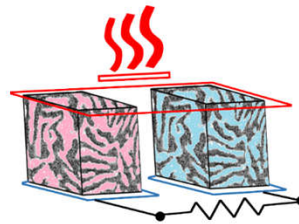
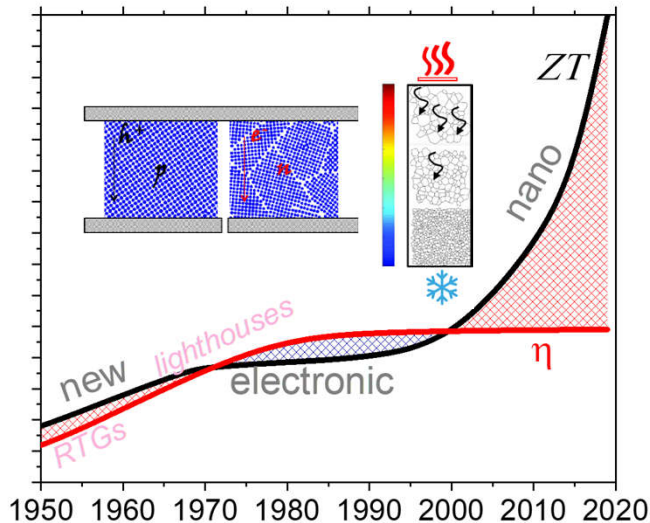




Ben-Gurion University  
of the Negev

# Thermal energy conversion and storage (thermoelectrics)



Diffusion  
Oxidation  
Coarsening  
Sublimation  
Phase transition  
CTE matching  
Mechanical properties

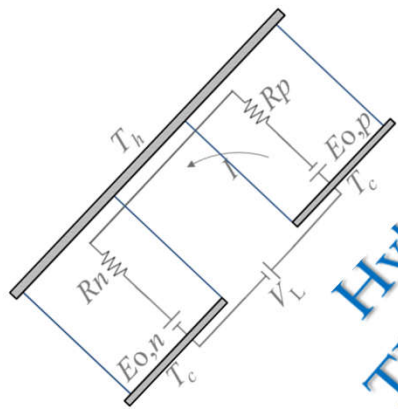
Presented by:

**Prof. Yaniv Gelbstein**

TRL	9	Commercialized
	8	Pre-production
	7	Field Test
	6	Prototype
	5	Bench / Lab Testing
	4	Detailed Design
	3	Preliminary Design
	2	Conceptual Design
	1	Basic Concept

The Samuel Ayrton Chair in Metallurgy, Head of the Department of Materials Engineering

Dutch Israeli renewable energy conversion mini symposium, ZOOM, Jan. 13 (2021)



# Thermoelectrics

Hybrid  
TE-SOFC

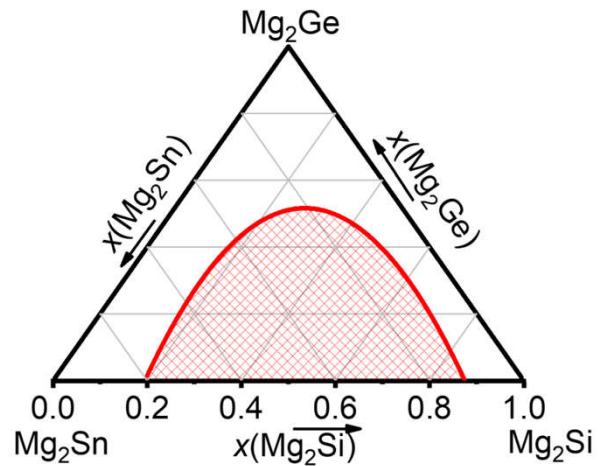
TE-H<sub>2</sub> (TEP)

*Materials  
for Energy*

SOFC

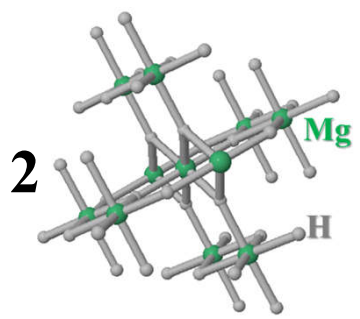
Hydrides  
(MgH<sub>2</sub>)

F.C. fuels

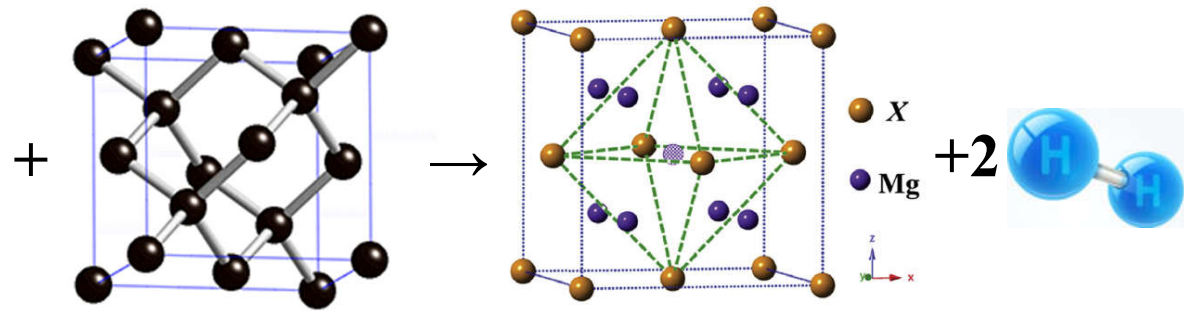


Juri Grin – U.S. Patent PCT/EP02/03953 (2002)

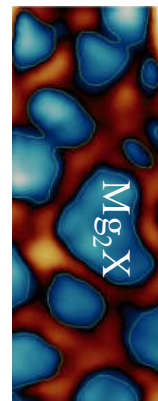
Diamond (Si/Ge) Franck Gascoin - Powder Technology 228 295-300 (2012)



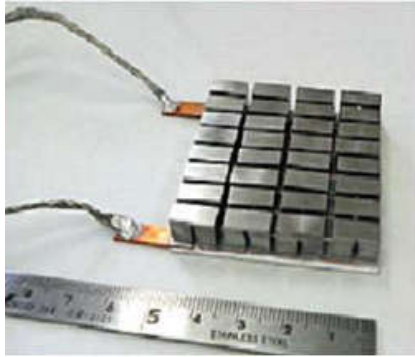
MgH<sub>2</sub> (rutile)



Mg<sub>2</sub>X (X=Si,Ge,Sn) (anti-fluorite, Fm $\bar{3}$ m)  
X. Liu et al. *Adv. Electr. Mater.* 2 1500284 (2016)



*p*-GeTe or *n*-PbTe matrix



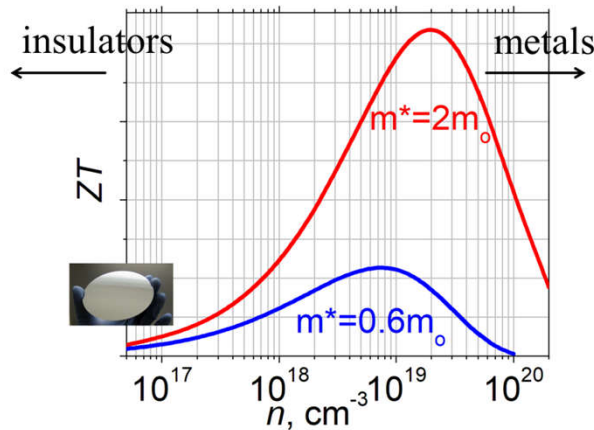
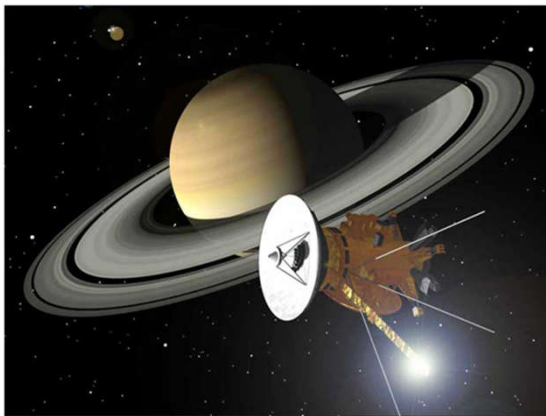
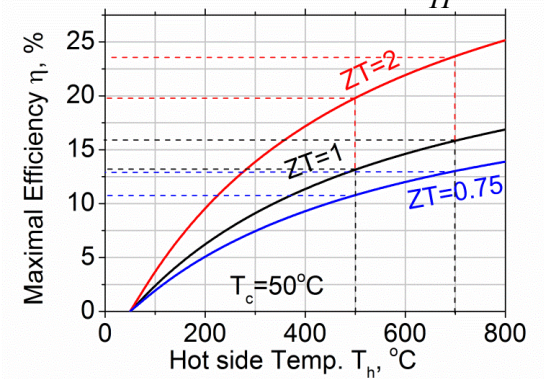
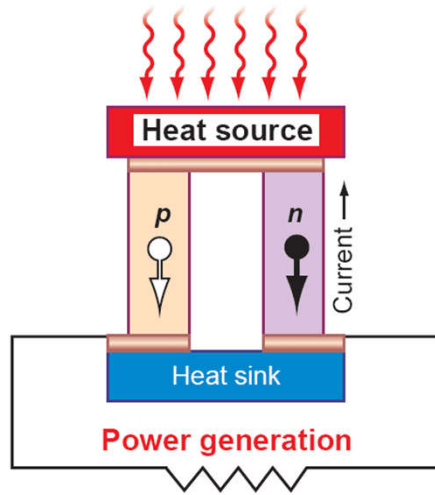
# Power Generation

