Glass-like thermal conductivity in high efficiency thermoelectric materials

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Funding:
Beckman Foundation
NASA-JPL
ARPA-E
DARPA
ZT Plus
BSST

Outline

$$\kappa_L = \frac{1}{3}\int C v_g^2 \tau \, d\omega$$

v_g - phonon group velocity
τ - phonon relaxation time

Group velocity (v_g)

- Structural complexity
  - $Yb_{14}MnSb_{11}$
  - $Ca_5Al_2Sb_6$
  - Ca_3AlSb_3

Scattering (τ)

- Intrinsic point defects
  - $La_{3-x}Te_4$
  - Zn_4Sb_3
- Nanostructures
  - Zn_4Sb_3
  - PbTe

Designing low κ_L materials – group velocity

$$\kappa_L = \frac{1}{3}\int C v_g^2 \tau \, d\omega$$

v_g - phonon group velocity
τ - phonon relaxation time

$$v_s = \sqrt{\frac{B}{d}}$$

v_s – acoustic speed of sound
B – elastic modulus
d - density

New materials should have ‘soft’ bonding and be composed of heavy atoms

Designing low κ_L materials – group velocity

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v_g - phonon group velocity
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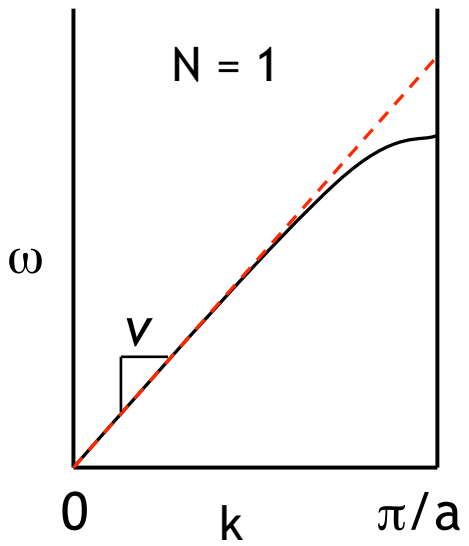
v_s - acoustic speed of sound
B - elastic modulus
d - density

$$v_g(\omega) = v_s$$

Valid only for phonons at long wavelengths!

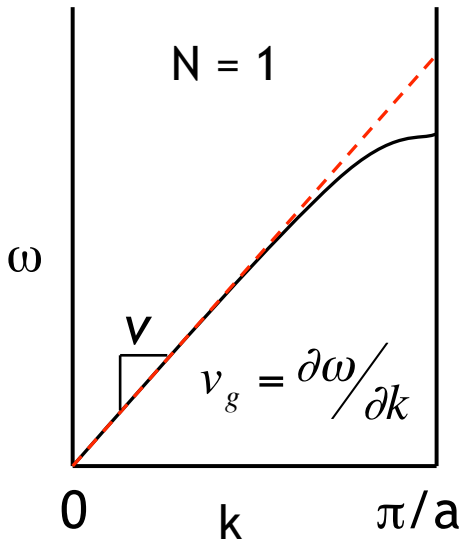


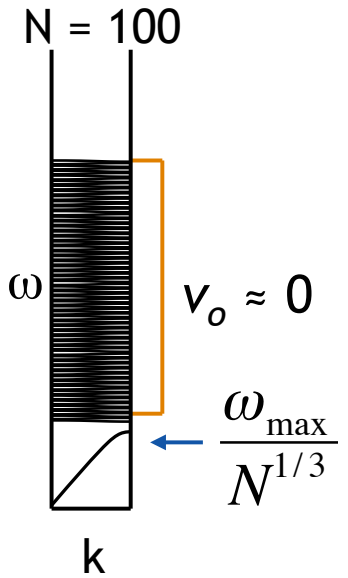
$$v_g = \partial\omega / \partial k$$

Lattice thermal conductivity prediction

In complex materials:

- 3 acoustic branches (2 transverse, 1 longitudinal)
- 3(N-1) optical branches, where N is # atoms in primitive cell





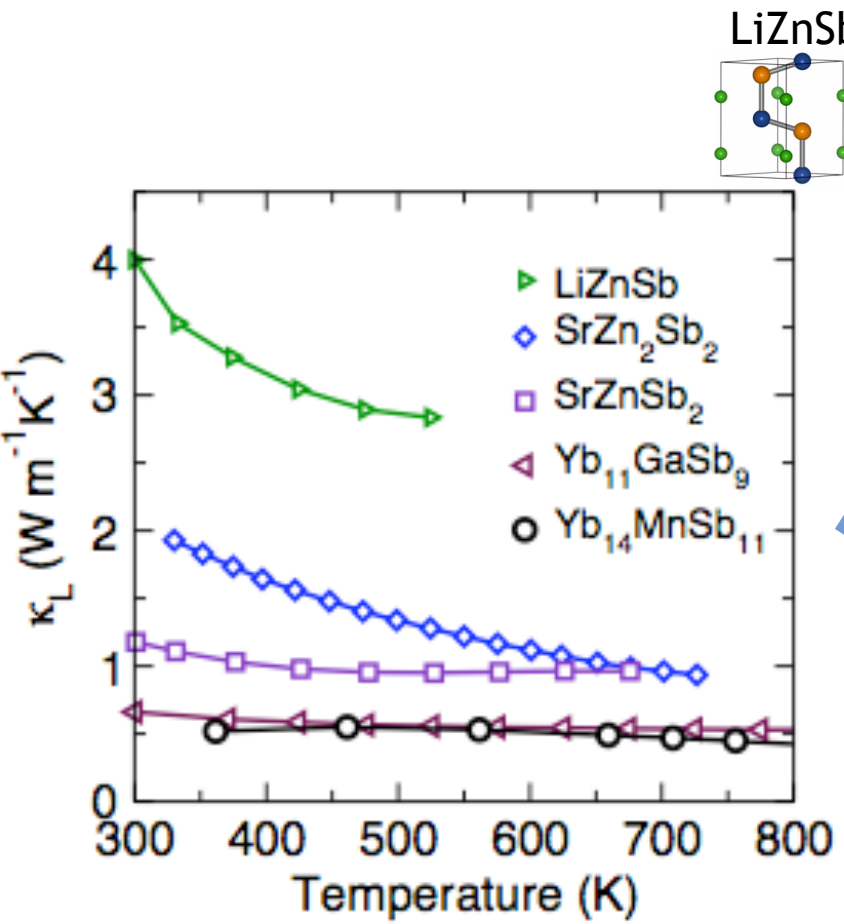
$$\kappa_a = \frac{c\overline{M}\theta_D^3 a}{N^{1/3}\gamma^2 T}$$

True in practice?

Roufosse and Klemens, *Phys Rev B* (1973), 7, 5379
Slack, *Solid State Phys* 1979

Antimonides and thermal conductivity

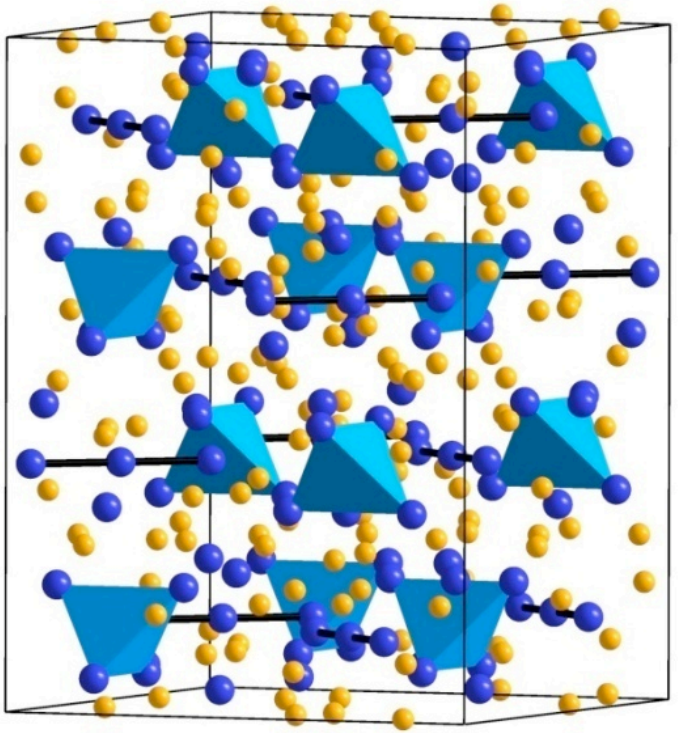
Primitive unit cell complexity good indicator for κ_L



Yi et al *Chem Mater* (2010)
Toberer et al *Dalton Trans* (2010)

May et al *J. Appl. Phys* (2009)
Toberer et al *J. Appl. Phys.* (2009)
Toberer et al *Adv. Funct. Mater.* (2008)

$Yb_{14}Mn_xAl_{1-x}Sb_{11}$ - Glass like thermal conductivity



Low κ_L arises from:

Complexity (N = 104)

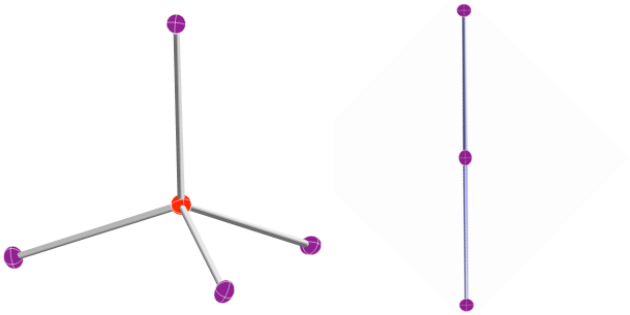
Density

Mass contrast

Anharmonicity (γ = 1.5)

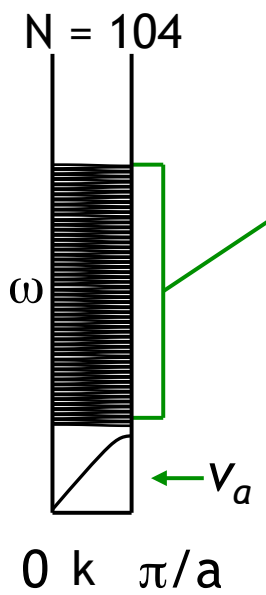
No evidence of rattling:

Single crystal XRD thermal ellipsoids



Understanding thermal conductivity in $Yb_{14}MnSb_{11}$

v_{optic} so low, we will use the theory developed for glassy materials.



$$\kappa_{optic} = \kappa_{glass}$$

300 K

0.3 W m^{-1} K^{-1}

$$\kappa_{acoustic} = \frac{1}{3}\int_0^{\omega_{acoustic}} C v^2 \tau \, d\omega$$

0.5 W m^{-1} K^{-1}

$$\kappa_{lattice} = \kappa_{acoustic} + \kappa_{optic}$$

300K

Prediction: 0.8 W m^{-1} K^{-1}

Reality: 0.6 W m^{-1} K^{-1}

Zintl $Yb_{14}Mn_xAl_{1-x}Sb_{11}$ - Next generation power source

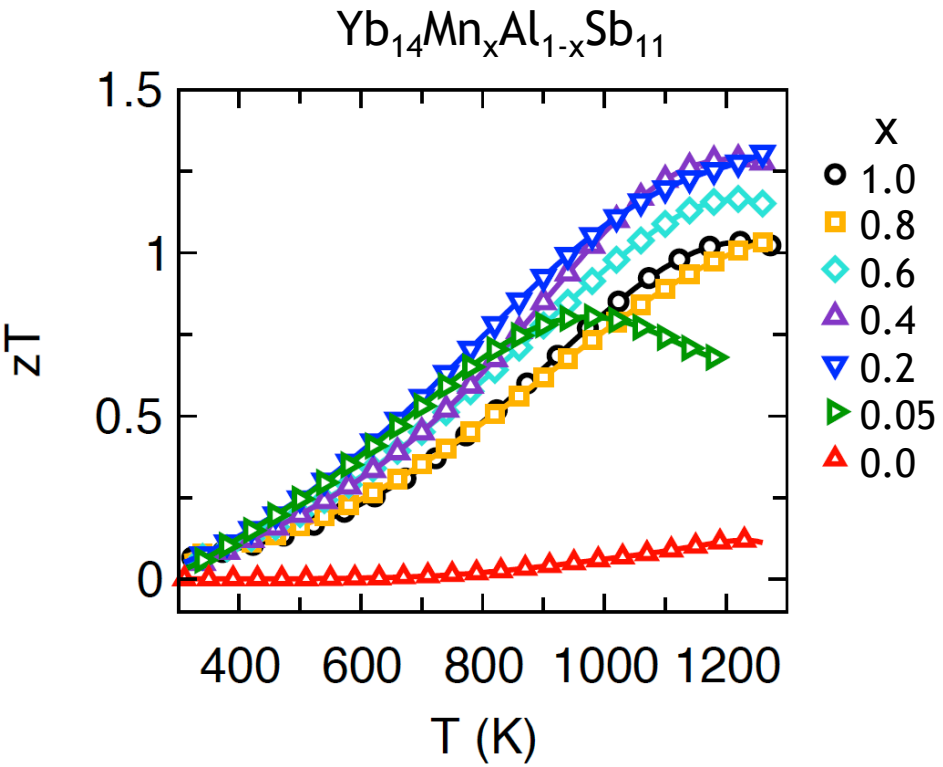


Figure of merit (zT) >1 at 1200K!

