Solar Thermoelectrics

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Materials Science Division

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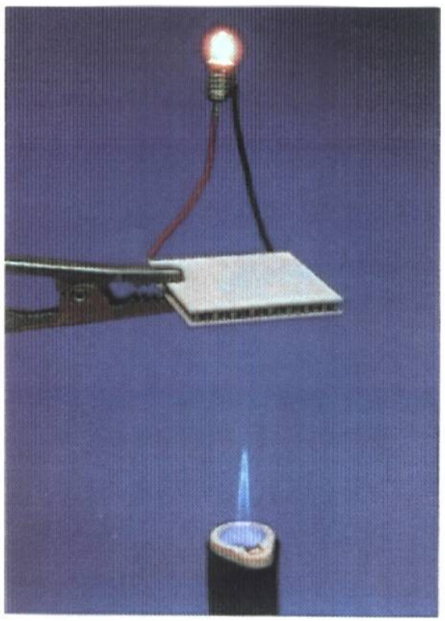
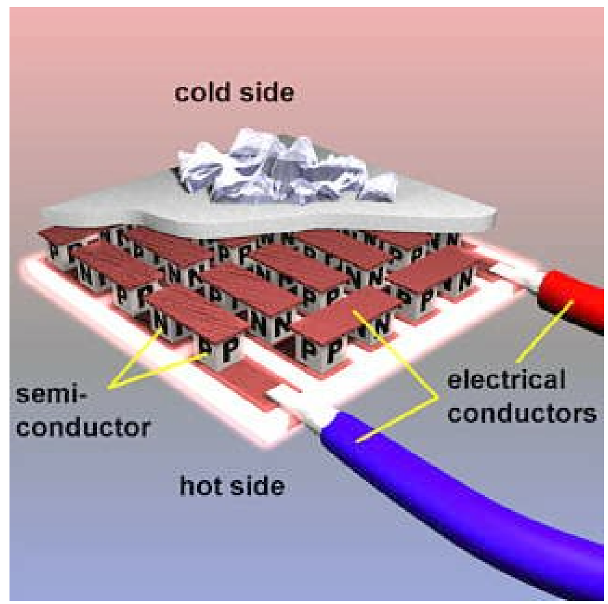
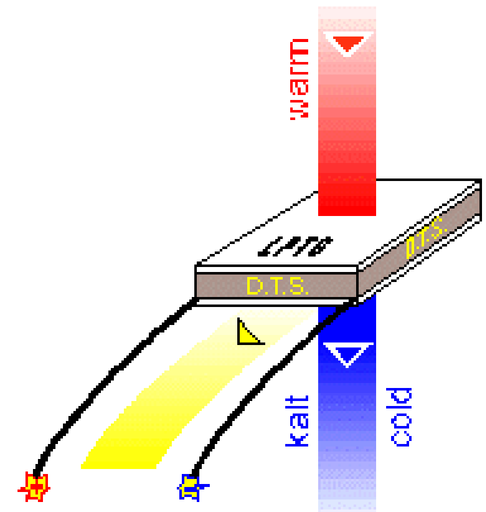
Heat to Electrical Energy Directly

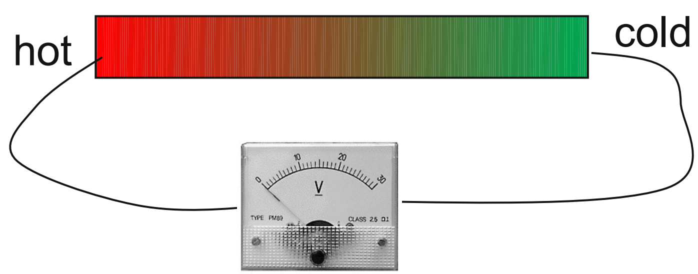
Up to 20% conversion efficiency with right materials



Electrical Power Generation





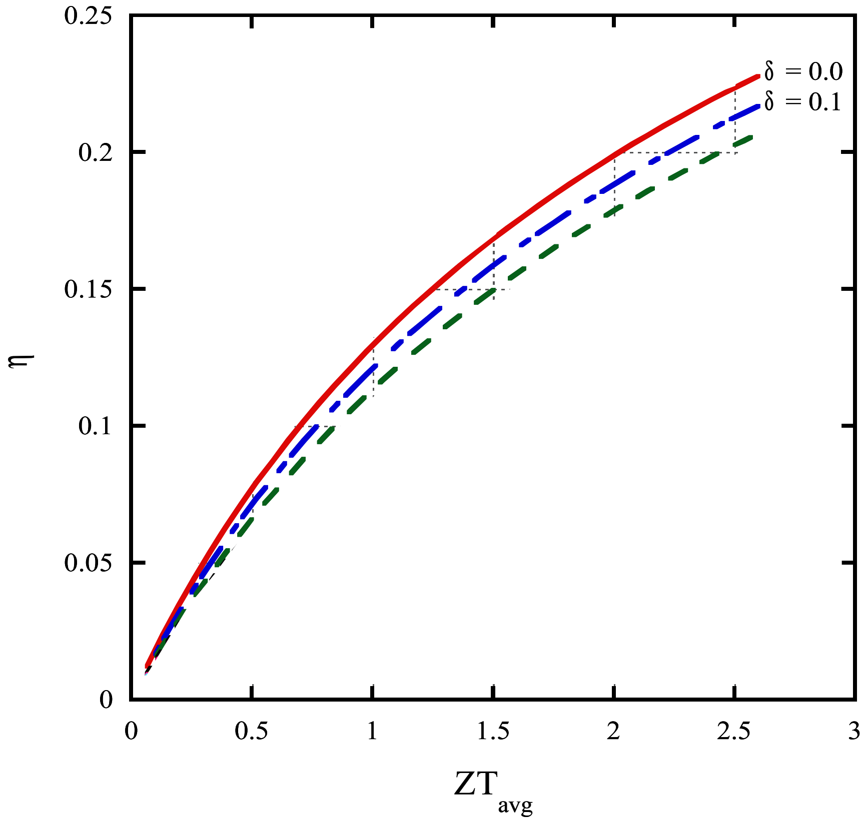


TE devices have <u>no moving parts, no noise, reliable</u>

Thermopower $S = \Delta V / \Delta T$

http://www.dts-generator.com/

Figure of Merit



$$\eta = \frac{T_h - T_c}{T_h} \cdot \frac{\sqrt{1 + z\overline{\overline{T}}} - 1}{\sqrt{1 + z\overline{\overline{T}}} + T_c / T_h}$$

Carnot efficiency

electrical conductivity

thermopower

$$ZT = \frac{\sigma \cdot S^2}{\kappa_{total}} \bullet T$$

Total thermal conductivity

Power factor

$\sigma \cdot S^2$

$\delta = R_c/R$

For T_h = 800K

T_c = 300K

ZT and Electronic Structure

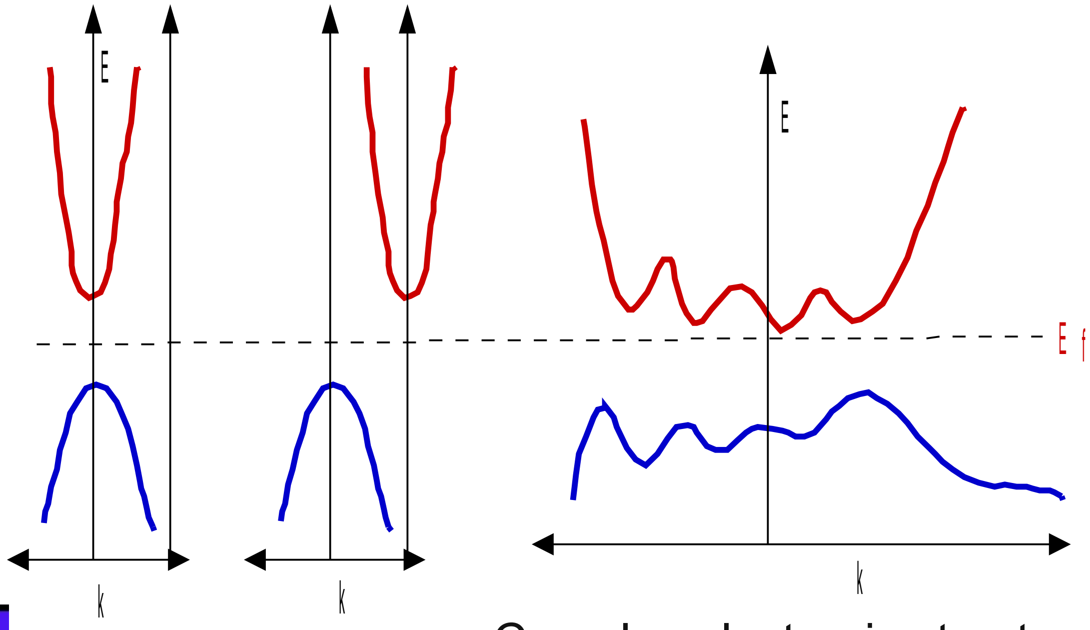
Isotropic structure

Anisotropic structure

$$Z_{\max} \propto \gamma \frac{T^{3/2}\tau\sqrt{\dfrac{m_x m_y}{m_z}}}{\kappa_{latt}} e^{(r+1/2)}$$

For acoustic phonon scattering
r=-1/2

m= effective mass
τ=scattering time
r= scattering parameter
κ_{latt}= lattice thermal conductivity
T = temperature
γ= band degeneracy



Complex electronic structure

Large γ comes with
(a) high symmetry e.g. rhombohedral, cubic
(b) off-center band extrema

Selection criteria for candidate materials

- Narrow band-gap semiconductors
- Heavy elements
  - High μ, low κ
- Large unit cell, complex structure
  - low κ
- Highly anisotropic or highly symmetric…
- Complex compositions
  - low κ, complex electronic structure

Investigating the A/Bi/Q system

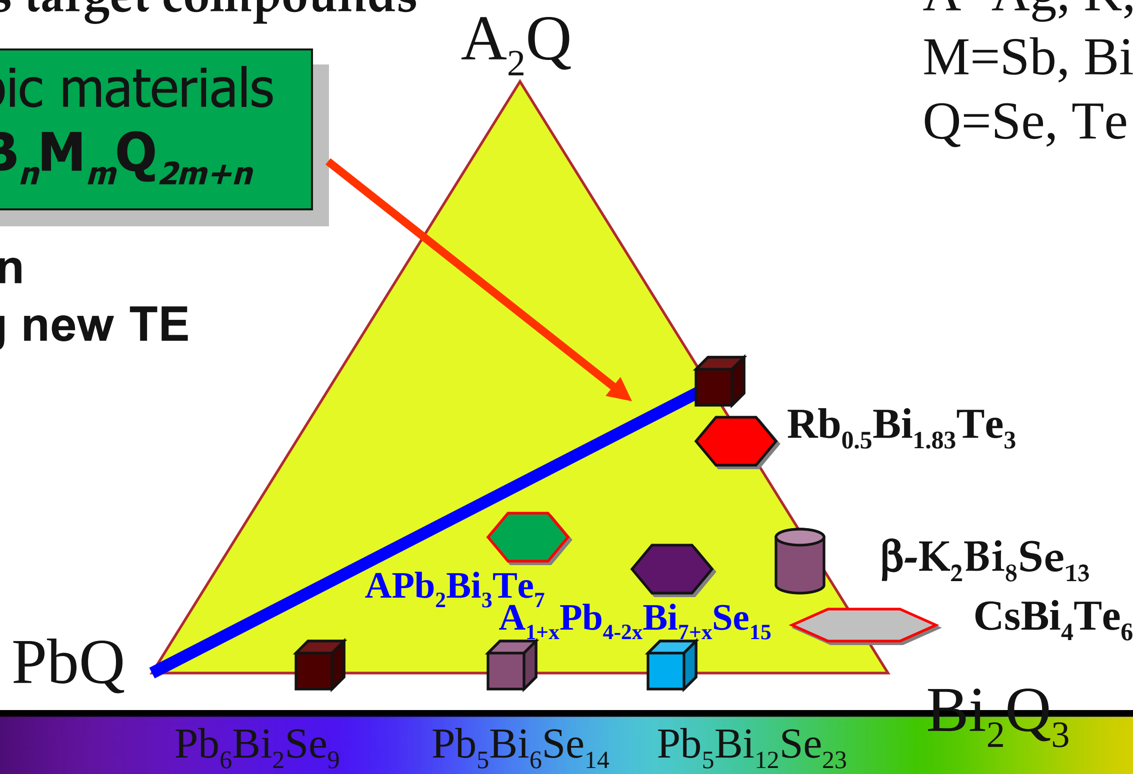
$$A_2Q + PbQ + M_2Q_3 \longrightarrow (A_2Q)_n(PbQ)_m(M_2Q_3)_p$$