$$Z = \alpha^2 / \kappa \rho$$

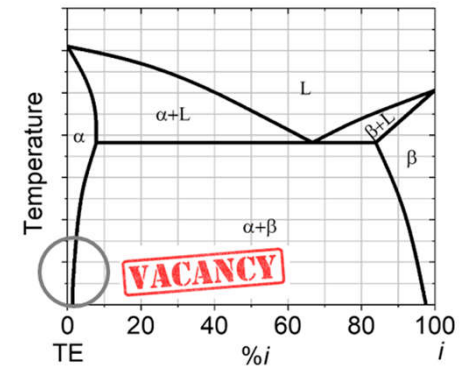
$$\eta_{opt} = \frac{\Delta T}{T_H} \frac{(\sqrt{1 + Z\bar{T}} - 1)}{\sqrt{1 + Z\bar{T}} + \frac{T_C}{T_H}}$$

$$V = \alpha \cdot (T_h - T_c)$$

$$K = K_L + K_e$$



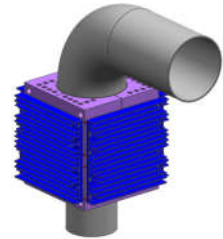
NASA deep space – Cassini ([www.nasa.gov](http://www.nasa.gov))



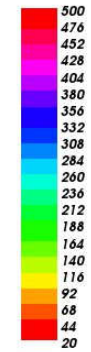
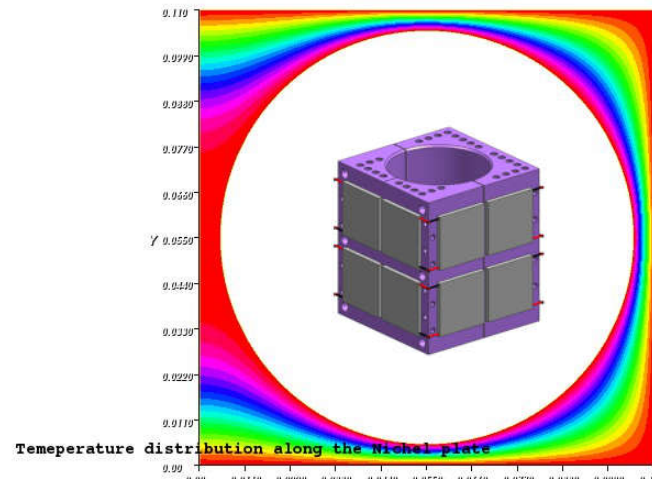
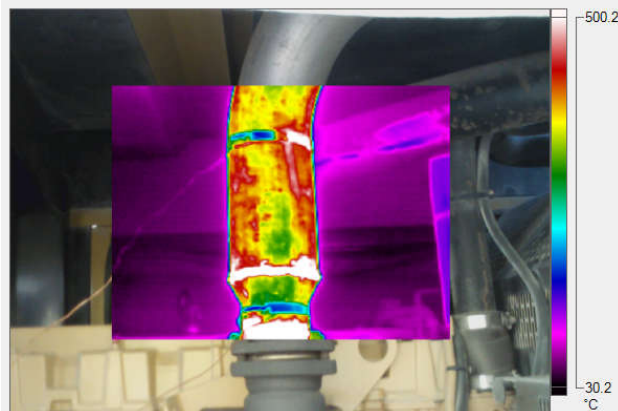


**CATERPILLAR®**

**ZOKO**  
0 217 1 111

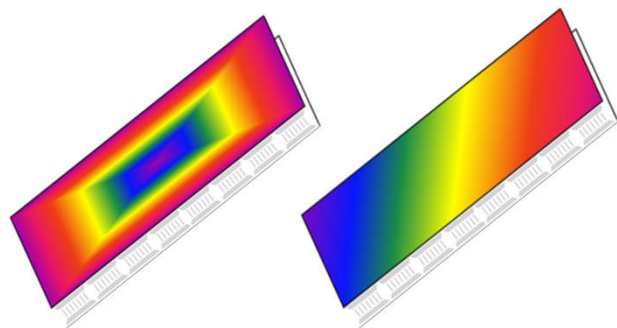
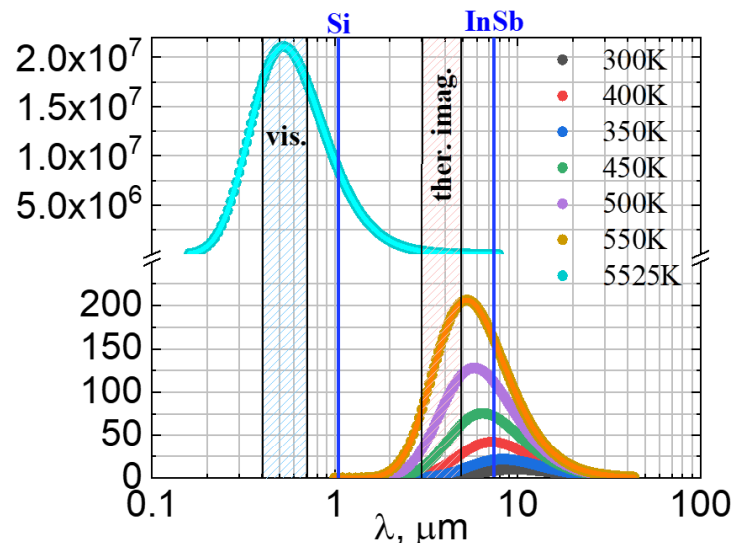
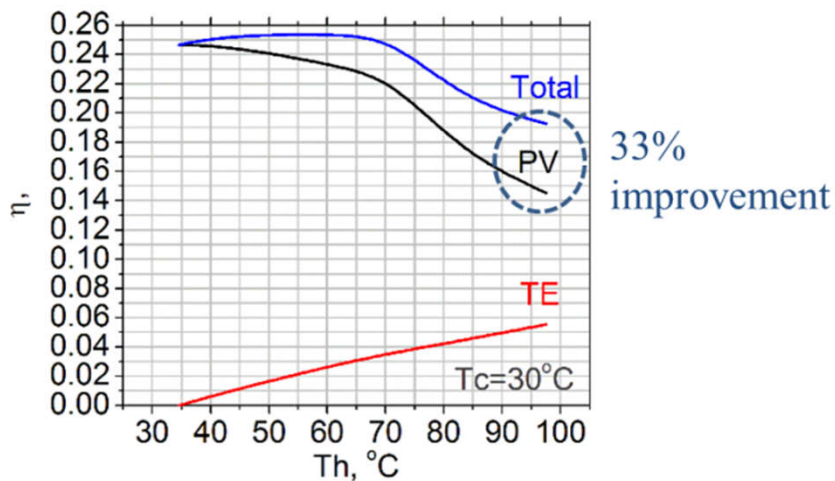


400°C @ 250kW load

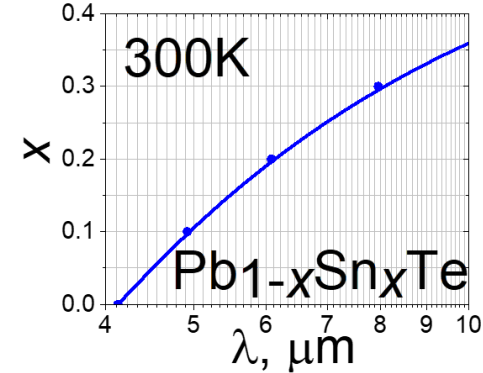
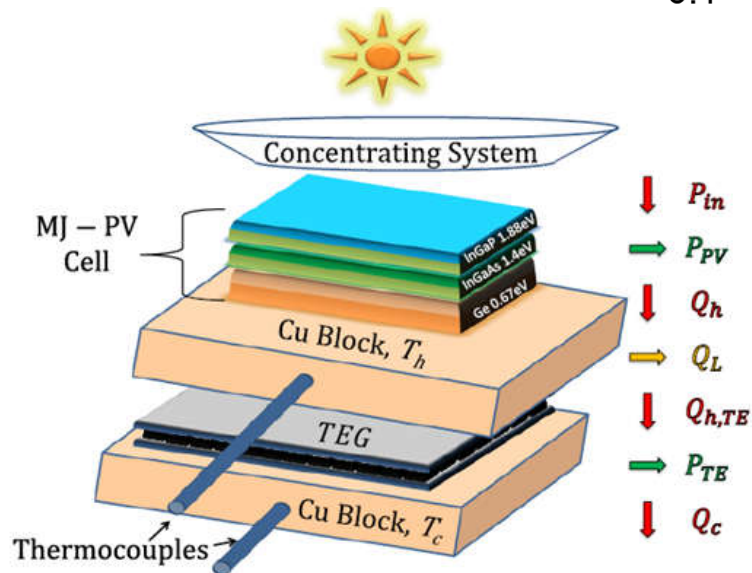


