High performance Zintl phase TE materials with embedded nanoparticles

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In collaboration with

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Lon Bell; BSST, Amerigon

Acknowledgement:

NSF-DOE,

ONR, DARPA DSO

DOE Thermoelectric Applications Workshop, San Diego; 4 January 2011

Thermoelectric figure of merit, ZT

Power factor

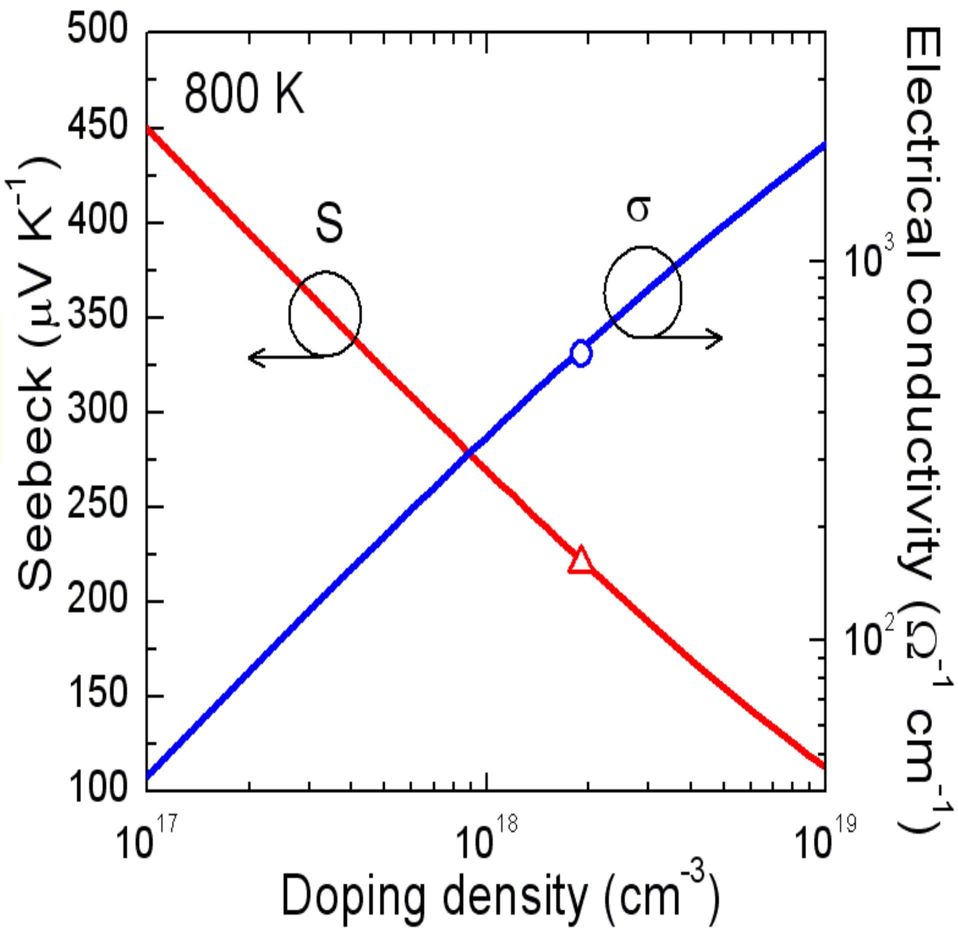
$$ZT = \frac{\boxed{S^2\sigma}}{\kappa} T$$

S: Seebeck coefficient

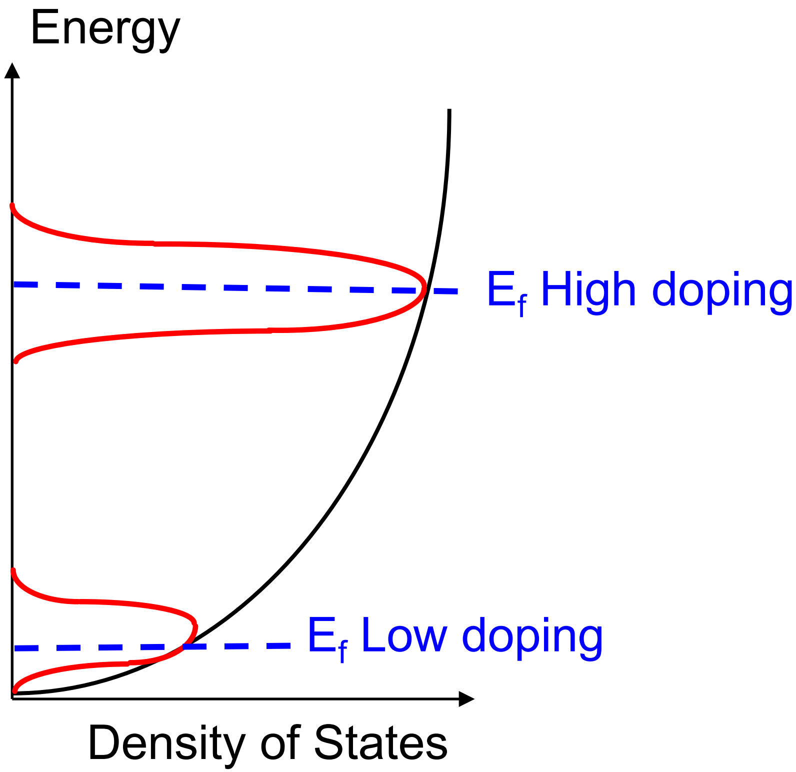
σ: Electrical conductivity

κ: Thermal conductivity (e + phonon)

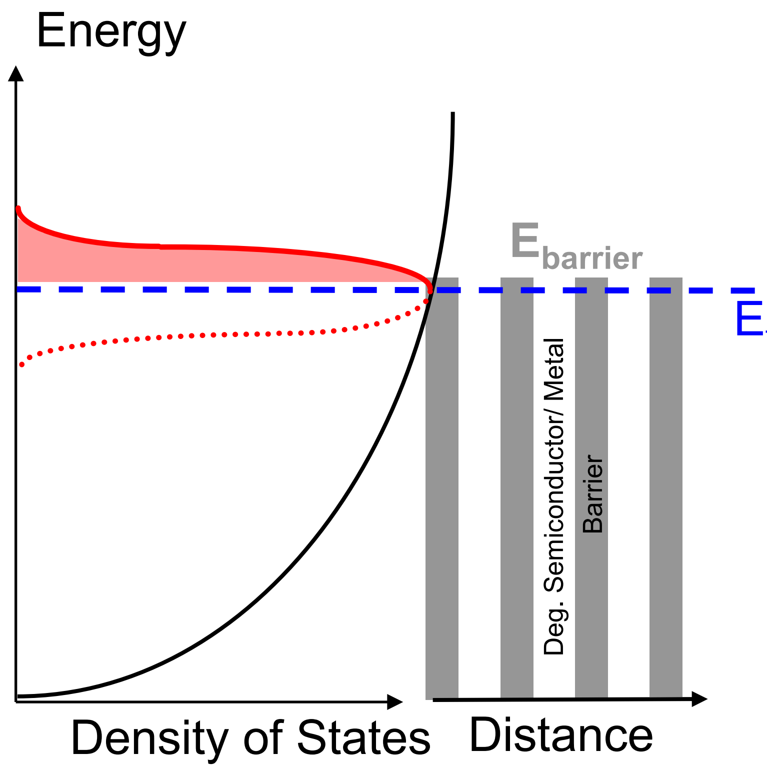
Example: Si-doped $(InGaAs)_{0.8}(InAlAs)_{0.2}$



Seebeck-conductivity trade-off



Doped Bulk Semiconductor



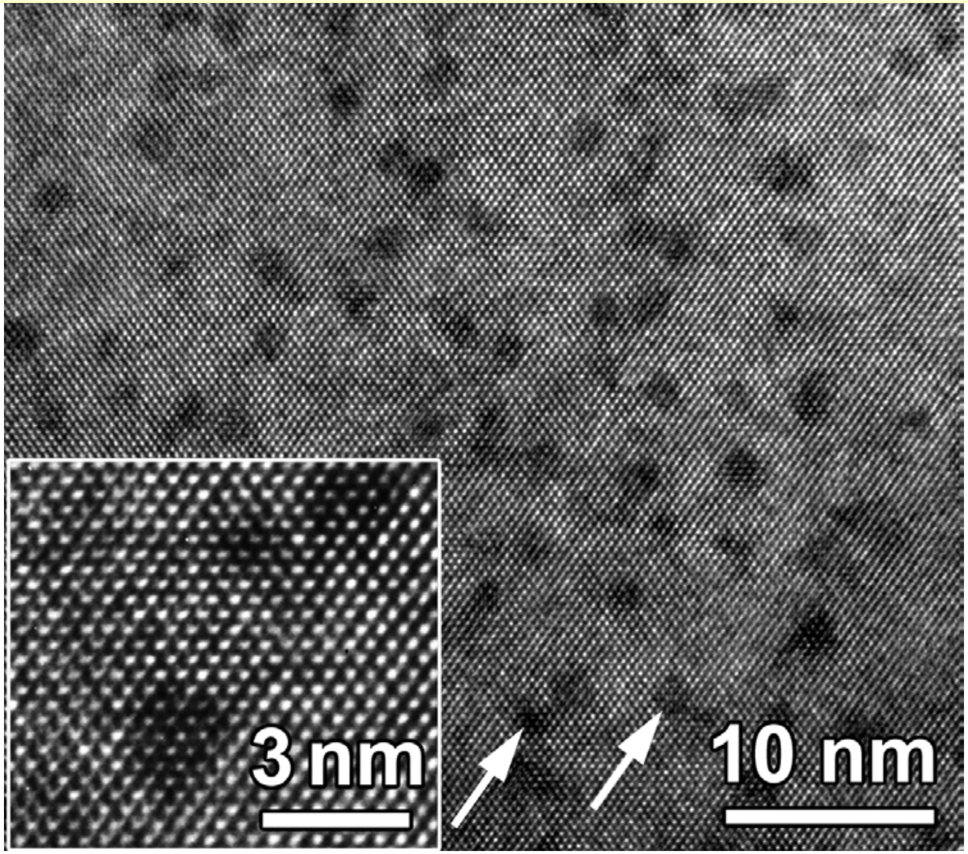
Deg. Semiconductor/Metal + Energy Filter (Thermionic emission)