Map generates target compounds

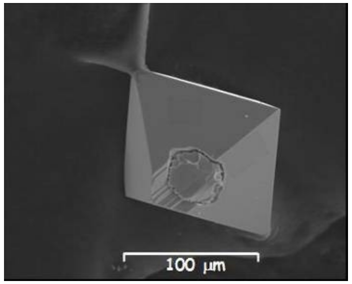
A=Ag, K, Rb, Cs
M=Sb, Bi
Q=Se, Te

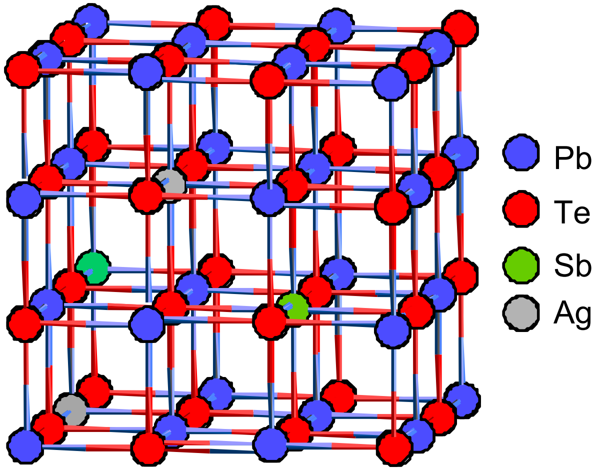
Cubic materials
$\mathbf{A_mB_nM_mQ_{2m+n}}$

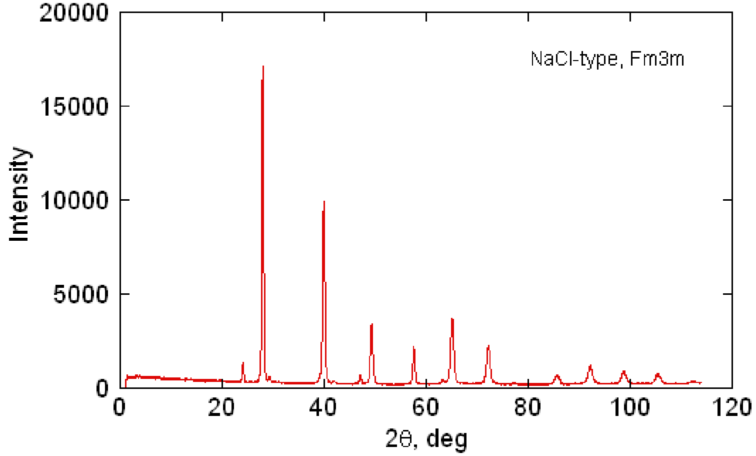
Phases shown are promising new TE materials

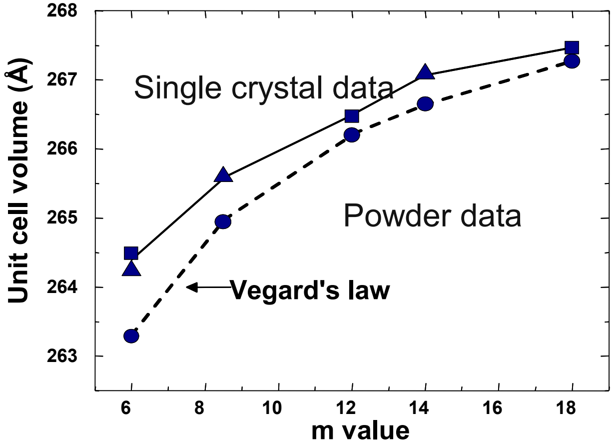


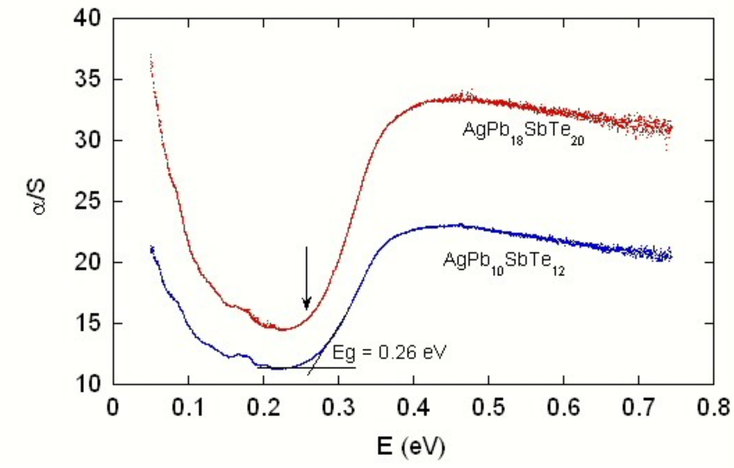
$AgPb_mSbTe_{2+m}$ (LAST-m)
$NaPb_mSbTe_{2+m}$ (SALT-m)









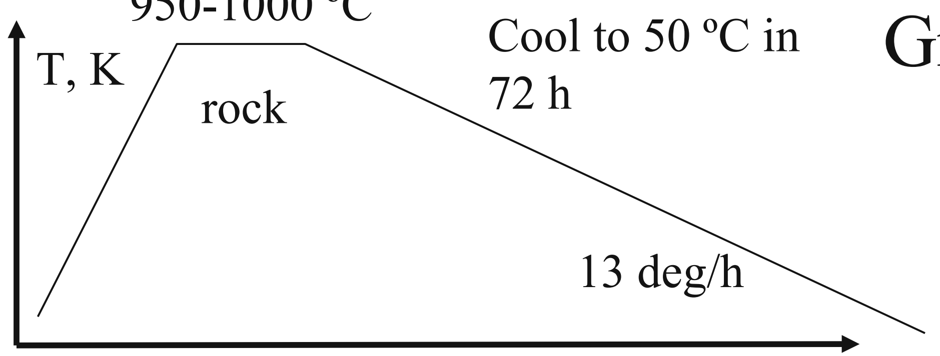


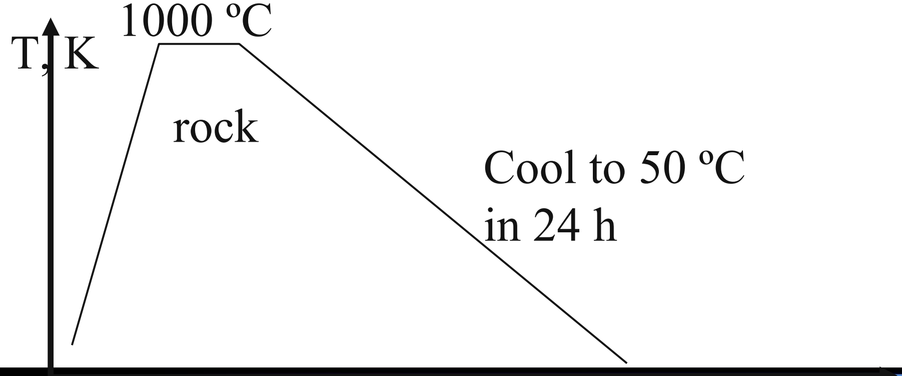
(1) (a) Rodot, H. *Compt. Rend.* **1959**, *249*, 1872-4.
(2) (a) Rosi, F. D.; Hockings, E. S.; Lindenblad, N. E. *Adv. Energy Convers.* **1961**, *1*, 151.

- No phase transitions to melting point

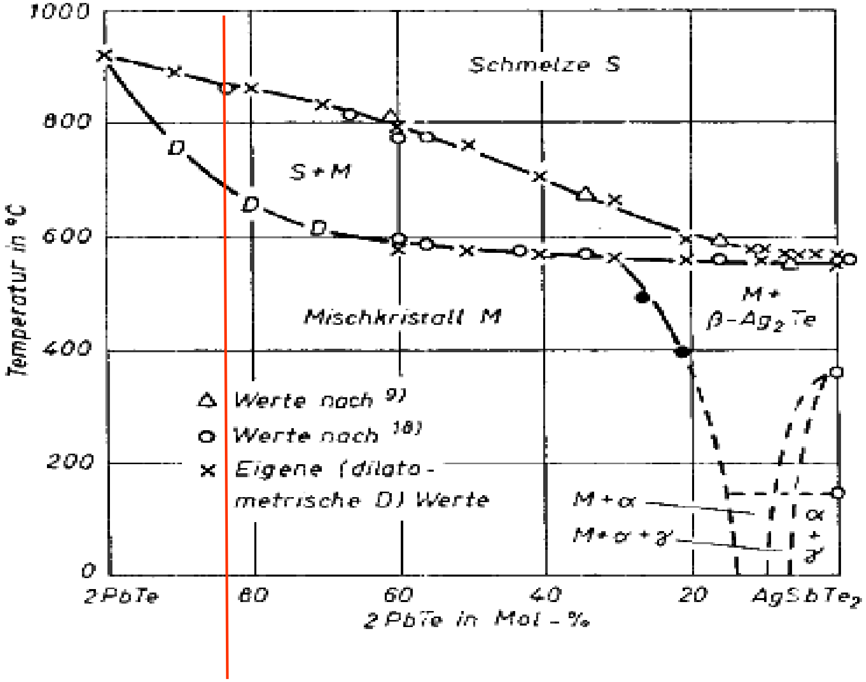
Synthesis

Ingot properties very sensitive to cooling profile





Gravity induced inhomogeneity



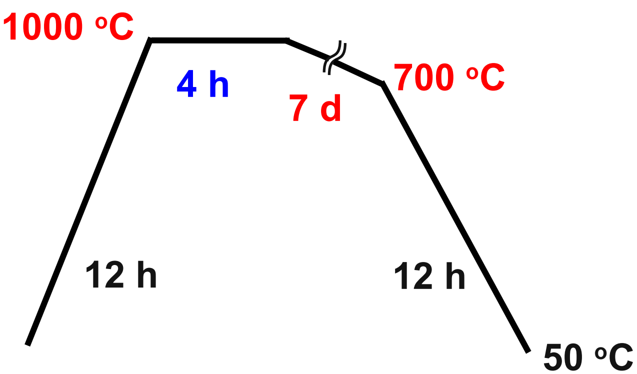
Wernick, J. H.. *Metallurg. Soc. Conf. Proc*. (1960), 5 69-87.

