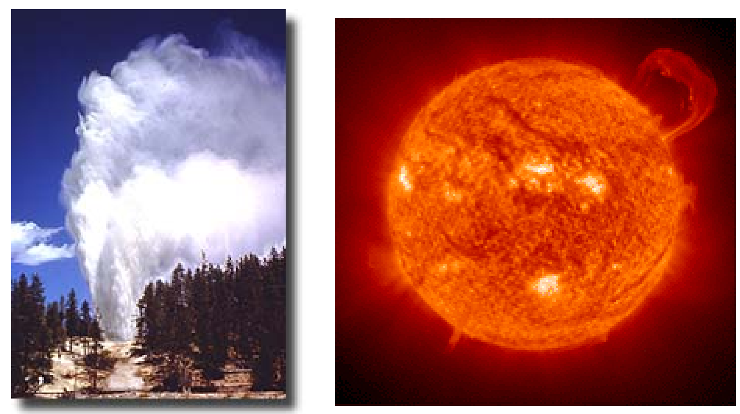


Transportation

Industrial Waste Heat (DOE/ITP)



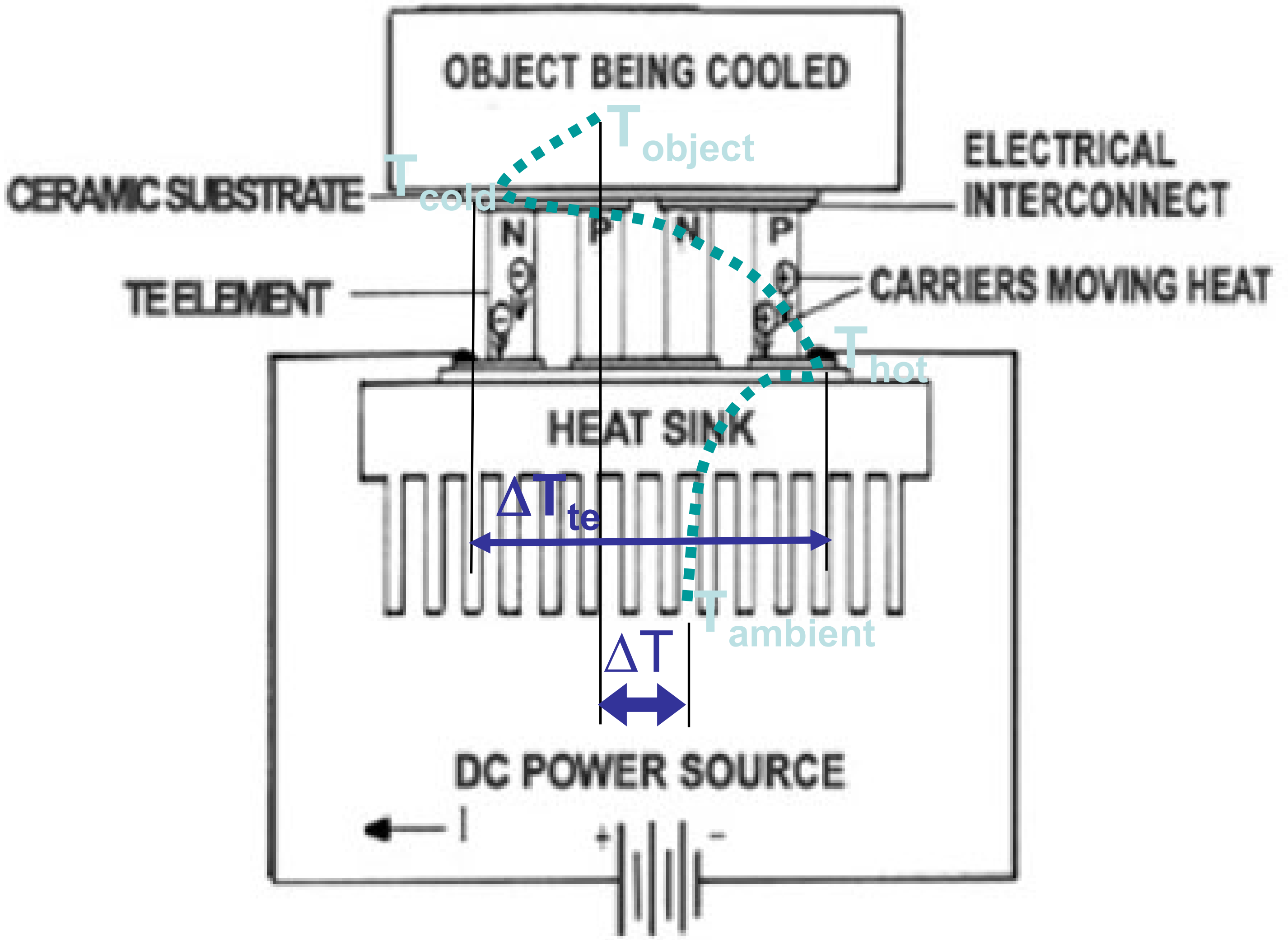
Buildings



Renewables