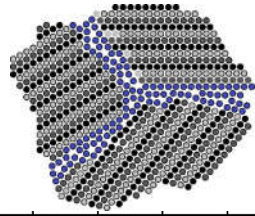
FEM

# PV-TE applications

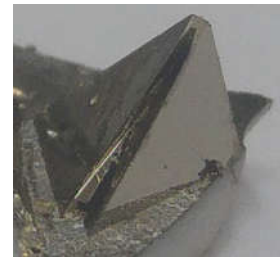
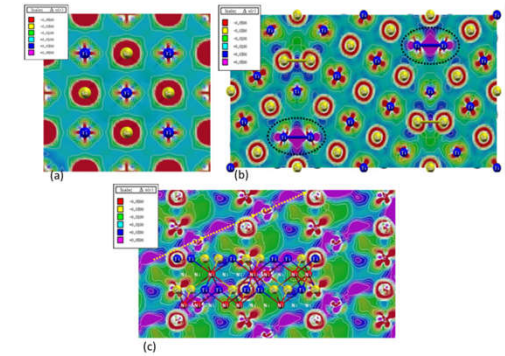
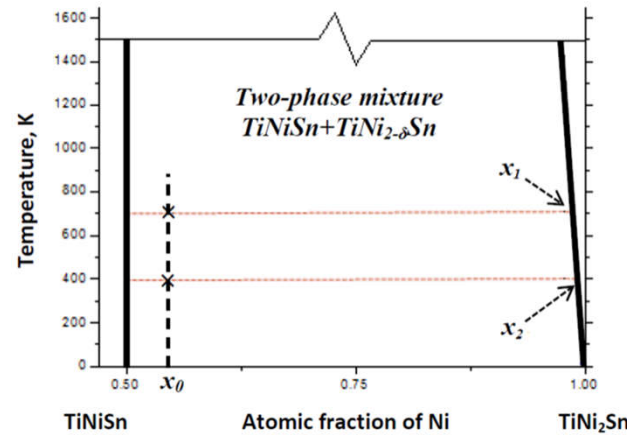
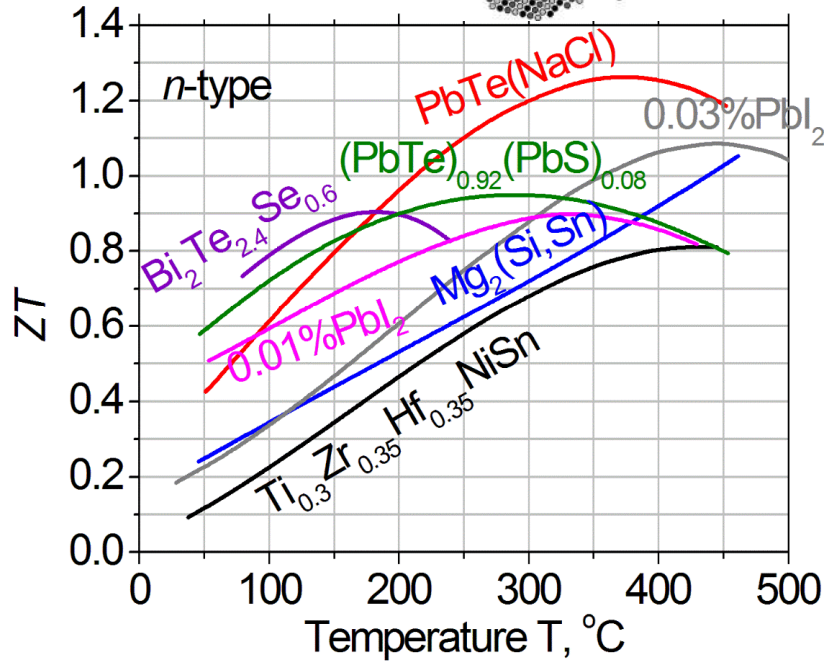
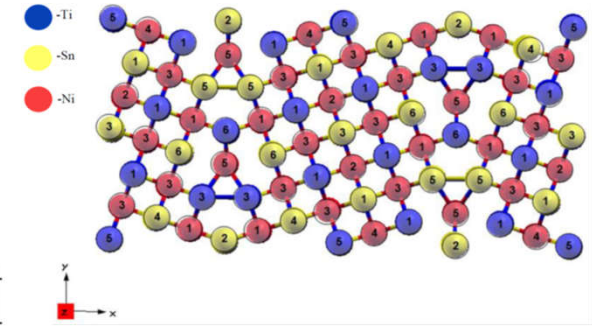


*J. Appl. Phys.* **118** 115104 (2015)





G.B.  
+  
Sn segregation



HH-

*Journal of Materials Research* **26**(15) 1919-1924 (2011)  
*Journal of Electronic Materials* **42**(7) 1340-1345 (2013)  
*Journal of Solid State Chemistry* **203** 247-254 (2013)  
*Journal of Electronic Materials* **43**(6) 1976-1982 (2014)  
*Physical Chemistry and Chemical Physics* **16** 20023 (2014)

PbTe-PbS-

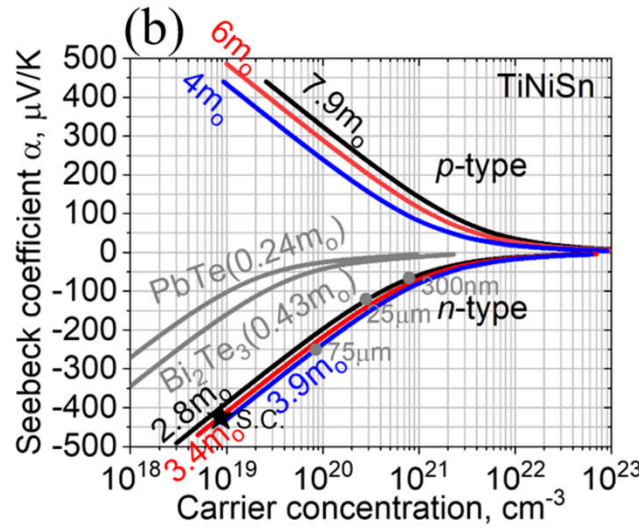
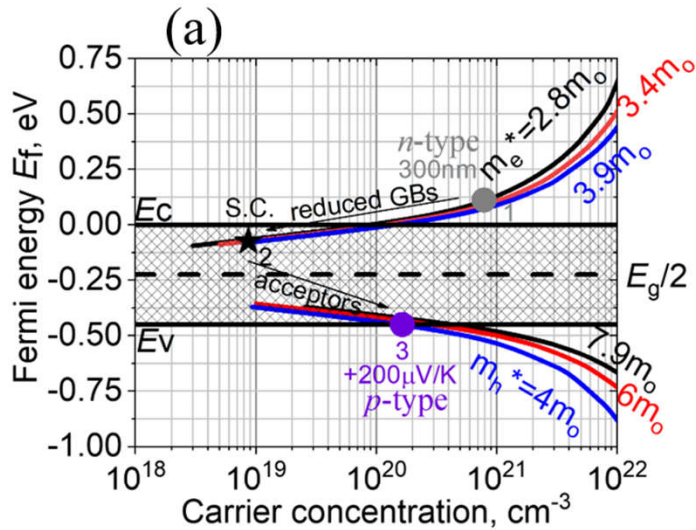
*Adv. Energy Mater.* **5**(11) 1500272 (2015)