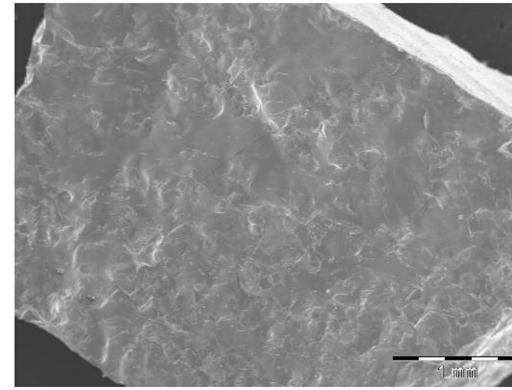
R. G. Maier *Z. Metallkunde* 1963, 311

LAST-18: Synthesis with Slow Cooling

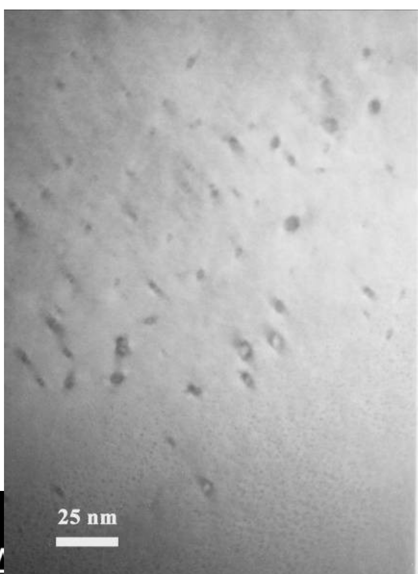
~2deg/hr

Ag	Sb	Pb	Te	amount
0.86	1	19	20	105 g

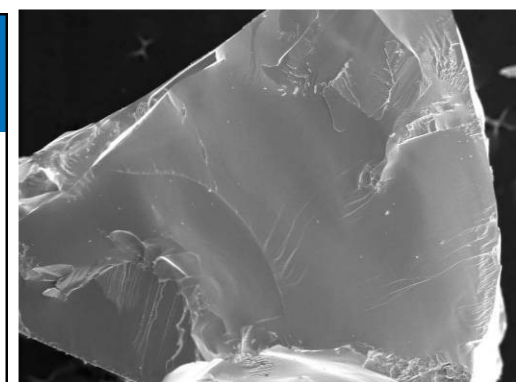




fast cooled sample

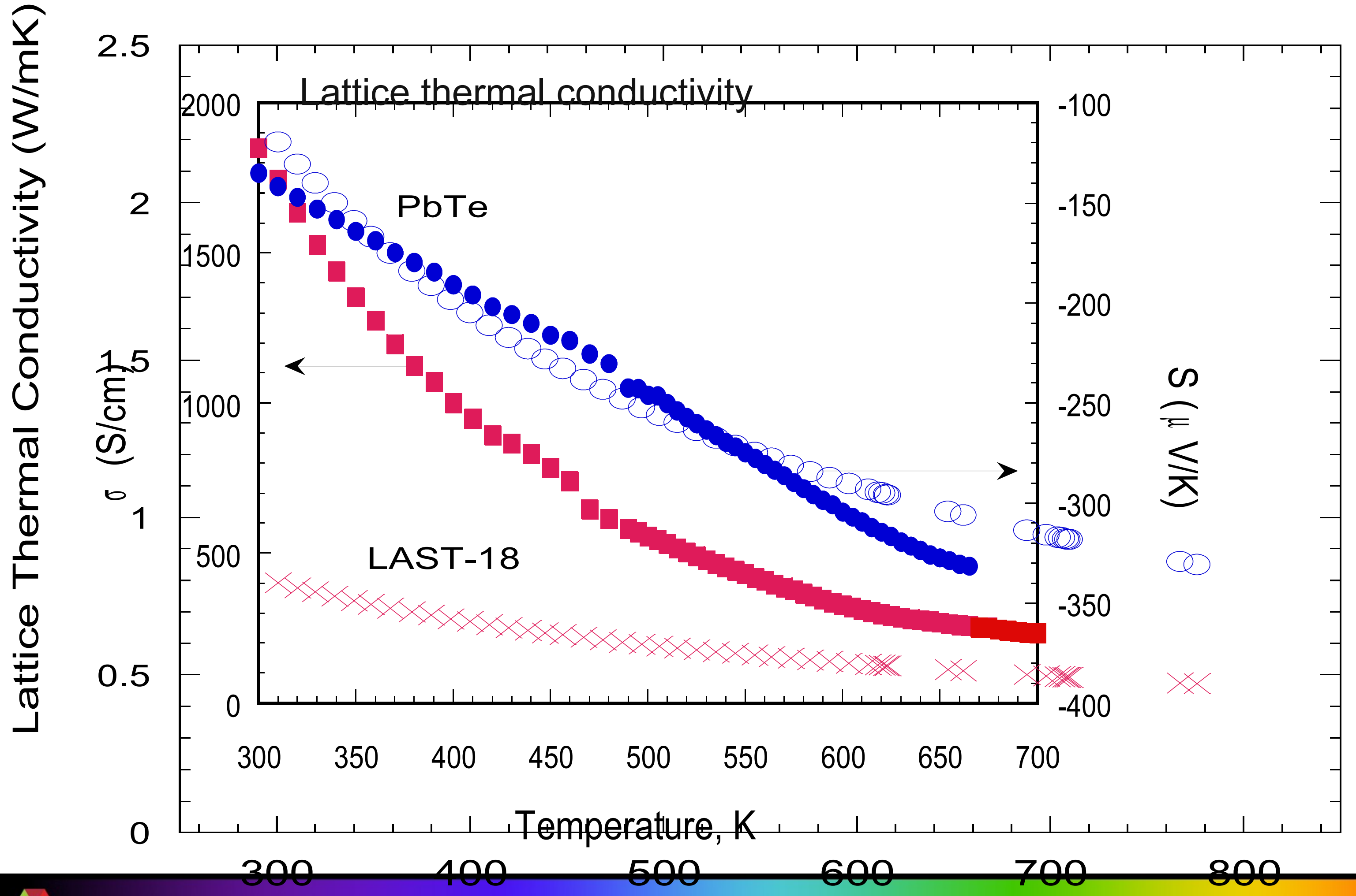


ETN125	σ (S/cm)	S (µV/K)	PF (µW/cm·K²)
A	535	-121	7.8
B	959	-128	15.7
C	1026	-158	25.6
D	1341	-180	43.4