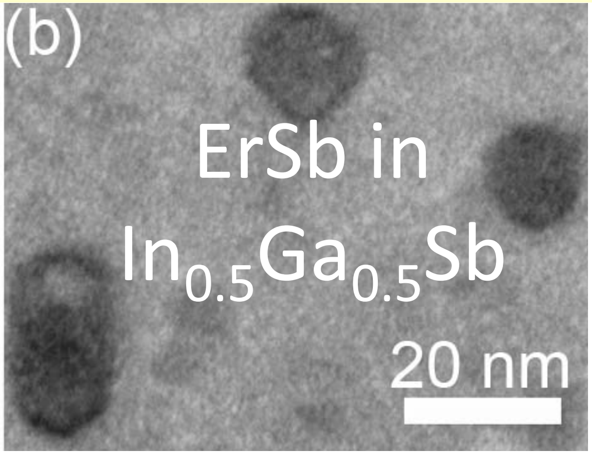
=> Potential to reach ZT~4-5 *(with $k_{lattice}$~1W/mK)*

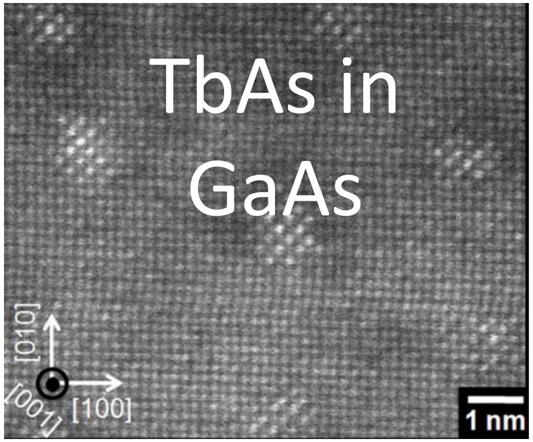
D. Vashaee and A. Shakouri, *Phys. Rev. Lett.* **92**, 106103/1 (2004)

ErAs Semi-metal Nanoparticles embedded in InGa(Al)As Semiconductor Matrix

- Erbium is co-deposited at a growth rate which is a fixed fraction of the InGaAlAs growth rate (MBE growth)
- Solubility limit is exceeded → islands are formed (2-3nm ErAs)



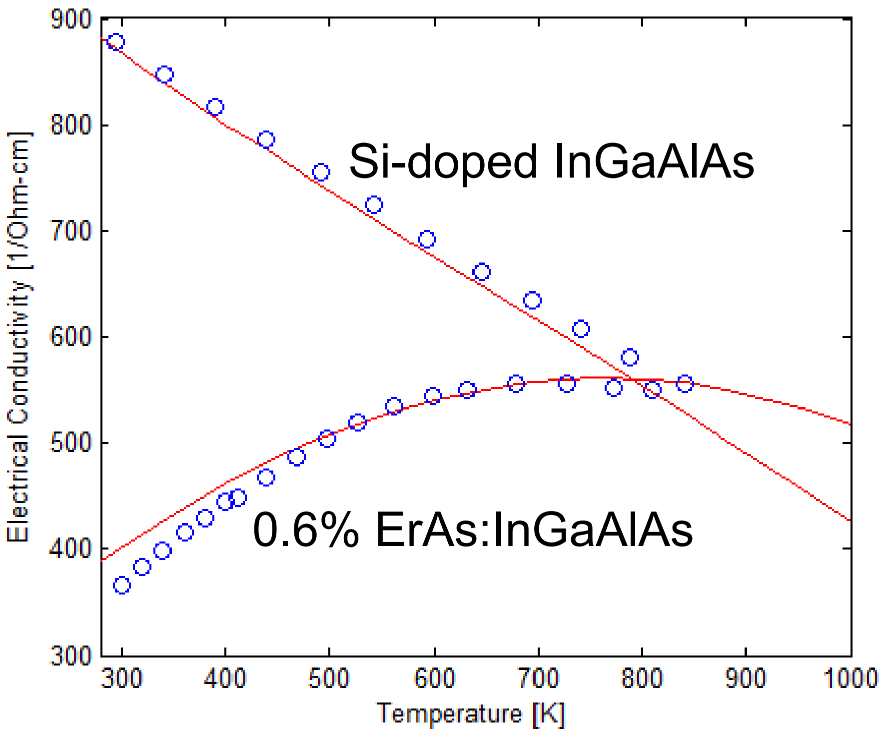




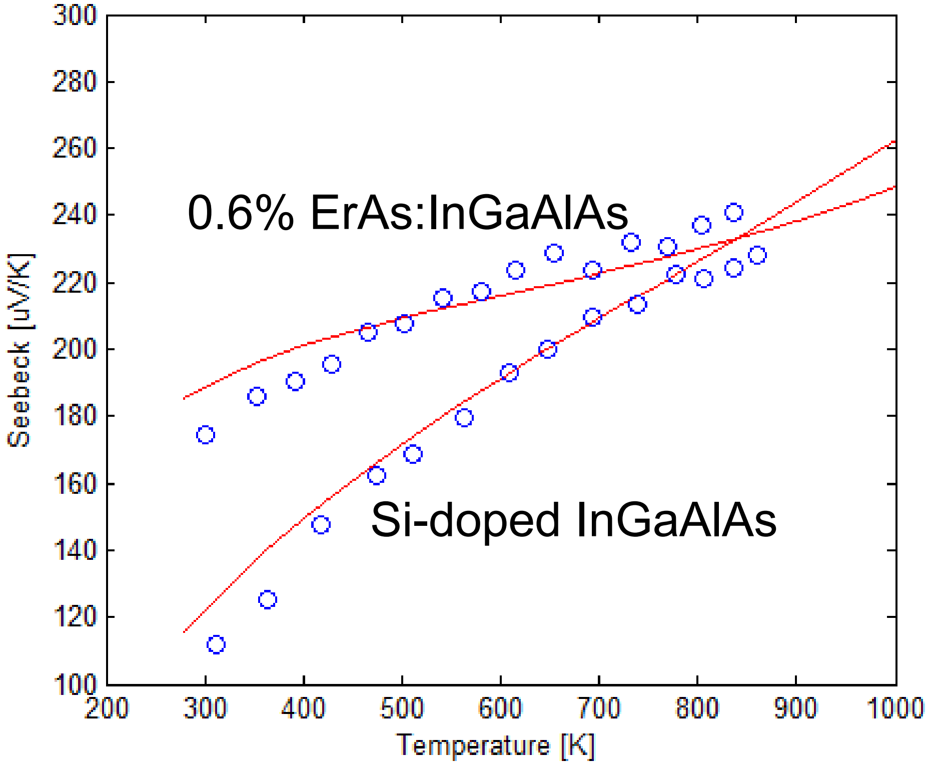
Josh Zide, Art Gossard and Chris Palmstrøm (UCSB and Delaware)

Electrical conductivity and Seebeck (theory/experiment)

Electrical Conductivity



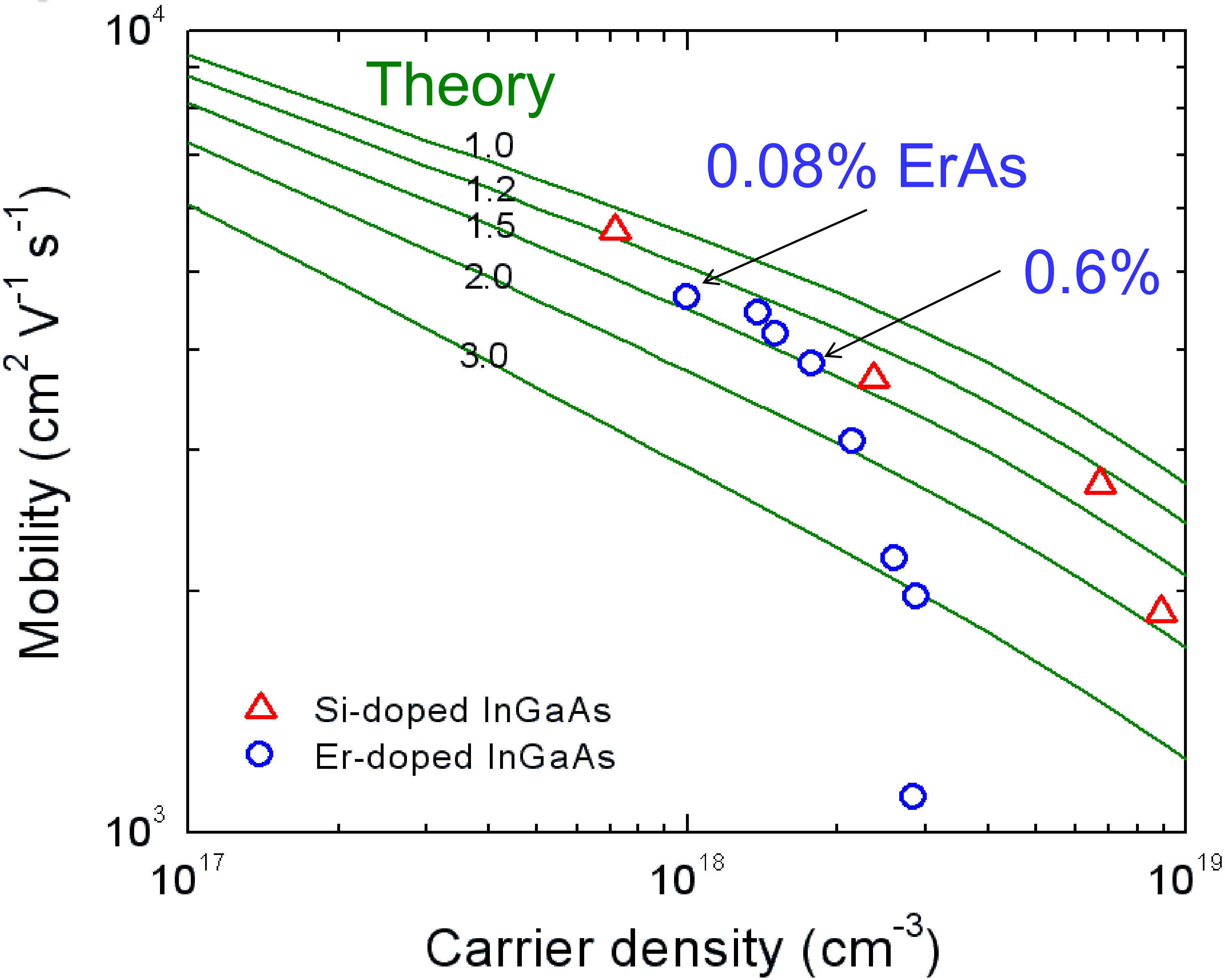
Seebeck



M. Zebarjadi, et al., Appl. Phys. Lett. 2009
J.-H. Bahk et al., Phys. Rev. B 2010 (Si-doped)
J. Zide et al., J. Appl. Phys. 2010