Factors contributing to good thermoelectric performance:

- Band gap (0.5 eV) and moderate mobility
- robust carrier concentration control
- glass-like κ_L

Rauscher, et al, *Chem. Mater* (2010)
Cox, et al, *Chem. Mater.* (2009)
Toberer et al *Appl. Phys.* Lett. (2008)
Brown et al, *Chem. Mater. (*2008)
Toberer et al, *Adv. Funct. Mater.* (2008)
Brown et al *Chem. Mater.* (2006)

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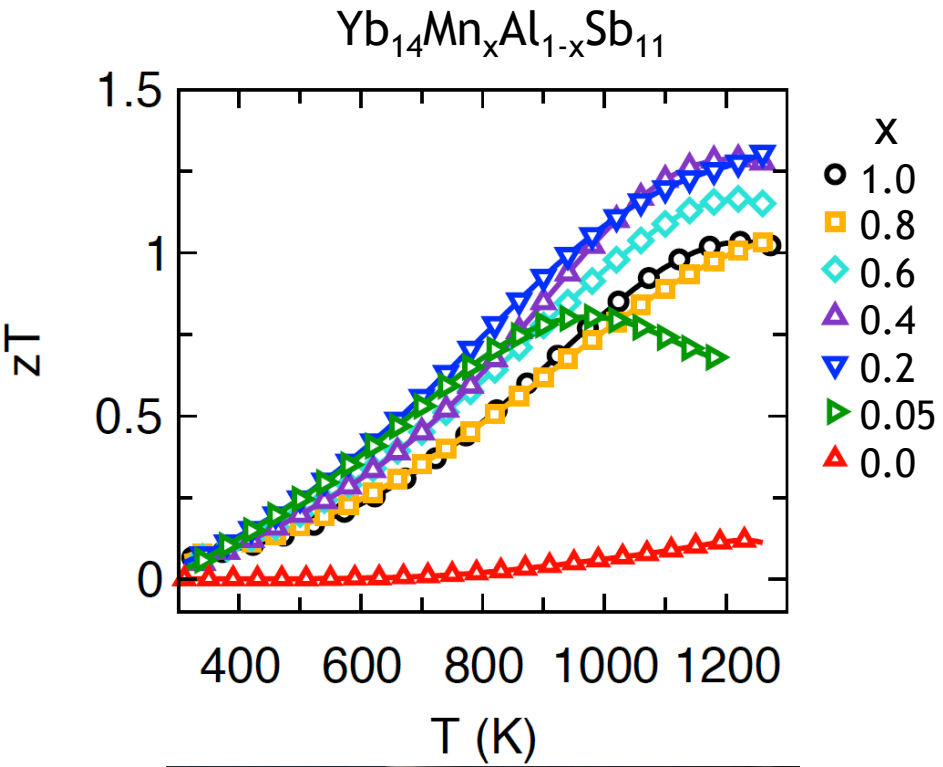


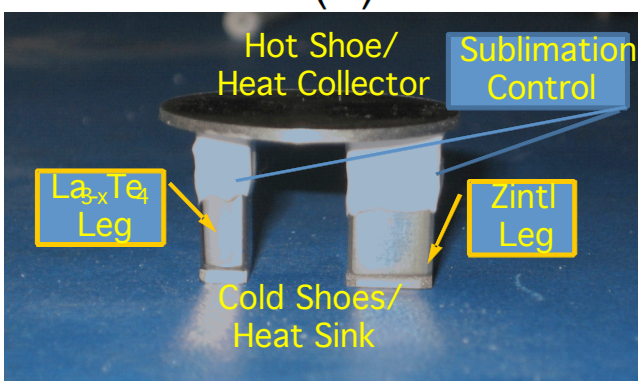


Figure of merit (zT) >1 at 1200K!

NASA has been flying $Si_{0.8}Ge_{0.2}$ for the last 30 years with a peak zT of 0.6 at 1100K.

JPL:

14-1-11/$La_{3-x}Te_4$ (BOL)

10% efficient at 1000°C

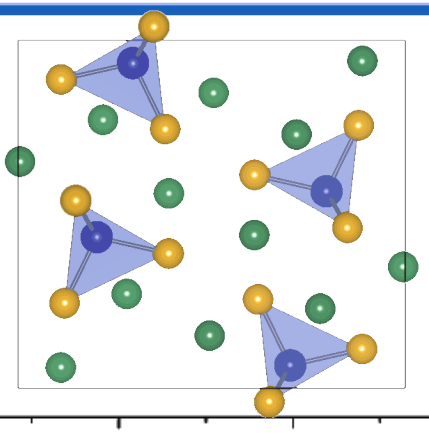
3000 hours of test

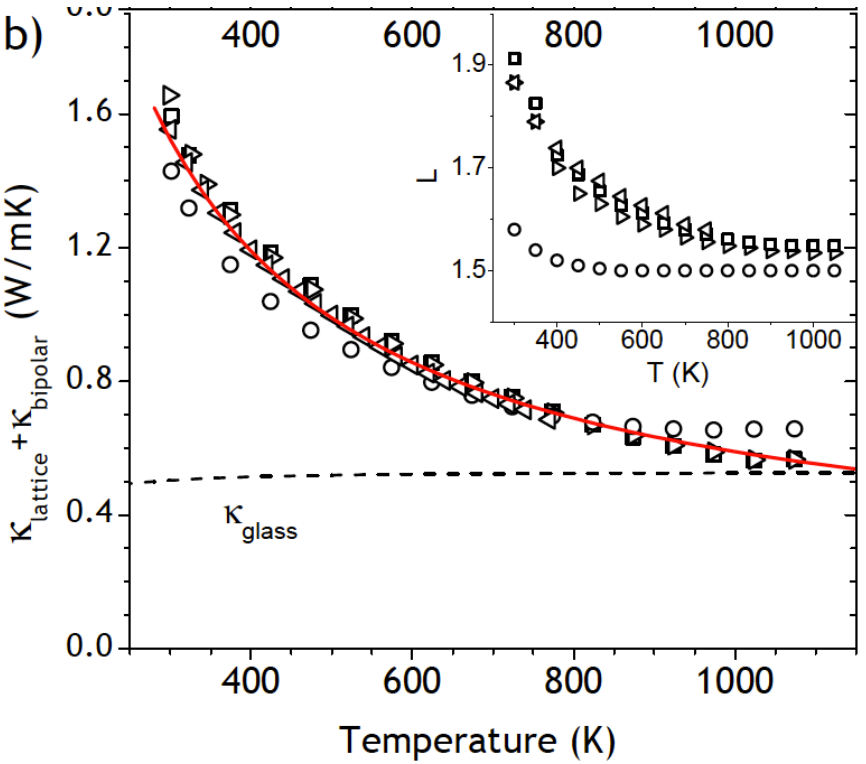
Segmented with skutterudite:

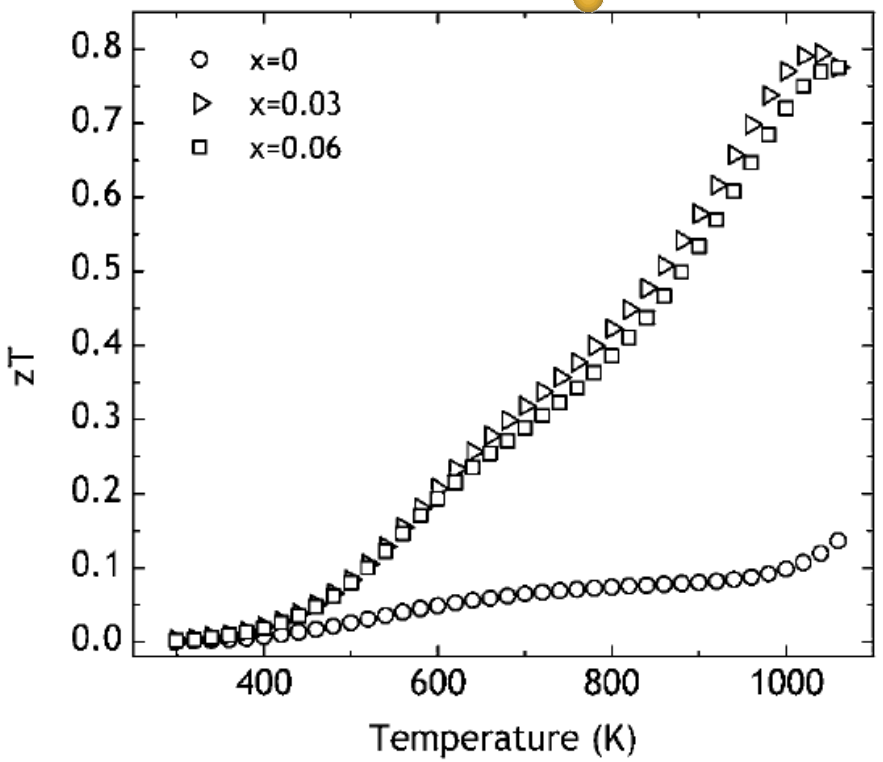
15% efficient (180/1000°C, BOL)

New Earth-abundant complex semiconductors

$Ca_5Al_2Sb_6$ (N = 26) and **Ca_3AlSb_3** (N = 28):







E. Toberer, A. Zevalkink et al, *Adv. Func. Mat.* **20**, 2010

A. Zevalkink, E. Toberer, et al, *Energy Environ. Sci.* in press

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- Nanostructures
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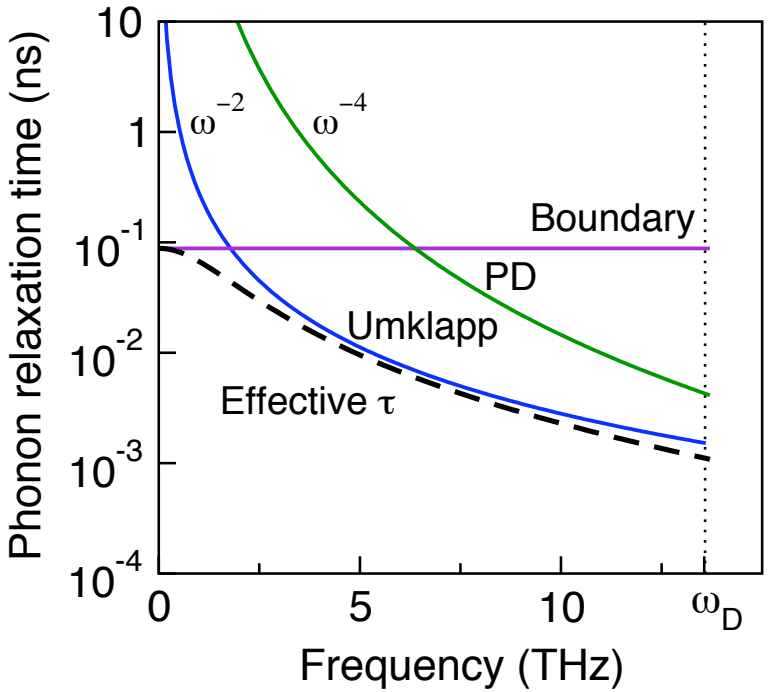
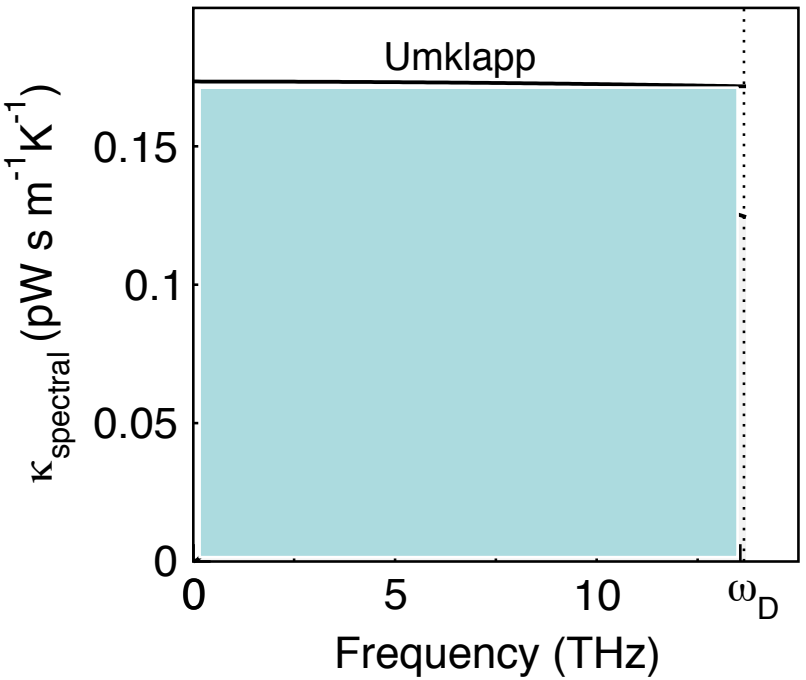
Scattering: Relevant phonon relaxation times

$$\kappa_L = \frac{1}{3}\int C v_g^2 \tau \, d\omega \quad \rightarrow \quad \tau^{-1} = \sum_i \tau_i^{-1}$$