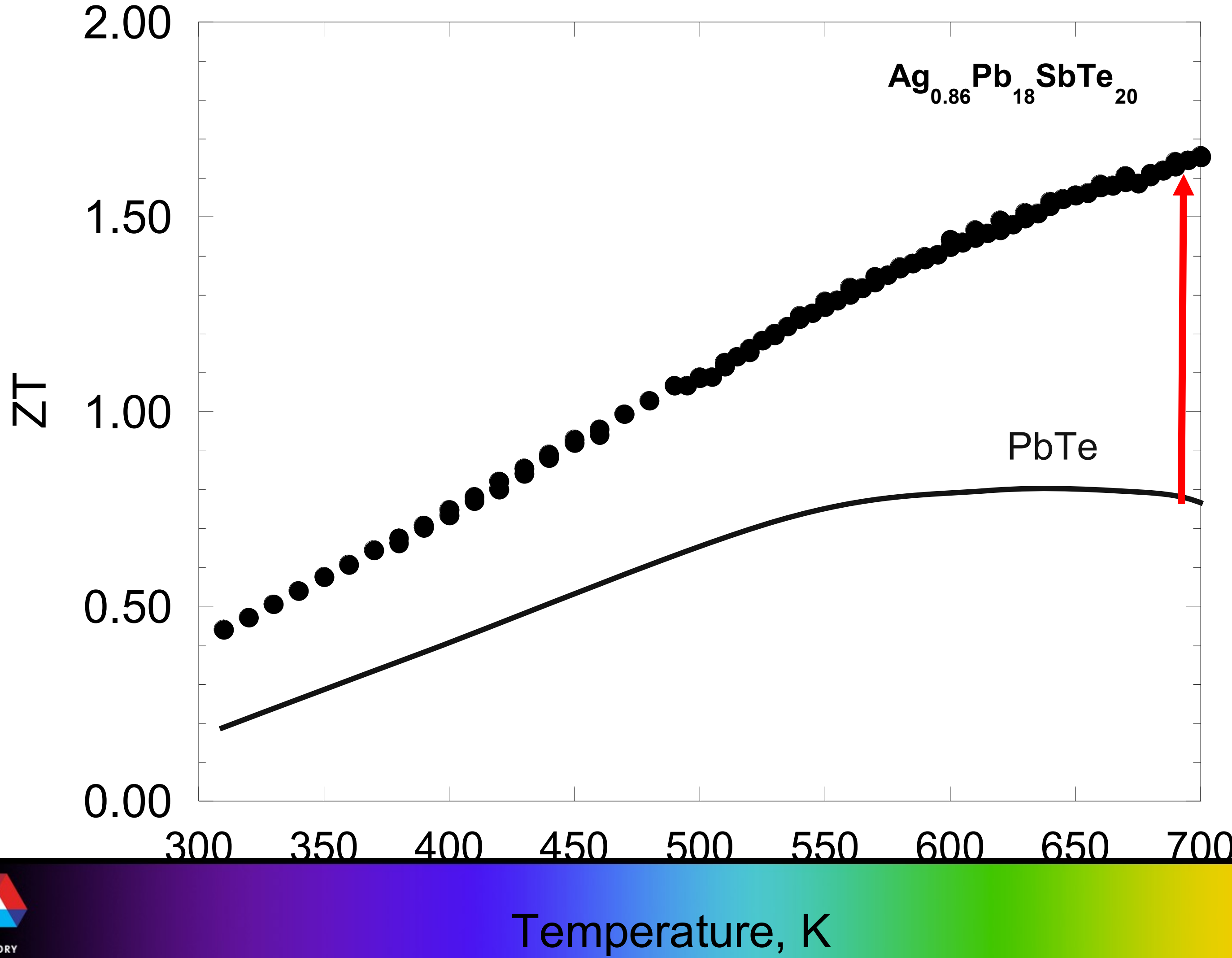


slow cooled sample

Properties of $Ag_{1-x}Pb_{18}SbTe_{20}$

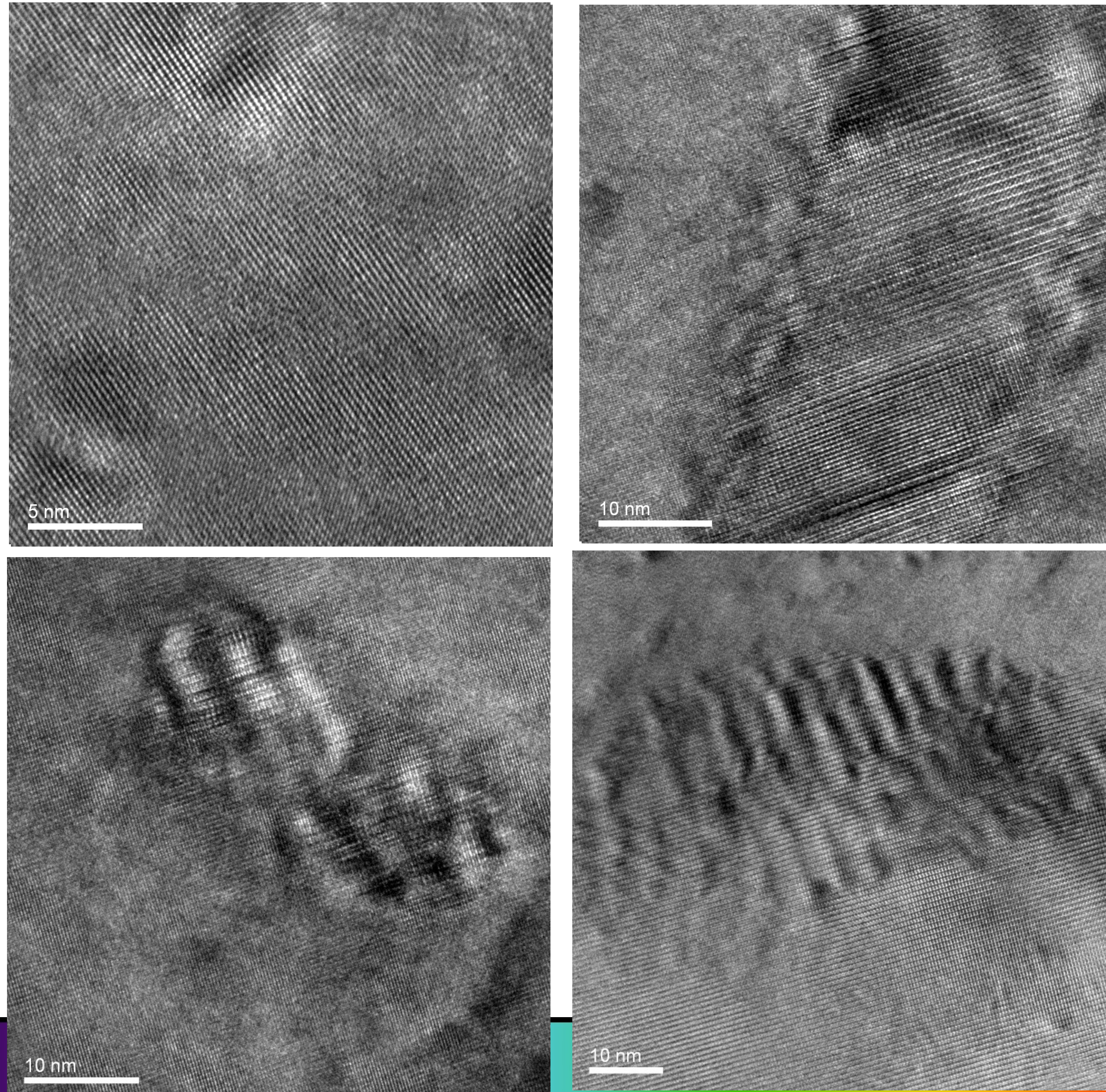


LAST-18 ZT~1.6

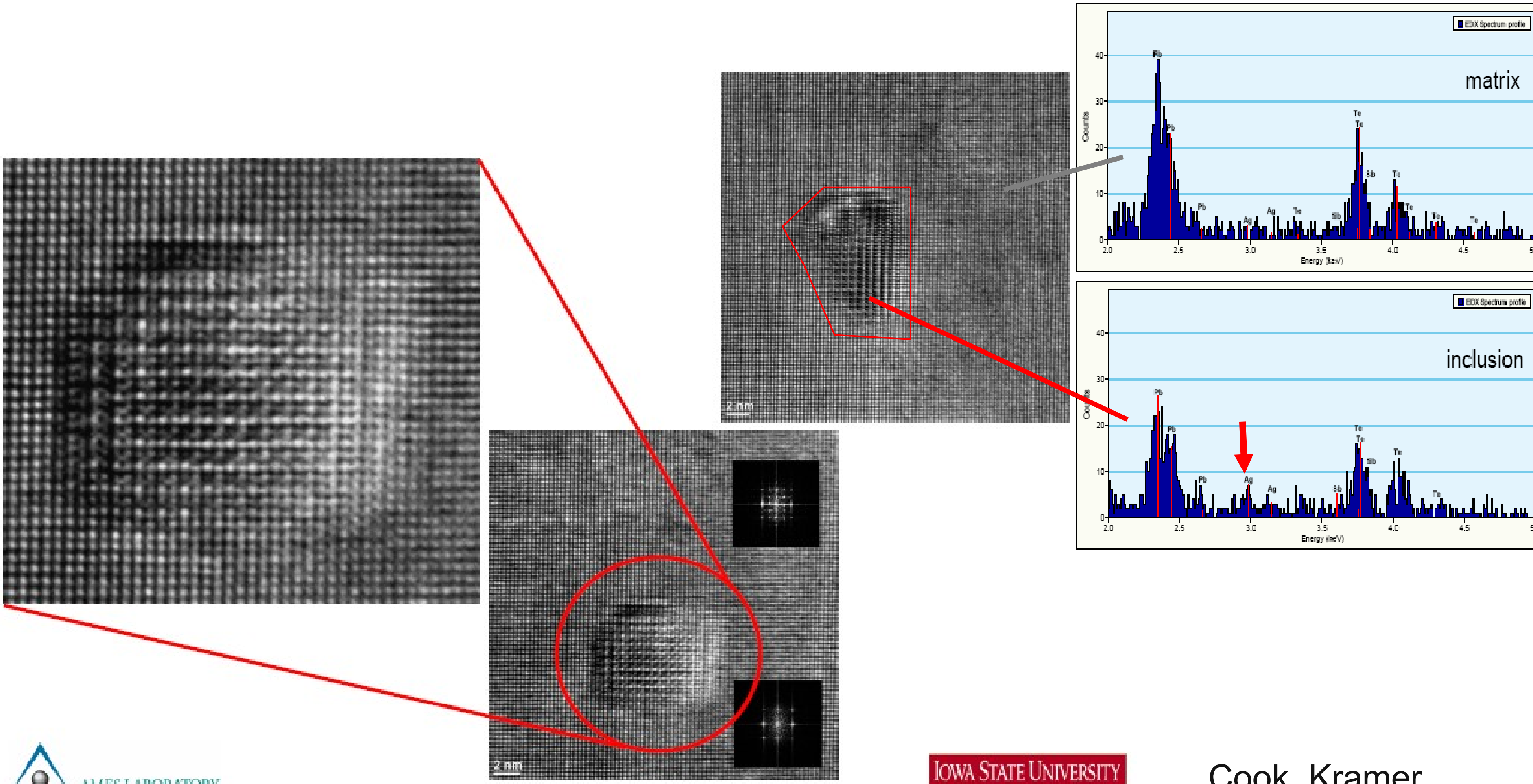


2.00
1.50
1.00
0.50
0.00
ZT
Ag0.86Pb18SbTe20
PbTe
300
350
400
450
500
550
600
650
700
Temperature, K

HRTEM
of LAST-18

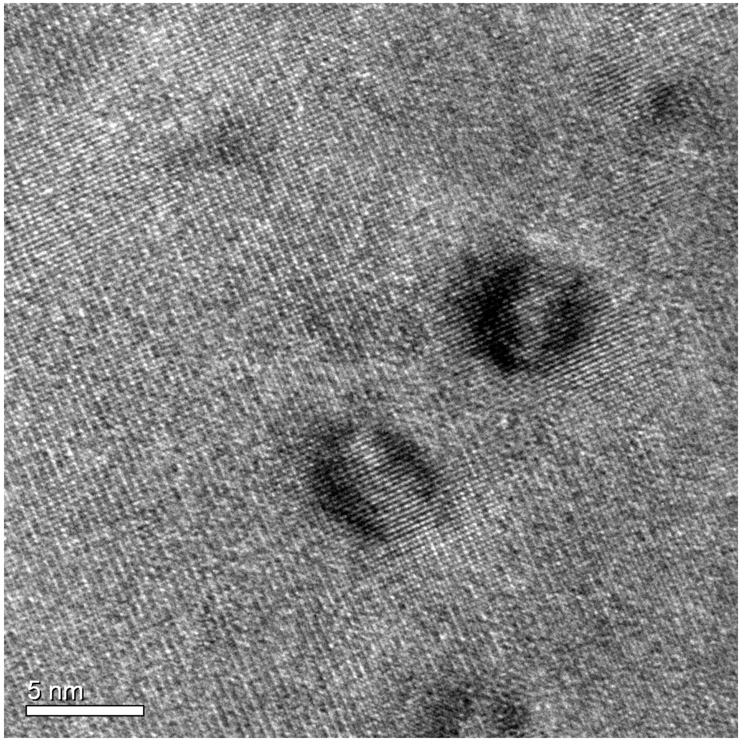


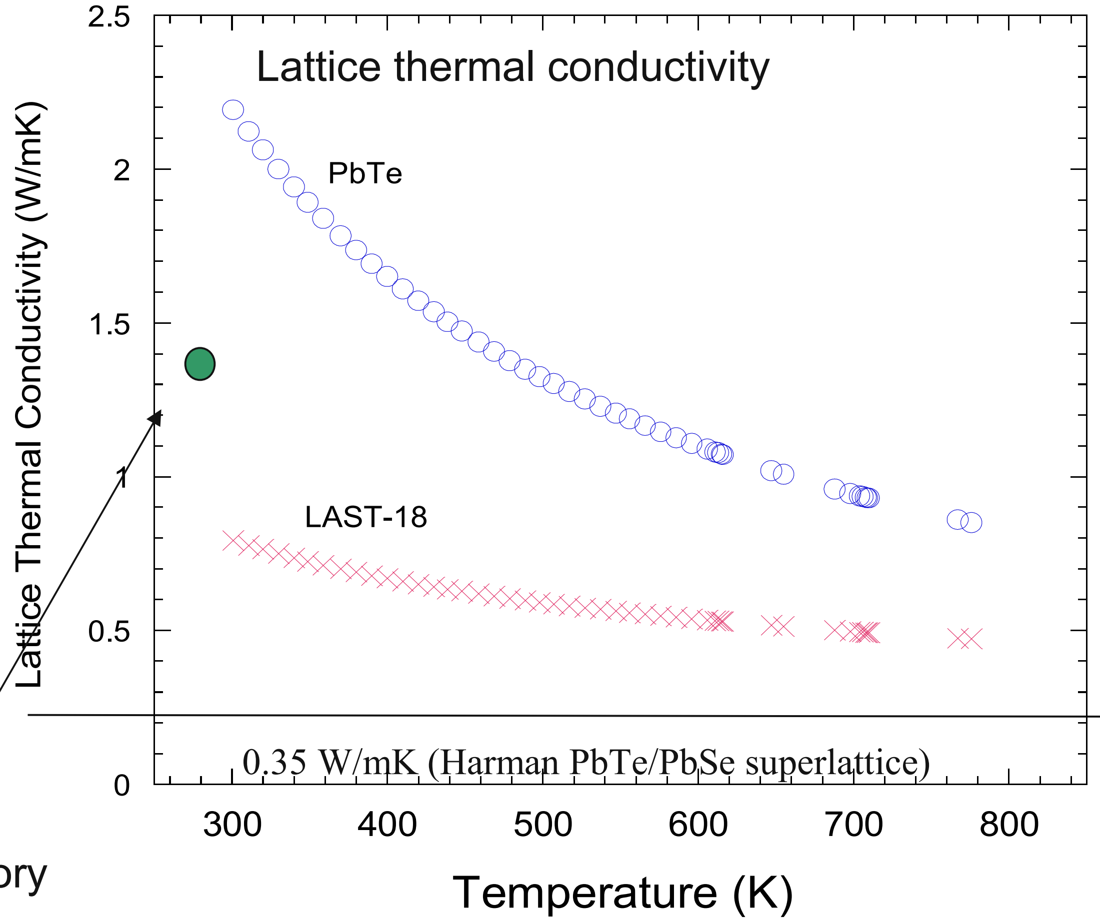
What is the dot made of?



Cook, Kramer

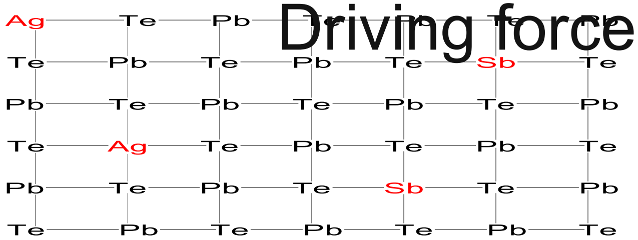
Nanostructures reduce the lattice thermal conductivity

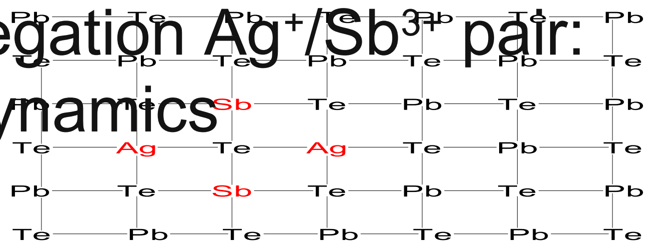




Why do the LAST materials nanostructure?

