Micromechanical Design of Novel Thermal Composites for Temperature Dependent Thermal Conductivity

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ATOA

- **Engineering Design Solution Provider**
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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

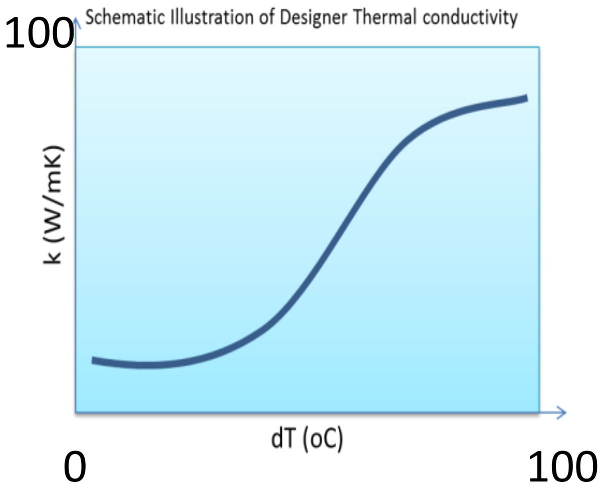


Figure 1. Schematics of Temperature dependent thermal conductivity Material Design.

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

$$\varepsilon(\mathbf{x}) = \mathbf{A}(\mathbf{x})\langle\varepsilon\rangle$$
$$\sigma(\mathbf{x}) = \mathbf{B}(\mathbf{x})\langle\sigma\rangle$$

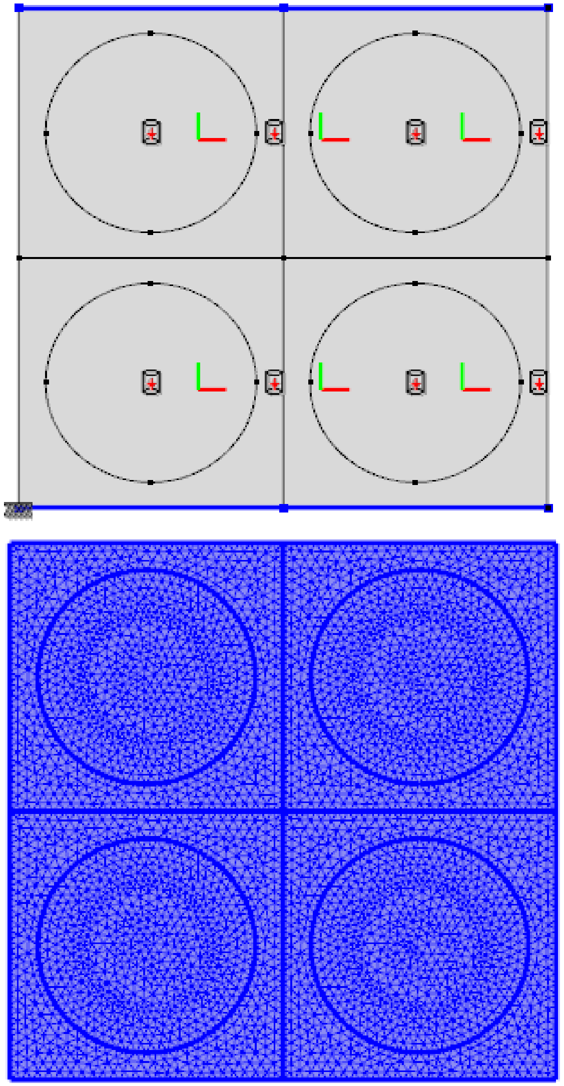
Macro fields

Homogenization relationship

$$\langle\varepsilon\rangle = \frac{1}{\Omega_s}\int_{\Omega_s}\varepsilon(\mathbf{x})\,d\Omega = \frac{1}{2\Omega_s}\int_{\Gamma_s}(\mathbf{u}(\mathbf{x})\otimes\mathbf{n}_\Gamma + \mathbf{n}_\Gamma\otimes\mathbf{u}(\mathbf{x}))\,d\Gamma$$
$$\langle\sigma\rangle = \frac{1}{\Omega_s}\int_{\Omega_s}\sigma(\mathbf{x})\,d\Omega = \frac{1}{\Omega_s}\int_{\Gamma_s}\mathbf{t}(\mathbf{x})\otimes\mathbf{x}\,d\Gamma$$

Where,
Ω –volume, Γ-surface,
$u(x)$– deformation vector
$t(x)$– surface traction vector
n_Γ – surface normal vector

