Application of a multiscale Boltzmann transport solver to characterize thermal resistance from irradiation induced morphological changes in graphite

Jackson Harter, Laura de S. Oliveira, Todd Palmer and P. Alex Greaney

Oregon State University College of Engineering

April 8th, 2015

Motivation

- Effort to use predictive simulation to extend the certification of nuclear reactors
- Graphite is still an important moderating material
- Restart of TREAT (Transient Reactor Test Facility)

Defect thermal conductivity (κ)

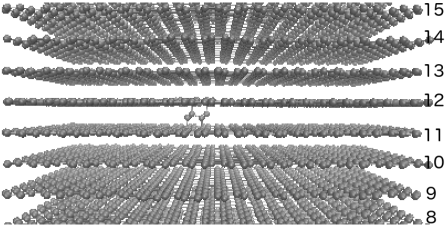
Molecular dynamics simulation

- Classical molecular dynamics
  - LAMMPS
- Equilibrium MD
  - Green-Kubo Method

$$K_x = \frac{V}{k_B T^2} \int_0^\infty \; C \; dt$$

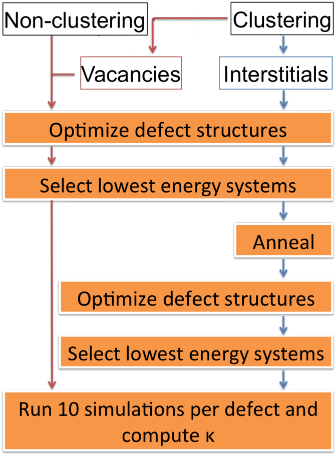
$$C = \langle J_x(t) J_x(t + \Delta t) \rangle$$

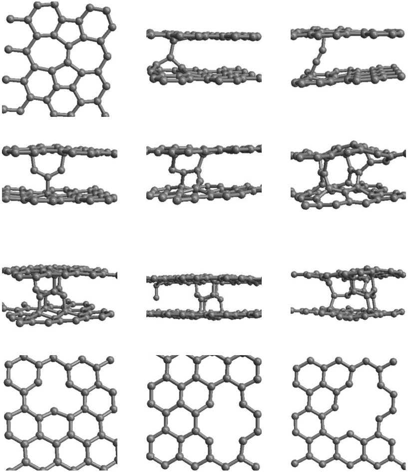
- Supercell volume: 2.71 $\times$ 4.69 $\times$ 7.38 nm^3



Defect thermal conductivity (κ)

Molecular dynamics simulation

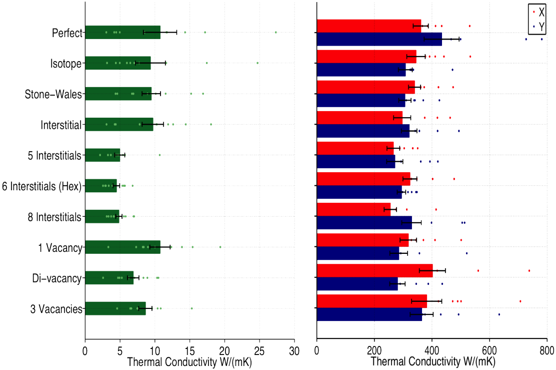




Oregon State University

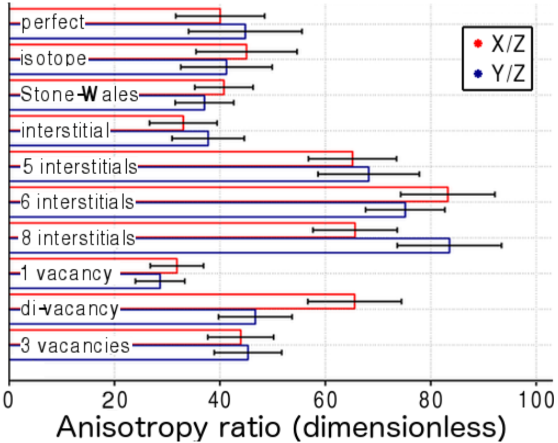
Defect thermal conductivity (κ)

Results



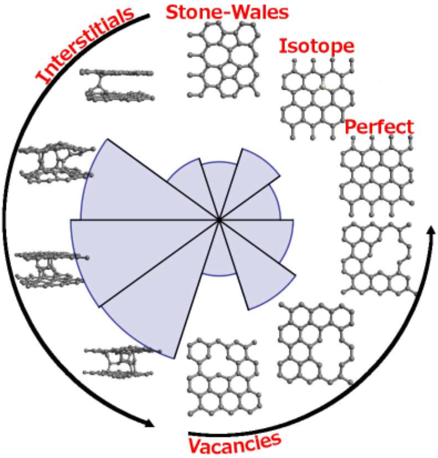
Defect thermal conductivity (κ)

Results



Defect thermal conductivity (κ)

Thermal resistance along the C-axis



Defect thermal conductivity (κ)

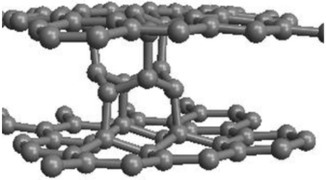
Thermal resistance along the C-axis

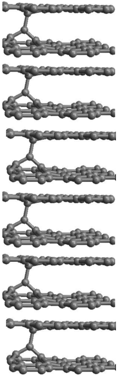
$$\frac{1}{\mu} = \frac{1}{\mu_{\text{impurities}}} + \frac{1}{\mu_{\text{lattice}}} + \frac{1}{\mu_{\text{defects}}} + \cdots$$

$$r_{\text{defective}} = r_{\text{perfect}} + r_{\text{defects}}$$

Defect thermal conductivity (κ)