$$\kappa_L = \int \kappa_{spectral} \, d\omega$$





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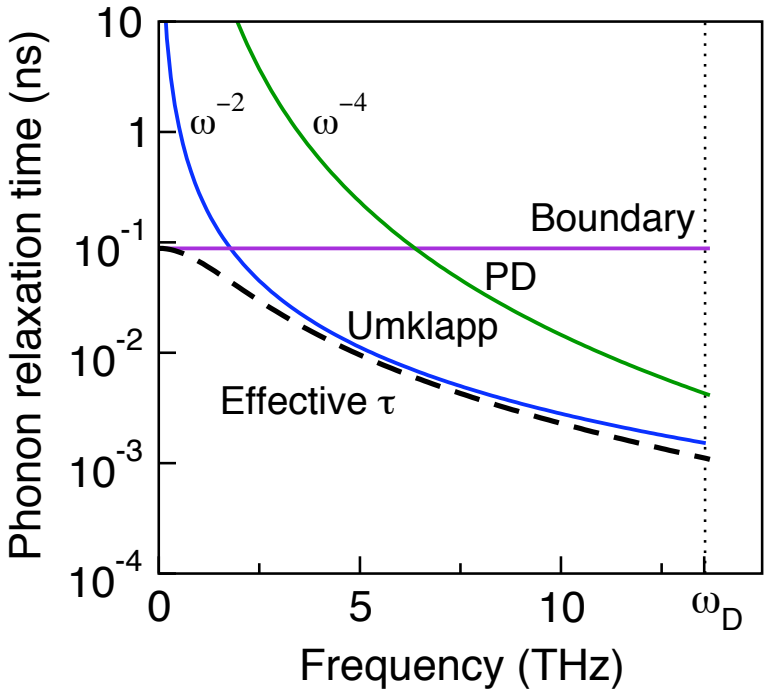
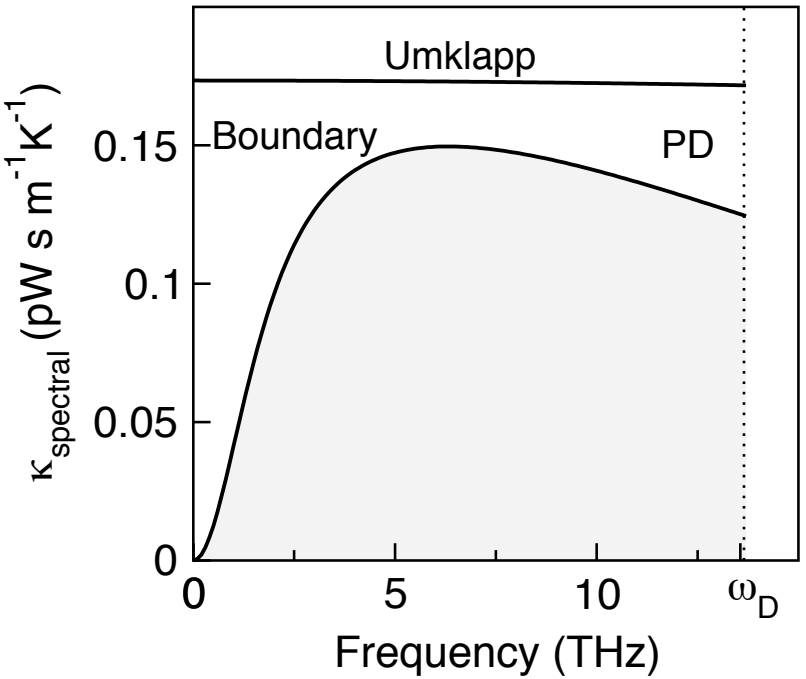
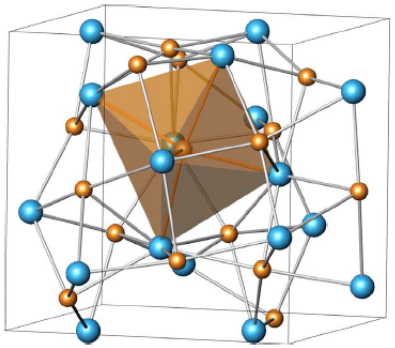




$La_{3-x}Te_4$ – High T *n*-type material

Charge balance: $La_2^{3+}Te_3^{2-}$

Th_3P_4:



Cutler et al, Phys. Rev. (1964)
Wood, Rep. Prog. Phys. (1988)

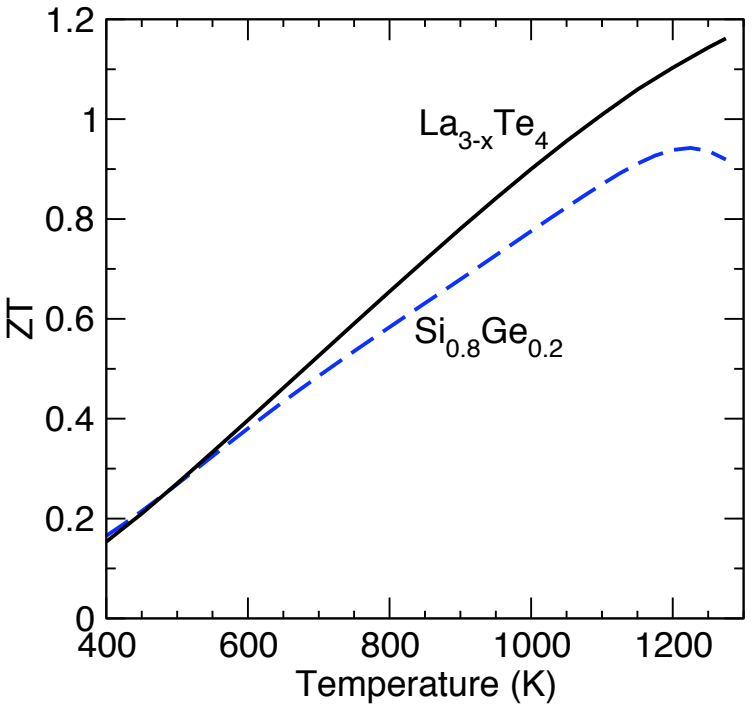
Conflict between structure type and charge balanced composition:

- **vacancies**!

Other sources of low κ_L:

- Anharmonicity (1.7)
- High density
- N = 14
- Moderately soft bonding

  v = 3580 (l) and 2010 (t) m/s



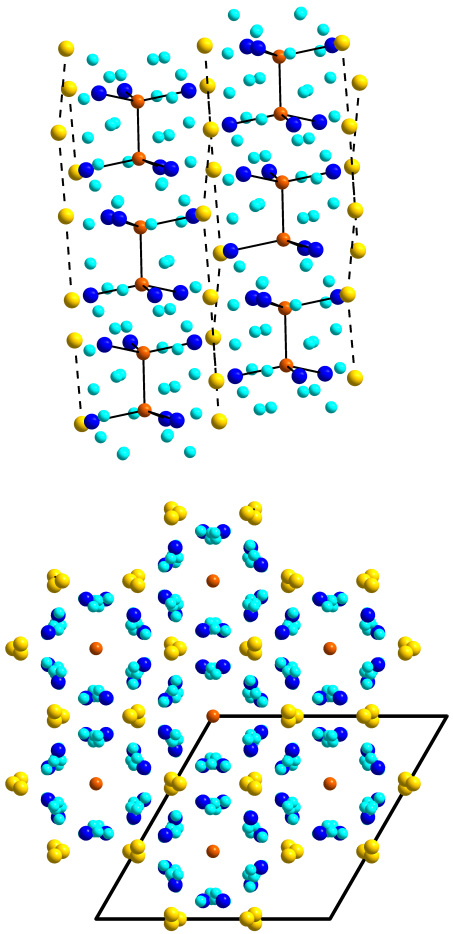
May et al, Chem. Mater. (2010)
May et al, Phys. Rev. B (2010)
Delaire et al, Phys Rev B (2009)
May et al Phys. Rev. B (2009)
May et al Phys. Rev. B (2008)

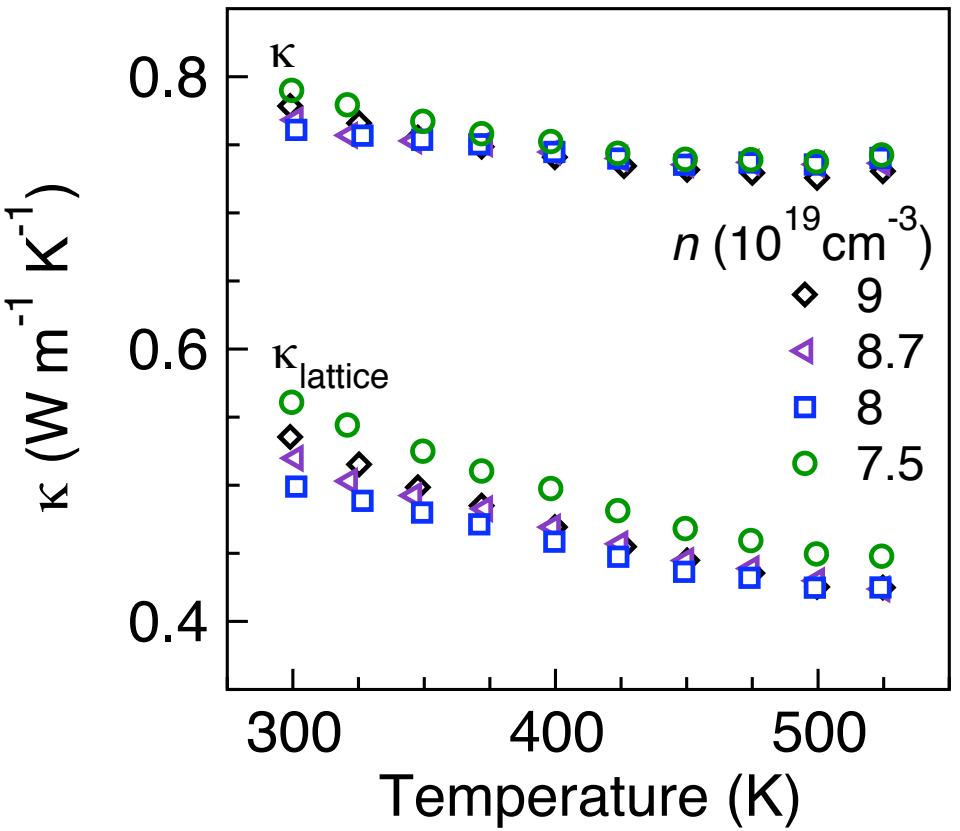
Point defect scattering in Zn_4Sb_3

Like $La_{3-x}Te_4$, conflict between **structure** and **charge balance**

Structure: $Zn_{36}Sb_{30}$ Charge balance: $Zn_{39}Sb_{30}$

3 additional Zn - interstials





Toberer et al, J. Mater. Chem (2010)

Zn_4Sb_3

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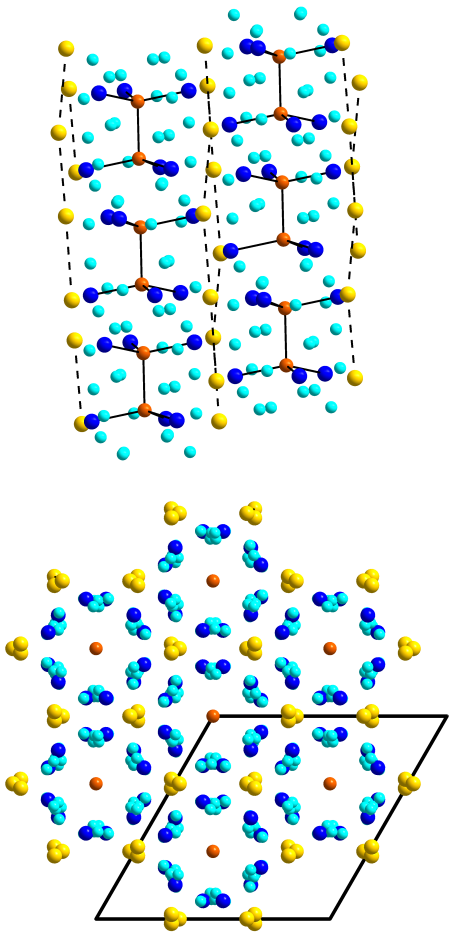

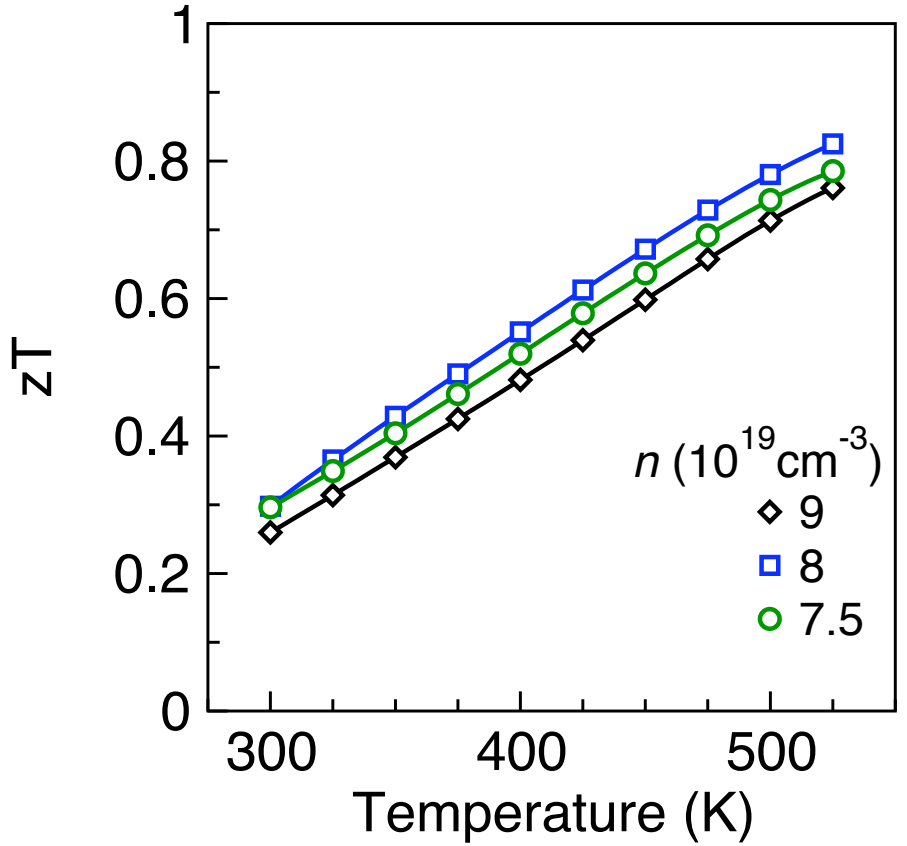

Toberer et al, J. Mater. Chem (2010)

