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# Development of High–ZT, Bulk Thermoelectric (New Program)

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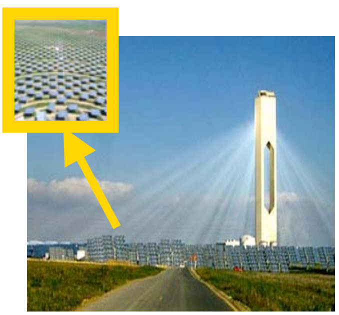
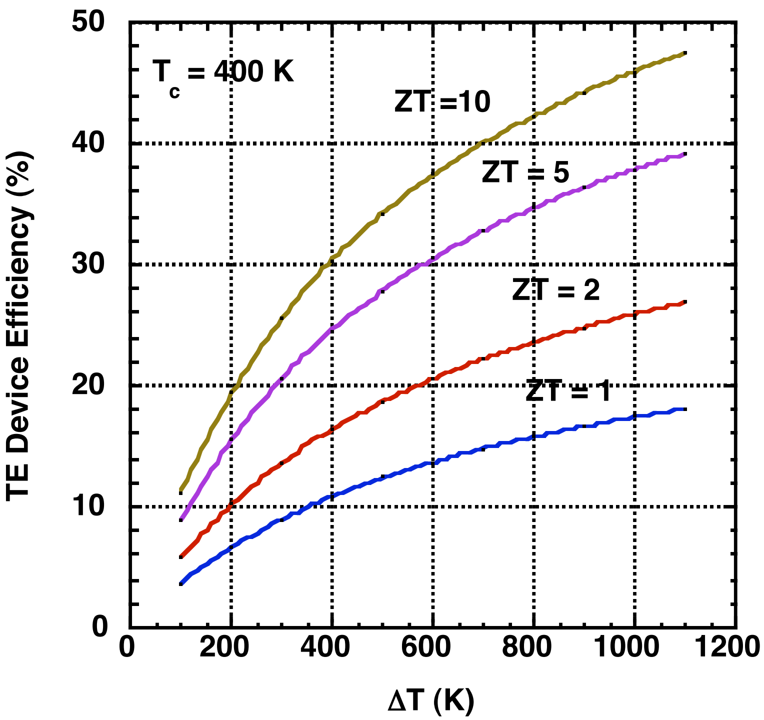
*This presentation does not contain any proprietary or confidential information*