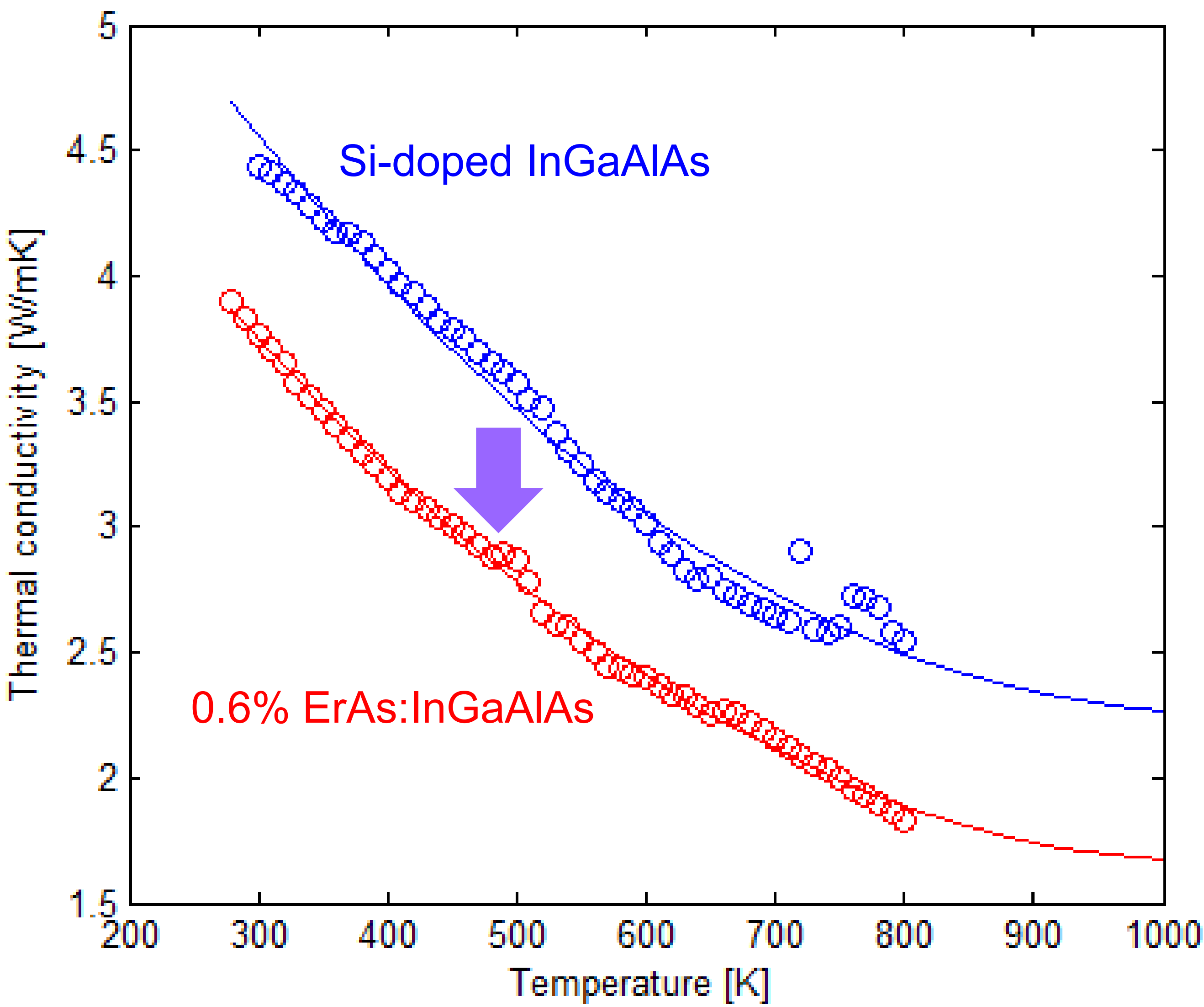
The nanoparticle material is not optimized.