Silicides-

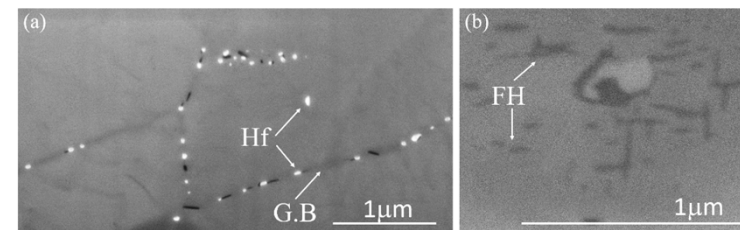
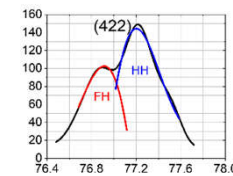
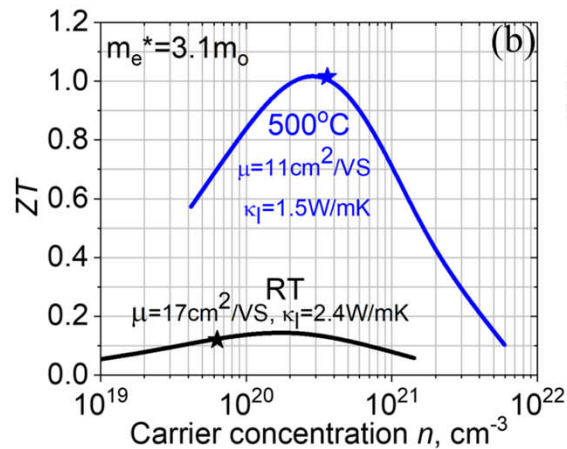
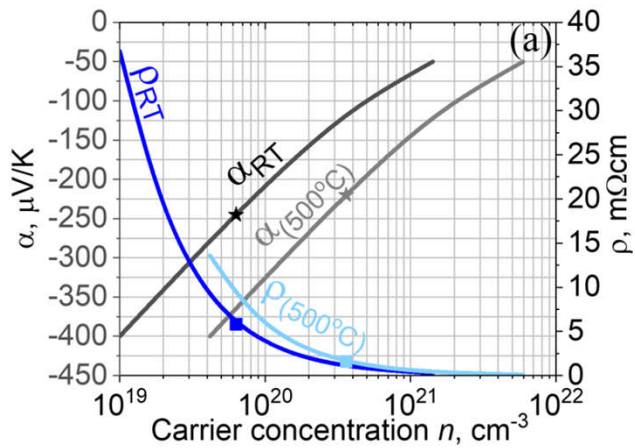
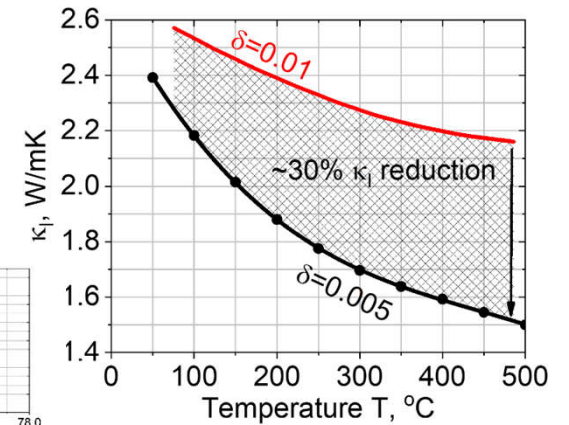
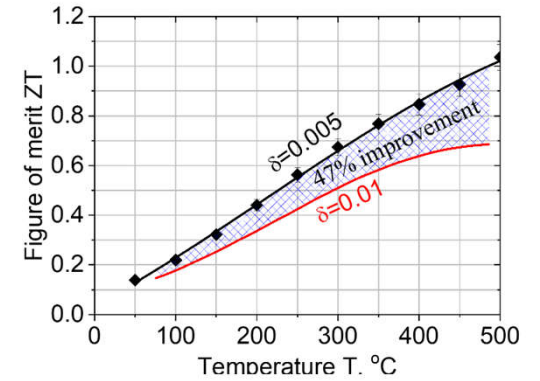
*Journal of Electronic Materials* **41**(6) 1504-1508 (2012)  
*Journal of Electronic Materials* **42**(7) 1926-1931 (2013)  
*Journal of Nanomaterials* **701268** (2013)  
*Journal of Electronic Materials* **43**(6) 1703-1711 (2014)



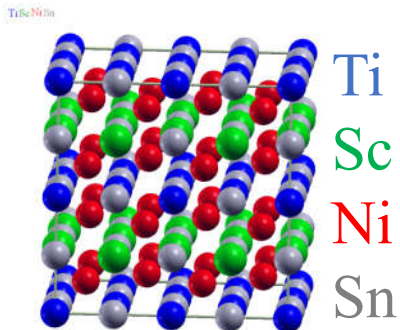
# Half-Heusler – TiNiSn & $\text{Ti}_{0.3}\text{Zr}_{0.35}\text{Hf}_{0.35}\text{Ni}_{1+\delta}\text{Sn}$



JAP 126 085110 (2019)



Journal of Alloys and Compounds 781 1132-1138 (2019)

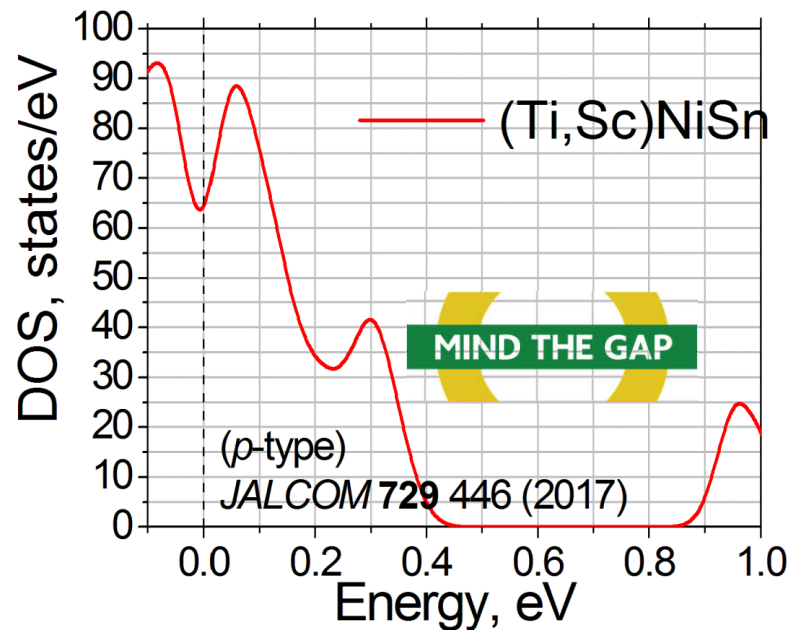
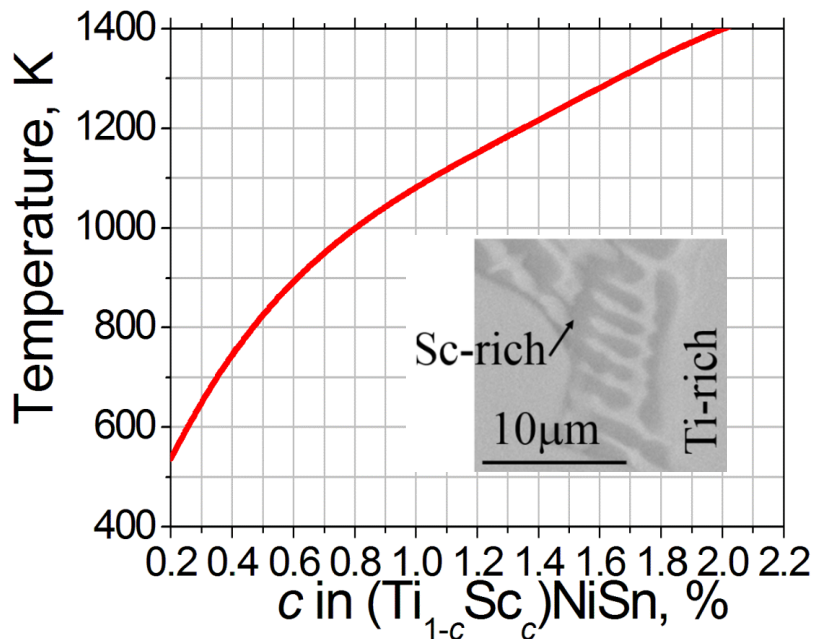
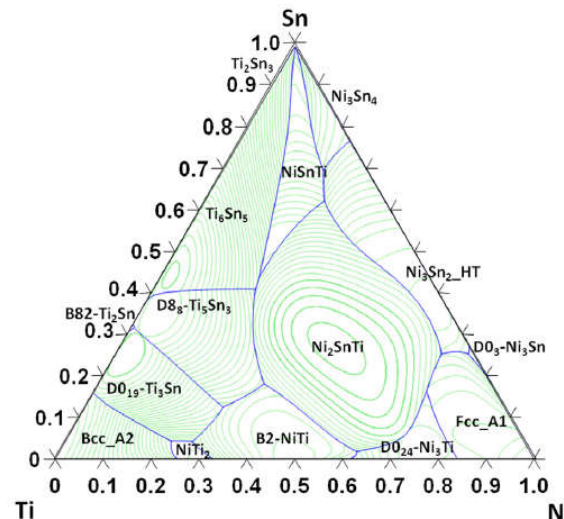