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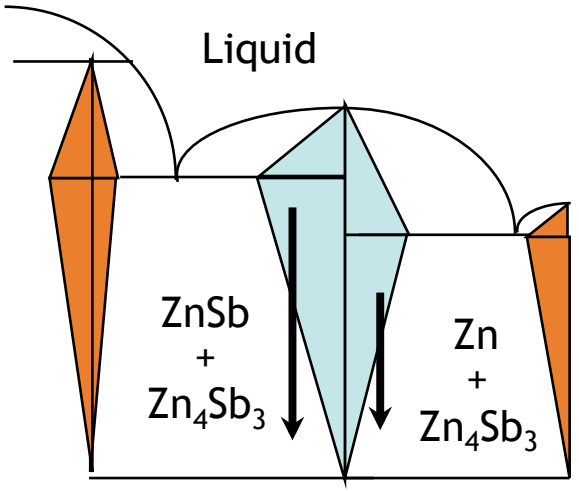
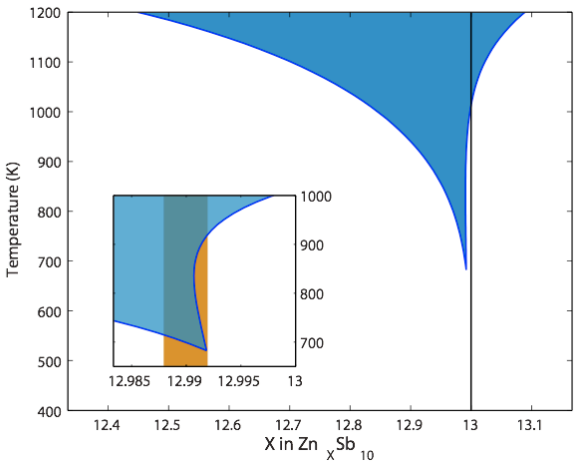
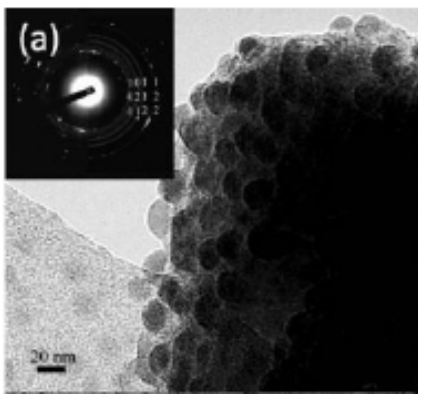
Nanostructured Zn_4Sb_3



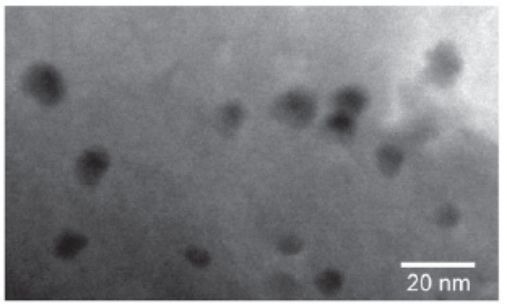


ZnSb $Zn_{3.9}Sb_3$ Zn

x in Zn_xSb_3



ZnSb precipitates (10nm) found in Sb rich samples of Zn_4Sb_3

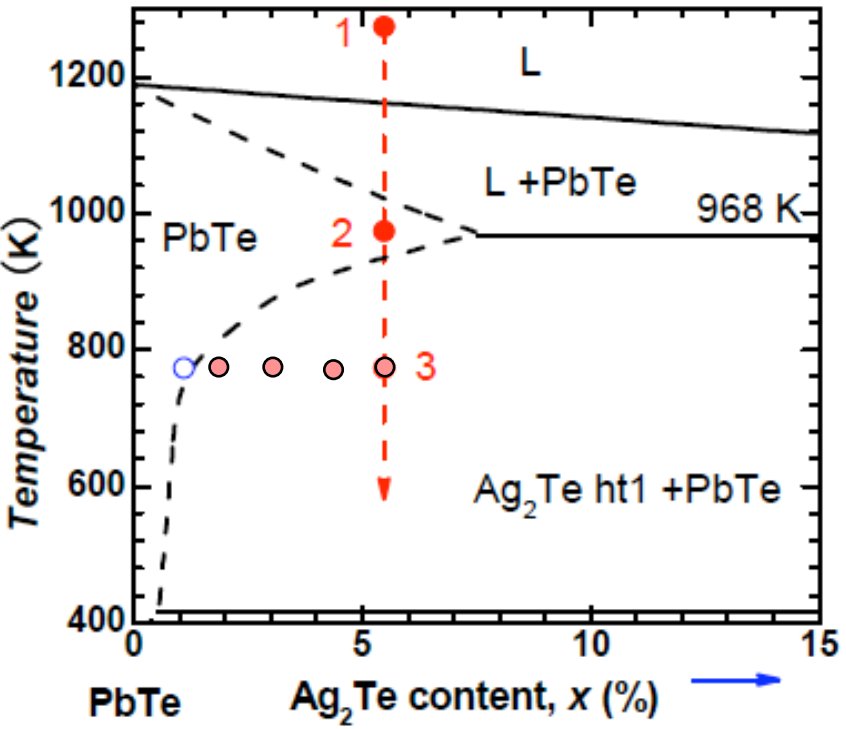


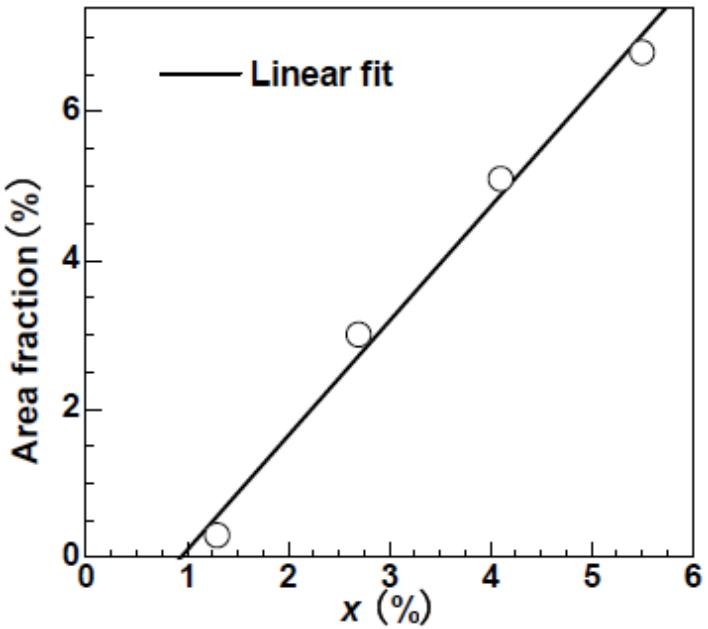
Coherent Zn precipitates found in some samples of Zn_4Sb_3

Prytz et al. Phil. Mag. Lett. (2009)
Toberer et al, J. Mater. Chem (2010)
Pohmrehn et al Phys. Rev B in press

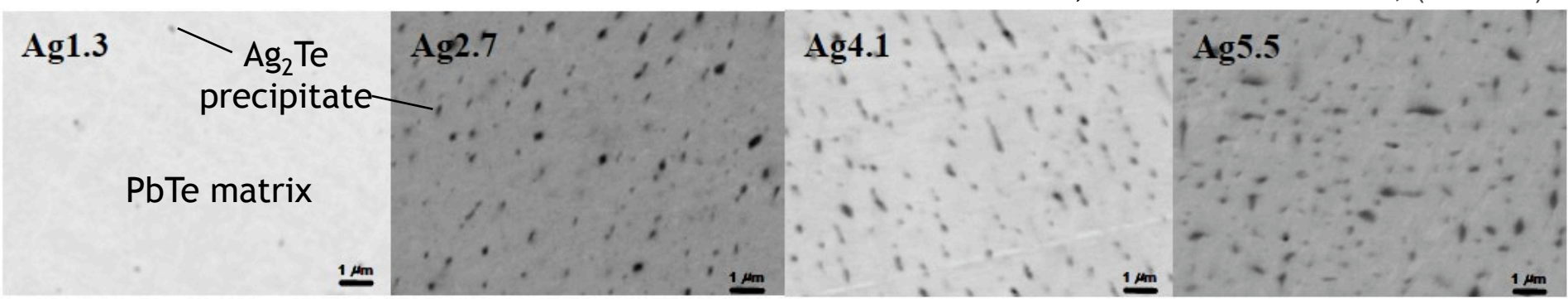
PbTe-Ag_2Te Composite Formation

Ag_2Te precipitates form as expected from equilibrium phase diagram

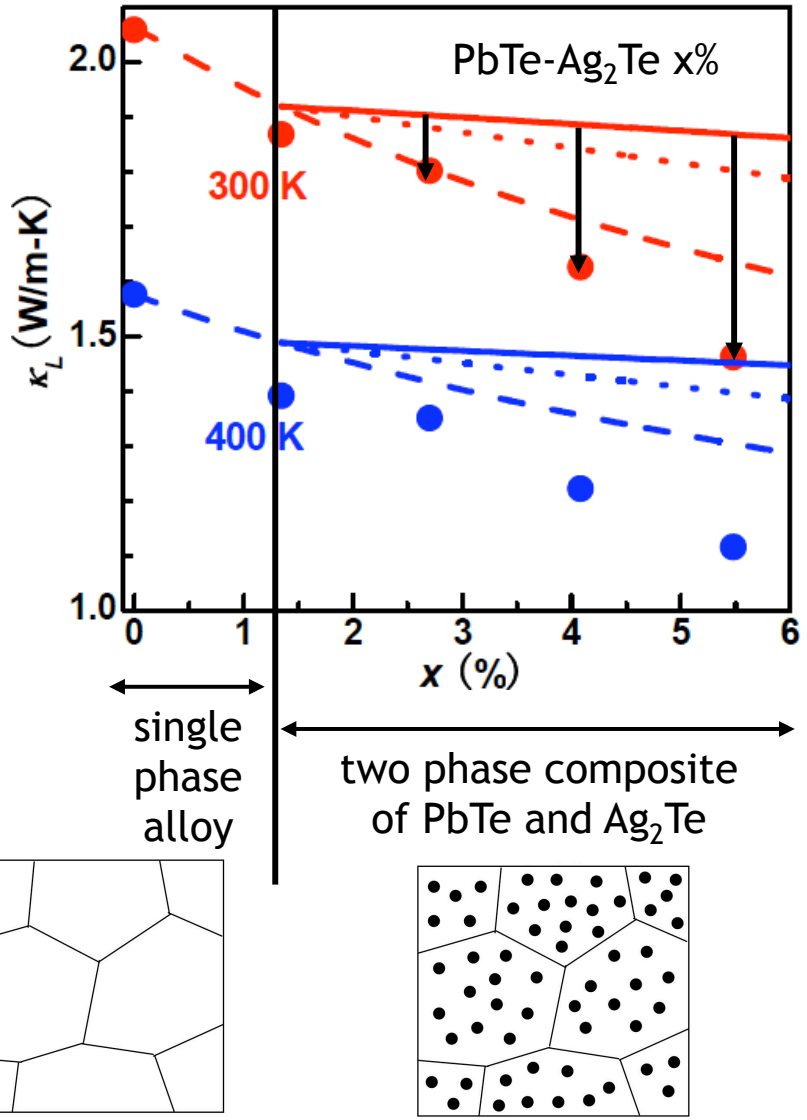




Pei, et al *Adv. Funct. Mat.*, (in Press)

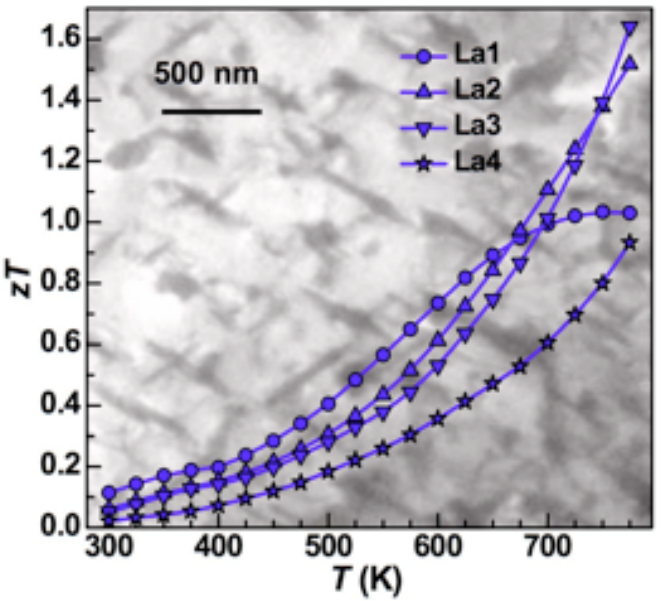


Nanoscale Effects



- Thermal conductivity reduction ~20%
- Must be reduced in matrix

- Reduction due to Nanoscale Effects
- even from ~100nm microstructure!



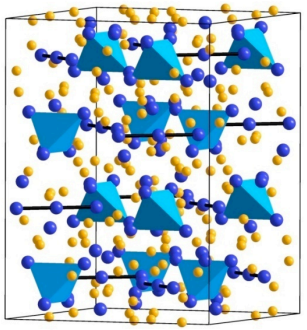
Pei, et al *Adv. Funct. Mat.*, (in Press)

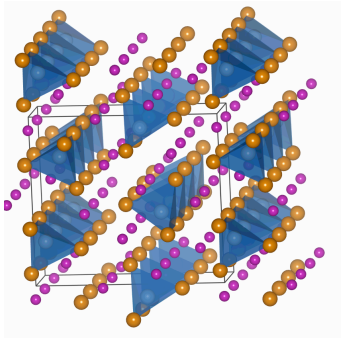
Outlook

Successful strategies for targeting low κ_L materials must utilize both **group velocity** and **scattering**!

