Micromechanical Design of Novel Thermal Composites for Temperature Dependent Thermal Conductivity

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ATOA

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Introduction

- Material with an order variable in thermal conductivity as a function of temperature is desirable for thermoelectric heat energy recovery, building thermal insulation and solar thermal applications.

- Micromechanics + Thermal Conduction

- Thermal + Structural

- Focus is on the commercially available constituent materials

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Micromechanics

• Continuum Micromechanics based on homogenization theory
  – Aims at finding a volume elements (Representative Volume Element – RVE, periodic Micro field- PMA) response to prescribed mechanical loads.

  – Prediction of macro properties from micro structure and constituents.

Localization relationship

Micro fields
\[ \varepsilon(x) = A(x) \langle \varepsilon \rangle \]

Macro fields
\[ \sigma(x) = B(x) \langle \sigma \rangle \]

Homogenization relationship

\[ \langle \varepsilon \rangle = \frac{1}{\Omega_s} \int_{\Omega_s} \varepsilon(x) \, d\Omega = \frac{1}{2\Omega_s} \int_{\Gamma_s} (u(x) \otimes n_{\Gamma} + n_{\Gamma} \otimes u(x)) \, d\Gamma \]

\[ \langle \sigma \rangle = \frac{1}{\Omega_s} \int_{\Omega_s} \sigma(x) \, d\Omega = \frac{1}{\Omega_s} \int_{\Gamma_s} t(x) \otimes x \, d\Gamma \]

Where,
\( \Omega \) – volume, \( \Gamma \) -surface,
\( u(x) \) – deformation vector
\( t(x) \) – surface traction vector
\( n_{\Gamma} \) – surface normal vector
Numerical Implementation

• Periodic boundary condition
  • \( u_{xl} = u_{x0} + e_x \)
  • \( v_{yl} = u_{y0} + e_y \)

• Global (macro) vs local (micro) stress and strain
  – Integration of variables
  – Coupled Thermal + Structural

• Parametric model to predict the Thermo Elastic property prediction

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Simulation Results

- Thermo elastic
- Micromechanical model
  - Vf
  - Constituent Properties
- Differential Thermal Expansion
- Thermal Expansion = Changes in morphology
- Insulator to conductor Transition
Simulation Results

- Thermal conductivity (predicted as per ASTM standard)
  - At room temperature: (~22 °C)
    - \((11.73) \text{ W/m} \cdot \text{K}\)
  - At Service Temperature (~100°C)
    - \((92.57) \text{ W/m} \cdot \text{K}\)

- 1 order/10X change in Thermal conductivity wrt Temperature

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Conclusions

• Novel Composite material Design
• Engineered Thermal conductivity
• DoE with commercially available materials.
• Next steps
  – Optimization for product application
  – Waste heat recovery
  – Solar Thermal