# $p$ -type HH $(\text{Ti}_{1-c}\text{Sc}_c)\text{NiSn}$

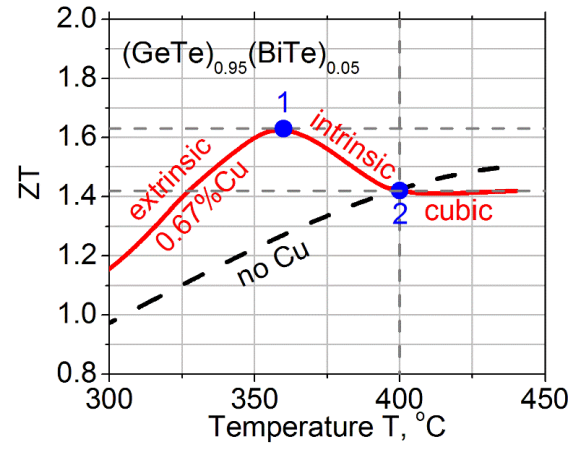
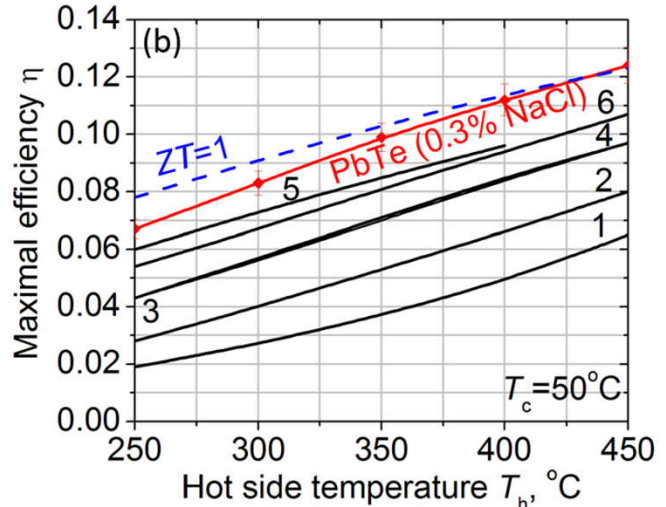
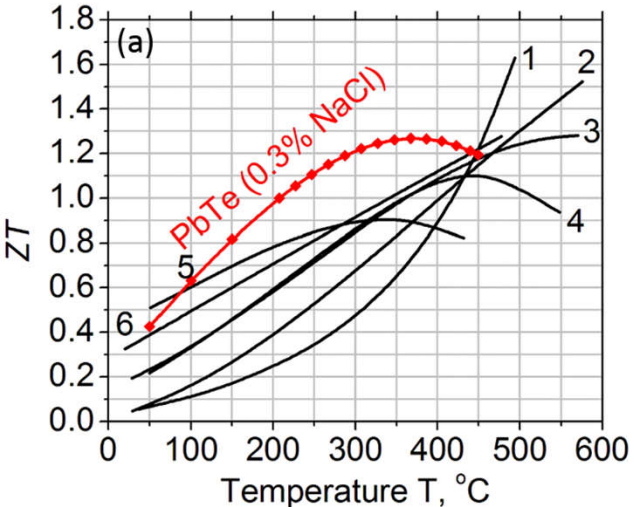
Solidification sequence:  
 FH  $\rightarrow$  HH,  $\text{Sn}_5\text{Ti}_6$ , minority phases  $\rightarrow$  HH

*Effects of Fe (acceptor) & Cu (donor) in TiNiSn - Intermetallics 98 154-160 (2018)*

$p$ -type  $(\text{Ti}_{1-c}\text{Al}_c)\text{NiSn}$  - *PCCP 21 7524 (2019) & PCCP 22(3) 1566 (2020)*

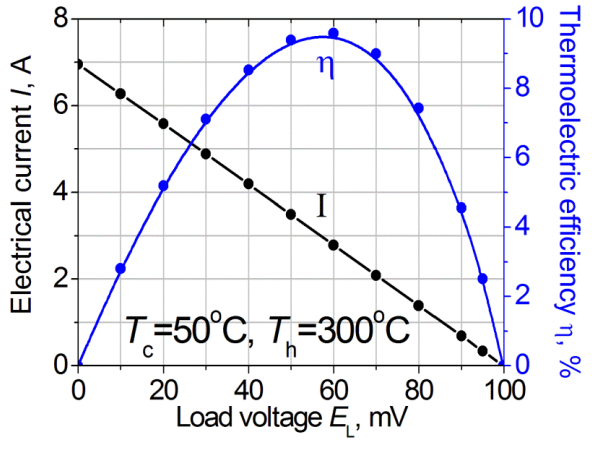
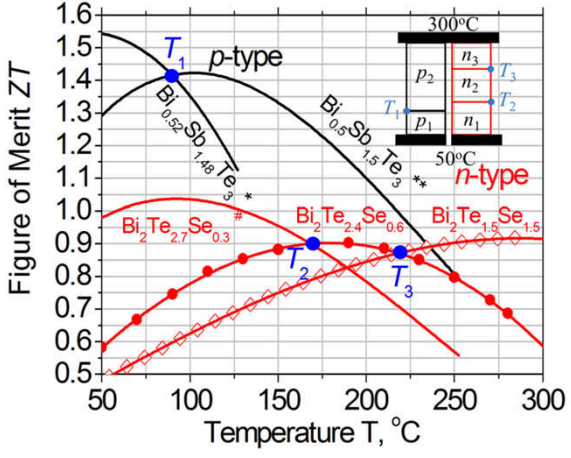




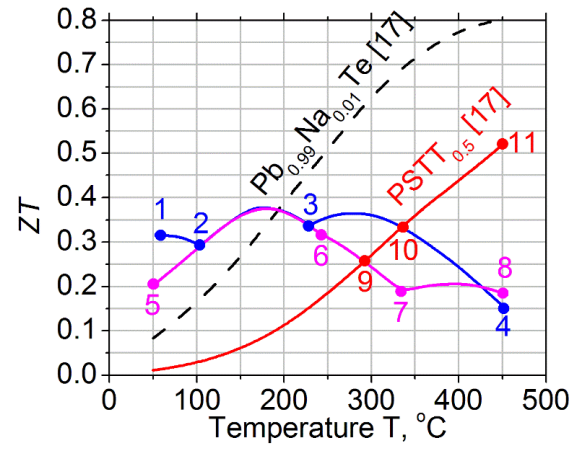


*J. Mater. Chem. C* **3** 9559-9564 (2015), *J. Sol. Stat. Chem.* **240** 91 (2016)

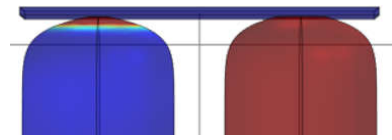
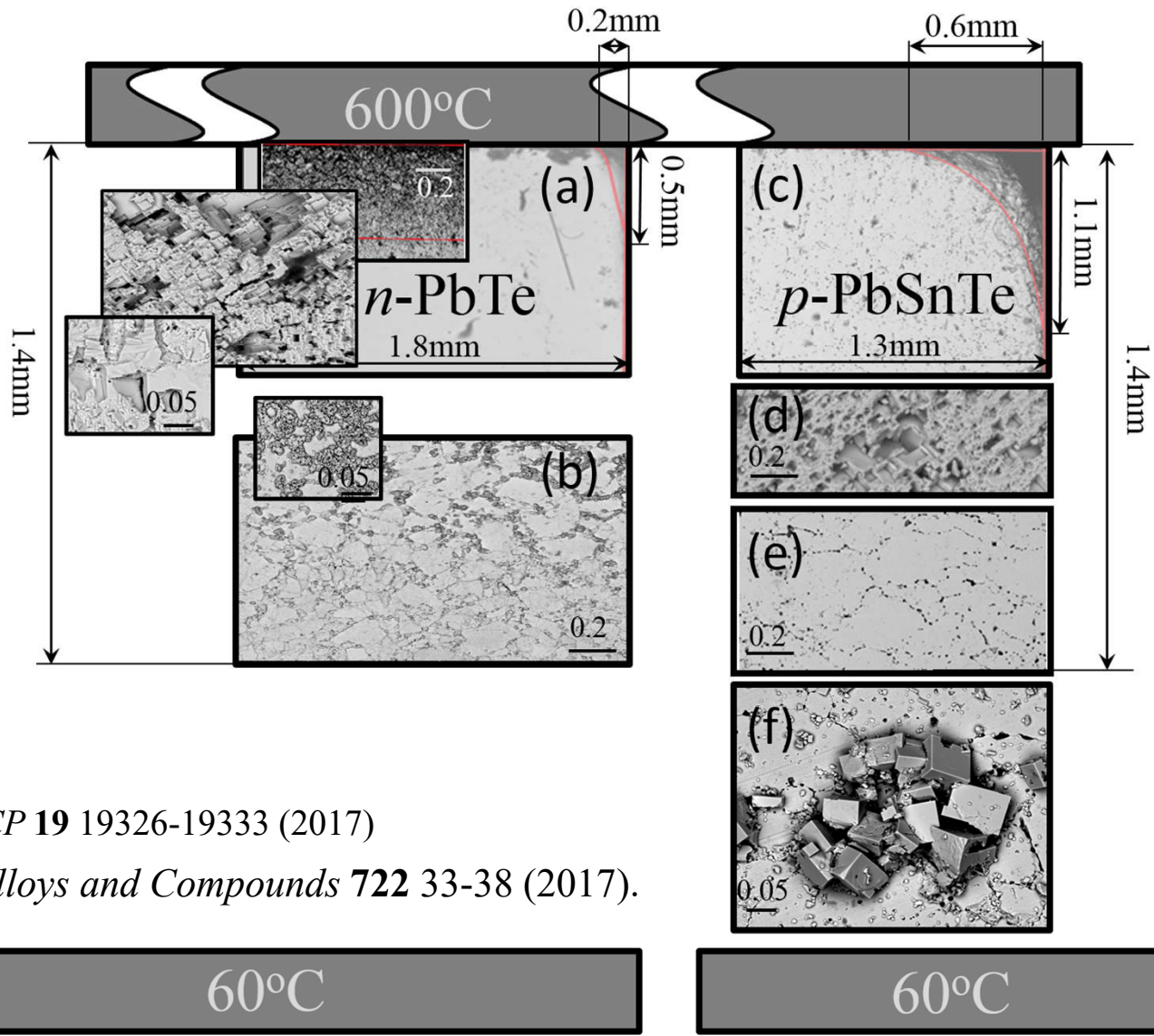
*Adv. Electron. Mater.* **1** 1500228 (2015)  
*J. Appl. Phys.* **120** (3) 035102 (2016)