Driving force for segregation Ag^{+}/Sb^{3+} pair: thermodynamics



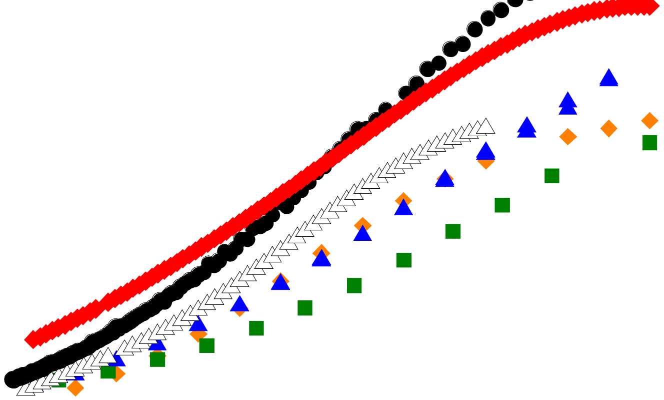


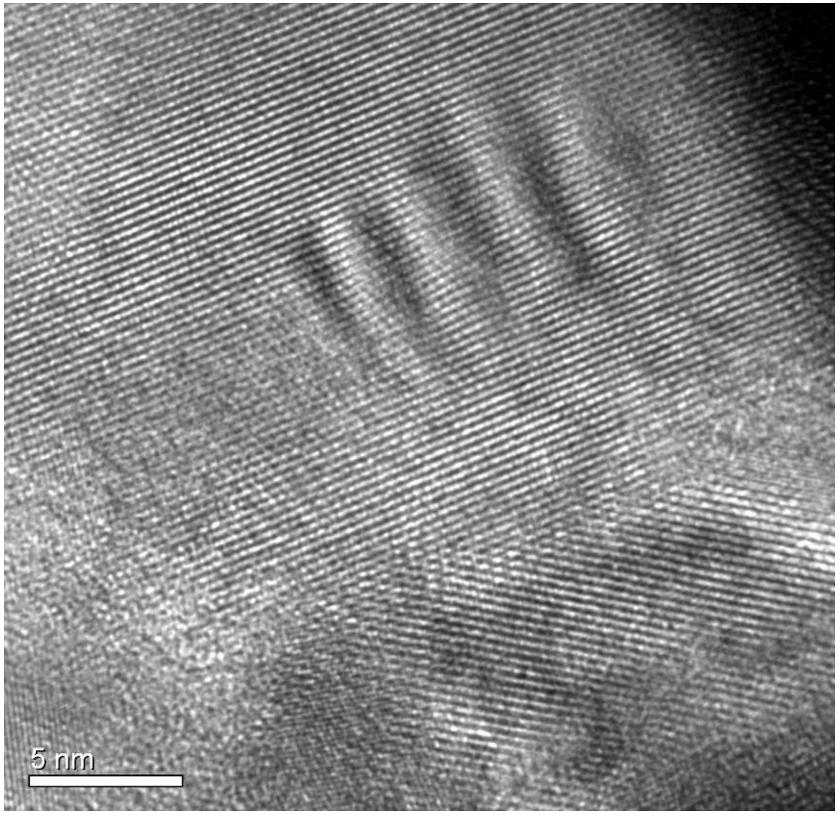
Dissociated state..unstable

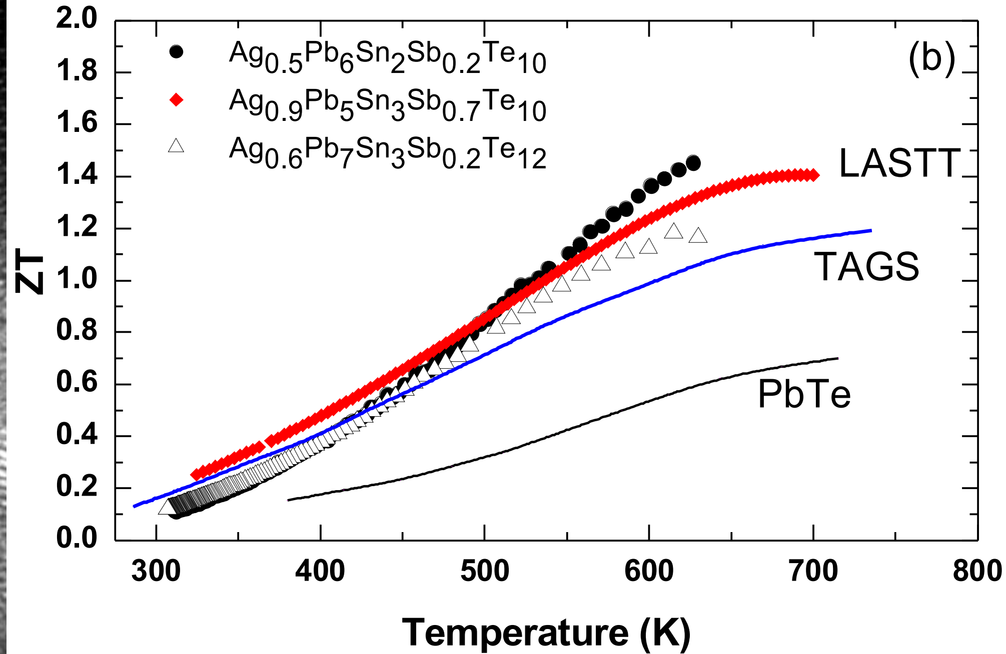
Associated state..stable

Any +1/+3 pair

Figure of Merit LASTT (p-type)







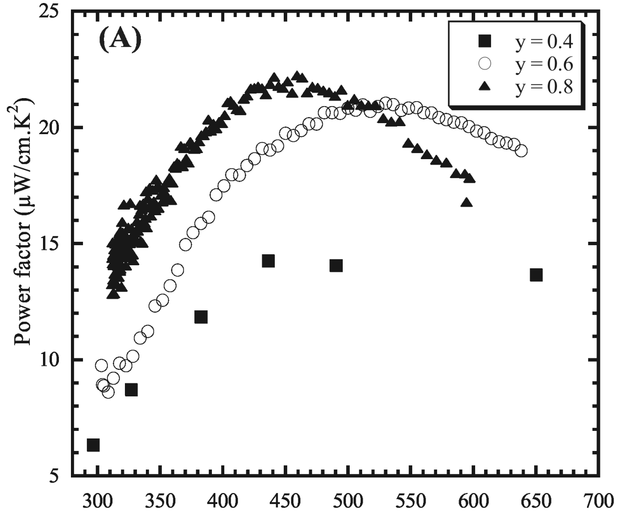
J. Androulakis, R. F. Hsu, R. Pcionek, H. Kong, C. Uher, J. J. D'Angelo, A. Downey, T. Hogan, M. G. Kanatzidis, *Advanced Materials* **2006**, 18, 1170

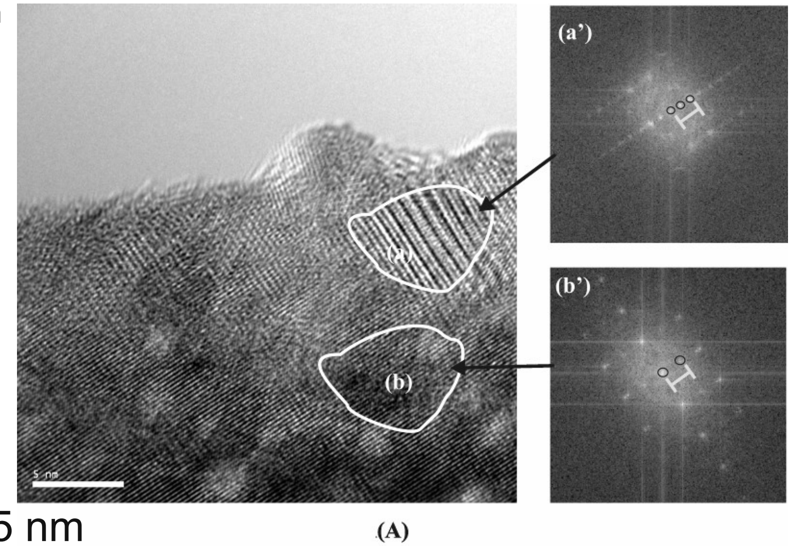
Na-based materials (SALT-m)