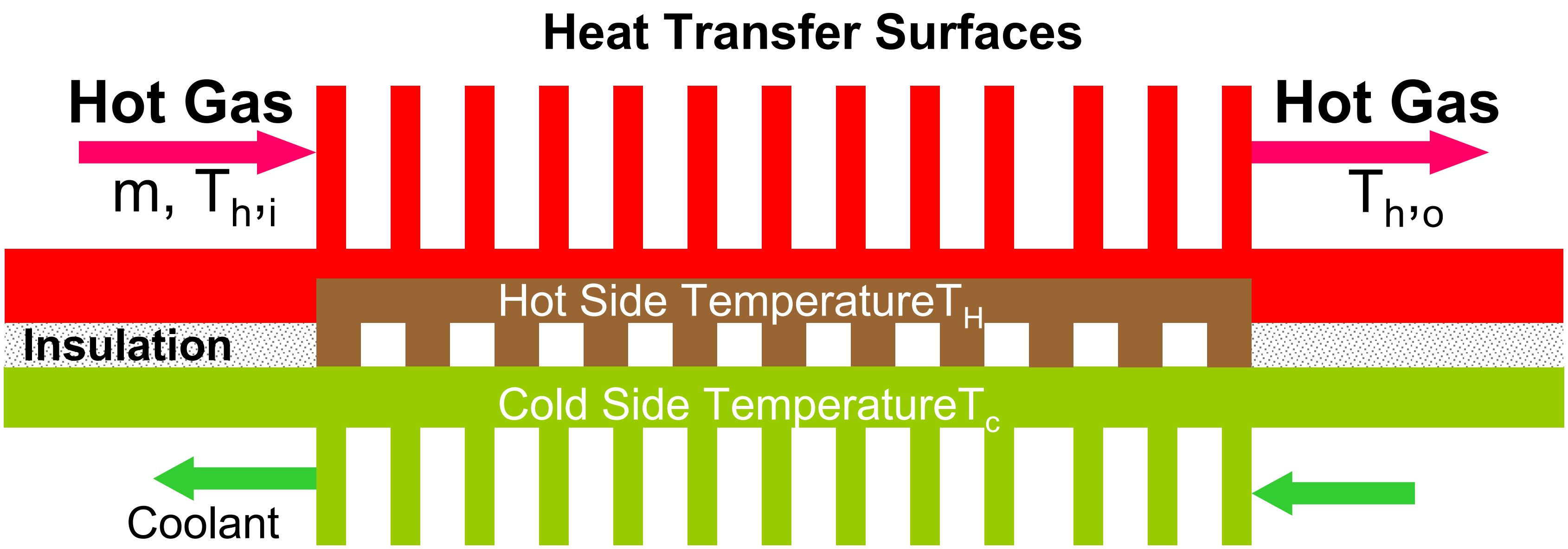
And Entropy is Generated

System Consideration



Sometimes, thermal systems more expansive

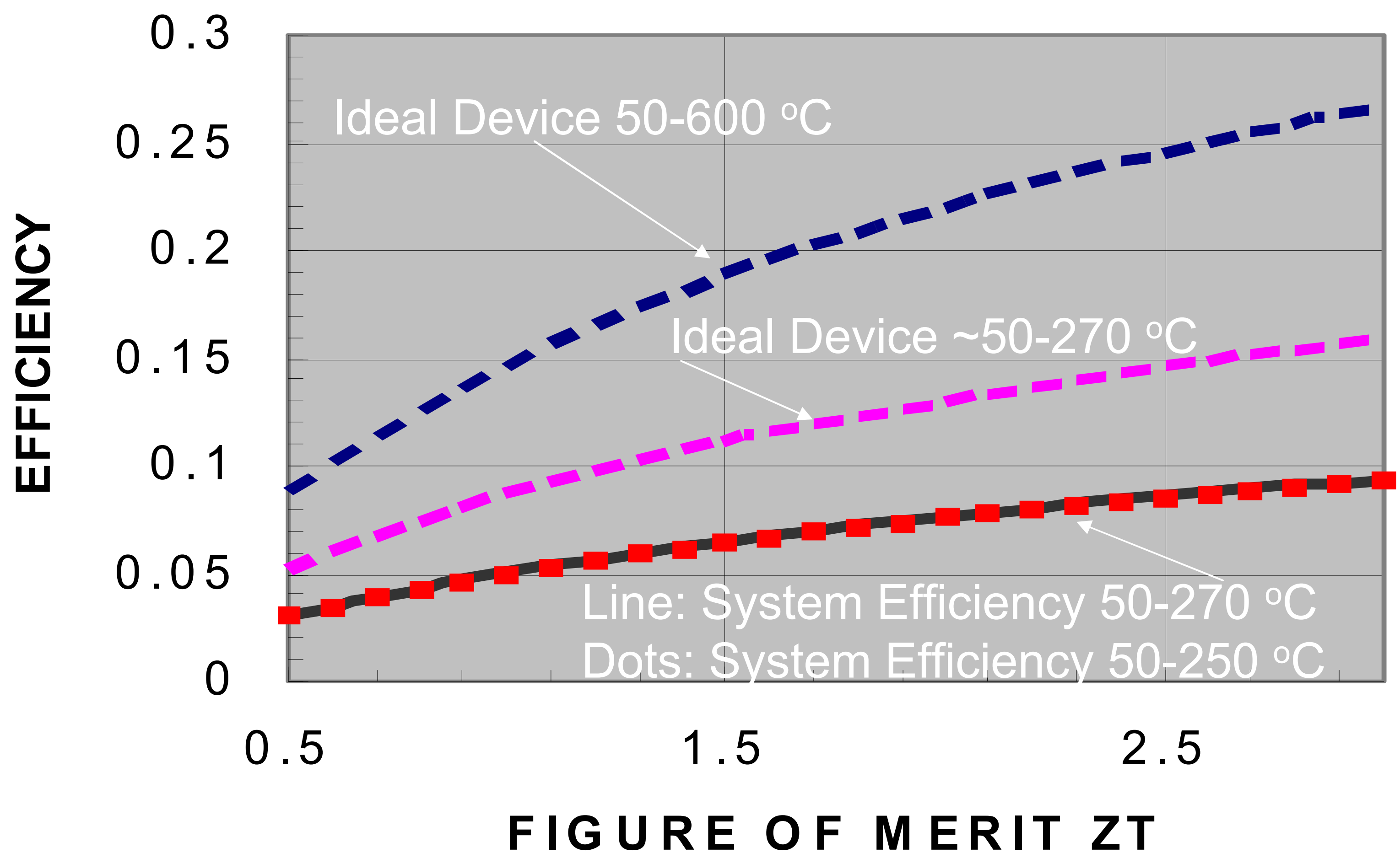
Heat to Electricity Recovery from Gas Stream



- **For thermoelectric devices, T_H higher is better**
- **However, maximum heat intercepted from hot gas stream, $mc_p(T_{h,i}-T_H)$, decreases with T_H**

