Microstructure Effects of Thermoelectric Nanowire Composites

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Motivation

Bookout, John F. (President of Shell USA), “Two Centuries of Fossil Fuel Energy”
\[ ZT = \frac{S^2 \sigma}{\kappa_{el} + \kappa_{ph}} T \]
Thermoelectricity

Seebeck ("Direct") Effect

\[ J_Q \rightarrow T_1 \]  
\[ T_2 \rightarrow J_\rho \]

Peltier ("Converse") Effect

\[ \phi_1 \rightarrow J_\rho \]  
\[ J_Q \rightarrow \phi_2 \]

\[ ZT = \frac{S^2 \sigma}{\kappa_{el} + \kappa_{ph}} T \]
Nanowire Composites

Sander et al., Chem. Mat., V. 15, 2002
Microstructural Effects

Wire diameter

Spacing between wires

Volume fraction of nanowire
Microstructural Effects

- Length of grains
- Grain boundaries
- Wire diameter

[Diagram showing microstructures and annotations]
Extending OOF2

\[ C_p \frac{\partial T}{\partial t} = -\nabla \cdot \vec{J}_Q \]

\[ \frac{\partial \rho}{\partial t} = -\nabla \cdot \vec{J}_\rho \]

\[ \vec{J}_Q = -\kappa \nabla T - T \vec{L} \nabla \phi \]

\[ \vec{J}_\rho = -\sigma \nabla \phi - \vec{L} \nabla T \]
Validation of Model

Non-Linear Properties for Bismuth Telluride

**Validation of Model**

Heat Flux as a Function of Temperature

*Nonlinear Seebeck Coefficient*

\[
J_Q = -\kappa \nabla T - T \cdot L \nabla V
\]

Analytical and numerical solutions differ by 1 part per 10 million.
\[ \vec{J}_\rho = - \sigma \nabla \phi \]
\[ \vec{J}_Q = - \kappa \nabla T \]

\[ \vec{J}_Q = - \kappa \nabla T - T \nabla \phi \]
\[ \vec{J}_\rho = - \sigma \nabla \phi - L \nabla T \]
Heat flux in the x direction

100 MW/m²

100 nm

MW/m²

0 MW/m²

MW/m²

−100 MW/m²
Charge flux in the $x$ direction

$-1.0 \times 10^{11} \frac{A}{m^2}$
Conclusions

- Thermoelectricity induces internal voltages in the composite
- Misorientations at grain boundaries act as sources and sinks of charge carriers
- Grains not perfectly aligned with the fiber axis induce flux in the y and z directions
- OOF2 was successfully extended to study the effect of microstructure on thermoelectric nanowire composites
Future Work

- Engineer the microstructure to optimize the thermoelectric figure of merit

Increasing Randomness

Increasing Diameter
Questions??

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March Dollase Texture Probability Distribution

\[ P(r, \Phi) = \left( r^2 \cos^2 \Phi + r^{-1} \sin^2 \Phi \right)^{-\frac{3}{2}} \]