Electron mobility in embedded nanoparticle material



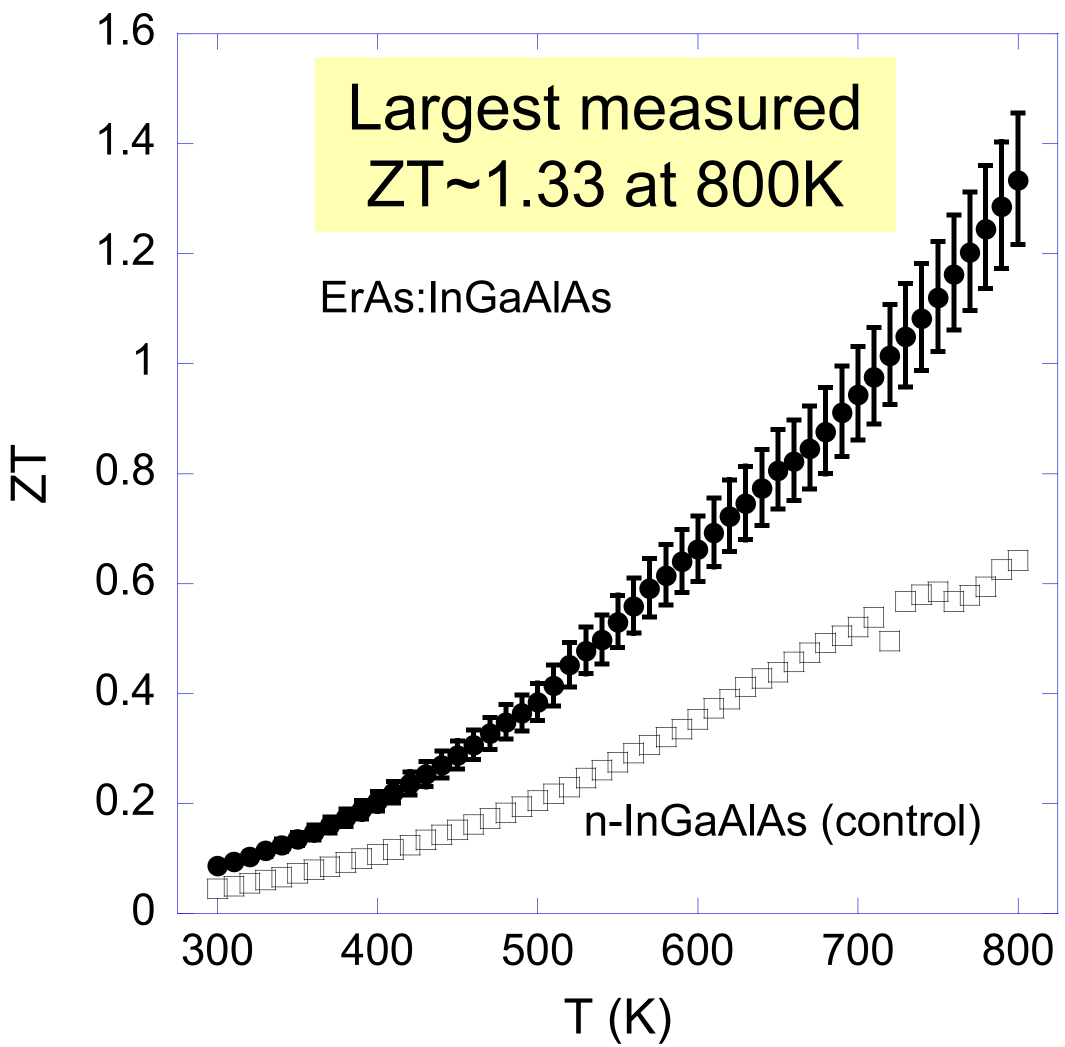
Je-Hyeong Bahk et al. 2010

Thermal conductivity reduction



UCSB, UCSC, UC Berkeley

Thermoelectric figure-of-merit

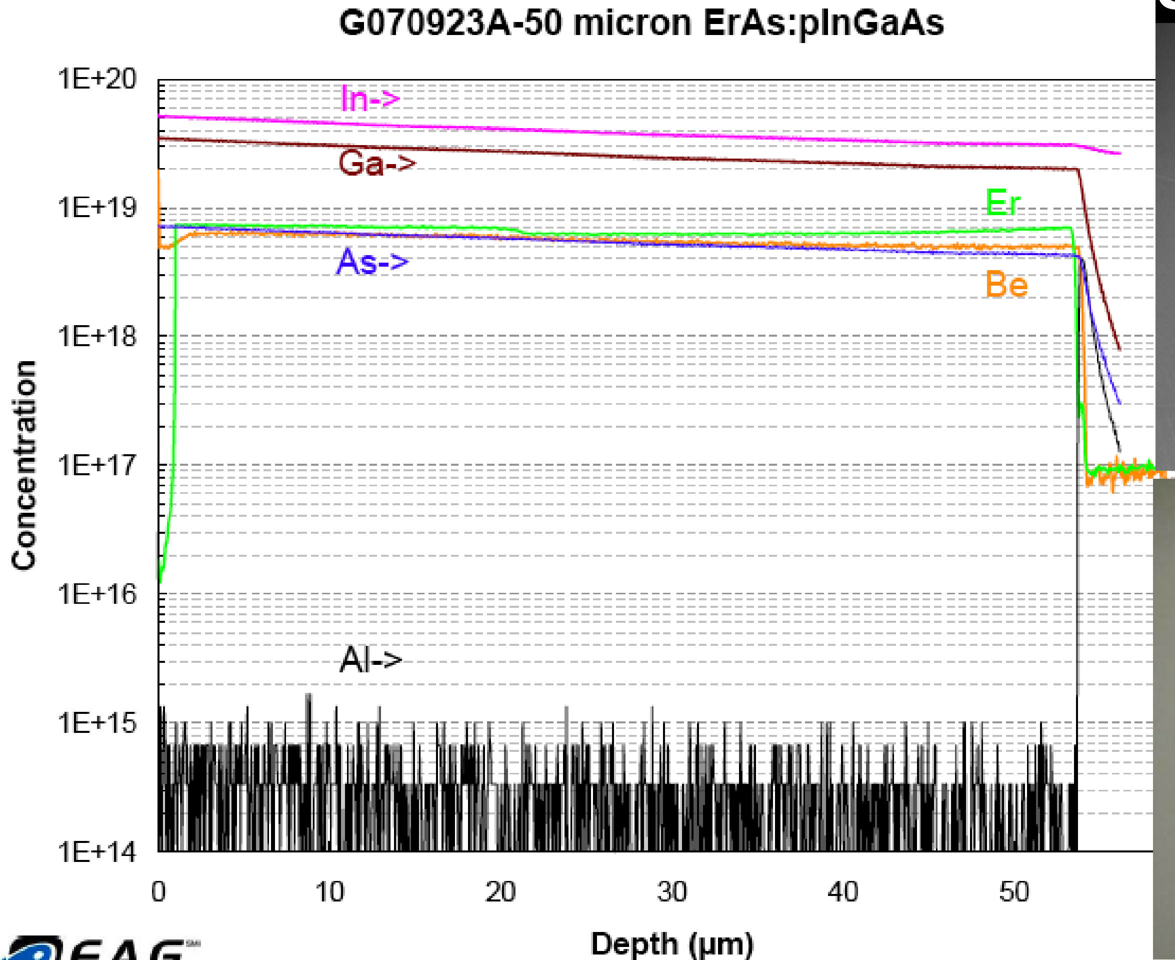


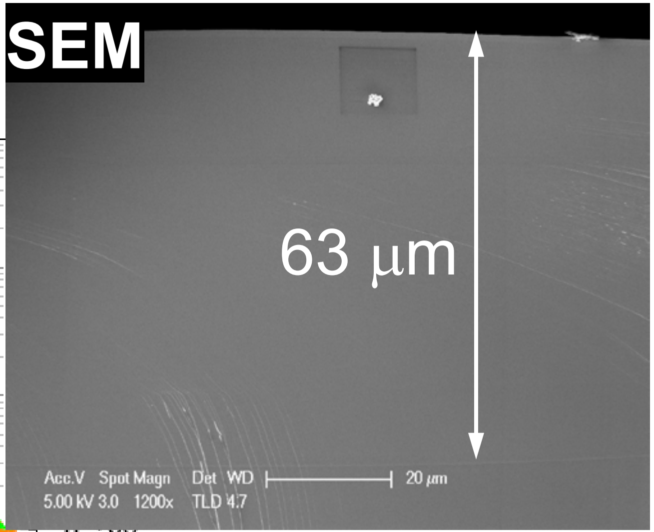
J. Zide et al. Journal of Applied Physics (Dec. 2010)

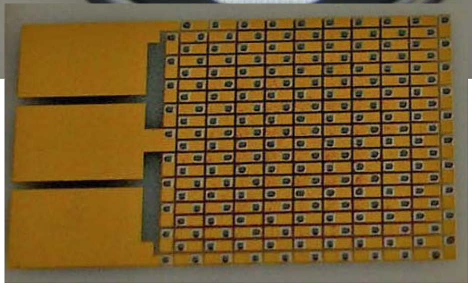
The majority of ZT enhancement is from thermal conductivity reduction.
5% power factor enhancement at 800K.