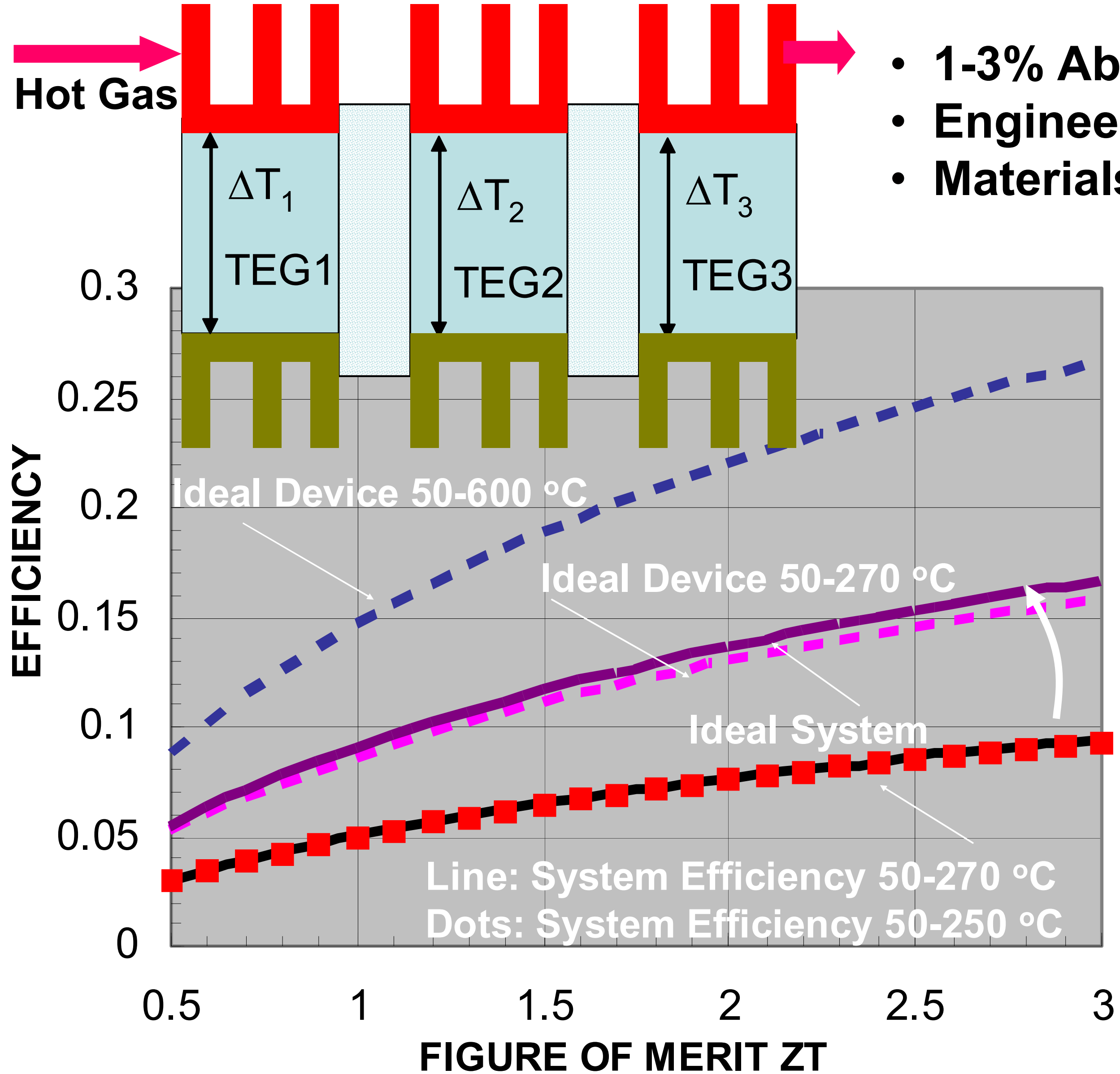
Efficiency Expectations

- $T_{h,i}$=600 °C, T_c=50 °C
- Optimal Hot Side Temperature ~ 270 °C



Locally Optimized Systems

- 1-3% Absolute Efficiency
- Engineering Room
- Materials Development



U.S. DEPARTMENT OF ENERGY

Solid-State Solar Thermal Energy Conversion Center (S³TEC)

Gang Chen (MIT)

S³TEC Center aims at developing transformational solid-state energy technologies to convert solar energy into electricity via heat, by advancing fundamental science of energy carrier coupling and transport, designing new materials, and inventing cost-effective manufacturing processes, and training energy workforce.

RESEARCH PLAN AND DIRECTIONS

(1) Engineering electron and phonon transport in nanostructures to achieve high performance thermoelectric materials, (2) controlling photon absorption and emission for materials working at high temperatures, and (3) device prototyping to demonstrate the high efficiency and low cost potential of the solar thermoelectric and solar thermophotovoltaic energy conversion technologies.