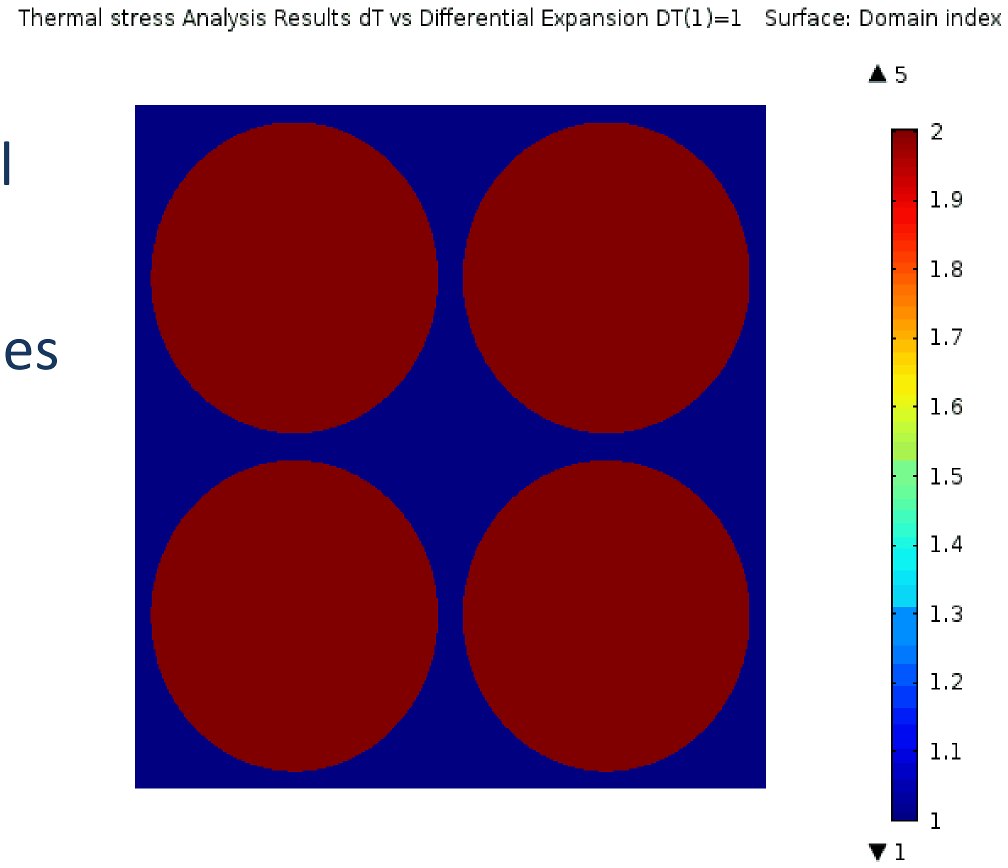
Numerical Implementation



- 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

Simulation Results

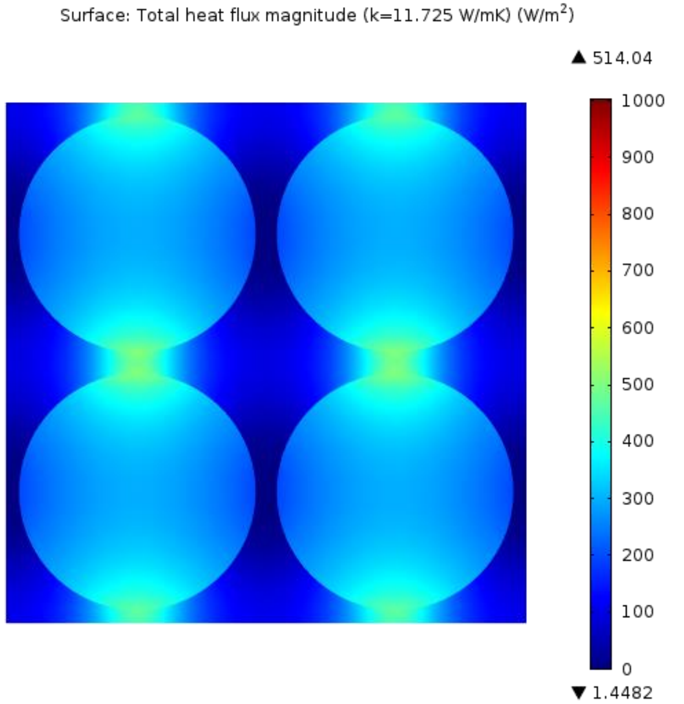
- Thermo elastic
- Micromechanical model
  - Vf
  - Constituent Properties
- Differential Thermal Expansion
- Thermal Expansion = Changes in morphology
- Insulator to conductor Transition

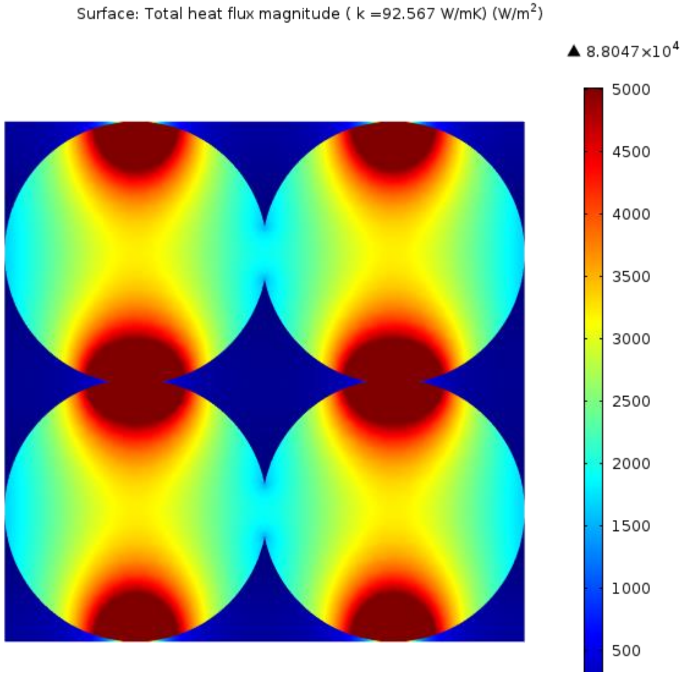


Simulation Results

- Thermal conductivity (predicted as per ASTM standard)
- At room temperature: (~22 oC)
    - (**11.73**) W/m·K
- At Service Temperature (~100oC)
    - (**92.57**) W/m·K

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





Conclusions

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