ErAs:InGa(Al)As thick growth approach

A. Shakouri 1/4/2011

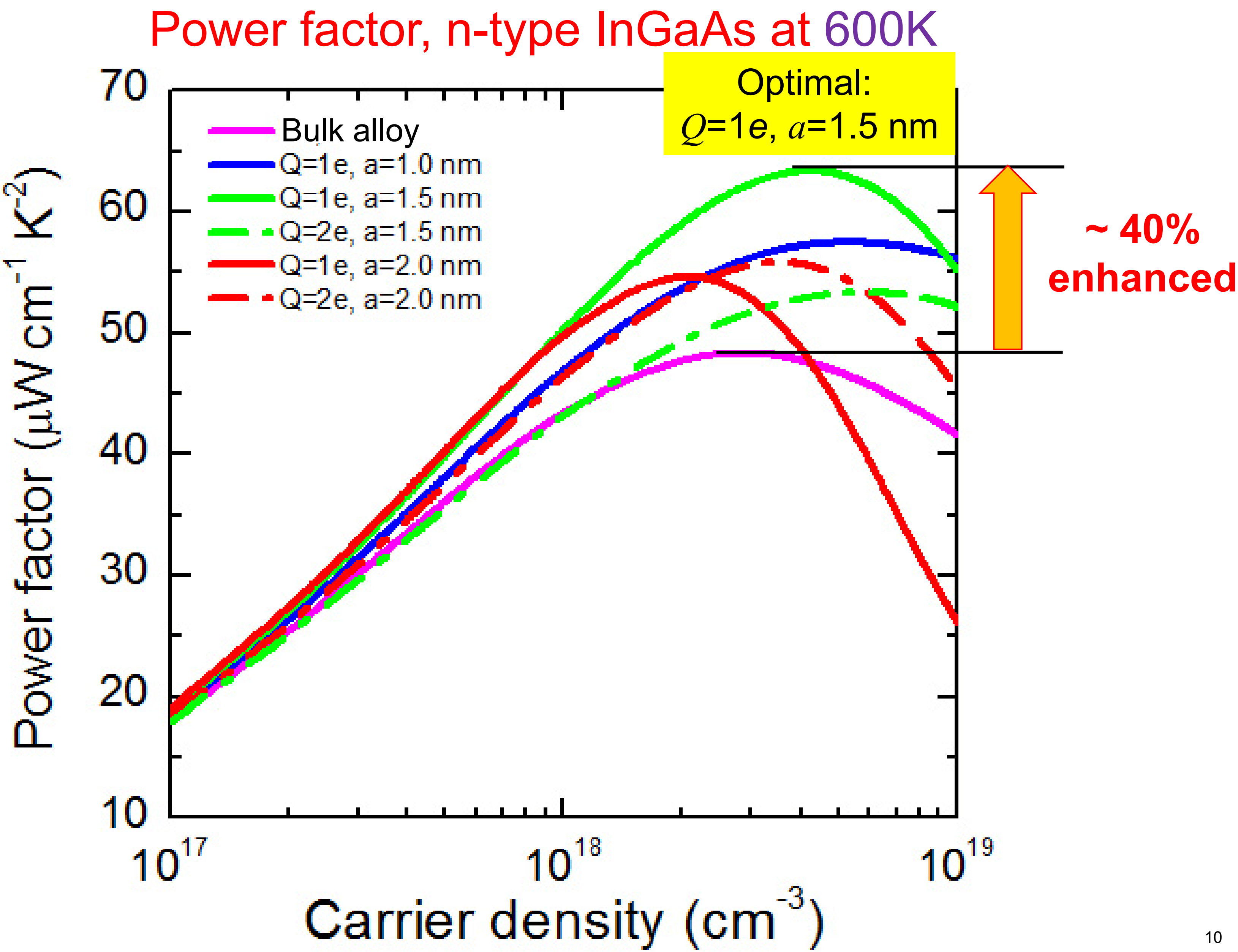




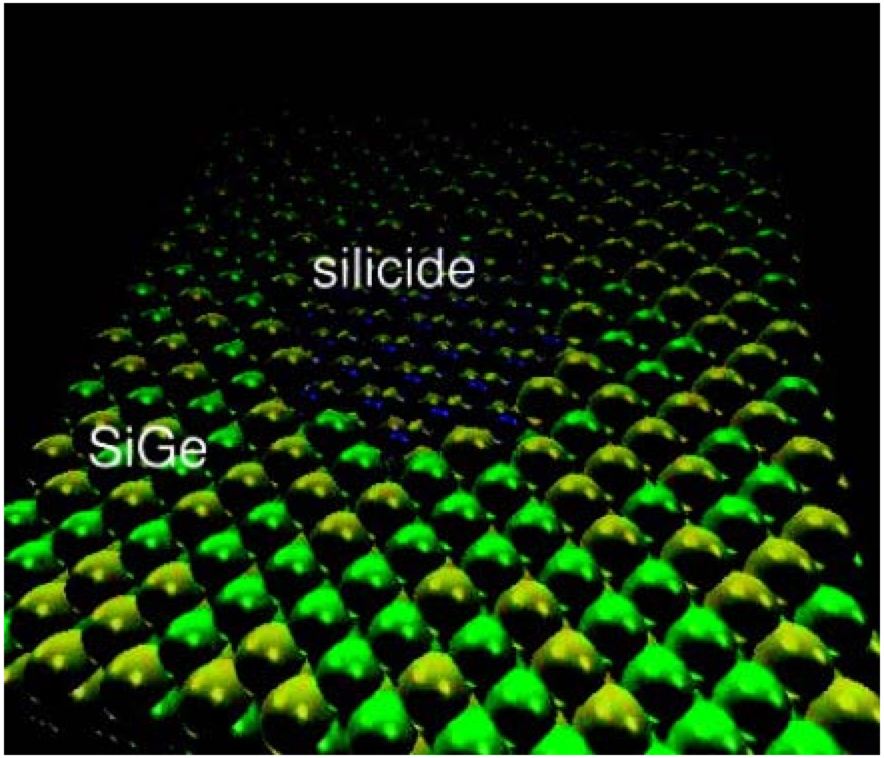


Hong Lu, Art Gossard, UCSB

Nanoparticle scattering optimization



Silicide nanoparticles in SiGe

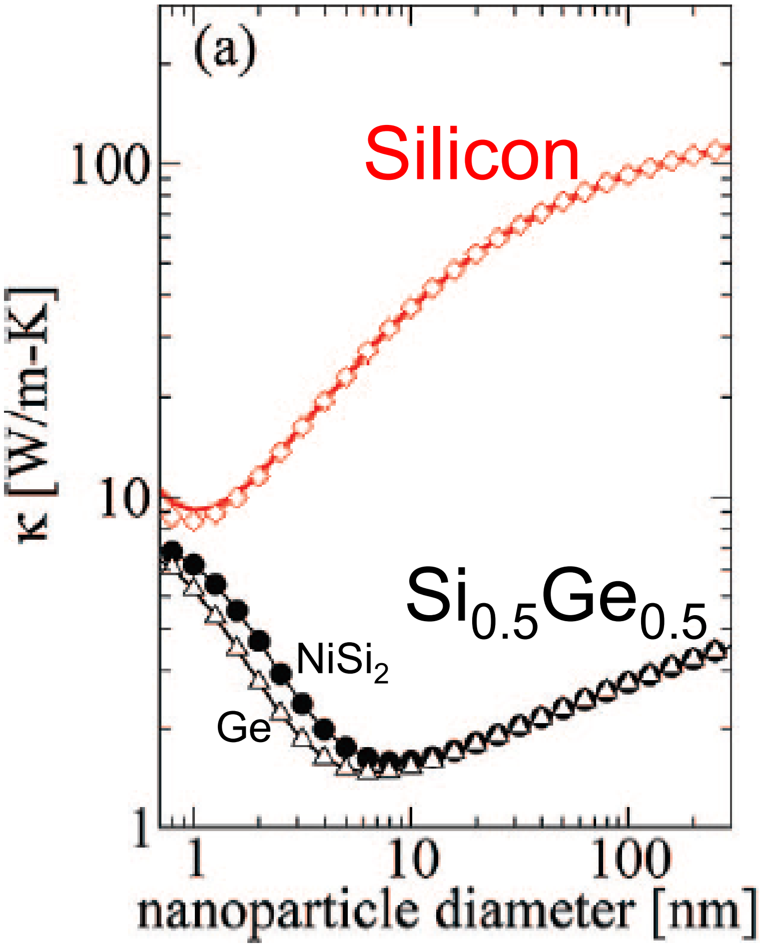


Predictions:

ZT (300K) ~0.5

ZT (900K) ~1.8

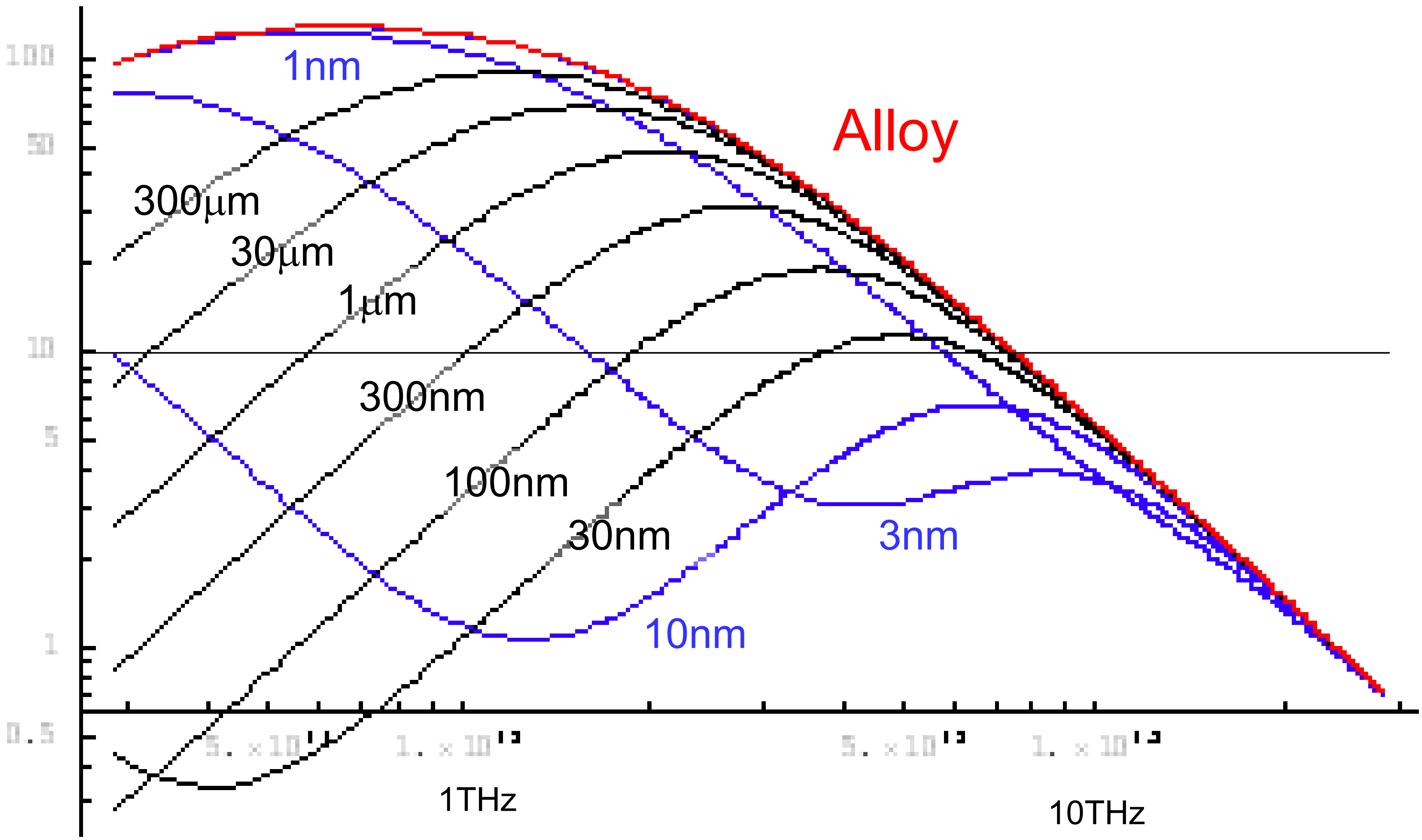
300K
3.4% nanoparticles



Natalio Mingo et al. Nano Letters 2009

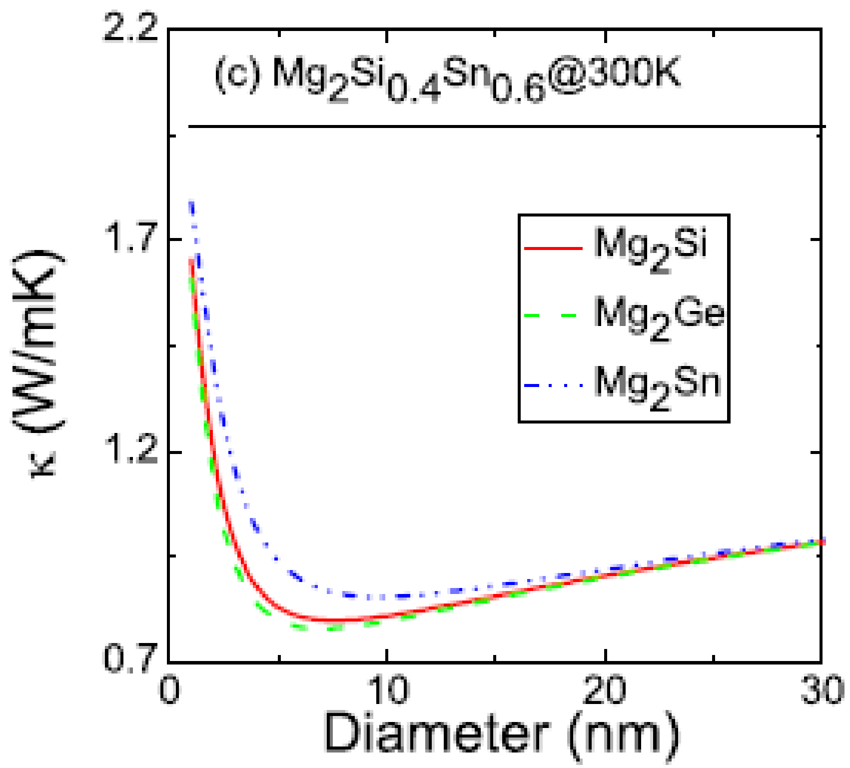
Frequency contributions to thermal conductivity in presence of Iron silicide nanoparticles at 300K

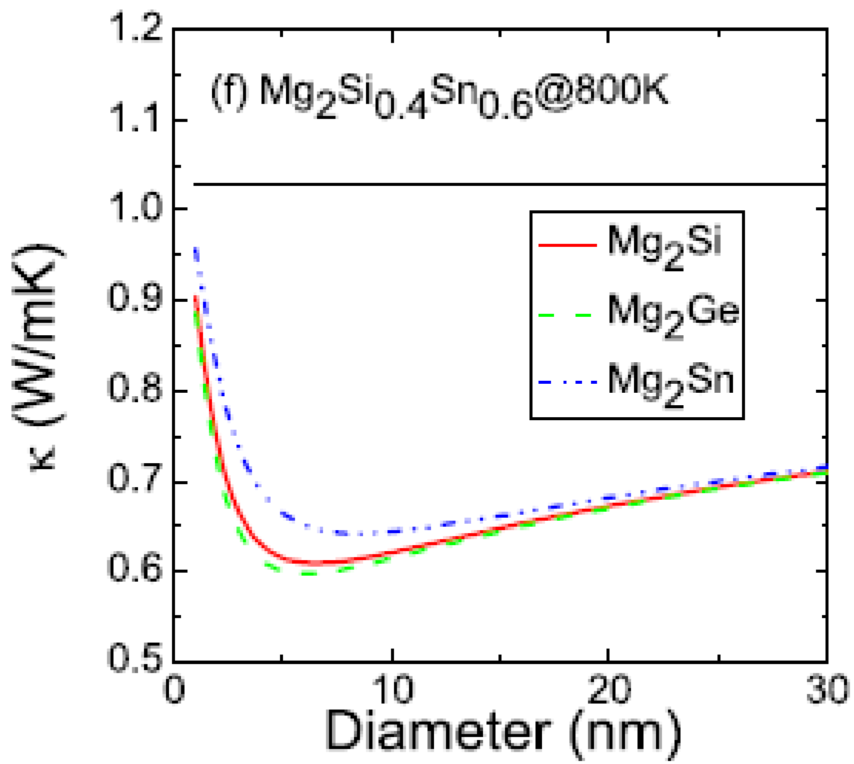
UC SANTA CRUZ
A. Shakouri 1/4/2011



Natalio Mingo 2009 (unpublished)

Nanoparticles in $Mg_2Si_xSn_{1-x}$





Wang and Mingo Applied Physics Letter 2009

Synthesis and Characterization of Mg_2Si/Si

Susan Kauzlarich's Group

Tanghong Yi

UC Davis

And

Jean-Pierre Fleurial's Group

Sabah Bux

JPL

Part of this work was performed at the Jet Propulsion Laboratory, California Institute of Technology under contract with the National Aeronautics and Space Administration.