Group velocity: heavy materials, soft bonding, low velocity optical modes

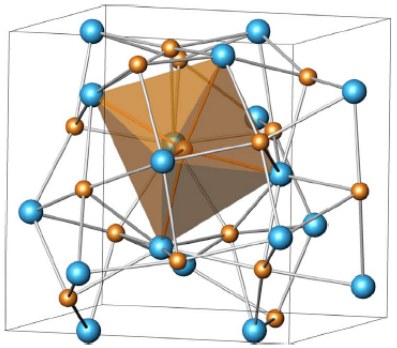
$Yb_{14}MnSb_{11}$



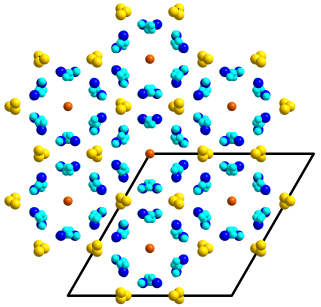


Ca_3AlSb_3

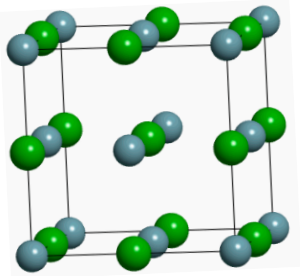
Scattering: spontaneously formation of point defects and nanostructures



$La_{3-x}Te_4$



Zn_4Sb_3

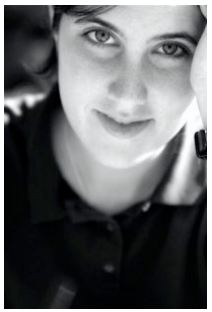


PbTe

Acknowledgements

Jeff Snyder

Andrew May



Alex Zevalkink

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Jean-Pierre Fleurial and Thierry Callait (Jet Propulsion Laboratory)

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Thermoelectric Materials

Review articles:

General: Snyder & Toberer, *Nature Mater.* 7 (2008) 105.
Zintl transport: Toberer, May, Snyder, *Chem. Mater.* 22 (2010) 624.

Lattice thermal conductivity model

Debye Model:

$$\kappa_L = \frac{1}{3}\int C(\omega)\nu_g(\omega)^2\tau(\omega)d\omega \qquad C_v = \frac{3\hbar^2}{2\pi^2 k_b T^2}\int_0^{\omega_m} \frac{\omega^4 \exp[\hbar\omega/kT]}{\nu_p^2\nu_g(\exp[\hbar\omega/kT]-1)^2}d\omega$$

$$\kappa_L = \frac{\hbar^2}{2\pi^2 k_B T^2}\int_0^{\omega_m} \frac{\omega^4 \exp[\hbar\omega/kT]}{\nu_p^2(\exp[\hbar\omega/kT]-1)^2}\nu_g\tau d\omega$$

Scattering:

$$\tau^{-1} = \sum_i \tau_i^{-1}$$

$$\tau_U(\omega) = \frac{\bar{M}\nu_g\nu_p^2}{Ca\gamma^2 k\omega^2}$$

$$\tau_{PD} = \frac{V}{4\pi\nu^3}\omega^4\sum_i f_i\left(\frac{\bar{m}-m_i}{\bar{m}}\right)^2$$

$$\tau_B = \frac{d}{\nu}$$

Cahill's glass model:

$$\kappa_g = \left(\frac{\pi}{6}\right)^{1/3}\frac{\hbar^4}{k_B^3 a^2 T^2}\sum_i \frac{\nu_i}{\Theta_i^2}\int_{\frac{\omega_D}{n^{1/3}}}^{\omega_D} \frac{\omega^3 \exp[\hbar\omega/kT]}{(\exp[\hbar\omega/kT]-1)^2}d\omega$$

Understanding thermal conductivity in $Yb_{14}MnSb_{11}$

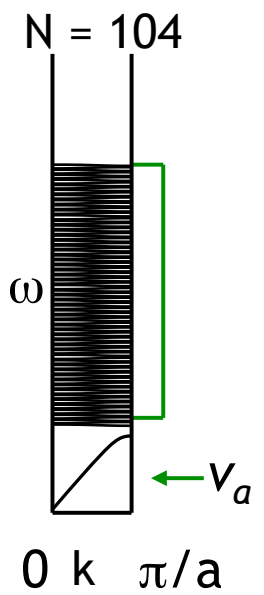
Phonon mean free path (l):

$$l^{-1} = \sum_i l_i^{-1}$$

$$l_{Umklapp}(\omega) = \frac{\overline{M} v_g^2 v_p^2}{C a \gamma^2 k \omega^2}$$

$$l_{Bounary}(\omega) = d$$

d = 1 micron



$$\kappa_{acoustic} = \frac{1}{3} \int_0^{\omega_{acoustic}} C v \, l \, d\omega$$

300 K

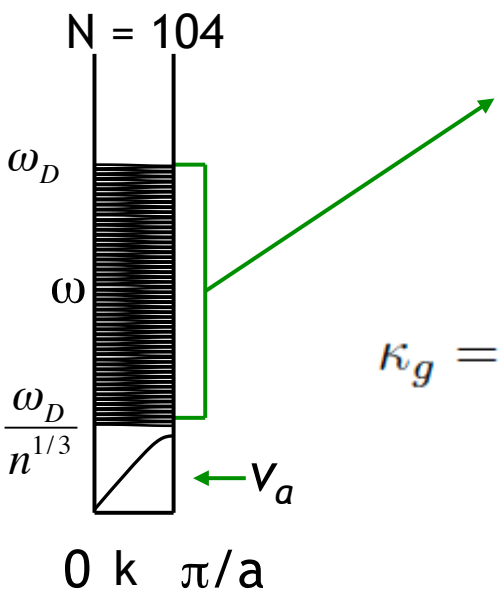
0.5 W m^{-1} K^{-1}

300K

Prediction acoustic: 0.5 W m^{-1} K^{-1}

Reality total: 0.6 W m^{-1} K^{-1}

Thermal conductivity in $Yb_{14}MnSb_{11}$



$$\kappa_{optic} = \kappa_{glass}$$

$$\kappa_g = \left(\frac{\pi}{6}\right)^{1/3} \frac{\hbar^4}{k_B^3 a^2 T^2} \sum_i \frac{\nu_i}{\Theta_i^2} \int_{\frac{\omega_D}{n^{1/3}}}^{\omega_D} \frac{\omega^3 \exp[\hbar\omega/kT]}{(\exp[\hbar\omega/kT]-1)^2} d\omega$$

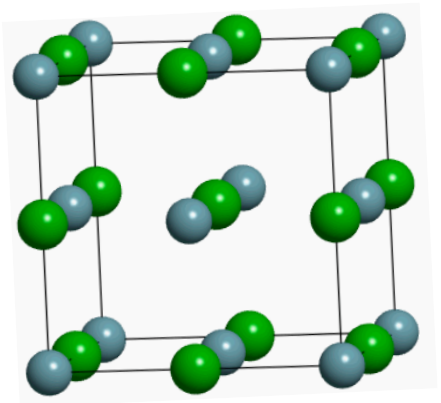
Here, heat transport is treated as a random walk of energy on a lattice. Coupling constant between the harmonic oscillators estimated by *v*.

Speed of sound (v)

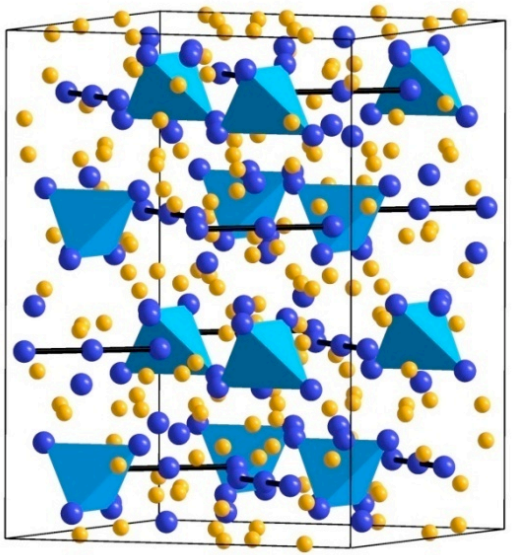
Despite similar speed of sounds between PbTe and $Yb_{14}MnSb_{11}$….
…… very different lattice thermal conductivities.

$$v = \sqrt{\frac{B}{d}}$$

	d g cm^{-3}	v_M m/s	κ_L (300 K) W m^{-1} K^{-1}
PbTe	8.2	1400	2.1
$Yb_{14}MnSb_{11}$	8.4	1600	0.6



PbTe (Fm-3m)



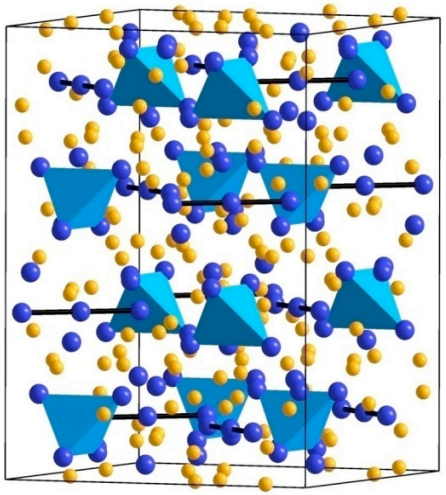
$Yb_{14}MnSb_{11}$ (I4/ammc)

$Yb_{14}AlSb_{11}$

Cations: 14 Yb^{2+}

Isolated anionic moieties:

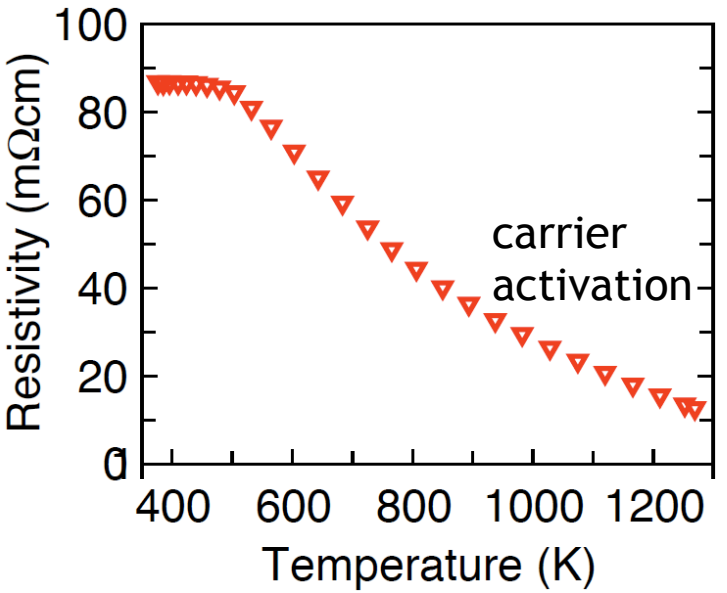
$AlSb_4^{9-}$ tetrahedra
Sb_3^{7-} linear trimer
4 isolated Sb^{3-}



104 atoms in the primitive cell.

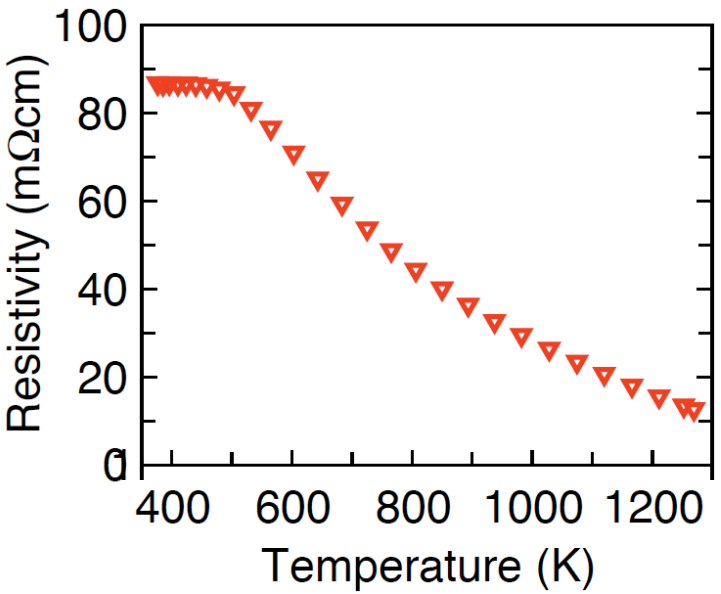
Intrinsic semiconductor due to precise valence balance

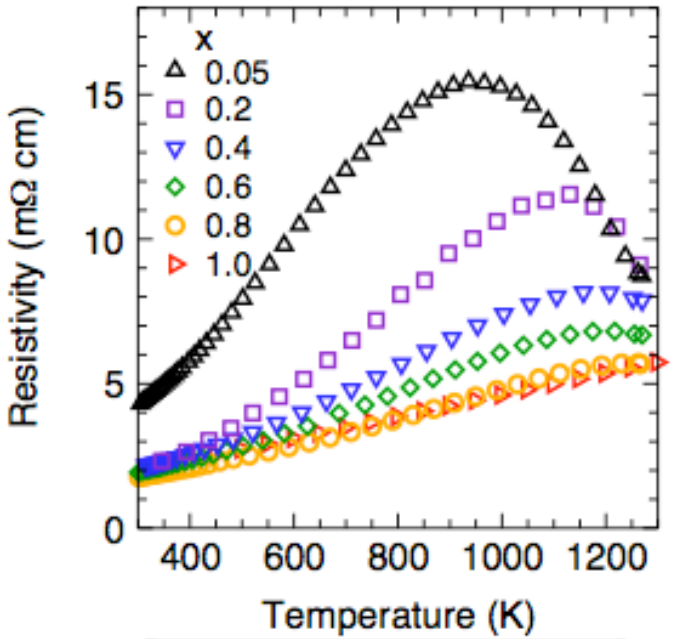
- Large, decreasing resistance with increasing T



Rauscher, Toberer, et al, Chem. Mater (2010)
Cox, Toberer, et al, Chem. Mater. (2009)
Toberer et al Appl. Phys. Lett. (2008)
Brown, Toberer, et al, Chem. Mater. (2008)
Toberer et al, Adv. Funct. Mater. (2008)
Brown et al Chem. Mater. (2006)

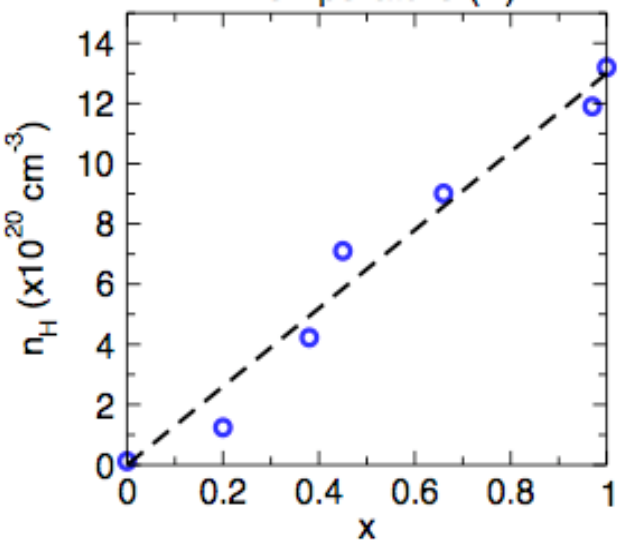
$Yb_{14}Mn_xAl_{1-x}Sb_{11}$ - Metallic resistivity!