New high ZT p-type material

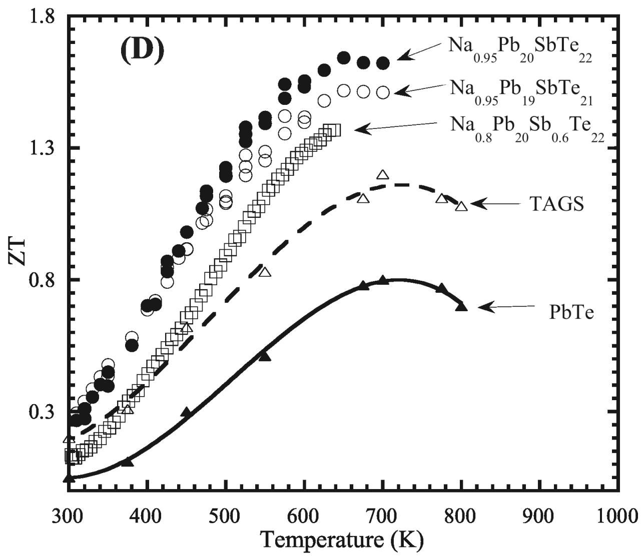
$Na_{1-x}Pb_mSbTe_{2+m}$

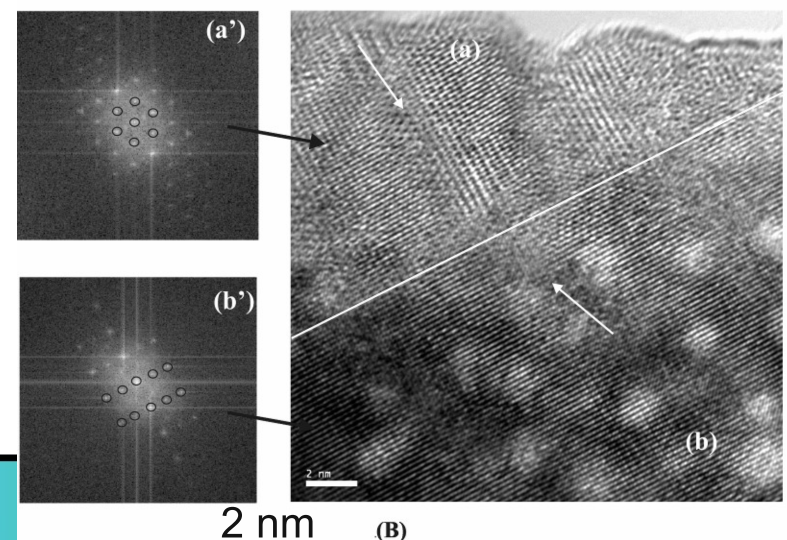
m~19-21





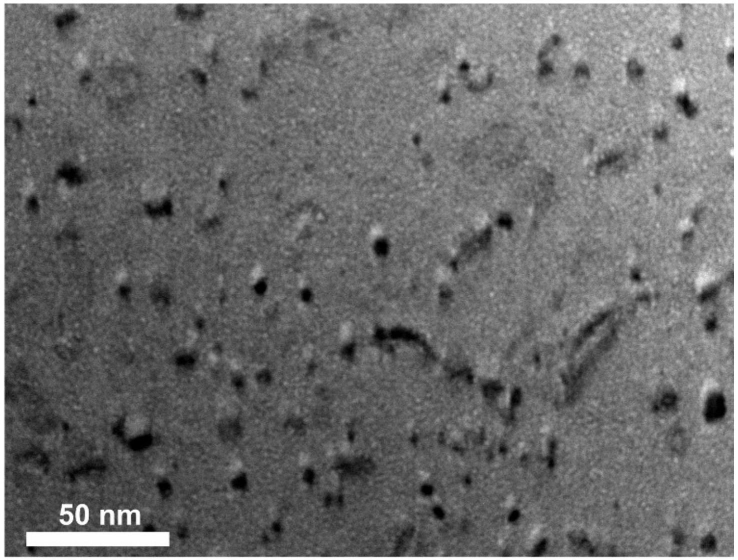
5 nm

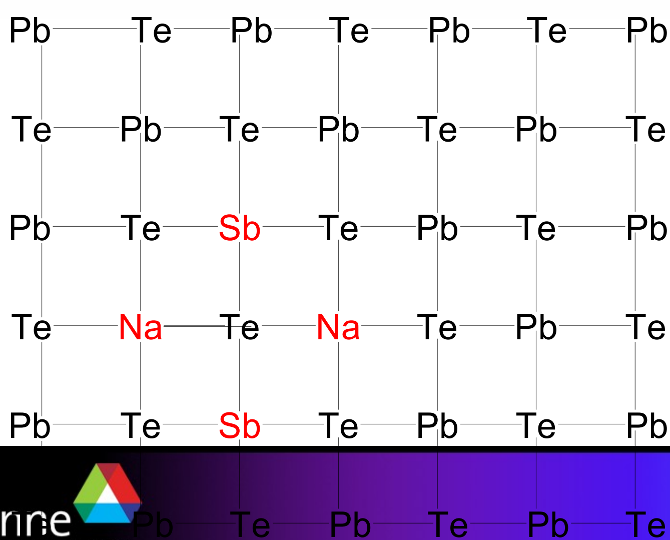


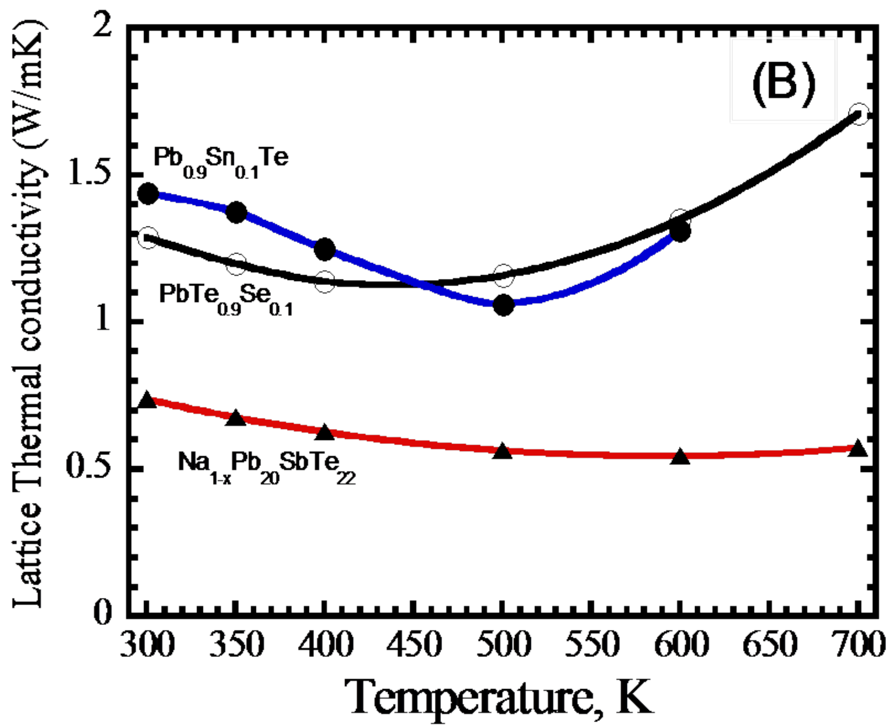


2 nm

What is nanostructuring worth?

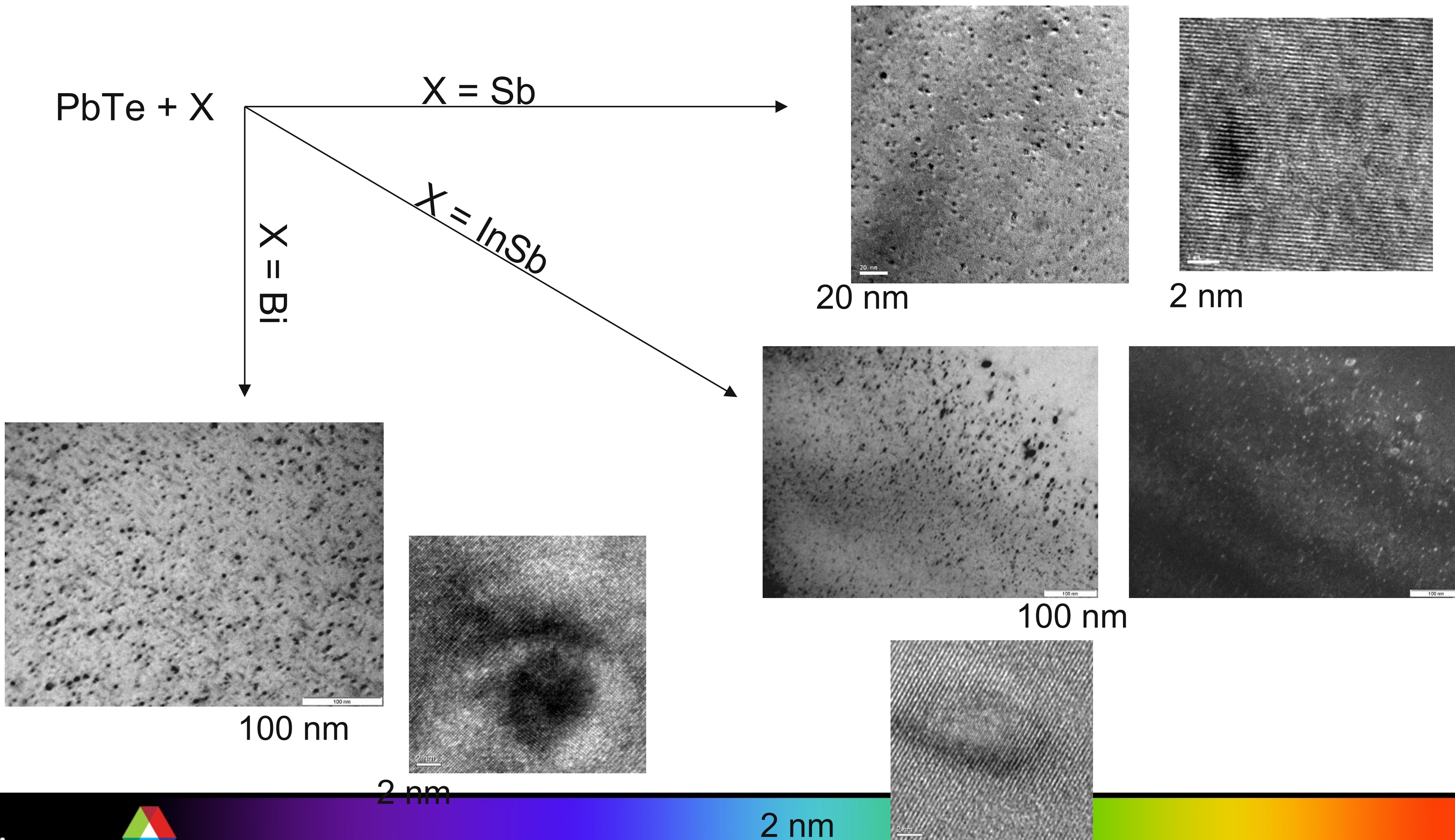




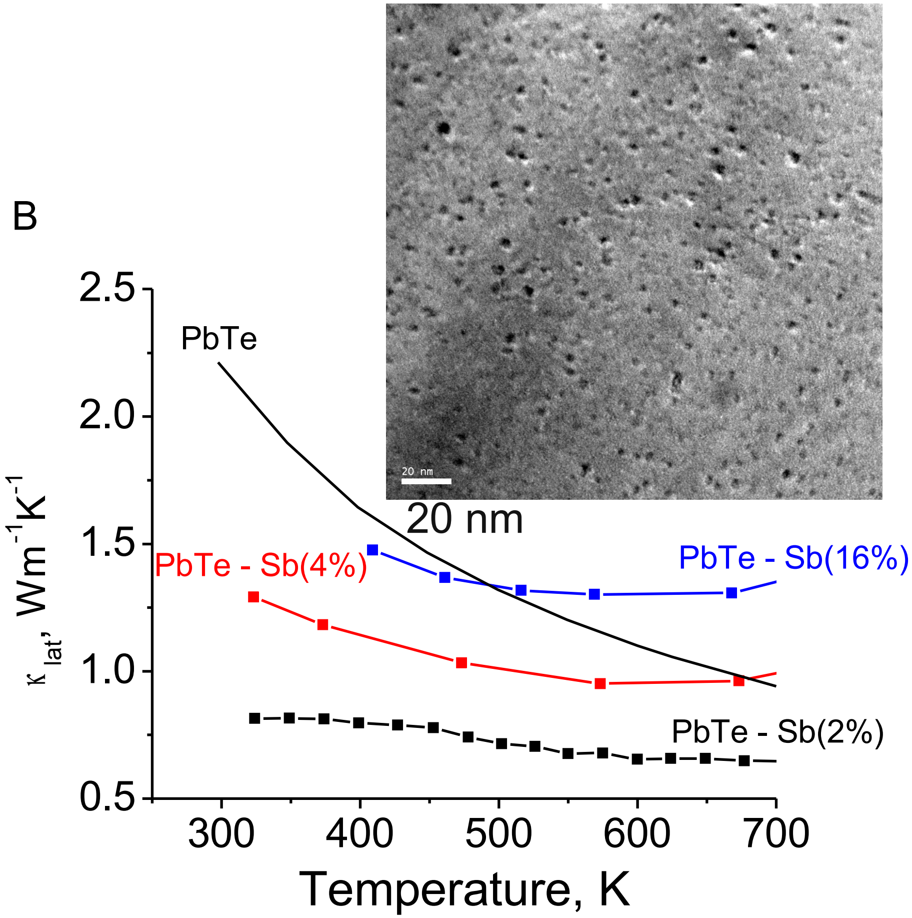


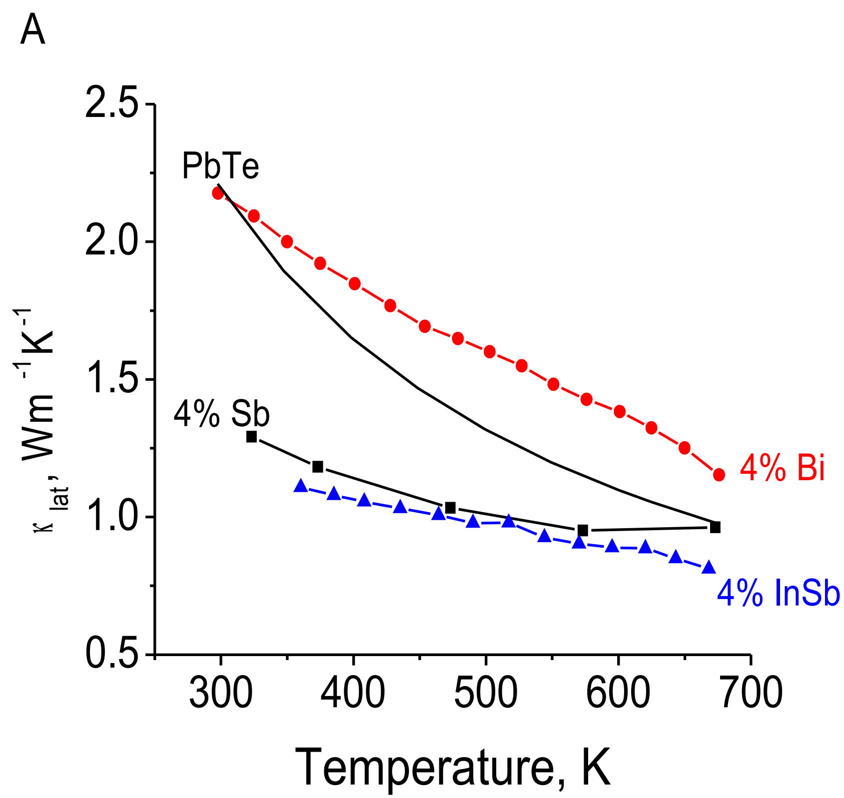
P. F. P. Poudeu, J. D'Angelo, A. D. Downey, J. L. Short, T. P. Hogan, M. G. Kanatzidis, *Angew. Chem. Int. Ed*. **2006**, 45, 1

