The Effects of Nanostructure on Thermoelectric Device Performance

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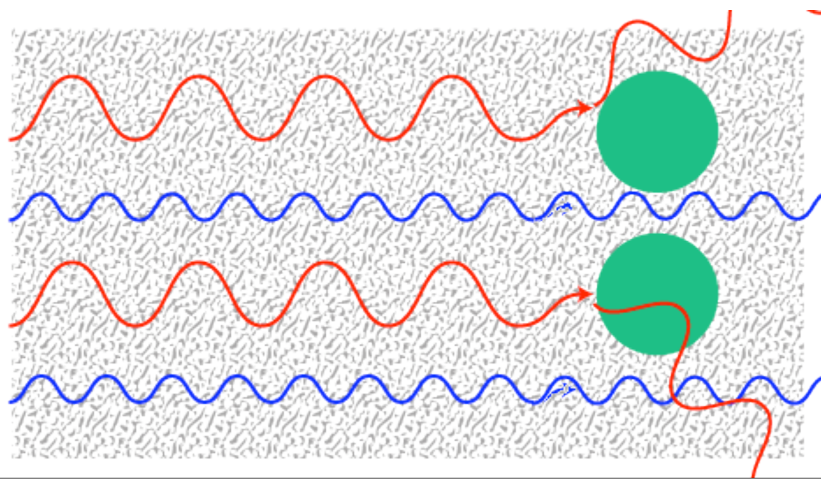
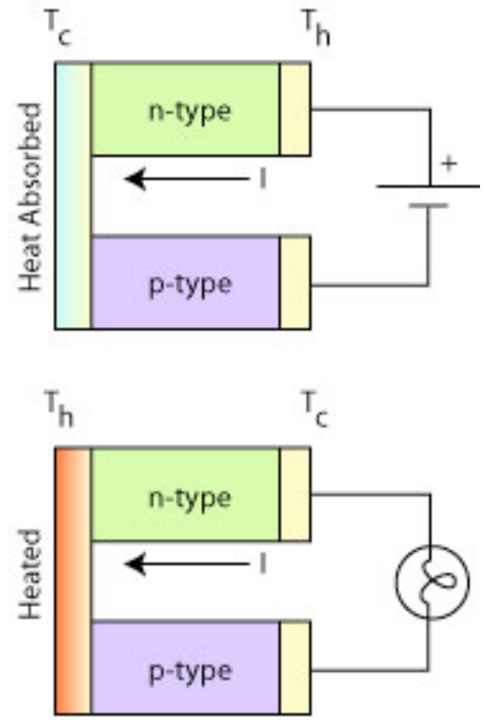
Refresher

- Figure of Merit

$$Z = \frac{\sigma \alpha^2}{\lambda_T}$$

- Slack's Proposal
  - Phonon-Glass, Electron-Crystal





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Where we left off...

- Bi_2Te_3 & Bi_2Se_3 (ZT ~0.8-1.0 at 300K)
- PbTe (ZT ~0.8 at 800K)
- SiGe (ZT ~0.6 at 1000K)

- LAST (ZT ~1.6 at 650K)
- SALT (ZT ~1.7 at 700K)

- Simple Goal: Look at some of the other materials out there.

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Outline

- Superlattice Thermoelectrics
- "Rattling Cage" Thermoelectrics
- Low-Dimensional Thermoelectrics