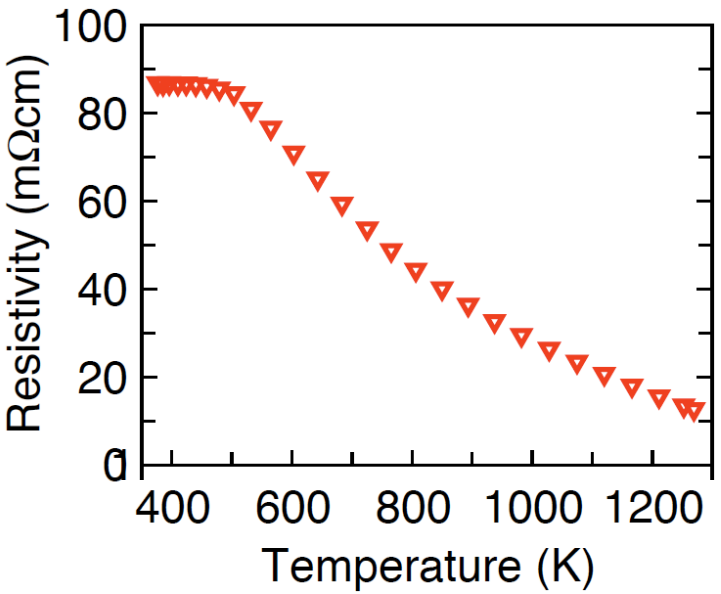
Successful *p*-type doping
with Mn^{2+} alloying on Al^{3+} site!

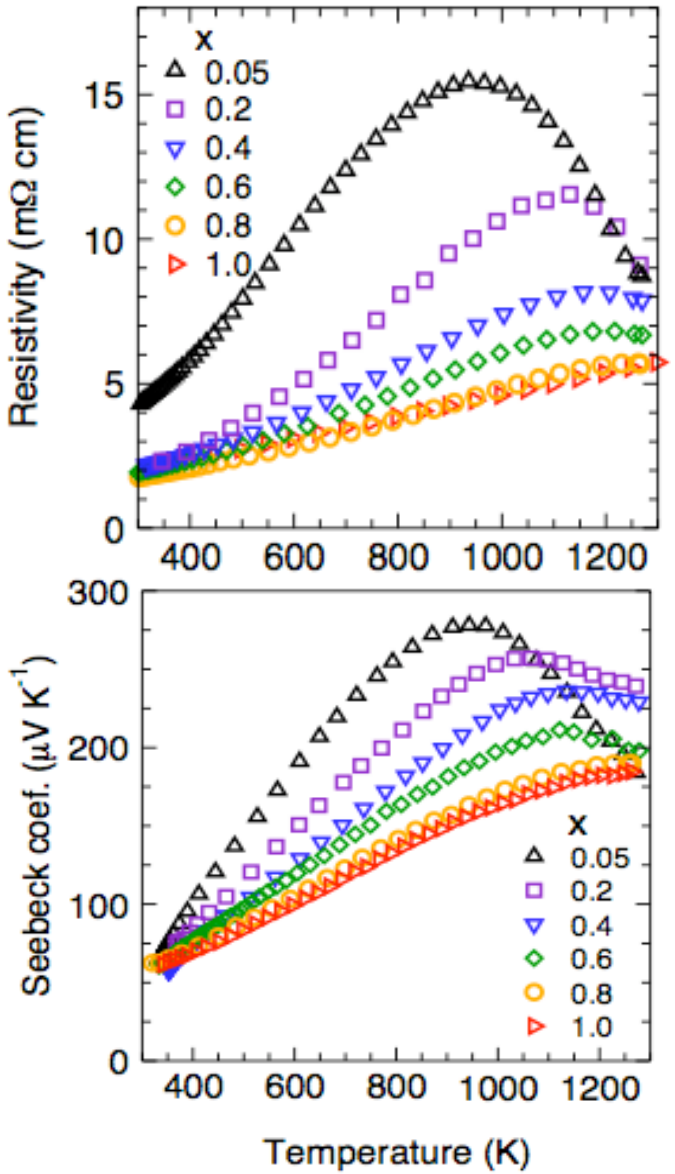
$Yb_{14}MnSb_{11}$ very metallic
(linear resistivity with temperature)



Toberer et al, Adv. Funct. Mater. (2008)

$Yb_{14}Mn_xAl_{1-x}Sb_{11}$ - Metallic resistivity!





$$\alpha = \frac{8\pi^2 k_B^2}{3eh^2} m^* T \left(\frac{\pi}{3n}\right)^{2/3}$$

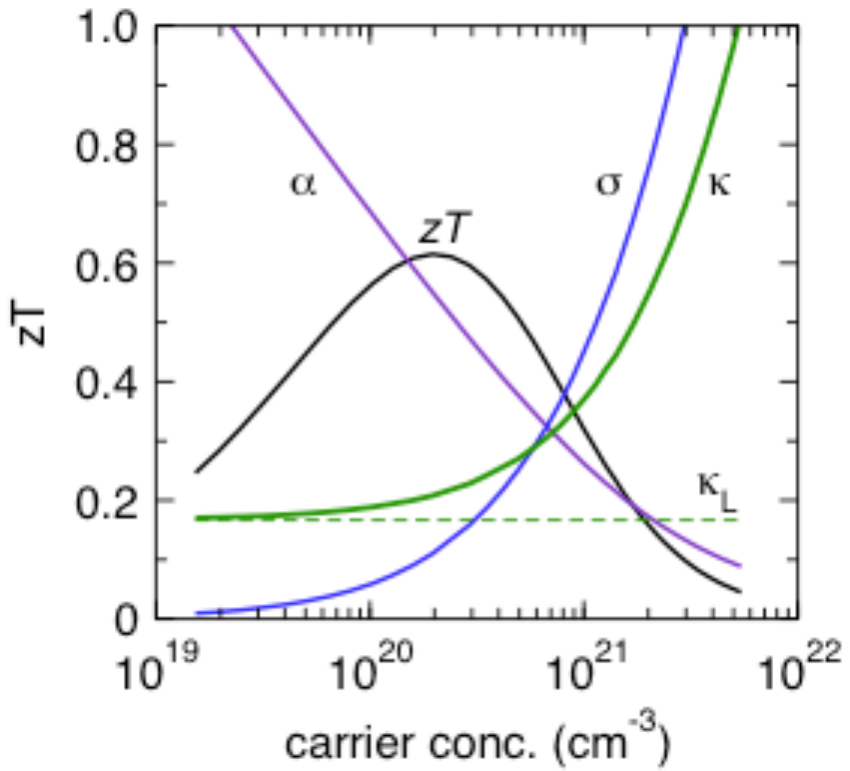
$m^* = 3\ m_e$

Massive for a band conductor!

Toberer et al, Adv. Funct. Mater. (2008)

Beyond the confines of a single parabolic band model

Transport within a single parabolic band will only get us so far - need a new approach!



$$\alpha = \frac{k}{e}\left(\frac{(2+\lambda)F_{1+\lambda}(\eta)}{(1+\lambda)F_{\lambda}(\eta)} - \eta\right)$$

$$F_r(\eta) = \int_0^{\infty} \zeta^r f_o(\eta) d\zeta$$

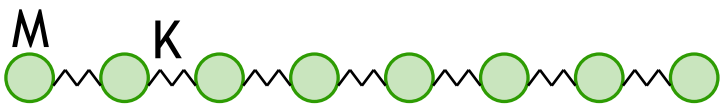
$$\mu_H = \frac{\mu_o \pi^{1/2} F_{\lambda}(\eta)}{2\Gamma(1+\lambda)F_{1/2}(\eta)}$$

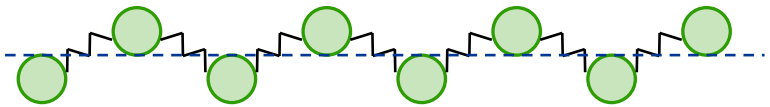
$$n = \frac{4}{\sqrt{\pi}}\left(\frac{2\pi m^* kT}{h^2}\right)^{3/2} F_{1/2}(\eta)$$

$$L = \left(\frac{k}{e}\right)^2 \frac{3F_0(\eta)F_2(\eta) - 4F_1(\eta)^2}{F_0(\eta)^2}$$

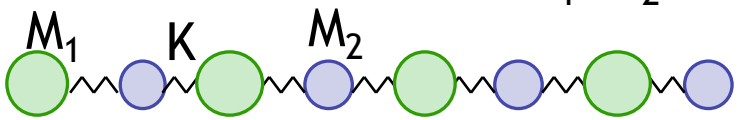
Formation of band gaps in the phonon dispersion

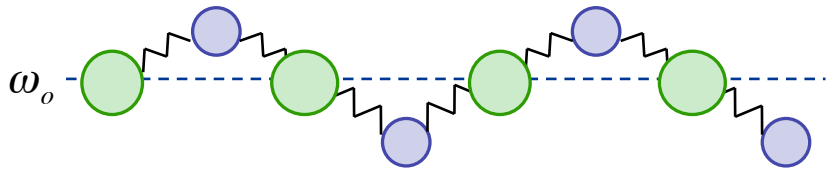
1D chain of atoms coupled via spring (*K*):

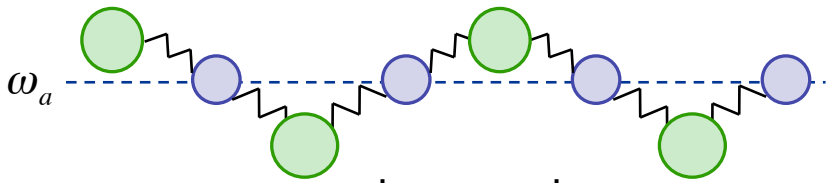


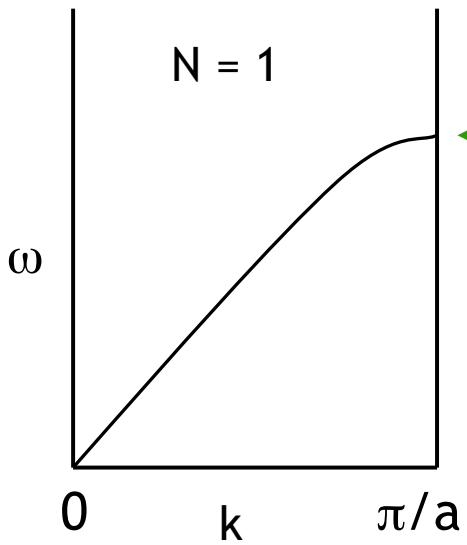


$M_1 > M_2$



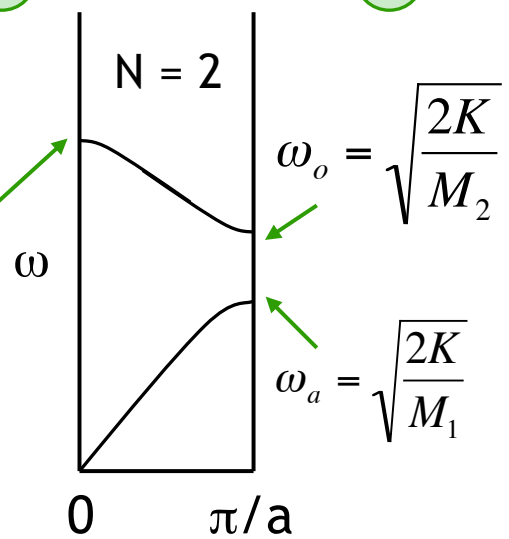






$$\omega_{\max} = \sqrt{\frac{4K}{M}}$$

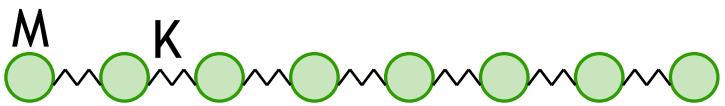
$$\omega_{\max} = \sqrt{\frac{2K}{M_1} + \frac{2K}{M_2}}$$