# *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


*From John Fairbanks*



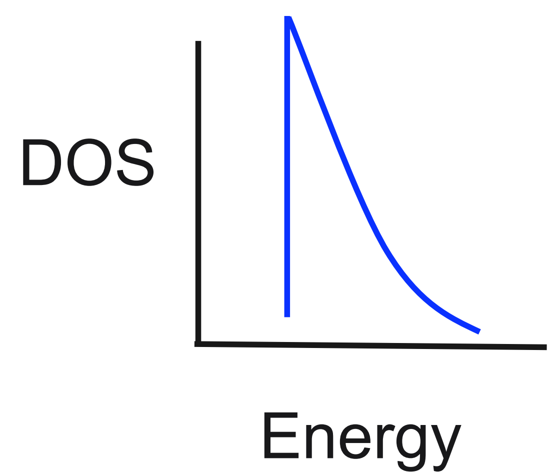



## Requirements for commercial applications

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

## *Ultra–nanocrystalline Dispersed Diamond - a composite*

$$ZT = S^2 \sigma T / \mathrm{K}$$



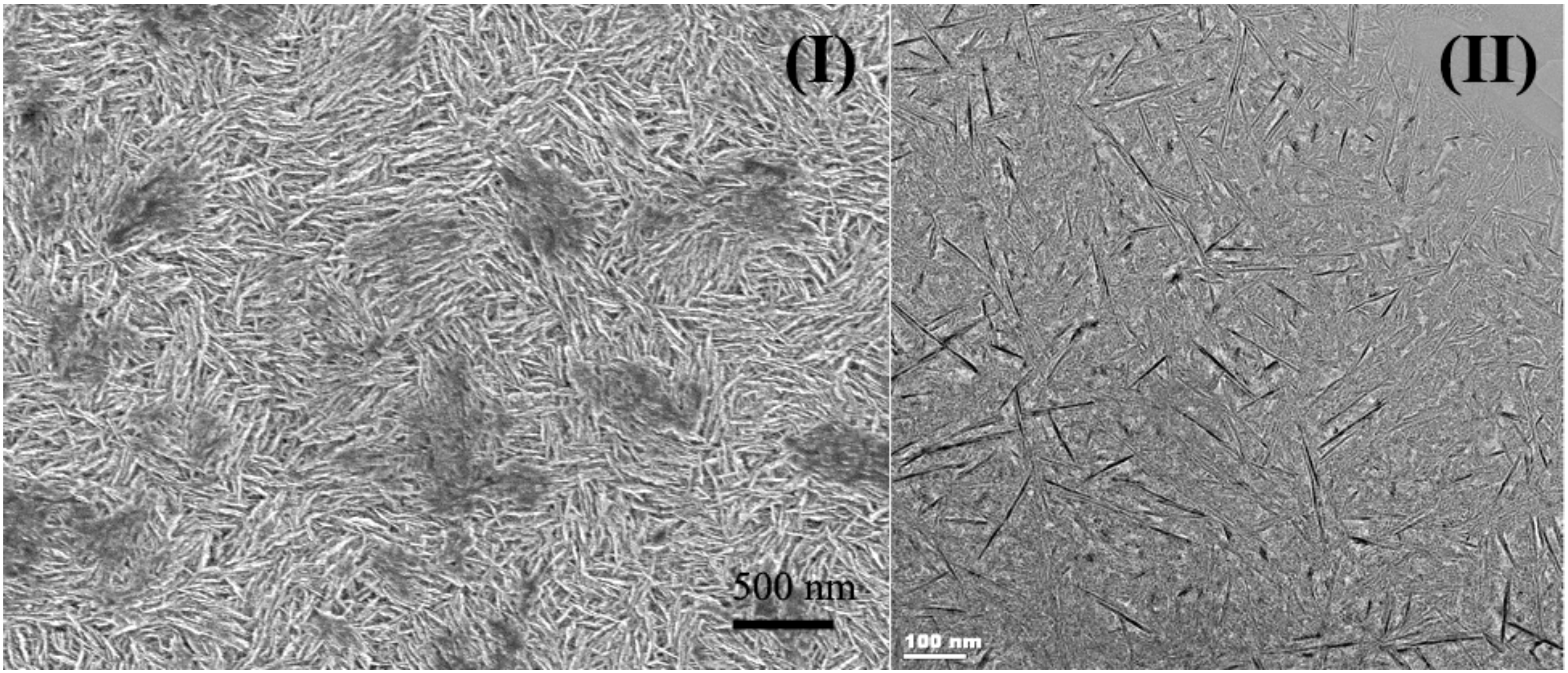

**Low dimensions give unique opportunities:**

- Enhanced density of states by doping
  ⇒ Increase S without reducing $\sigma$

- Boundary scattering at interfaces reduced $\kappa$ more than $\sigma$

# *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*

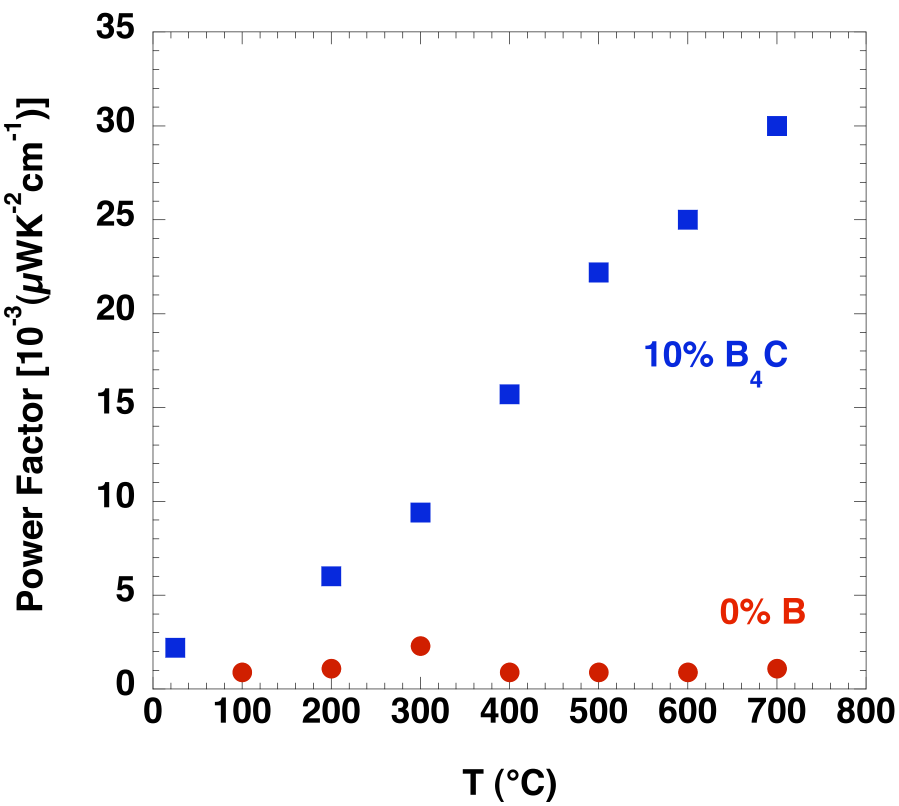
### *Apply low-dimensionality to production of bulk materials*

- Produced from ultrananocrystalline dispersed doped diamond (now available in kg quantities)
- Stable to > 1200°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