Man-Made Superlattice Thermoelectrics

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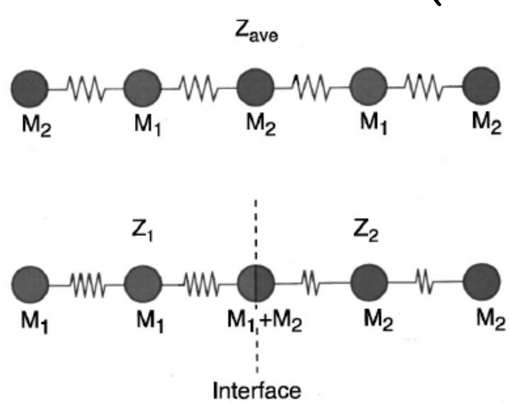
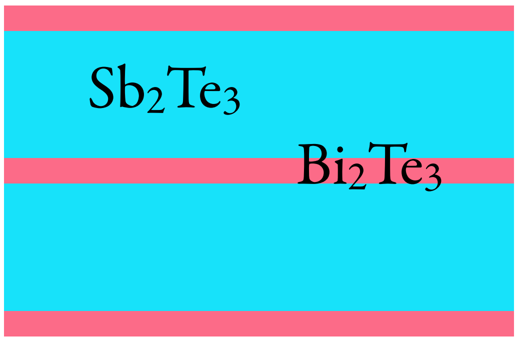
- Bi_2Te_3/Sb_2Te_3 Alternating Layers
  - Deposited using Metal Organic Chemical Vapor Deposition (MOCVD)
  - 10 Å Bi_2Te_3 / 50 Å Sb_2Te_3
  - ZT ~2.4 at 300K p-type, ZT ~1.2 for n-type
- Phonon reflection (mind the gap)





Venkatasubramanian, *Phys. Rev. B*, 2000

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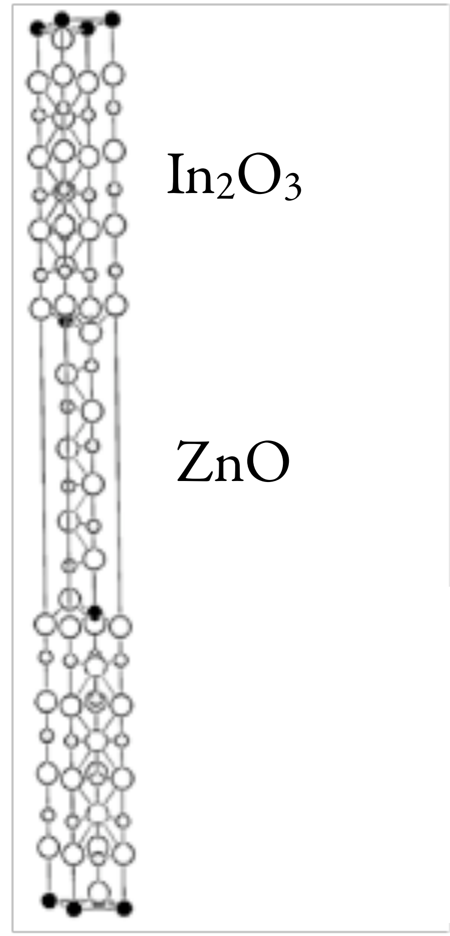
Nature-Made Superlattice Thermoelectrics

- Oxides
  - $(SrO)_m(SrTiO_3)$
    - ZT=0.34 at 1000K
    - Doping with Nb or La
  - $(ZnO)_m(In_2O_3)$, m=5
    - ZnO conducts heat too well
      - Dope Mg on Zn sites or Y on In sites
  - *Issues:* Need to better understand defect chemistry
  - *Benefits:* Oxidation resistance, low toxicity, high thermal stability