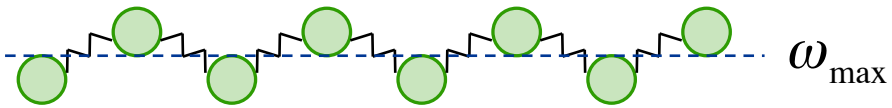


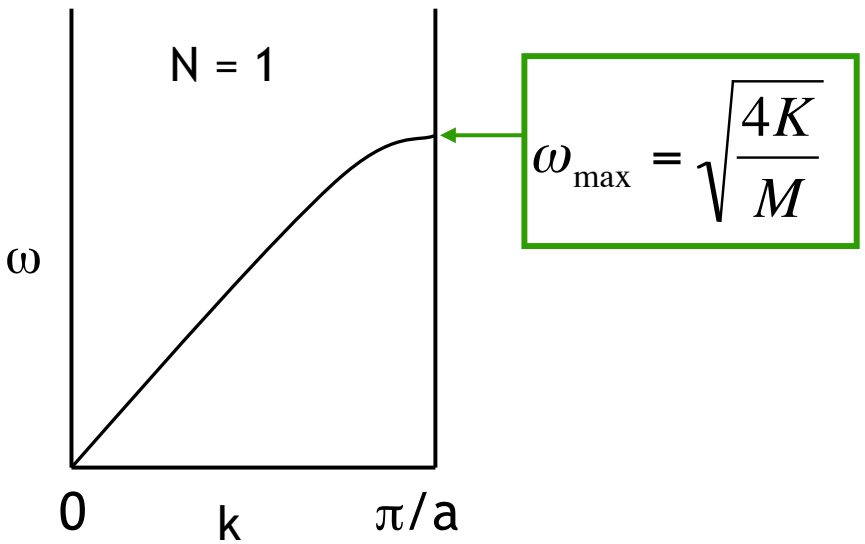
Phonon dispersion for 1-D chain

This approach to

1D chain of atoms coupled via spring (*K*):







$$\omega_{max} = \sqrt{\frac{4K}{M}}$$

$$\kappa_{lattice} = \frac{1}{3} C_v v l$$

Fine approximation, *if* *v* is constant

$$v_g = \partial\omega / \partial k$$

Formation of band gaps in the phonon dispersion

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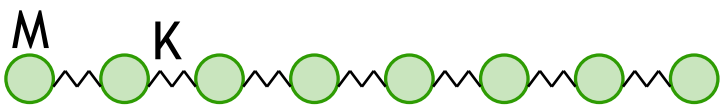

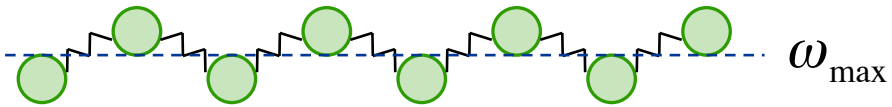

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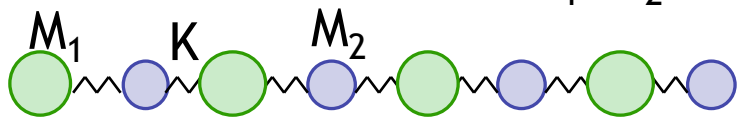

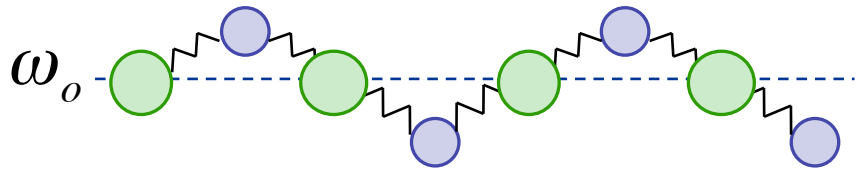

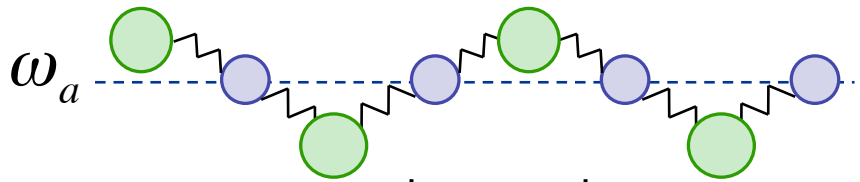

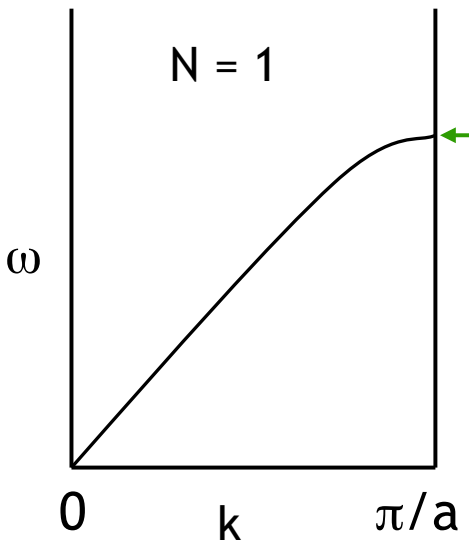

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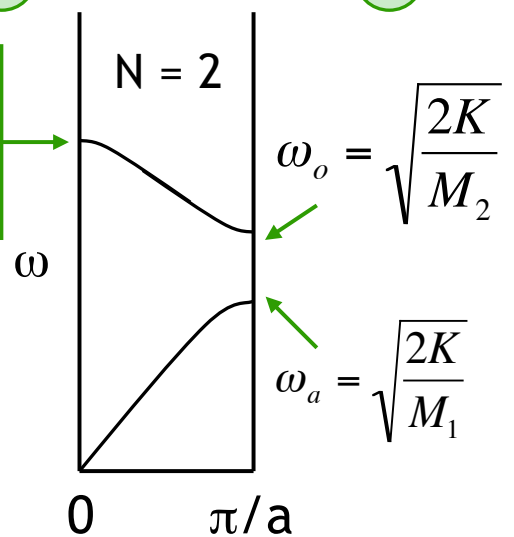
$$\omega_{max} = \sqrt{\frac{2K}{M_1} + \frac{2K}{M_2}}$$



Thermal conductivity estimation

$$\kappa_L = \frac{1}{3}\int C v_g^2 \tau \, d\omega$$

v_g - phonon group velocity
τ - phonon relaxation time
Umklapp, point defect...

Assumptions:

1- Acoustic branch: Debye solid, optical branches: phonon glass

2 – τ dominated by Umklapp scattering

$$\tau_{Umklapp} \propto T^{-1}\gamma^{-2}$$

Leibfried and Schlomann, *Nach. Akad. Wiss. Gottingen. Math. Phys. Klasse* (1954) 4, 71
Julian, *Phys. Rev.* (1965) 137, A128
Roufosse and Klemens, *Phys Rev B* (1973), 7, 5379

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v_g - phonon group velocity
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Umklapp, point defect…

Assumptions:

1- Acoustic branch: Debye solid, optical branches: phonon glass

2 – τ dominated by Umklapp scattering

$$\kappa_L = \frac{c\bar{M}\theta_D^3 a}{N^{1/3}\gamma^2 T}$$

$$\tau_{Umklapp} \propto T^{-1}\gamma^{-2}$$

M - mass
θ_D - Debye temperature
γ - Gruneisen parameter
a - interatomic distance
N – number of atoms in primitive cell

Good thermoelectric materials:
- heavy (low θ_D)
- anharmonic bonding (large γ)
- structurally complex (large N)

Recall $\theta_D \propto M^{-1}$

Leibfried and Schlomann, *Nach. Akad. Wiss. Gottingen. Math. Phys. Klasse* (1954) 4, 71
Julian, *Phys. Rev.* (1965) 137, A128
Roufosse and Klemens, *Phys Rev B* (1973), 7, 5379

Search for improved materials

Want to satisfy 2 requirements:

1 - Degenerate semiconductor w/ large $m^{*3/2}\mu$, high degeneracy

2 – Structural complexity to trap heat in low v optical modes

But where?

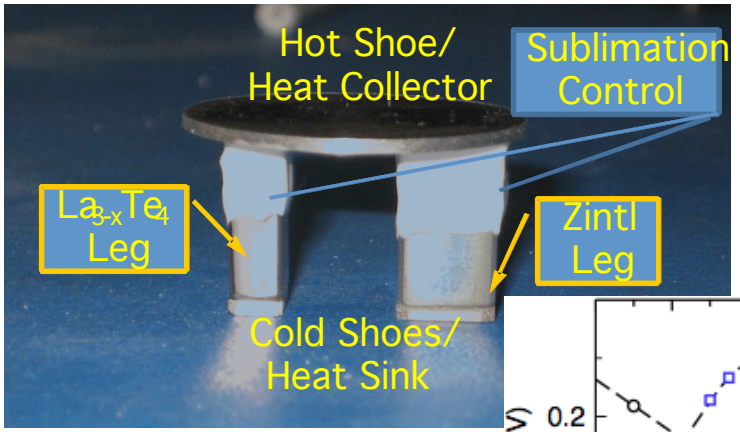
Unsegmented & Segmented Couples Under Development at JPL (10-15% eff.):

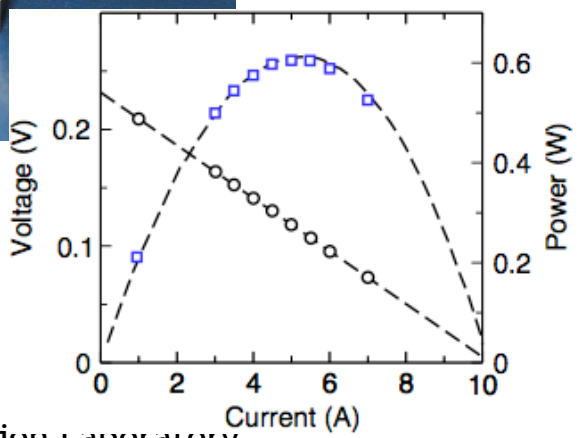
Uses novel materials developed in last few years:

- JPL and university collaborators
- 14-1-11 Zintls, $La_{3-x}Te_4$, nano bulk Si-Ge, filled Skutterudites

First set of couples built and tested at JPL in March 2009

- 10% efficient at 1000 C **14-1-11 Zintls/$La_{3-x}Te_4$** (BOL), 3000 hours of test





~ 6.3% Efficiency, 2.8 W/kg Multi-Mission RTG (MSL)

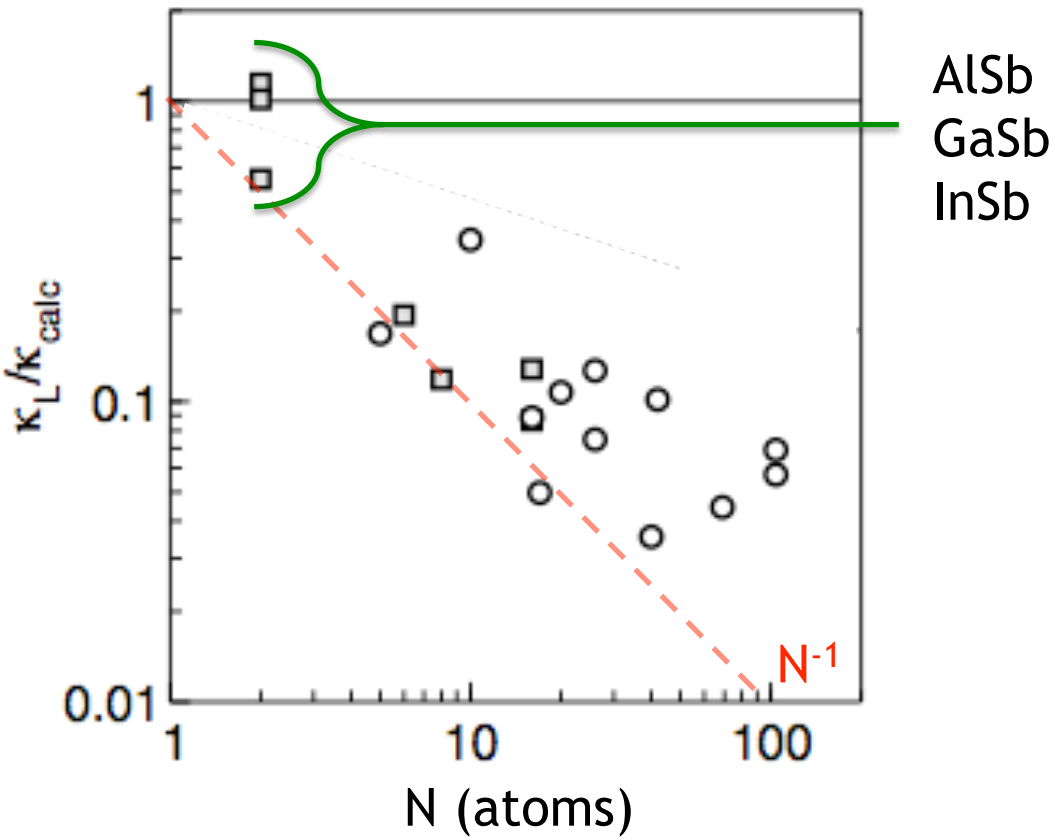
Near Term Goal:
> 10% Efficiency, 6 W/kg

Longer Term Goal:
> 15% Efficiency, 10 W/kg

Validating strong N dependence in antimonides

Strip N dependence from equation, compare to experiment:

$$\frac{\kappa_{L,\exp}}{\kappa_{L,calc}} = \frac{\kappa_L \gamma^2 T}{c\bar{M}\theta_D^3 a}$$



Validating strong N dependence in antimonides

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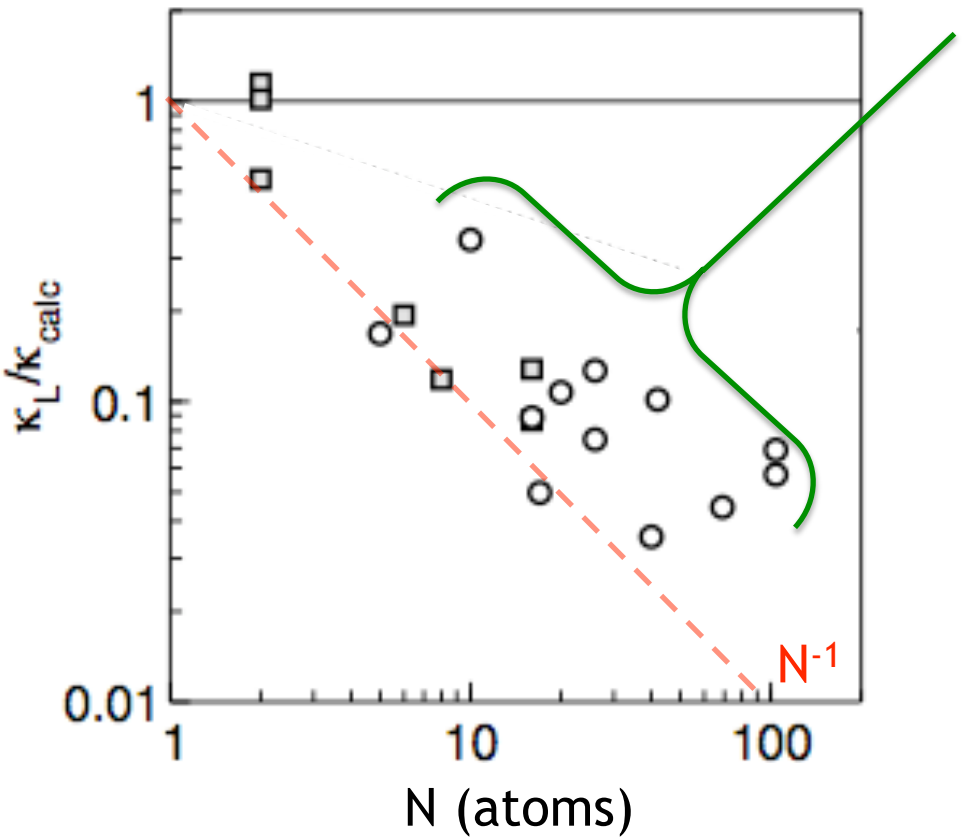

$IrSb_3$
$LiZnSb$
Mo_3Sb_7
$SrZn_2Sb_2$
$CeFe_4Sb_{12}$
$BaZn_2Sb_2$
$Ca_5Al_2Sb_6$
Mg_3Sb_2
$SrZnSb_2$
$Yb_{11}Sb_{10}$
$ZnSb$
$CdSb$
$Yb_{11}GaSb_9$
Zn_4Sb_3
$Yb_{14}MnSb_{11}$
$Yb_{14}AlSb_{11}$

N dependence is strong!