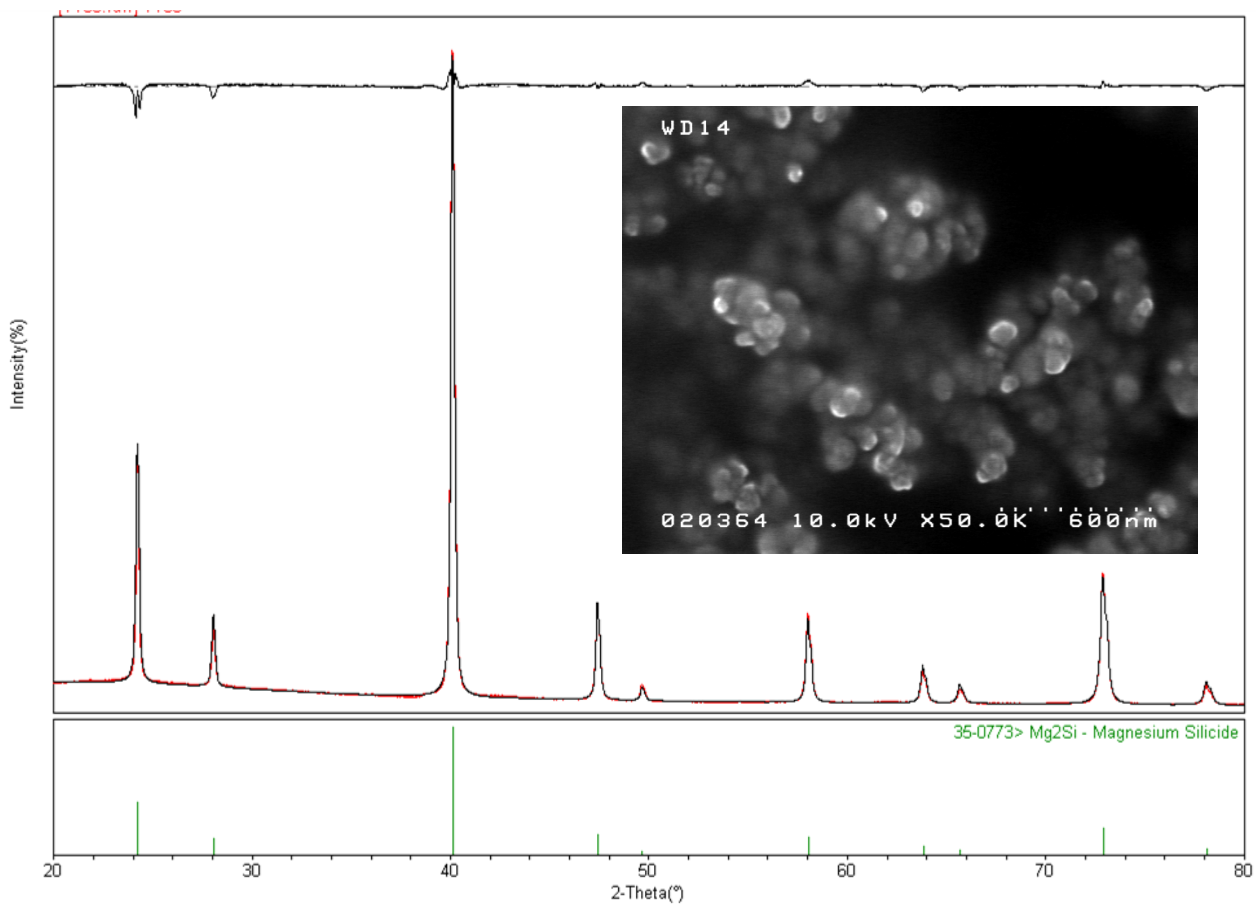
Synthesis Goals

- Develop non-toxic Zintl phase **magnesium silicide alloys with embedded nanoparticles**
- Optimizing the matrix alloy composition and the nanoparticles for maximum thermoelectric figure-of-merit in 500K ~ 800K range

Synthesis

S. Kauzlarich 1/4/2011

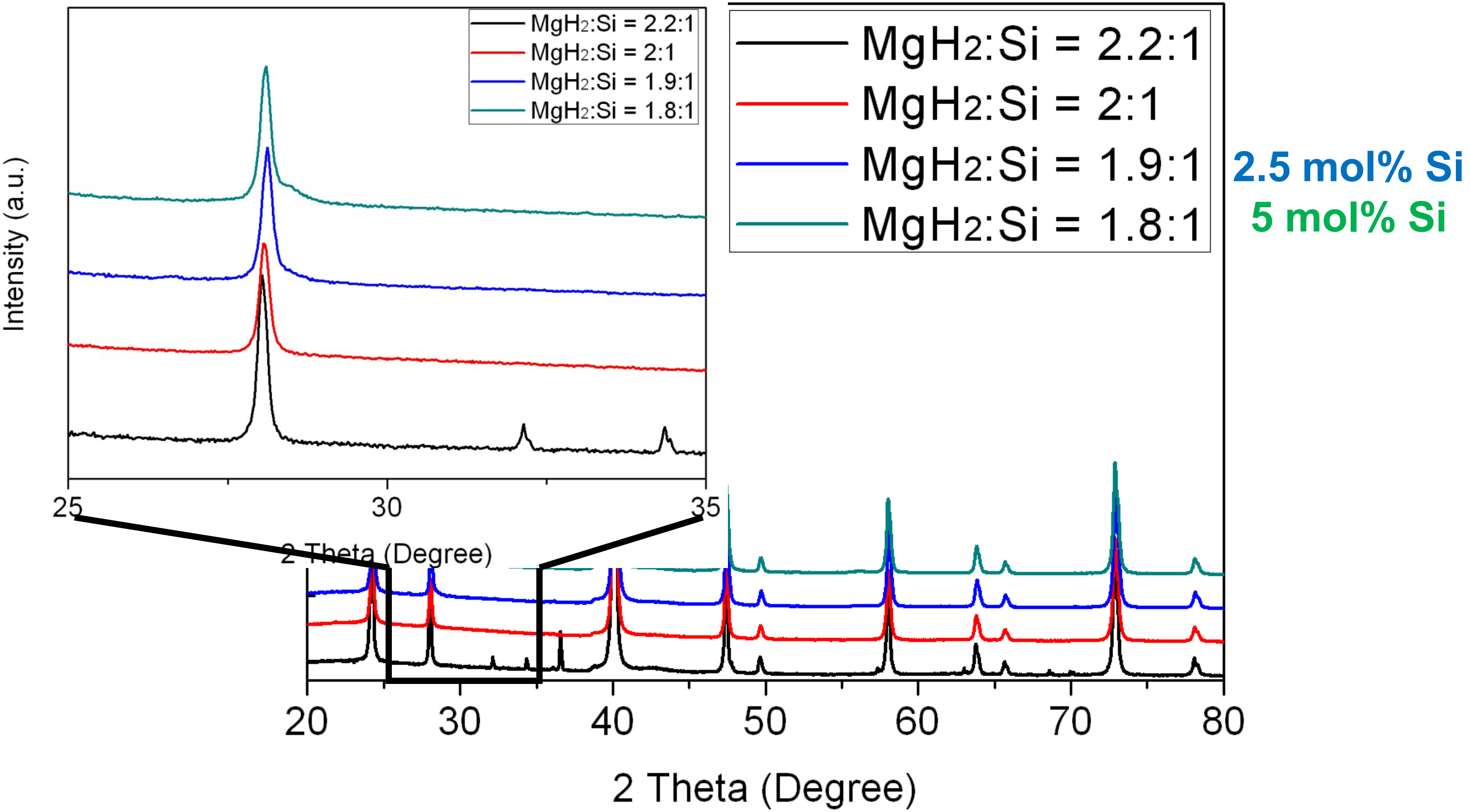
- $2MgH_2 + (1+x)$nano Si(Bi) → Mg_2Si/xSi(Bi)
  (x = 0%, 1.25%, 2.5%, 5%)