*J. Alloys and Compounds* **679** 196-201 (2016), *PCCP* **20**(6) 4092 (2018)



*J. Appl. Phys.* **118** 065102 (2015)  
*J. Appl. Phys.* **120** (5) 055104 (2016)

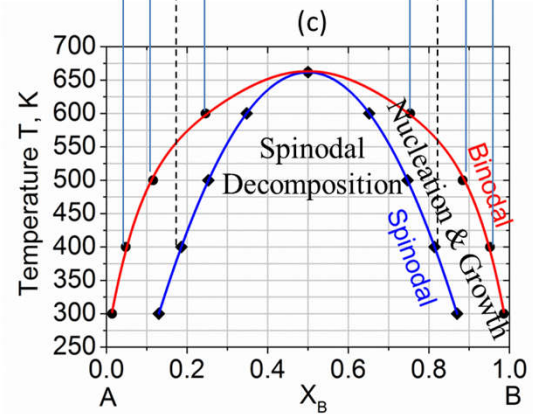
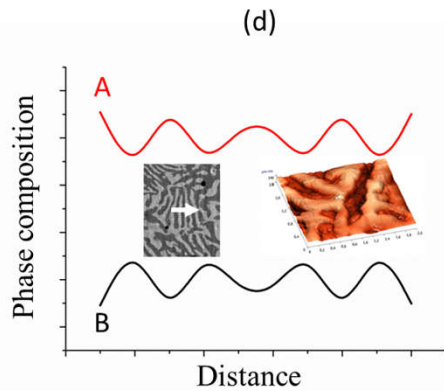
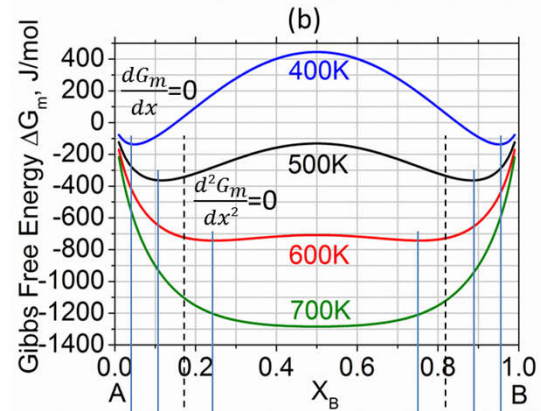
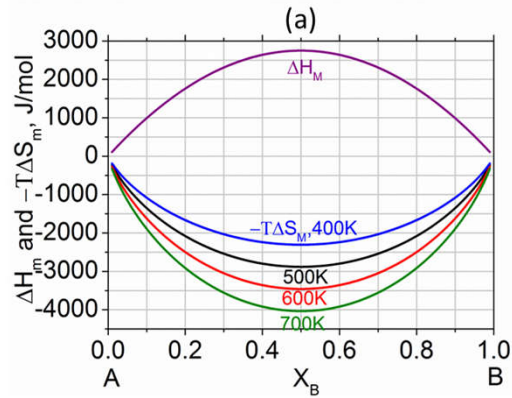


*PCCP* **19** 19326-19333 (2017)  
*J. Alloys and Compounds* **722** 33-38 (2017).

$(\text{SiO}_2)_{0.68}(\text{PbO})_{0.3}(\text{Na}_2\text{O})_{0.01}(\text{B}_2\text{O}_3)_{0.01}$   
**Sublimation coating-**  
*JMR* **34**(20) 3563-3572 (2019)  
**On PbTe-**  
*Metals* **10** 284 (2020)

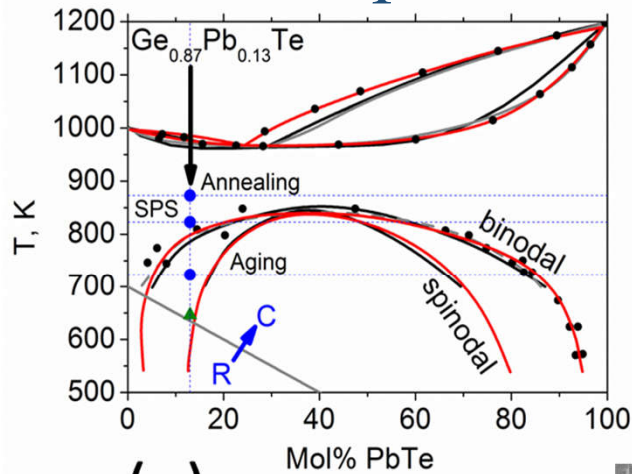
# Phase Separation - I

$$\Delta G_m = \Delta H_m - T\Delta S_m = \omega \cdot x \cdot (1 - x) + T \cdot R \cdot [(1 - x) \cdot \ln(1 - x) + x \cdot \ln(x)]$$

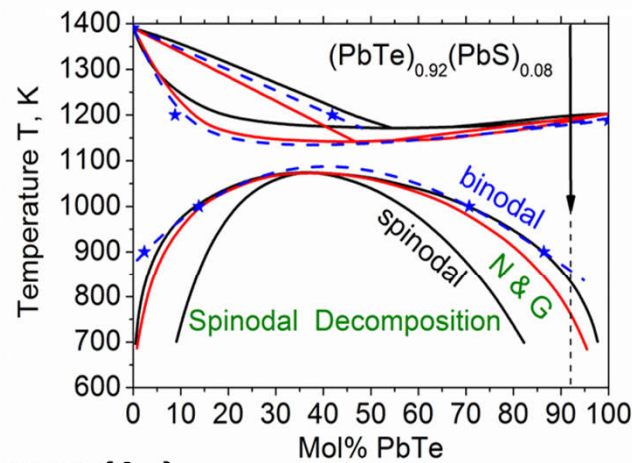




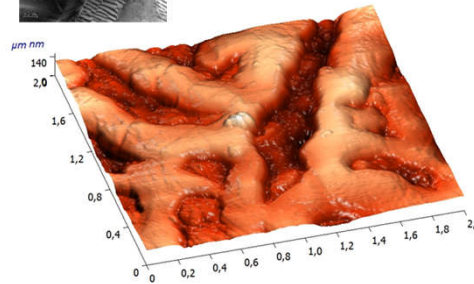
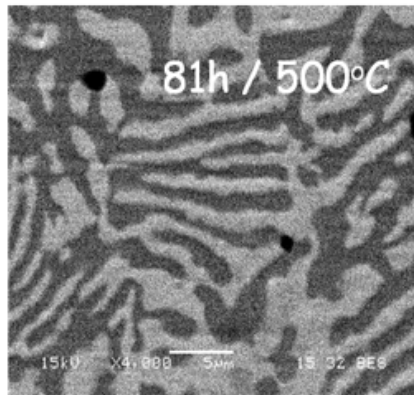
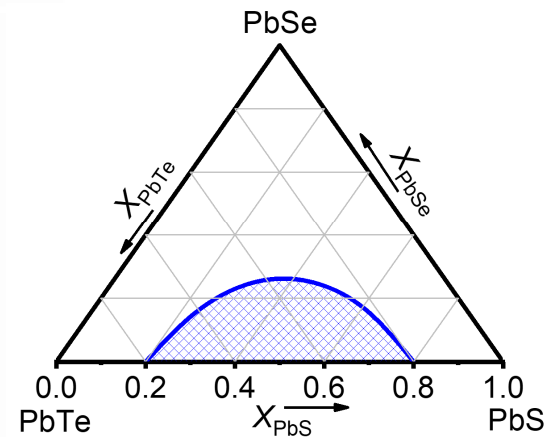
# Phase Separation - II