Matrix Encapsulation as a Route to Nanostructured PbTe



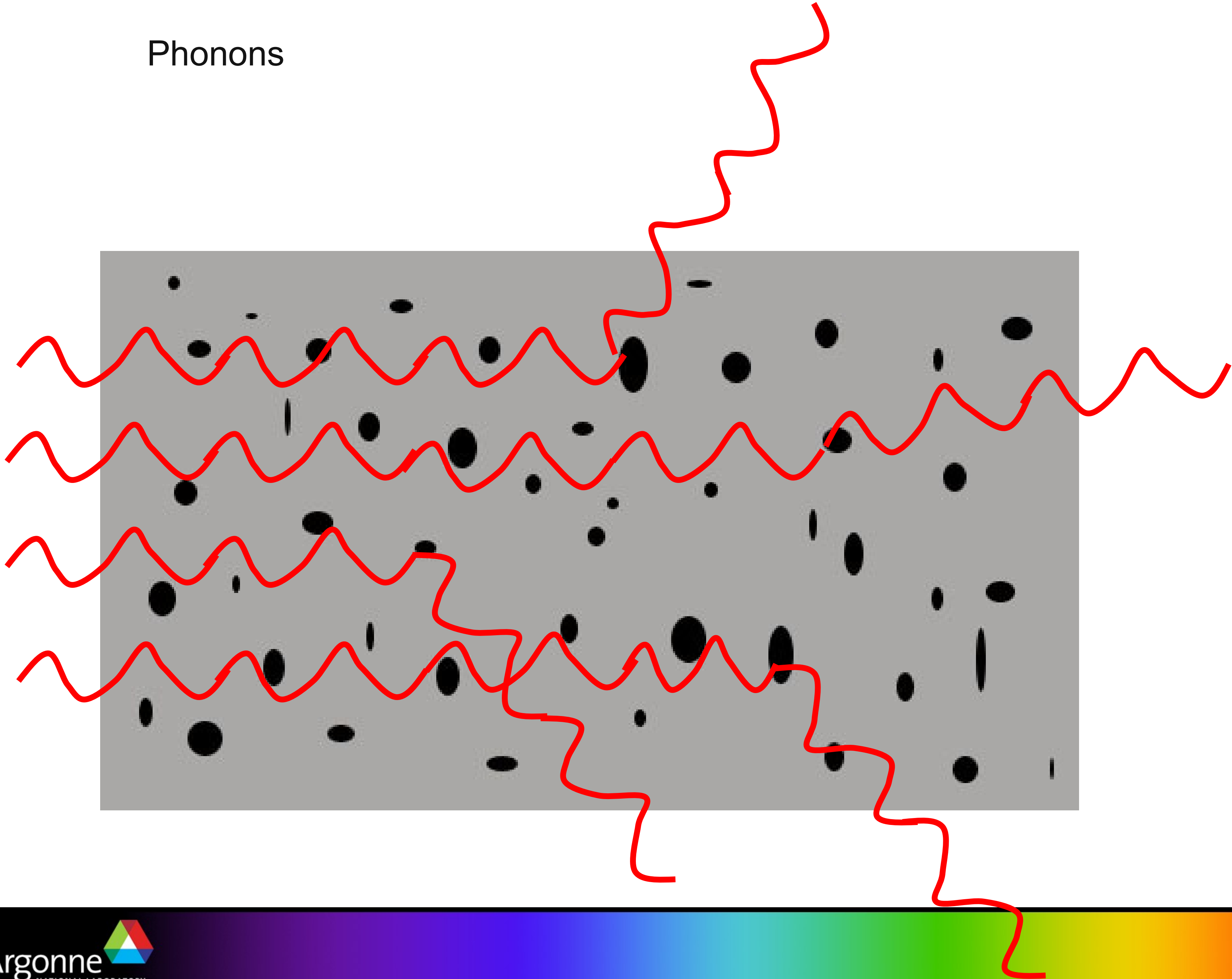
Nanocrystals of Sb in PbTe



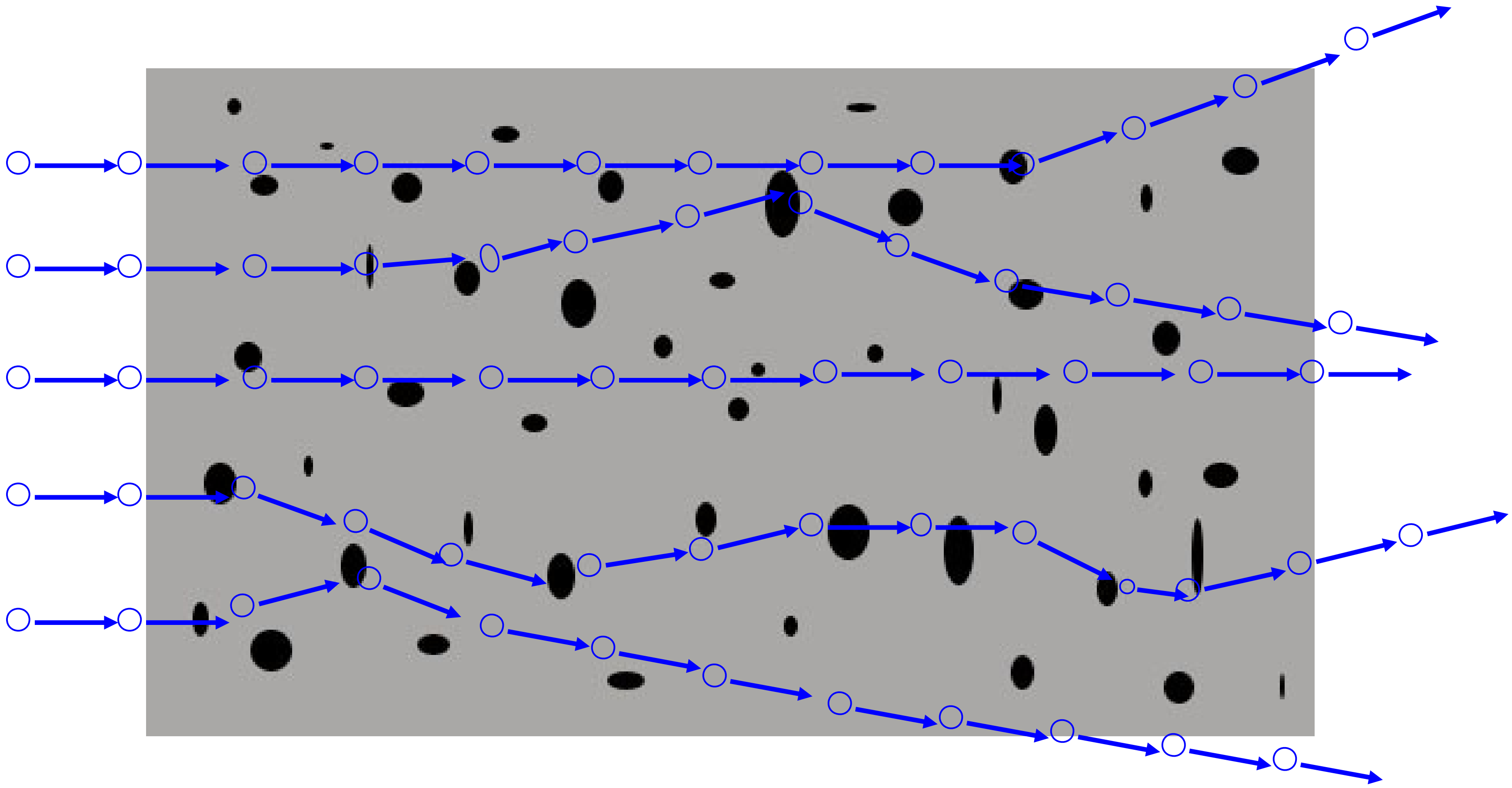


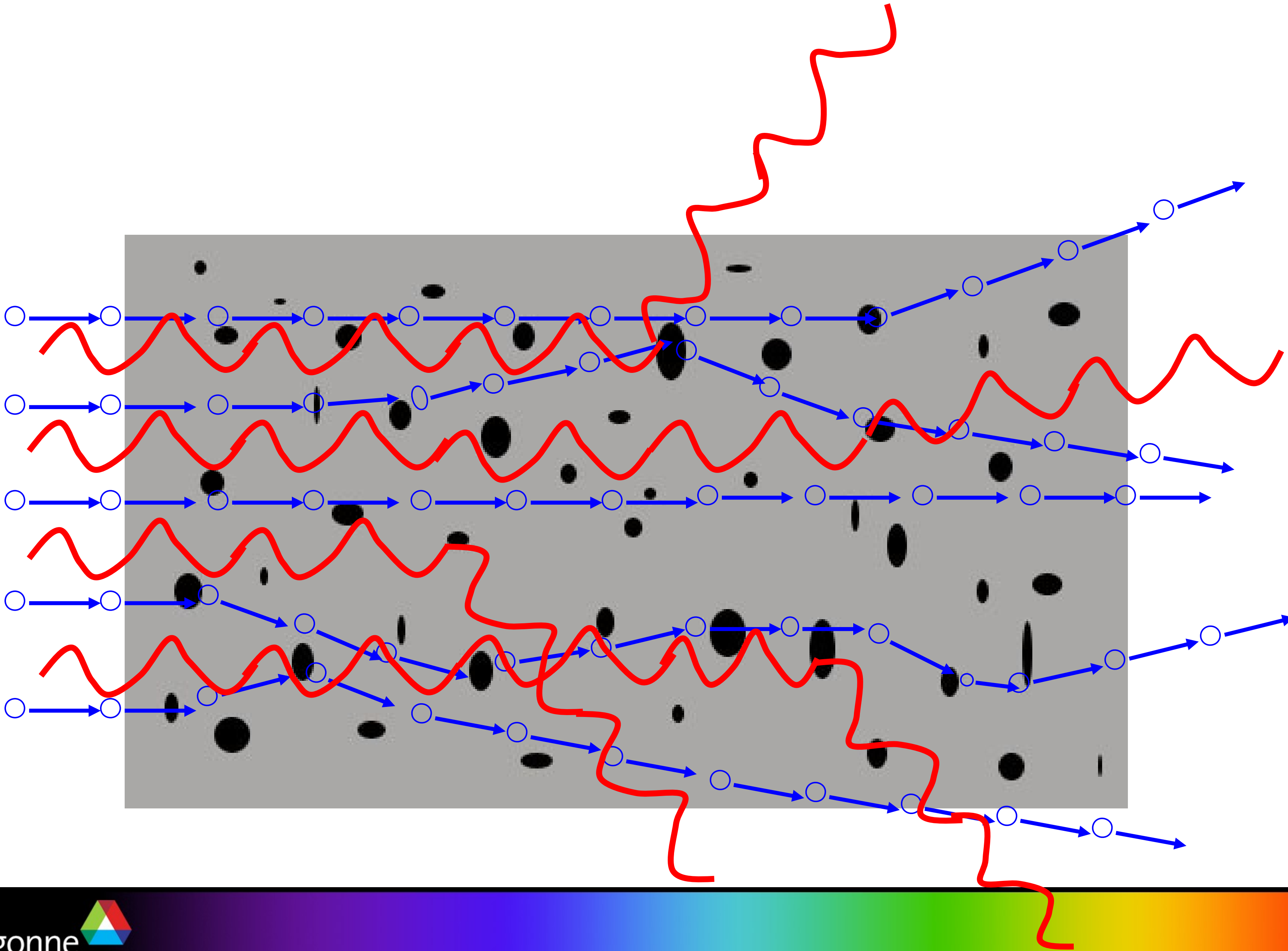
- An optimum concentration of nanoscale second phase is necessary
- Mass fluctuations play a role in thermal conductivity reduction
- Lattice thermal conductivity reduced, however ZT low due to small Seebeck