Wunderlich *et al.*, 24th International Conference on Thermoelectrics: 2005

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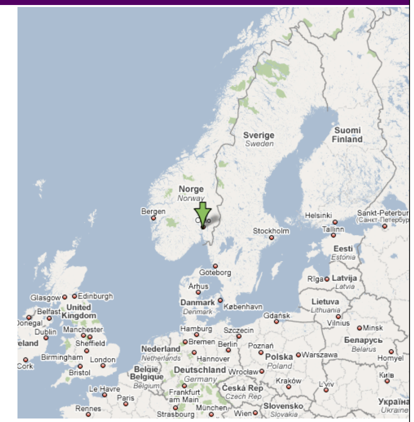
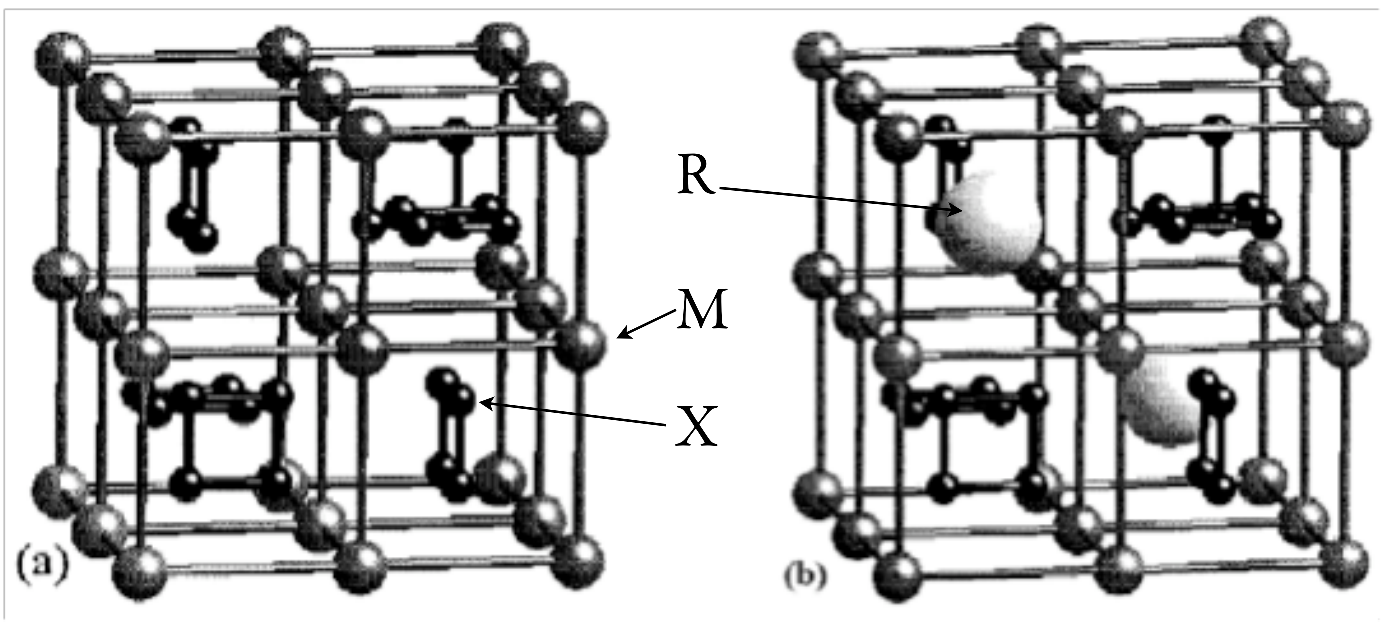
“Rattling Cage” Thermoelectrics



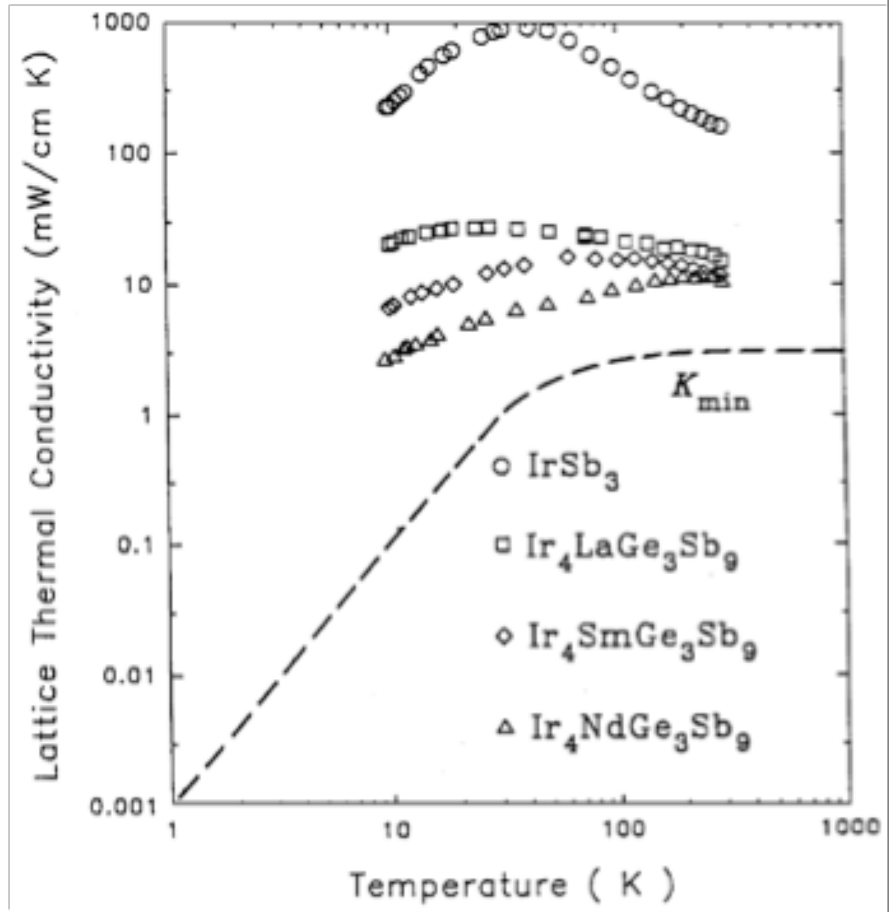
- Skutterudites (cubic, *Im3*)
  - *Binary:* MX_3 (M=Co,Rh,Ir, X=P, As, Sb)
  - *Ternary (filled):* RM_4X_{12} (R= Rare earth element)
    - (ZT ~1.8 at ~900K)



