



... for a brighter future



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Development of High-ZT, Bulk Thermoelectric (New Program)

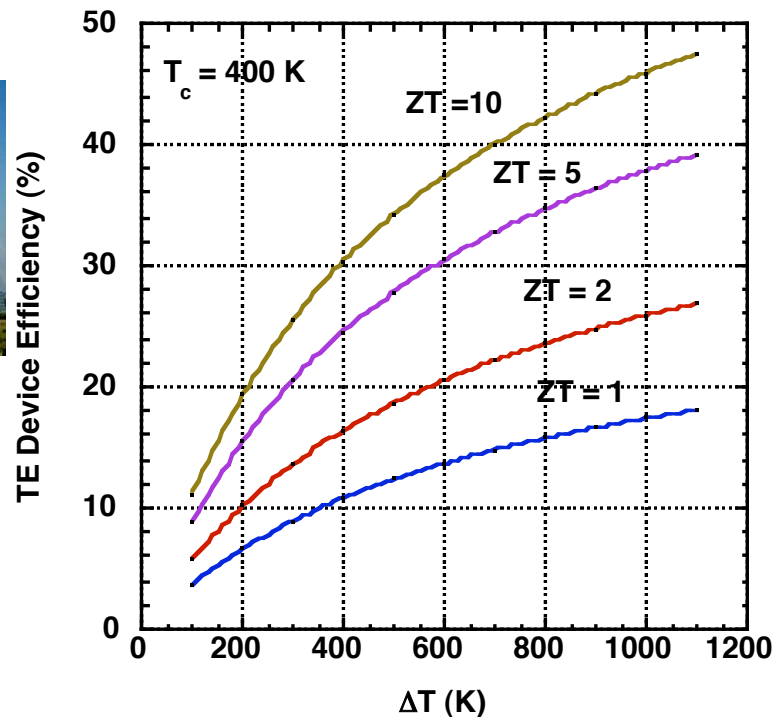
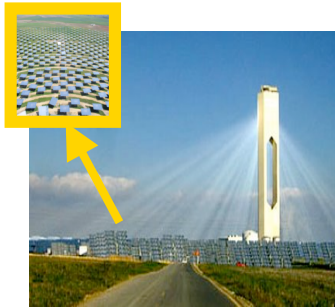
Dieter Gruen, Dileep Singh, Jules Routbort

VT Merit Review
February 26, 2008

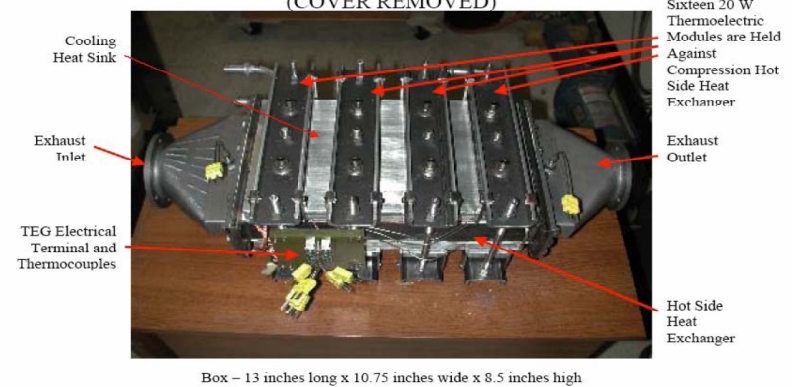
*This presentation does not contain any proprietary
or confidential information*

Potential Applications

- Recovery of waste heat for improved efficiency for transportation (7.1B gallons/y for HVAC for auto), steel, glass manufacturing, etc.
- Direct conversion of solar to electricity
- Ultimate – replace IC engine
- Cooling