Phonons



Electrons

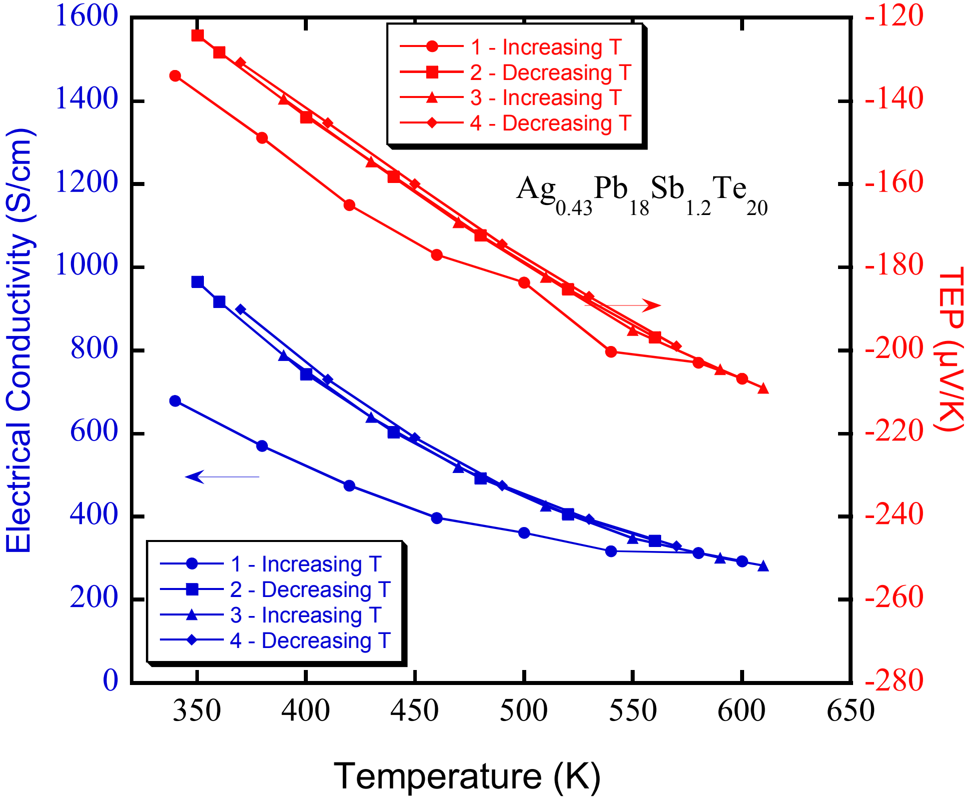


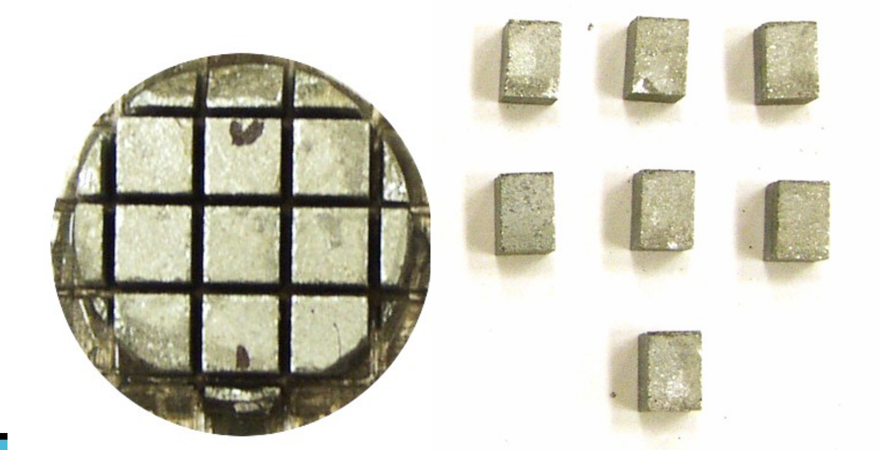


Completed and Processed Ingot

Schock

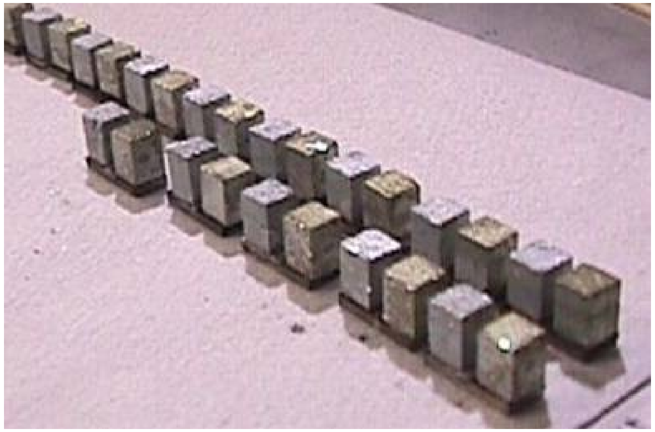
Composition: $Ag_{0.43}Pb_{18}Sb_{1.2}Te_{20}$ Weight: 200 grams

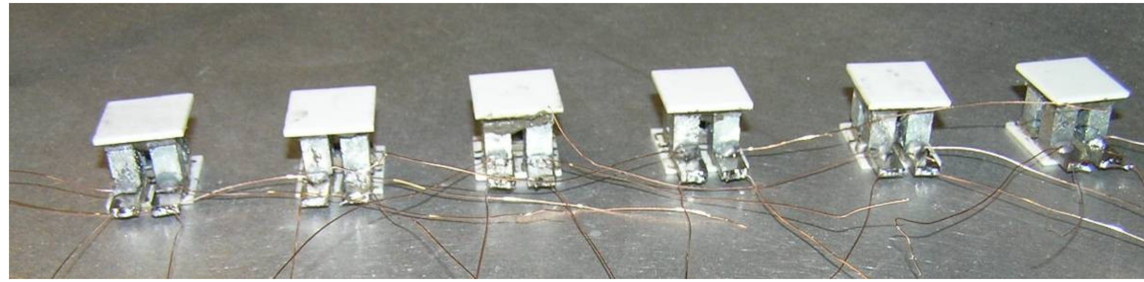




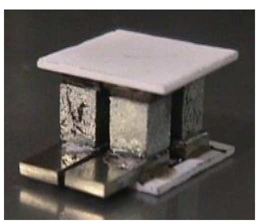
Temperature cyclability

Module Fabrication

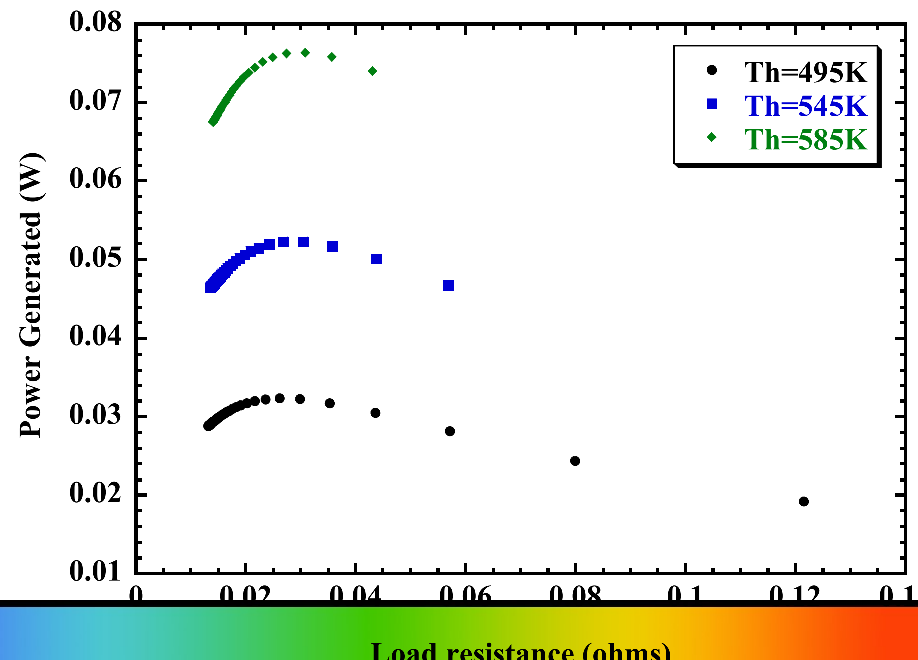




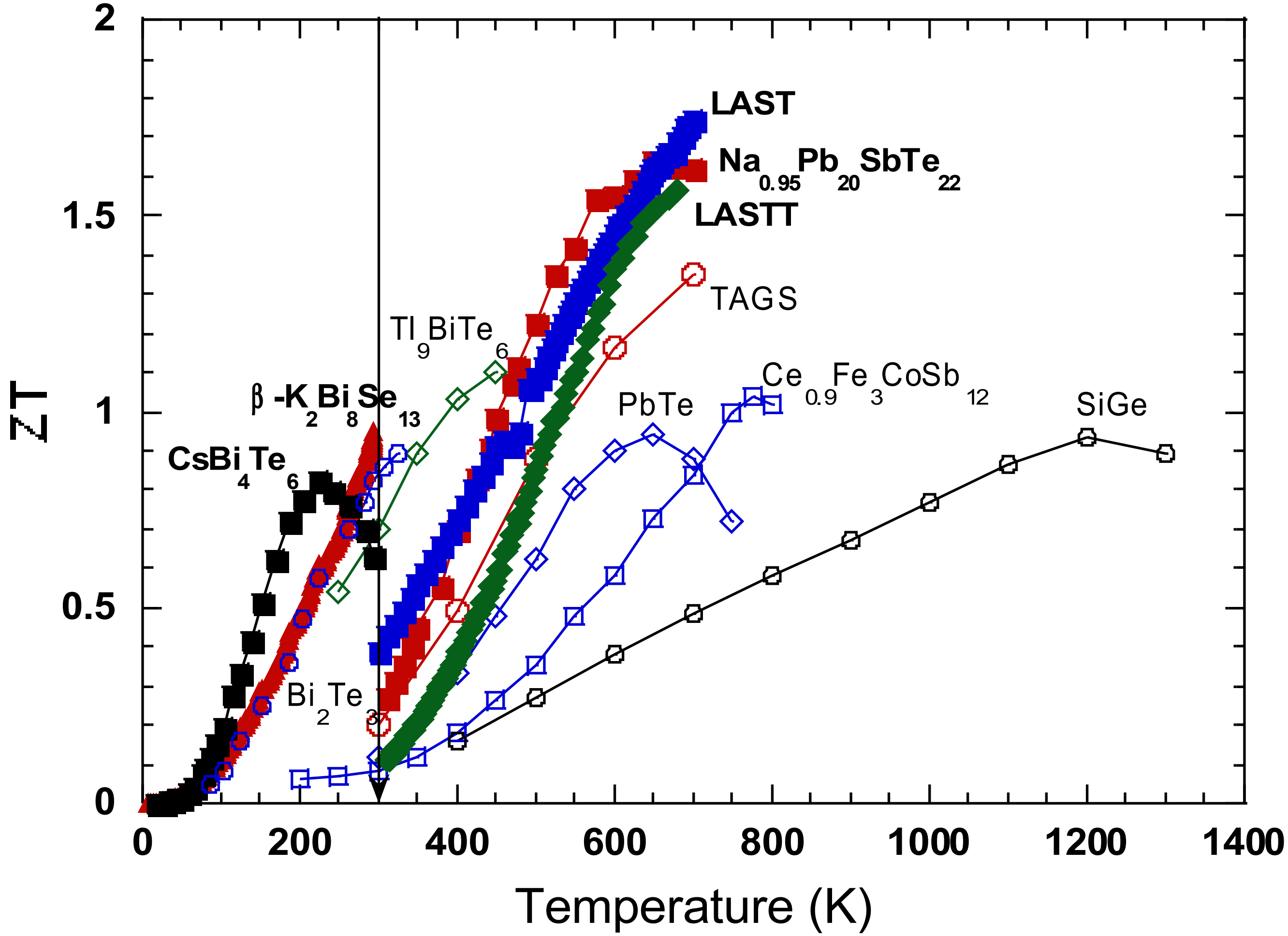
- Hot side diffusion contacts, and cold side solder contacts with <10 μW·cm2 have been achieved.



1.78mΩ total → 16.0μΩ·cm^2



Best ZT Materials



Conclusions

- LAST, LASTT and SALT: promising thermoelectric materials for next generation power generation modules. (expected device efficiency ~14%)
- Nanostructures strongly reduce thermal conductivity.
- Nanostructures are closely linked to high ZT.
- Scaleup successful in producing large quantities but material is brittle and contains microcracks.
- Hot pressing and powder processing yield 3x improvement in strength.
- Higher average ZT (>2) needed to reach 20% efficiency.