Nolas *et al.*, *J. Appl. Phys.*, 1996 || NASA Tech Briefs, 2001

"Rattling Cage" Thermoelectrics

- Example: Ternary $IrSb_3$
  - Rattlers: La, Sm, Nd
    - Reduce Thermal Conductivity by about an order of magnitude
- *Benefits:* abundance, low volatility, low cost, good thermoelectric properties



Dyck *et al.*, *Phys. Rev. B.*, 2002

Low-Dimensional Thermoelectrics

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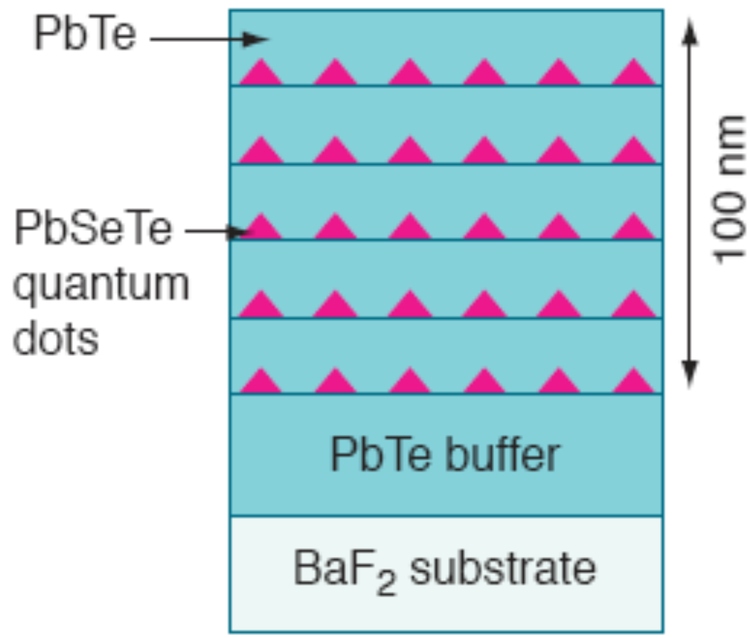
- PbSeTe Quantum dot superlattice
  - Dots ~1nm tend to produce an increase in ZT
  - Low dimensionality enhances Seebeck coefficient by increasing density of states near the Fermi level
  - Quantum wells create scattering interfaces for phonons



Sales, *Science*, 2002

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Other Factors

- Not just the material but also the design...
  - Contact resistances
  - Thermocouple length and number
  - Carnot Efficiencies
  - Manufacturing methods
    - Molecular beam epitaxy: slow and expensive
    - Natural nanostrucutring?
    - Self-assembly?