Crystallite~ 50 nm
Particle size ~200 nm

Powder X-ray Diffraction

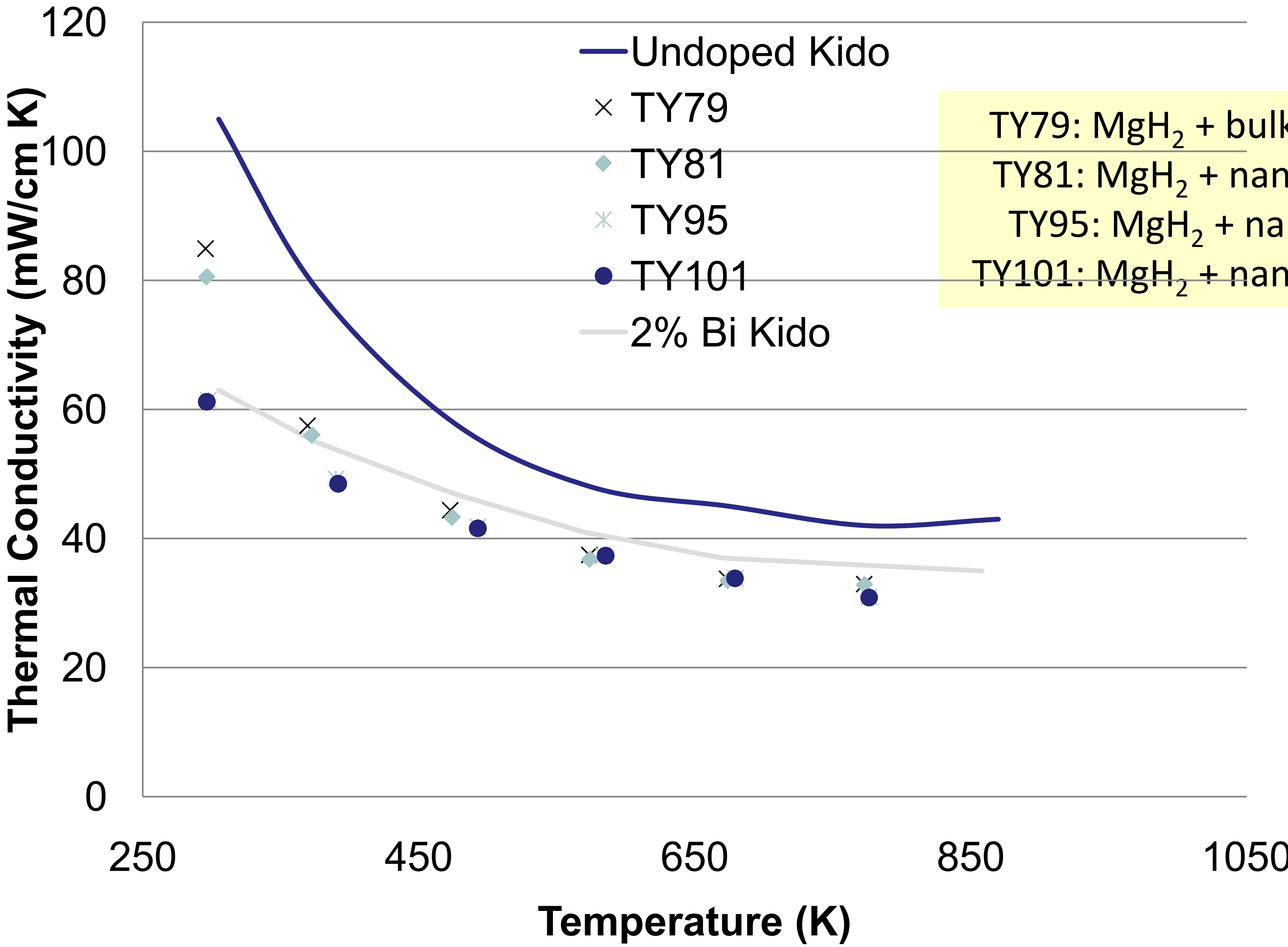
S. Kauzlarich 1/4/2011



Transport properties

S. Kauzlarich 1/4/2011

Sabah Bux and Jean-Pierre Fleurial (JPL)

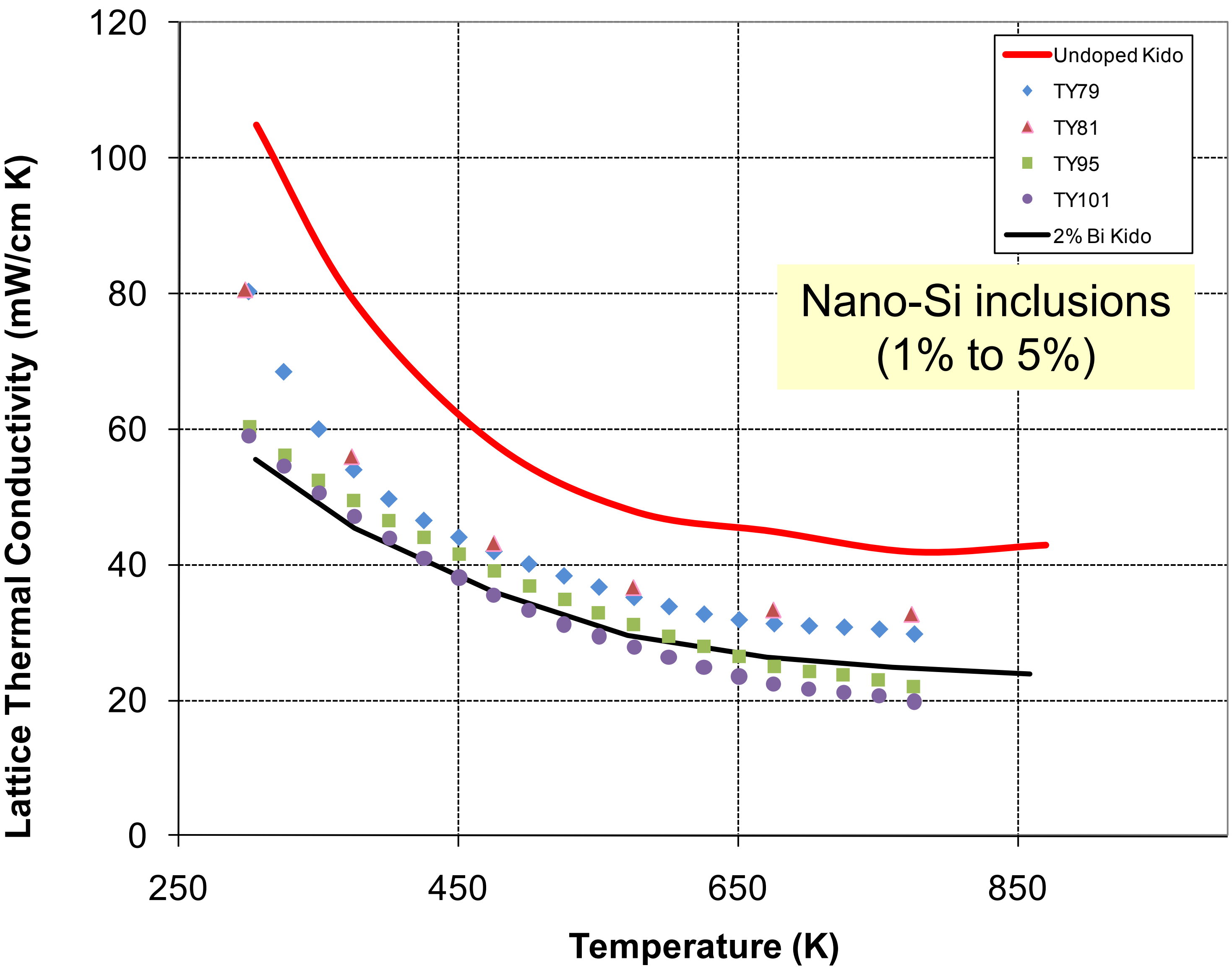


Tani and Kido, Physica B, 2005, 364, 218-224.

Transport properties

S. Kauzlarich 1/4/2011

Sabah Bux and Jean-Pierre Fleurial (JPL)



Summary and Future Directions

S. Kauzlarich 1/4/2011

❖ Demonstrated n-type Mg_2Si via a new synthetic method (MgH2 + Si) with naturally occurring Si nanoparticle inclusions.

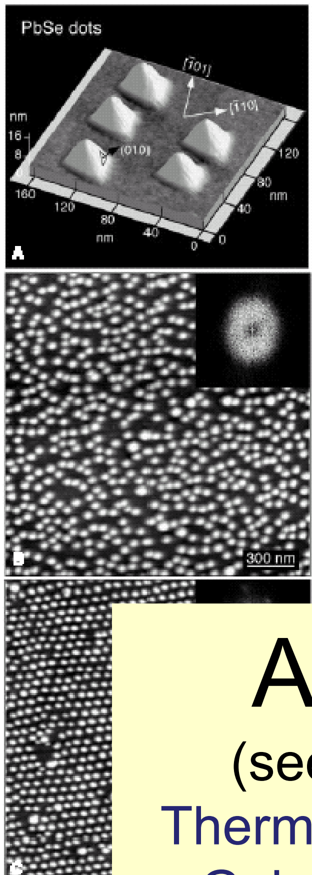
❖Preliminary measurements of thermoelectric properties by JPL

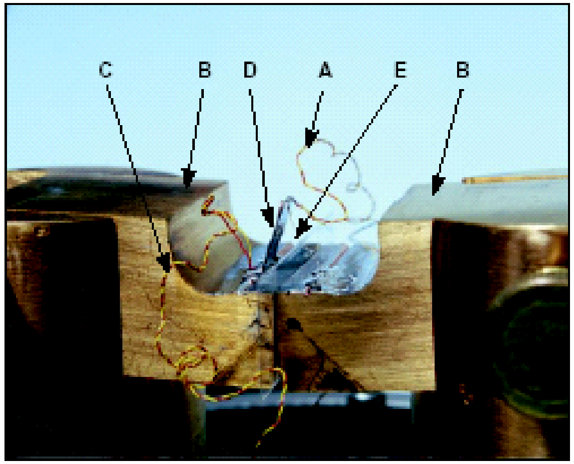
❖Carrier concentration changes vs nanoinclusions needs to be studied

❖Further characterization of the pressed pellets is necessary to determine if the nanoinclusions are isolated and randomly distributed.

❖Further efforts are underway to reduce particle size along with optimization of carrier concentration.