330 W THERMOELECTRIC GENERATOR FOR
GM SIERRA 1999 TRUCK
(COVER REMOVED)



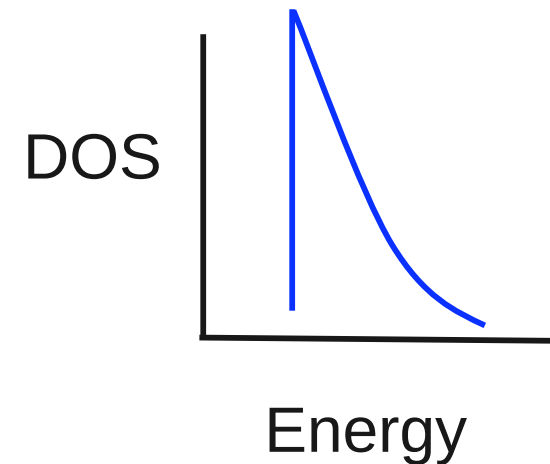
From John Fairbanks

Requirements for commercial applications

- high-T stability
- bulk
- cost-effective
- high ZT
- benign material

Ultra-nanocrystalline Dispersed Diamond - a composite

$$ZT = S^2 \sigma T / K$$

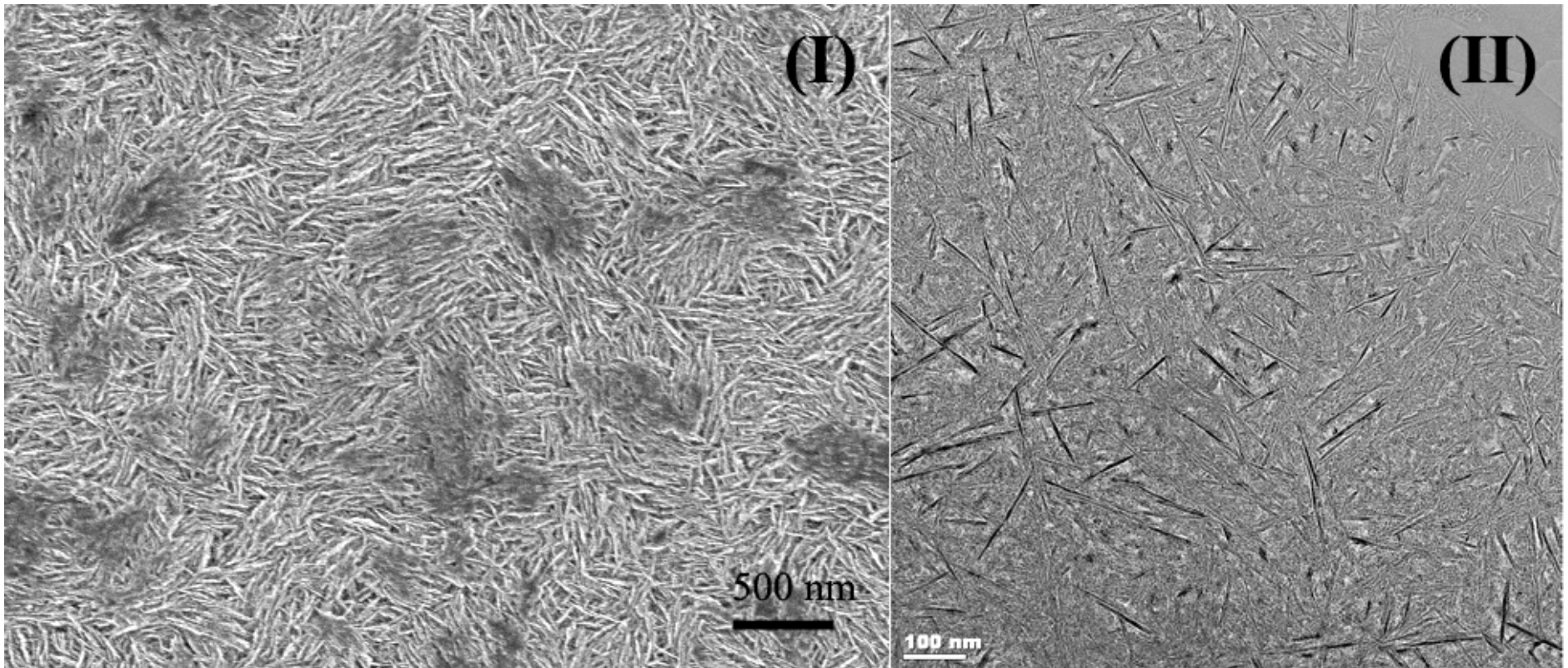


Low dimensions give unique opportunities:

- Enhanced density of states by doping
⇒ Increase S without reducing σ
- Boundary scattering at interfaces reduced κ
more than σ

Initial concept based on thin-film work sponsored by Office of Science

- Based on ultra nanocrystalline diamond (UNCD) coatings



(I) SEM and (II) low magnification TEM images of the samples showing the presence of nanowires.