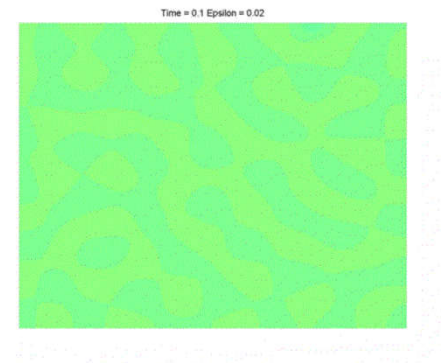
(a)



(b)



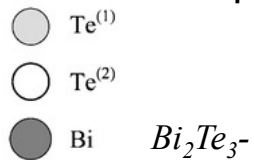
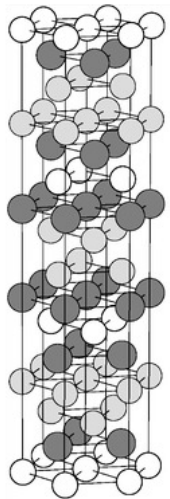
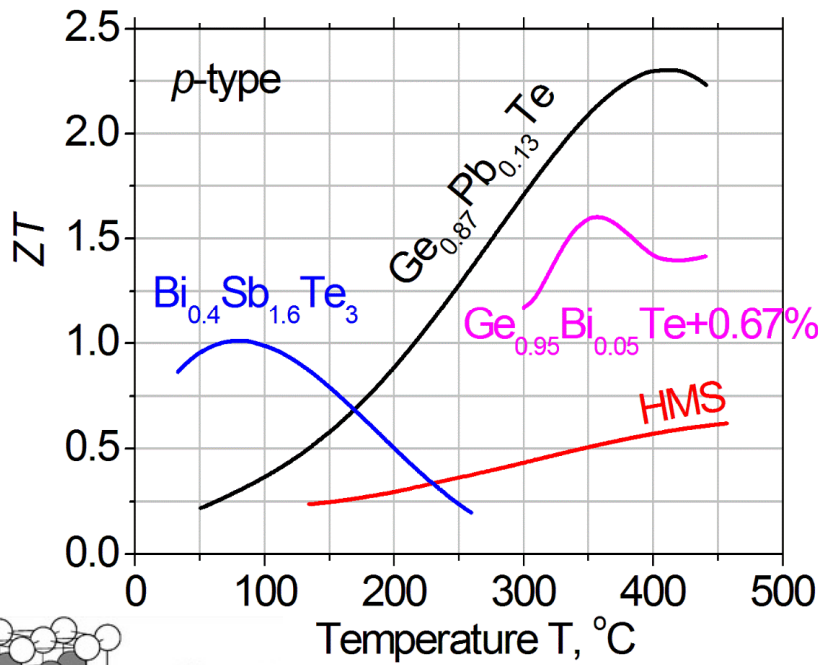
Cahn-Hilliard equation →



Evelyn Sander and Thomas Wanner, Monte-Carlo simulation

(a) Yaniv Gelbstein, Mercuri Kanatzidis et al., *Adv. Energy Mater.* **3** 815-820 (2013)

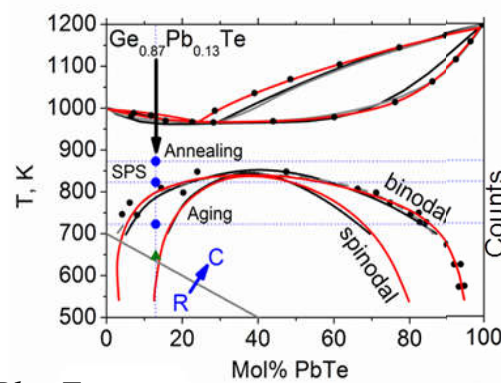
(b) John Androulakis et al., *J. Am. Chem. Soc.* **129** 9780-9788 (2007)



*Journal of Applied Physics* **101**, 113707 (2007)  
*Journal of Electronic Materials* **41**(6), 1546-1553 (2012)

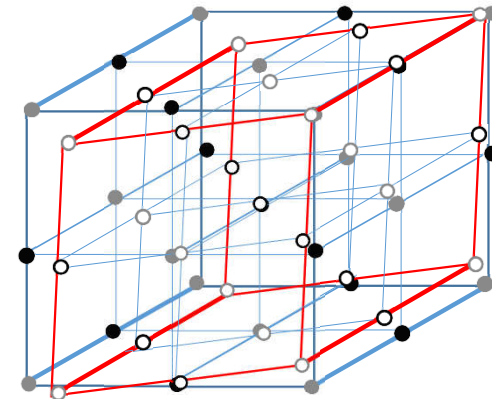
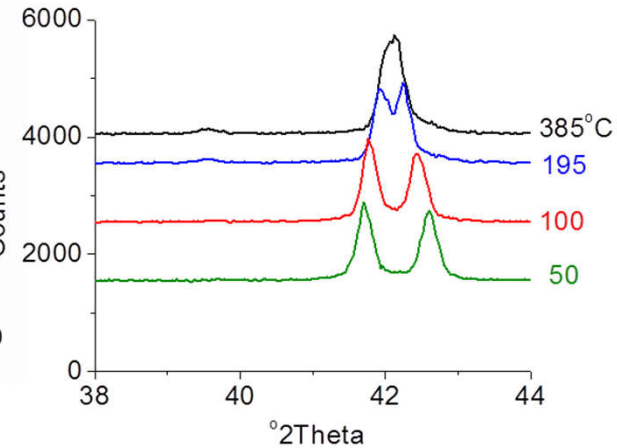
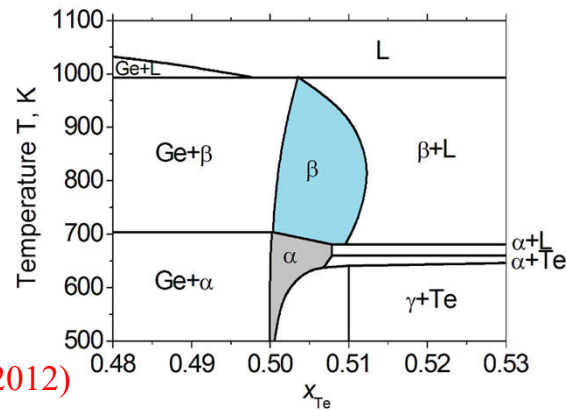
GeTe-

*Phys.Stat.Sol. (RRL)* **1**(6) 232-234(2007), *Powder Diffraction* **23**(2) 137(2008), *JEMS* **38**(7) 1478(2009), *Journal of Crystal Growth* **311** 4289(2009), *Chemistry of Materials* **22**(3) 1054 (2010), *JEMS* **39**(9) 2049,2165(2010), *Scripta Materialia* **62**(2) 89 (2009), *J. Phys. Chem. C* **114** 13126(2010), *J. Alloys and Compounds* **526** 31(2012), *JEMS* **42**(7) 1542(2013).