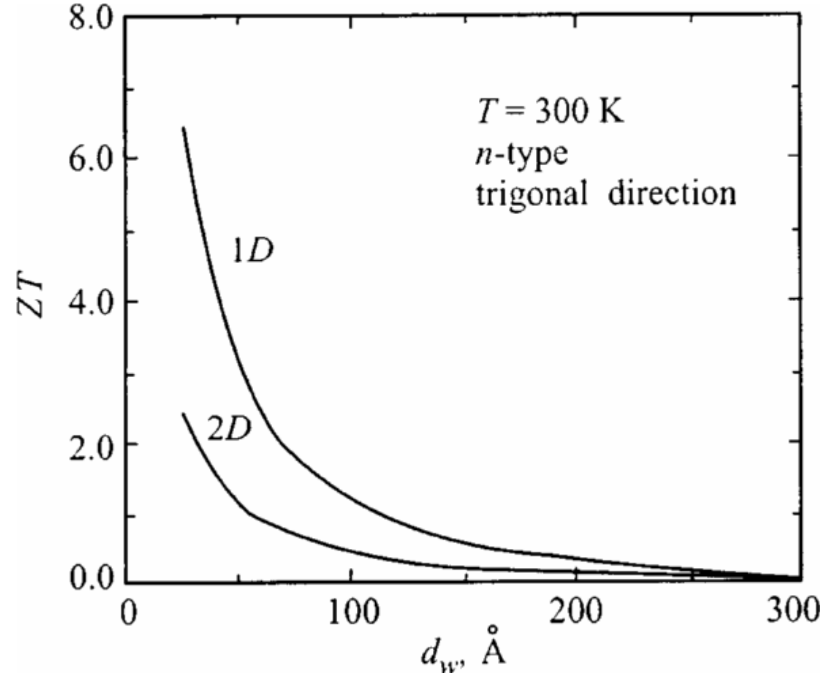
Recent Advances in Thermoelectric Materials:
Quantum Dot Superlattices (Science 2002), T. Harman et al.





PbTe/PbTeSe Quantum Dot Superlattices

– Dresselhaus et al. 1993



Actual ZT ~1

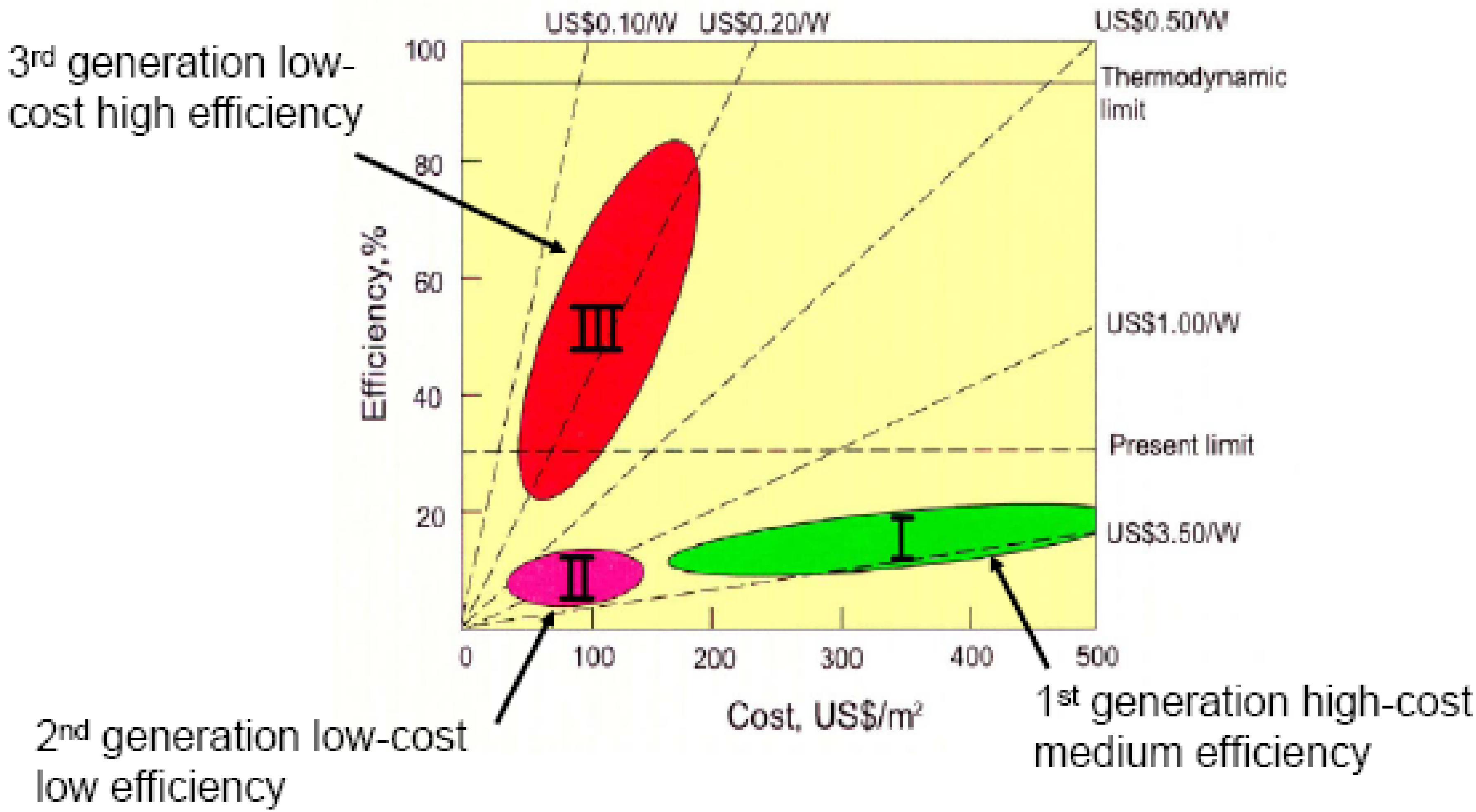
(see e.g. Nanostructured Thermoelectrics: Big Efficiency Gains from Small Features, *Vineis et al*. **Advanced Materials** 2010)

Difficulty

– Non-active barrier layers: Broido and Reinecke PRB ‘01, Mahan, etc.

– Improvement “per conduction channel” is 40-60%- Kim et Lundstrom J. Appl. Phys. 105, 034506 (2009)

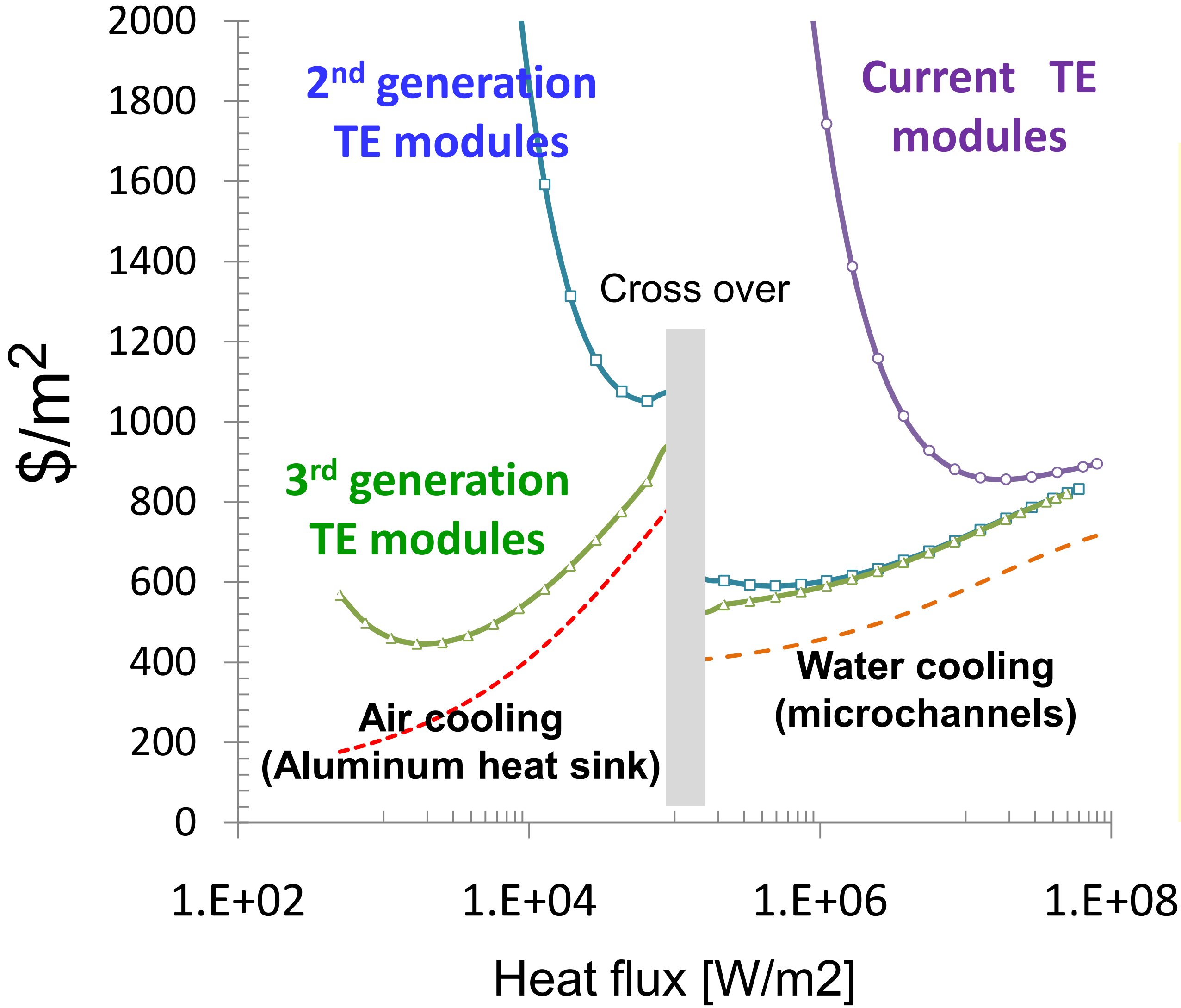
Solar Cells (Efficiency+ Cost → $/W)



An inconvenient truth about thermoelectrics

Cronin Vining, Nature Materials 2009

Material cost of TE power generation system



Today's TE power generation cost: $1-2/W

Potential to bring this down to: $0.1/W

See K. Yazawa's presentation on Wednesday

K. Yazawa and A. Shakouri, International Mechanical Engineering Congress Nov. 2010

Acknowledgement

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Collaborators: John Bowers, Art Gossard, Chris Palmstrom (UCSB), Tim Sands (Purdue), Rajeev Ram (MIT), Venky Narayanamurti (Harvard), Arun Majumdar (Berkeley), Josh Zide (Delaware), Lon Bell (BSST), Natalio Mingo (CEA/UCSC), Susan Kauzlarich (Davis), Sabah Bux, Jean-Pierre Fleurial (NASA JPL)