Research (started FY08) with seed funding from OFCVT

Apply low-dimensionality to production of bulk materials

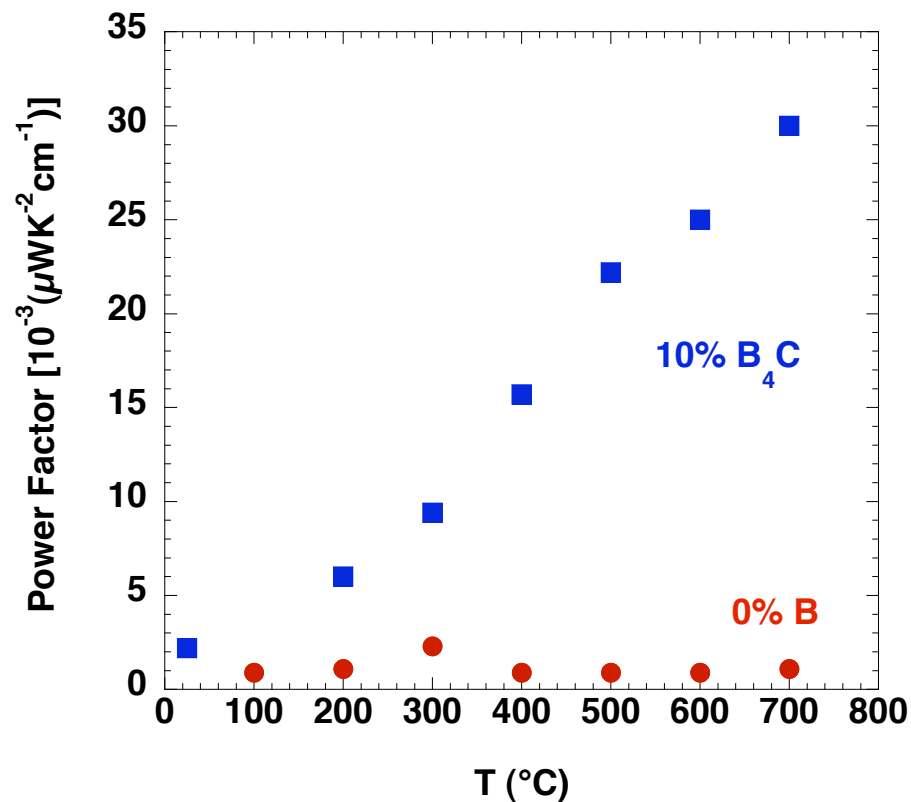
- Produced from ultrananocrystalline dispersed doped diamond (now available in kg quantities)
- Stable to $> 1200^{\circ}\text{C}$, mechanically robust
- Electrical conductivity increased by heat treatment and boron additions
- Seebeck and thermal conductivity measurements in progress
- Potential of $ZT > 4$
- Inexpensive, non-toxic, environmentally benign

Bulk TE produced by surface catalyzed reaction with hydrocarbon molecules binds UNCD particles together covalently in an sp^2 bonded nanocarbon network



Initial Results – Power Factor – $W = S^2\sigma(\Delta T=0)$

- Effect of annealing and doping
 - Power factor increases with T up to 1000K when nanocarbon ensembles are doped with boron
 - Needs further progress



Future Directions – Long-range program

- Processing
 - Powder consolidation
 - Atmospheres (argon initially, then methane, and hydrogen)
 - Temperature (might be as high as 2000°C)
 - Doping (p and n type)
- Properties
 - Seebeck coefficient
 - Electrical conductivity
 - Thermal Conductivity
 - Mechanical/thermal stability, thermal shock, and fracture strength
- Prototypic Device
- Systems Analysis
- Technology Transfer

B-doping of UNCD (for questions only)

- Large configurational entropy that results in high Seebeck coefficient
- Hybridization of B and C “p” orbitals contributes to strong electron/phonon coupling resulting in increased TE conversion efficiencies
- UNCD allows in-homogeneous doping of B which results in reversible TE performance, hence higher conversion efficiencies
 - boron doping in a temperature gradient
 - Humphrey & Linke, Phys. Rev. Lett., 2005, 94, 096601