Unsegmented & Segmented Couples Under Development at JPL (10-15% eff.):

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Segmented couples recently built, tested

- **14-1-11, $La_{3-x}Te_4$**, segmented with filled **Skutterudites**
- >11% efficient at 800 C/200 C (BOL demonstration completed)
- >13% efficient at 1000 C/200 C (BOL demonstration completed)
- >15% efficient at 1000 C/200 C demonstration planned for 9/2011

Advanced Segmented Couples

JP Fleurial, T. Callait, Jet Propulsion Laboratory

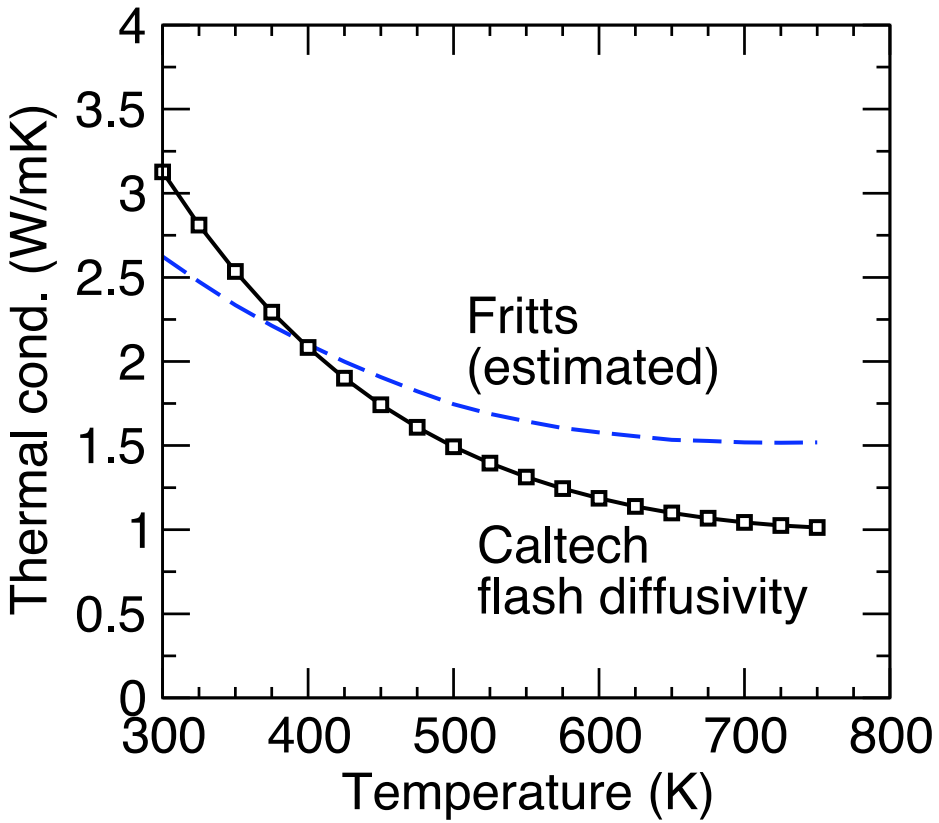
Reassessment of PbTe thermal conductivity

Classic 1960s work prior to development of laser flash diffusivity
High temperature κ was estimated!

Sources of low κ_L:

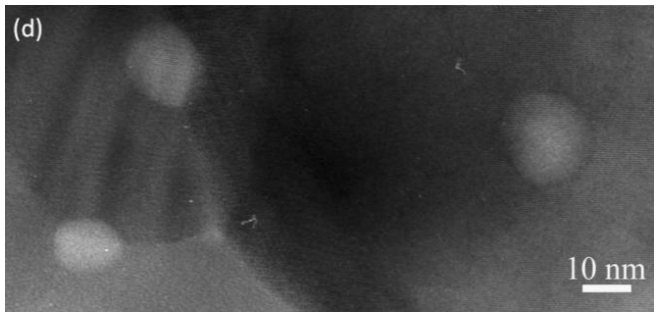
- Large Gruneisen parameter (1.5)
- High density
- Soft bonding

  v = XXXX (l) and YYyy (t) m/s

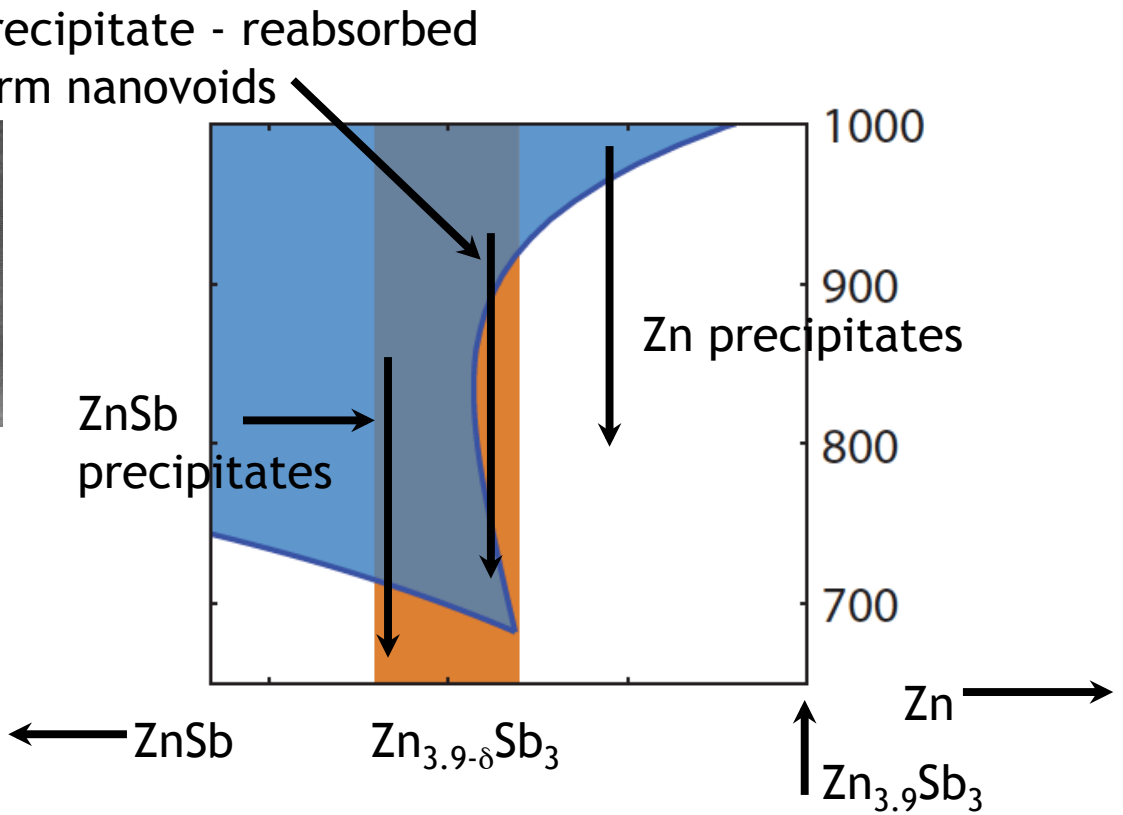


Pei et al Energy Env. Sci (2010) *in press*

Retrograde Solubility in Zn_4Sb_3



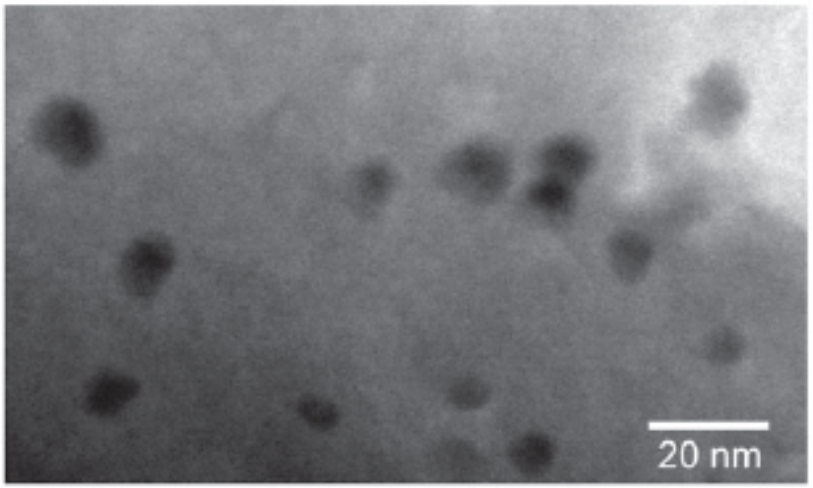
nanometer voids found in some samples of Zn_4Sb_3

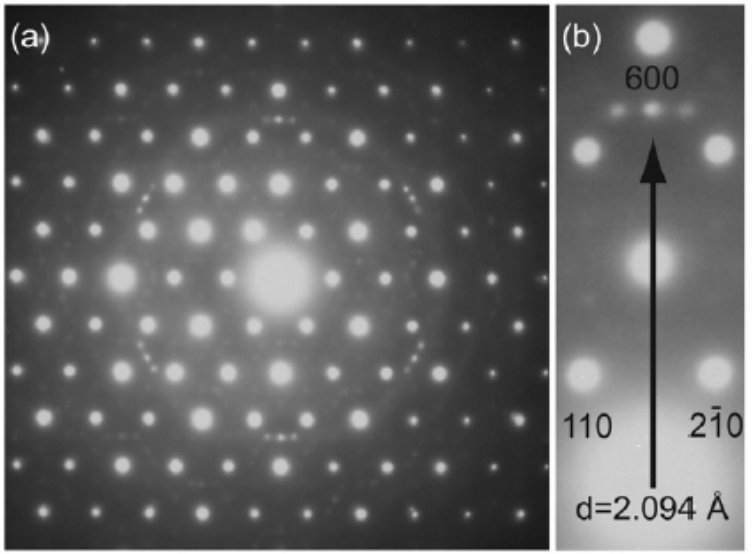


- Calculated phase diagram Zn_xSb_3 *ab initio*
- Confirms Zn_4Sb_3 stable due to configurational and Vibrational Entropy
- Correctly predicts phase should be Zn poor = *p*-type

Pomrhen, et al *Physical Review B* (in Press)

Zn Precipitates in Zn_4Sb_3





- Coherent Zn precipitates found in some samples of Zn_4Sb_3

Prytz, et al. *Phil. Mag. Lett.*,**89,** 362 (2009)

Fundamental material parameters

$$zT = \frac{\alpha^2 \sigma T}{\kappa} \rightarrow \beta = \frac{\mu m^{*3/2}}{\kappa_L}$$

Conflicts: Jeff Snyder's talk: $\mu = \frac{e\tau}{m^*}$

This talk: $\kappa_L >> \kappa_{glass}$

How do we find materials which have $\kappa_L \approx \kappa_{glass}$?

Chasmar and Stratton (1959)

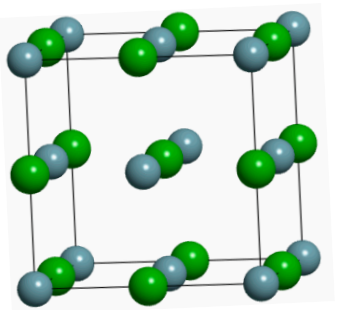
‘Simple’ example - PbTe thermal conductivity

PbTe known to have low κ_L – why?

Sources of low κ_L:

- Large Gruneisen parameter (1.5) → Increased Umklapp scattering
- High density
- Soft bonding → Low v_s
  - v = XXXX (l) and YYyy (t) m/s

No structural complexity
2 atoms in primitive cell



Outline

$$\kappa_L = \frac{1}{3}\int C v_g^2 \tau \, d\omega$$

Group velocity (v_g)

- Heavy atoms, soft bonding
  - PbTe
- Structural complexity
  - $Yb_{14}MnSb_{11}$
  - Ca_3AlSb_3

Scattering (τ)

- Intrinsic point defects
  - $La_{3-x}Te_4$
  - Zn_4Sb_3
- Nanostructures
  - Zn_4Sb_3