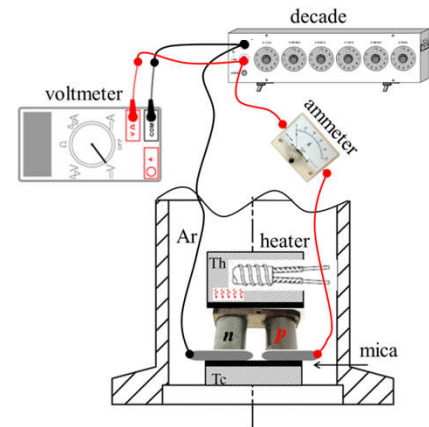
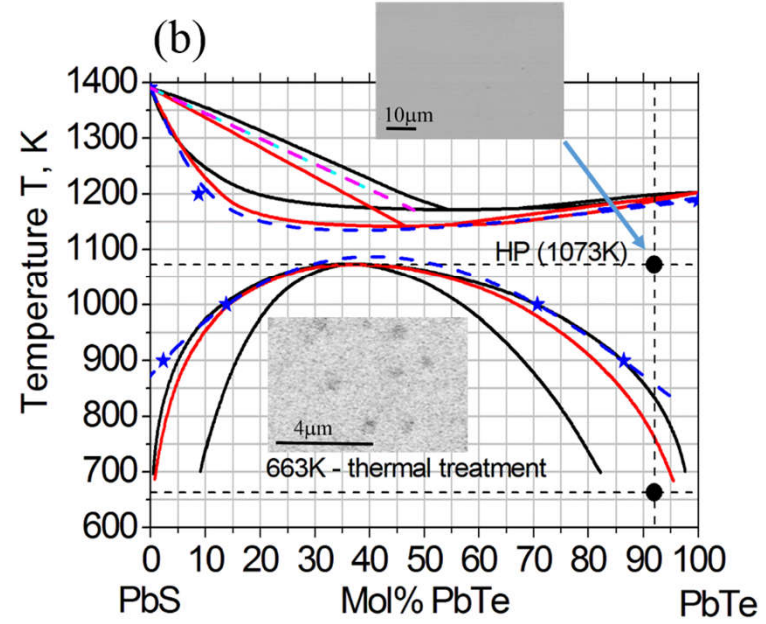
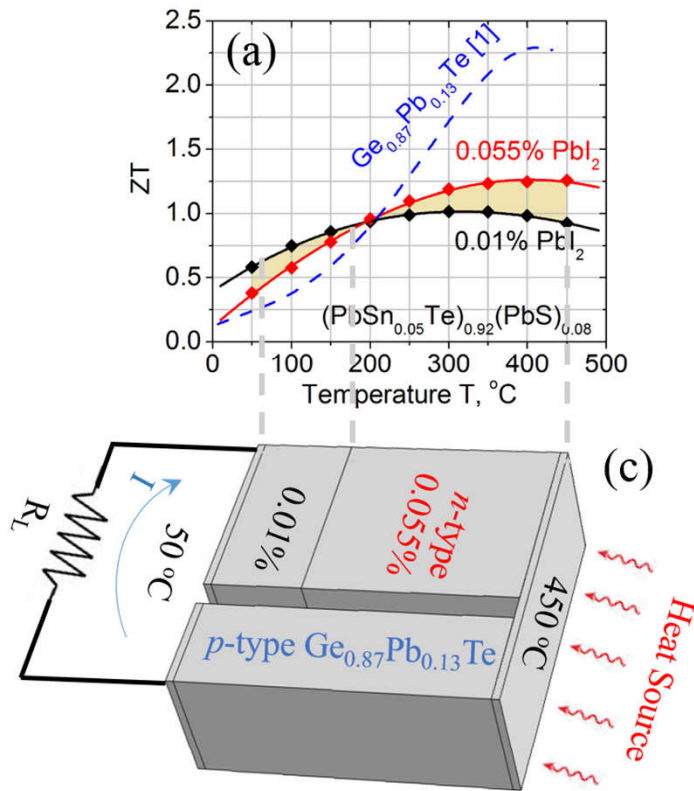


Ge<sub>x</sub>Pb<sub>1-x</sub>Te-

*Adv. Energy Mater.* **3** 815–820 (2013)  
*J. Am. Chem. Soc* **136** 11412-11419 (2014)

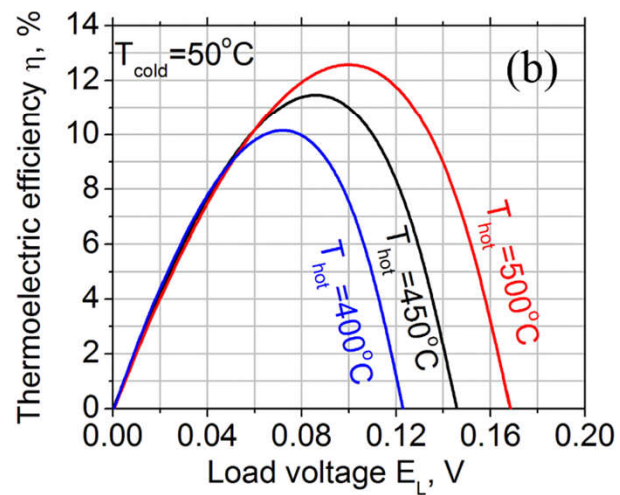
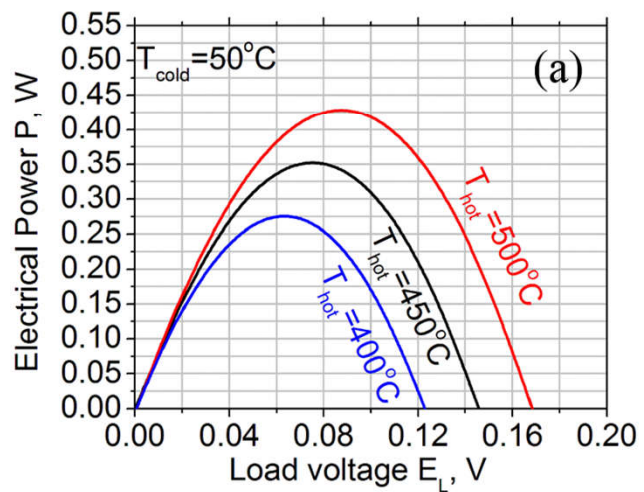
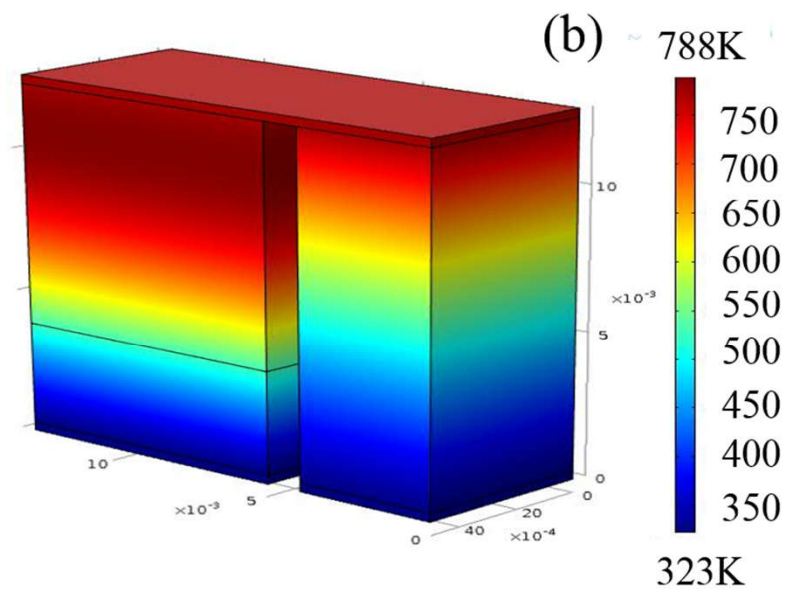
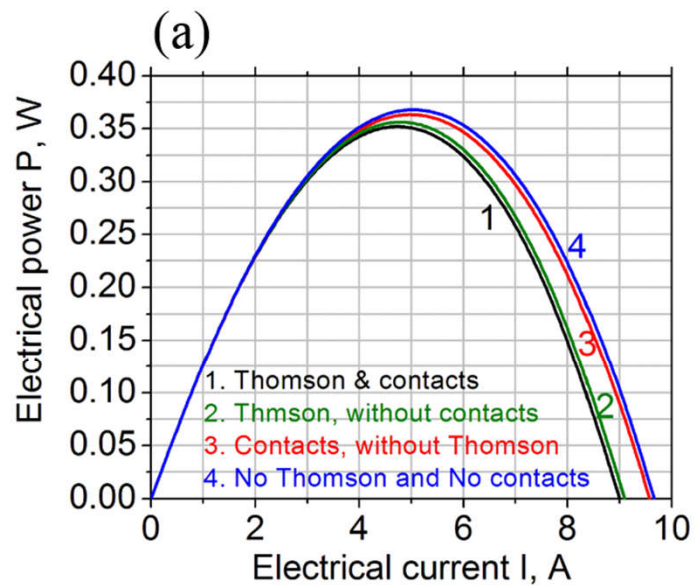


# GePbTe-PbTe/PbS



*Adv. Energy Mater.* **1500272** (2015)  
*Journal of Solid State Chemistry* **241** 79-85 (2016)





# Conclusions-

Practical TE design considerations should include:

- GB effects on **electronic** and phonon characteristics.
- Nano stabilization at the operating temperatures.
- Electronic optimization beyond the solubility limit.
- Mechanical properties (including CTE and  $H_V$ ) and their variation with the composition and temperature.
  - Correlation between mechanical and transport properties (incl. the piezoresistive effect\*).
- Minimization of degradation mechanisms.

$$\pi(\text{piezoresistive coeff.}) = (\Delta\rho/\rho) \cdot \sigma(\text{applied stress})$$

\* *Piezoresistive effect* – the change in the electrical resistivity when mechanical strain is applied