Thermal resistance along the C-axis





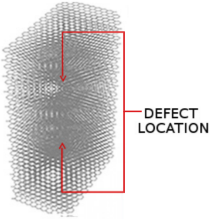
$$r_{\text{defect}-6\text{Int}} = 0.16 \pm 0.03 (mK/W)$$

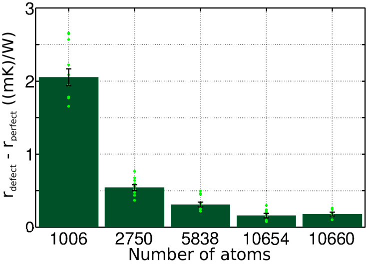
$$6 \cdot r_{\text{defect}-1\text{Int}} = 0.04 \pm 0.17 \ (mK/W)$$

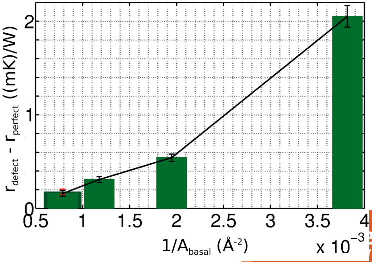
Oregon State UNIVERSITY

Defect thermal conductivity (κ)

Thermal resistance along the C-axis







Expected:

$r_{\text{defective}-2} = r_{\text{perfect}} + 2 \cdot r_{\text{defect}}$

$r_{\text{defective}-2} = 0.43 \pm 0.06$ W/(mK)

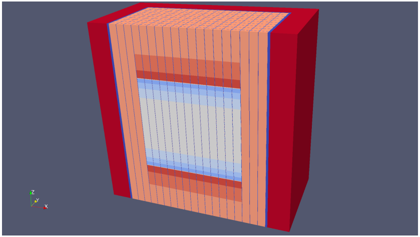
Actual:

0.29 ± 0.06 W/(mK)

Bridging the Gap

Connecting nanoscale simulations to the engineering scale

- Use MD to understand influence of defects on κ
- Can use this data to examine effects at larger scale, with reduced computational expense
- Use MD simulation values to reproduce κ with Rattlesnake



What is MOOSE?

- MOOSE
  - Multi-physics Object Oriented Simulation Environment
  - Sophisticated framework for solving coupled PDEs
  - Massively parallelizable
  - Unit agnostic finite element mesh discretization
- Rattlesnake
  - Solves the Boltzmann transport equation (BTE) for neutrons using the Self-Adjoint Angular Flux (SAAF) formulation
  - S_N, P_N angular discretization capability, may use diffusion acceleration

Oregon State University

Formulation of Phonon BTE

- Self-Adjoint Angular Flux formulation of BTE for phonons

$$-\Lambda\vec{\Omega}\cdot\vec{\nabla}\left[\Lambda\vec{\Omega}\cdot\vec{\nabla}f_\omega\right]+f_\omega=-\Lambda\vec{\Omega}\cdot\vec{\nabla}f_\omega^0+f_\omega^0$$

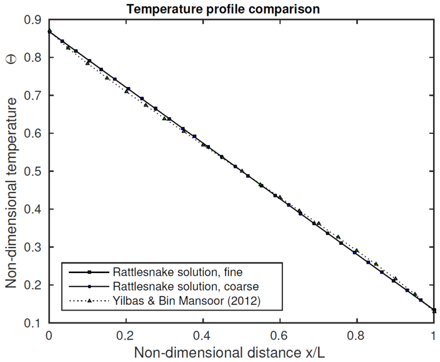
$$I\left(\vec{r},\theta,\phi\right)=\frac{1}{4\pi}\int_0^{\omega_{max}}\sum_p v_g f_\omega \hbar\omega\left(\vec{k}\right)D\left(\omega\right)d\omega$$

- Yields frequency independent gray medium Equation of Phonon Radiative Transport

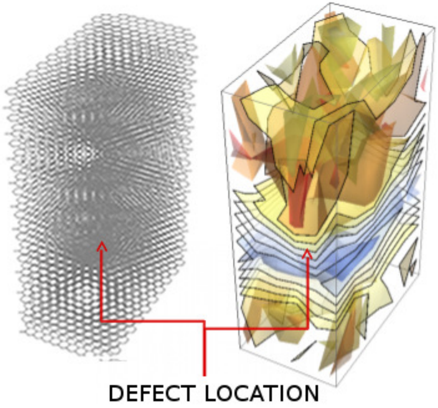
Oregon State UNIVERSITY

Validation

- Comparison to 1D results in silicon thin film of Yilbas and Bin Mansoor
  - Rattlesnake can model highly scattering problems
  - Results expected as exact solution of EPRT
  - Highly diffuse scattering behavior
  - Boundary scattering effects
- MOOSE is maintained at NQA-1 validation standard



Graphite Results



Concluding Remarks

- Not all defects are created equal
  - It is still unclear if they are additive
- Adapted Rattlesnake to transport phonons
- Learn from MD results and make predictions for engineering scale calculations

Acknowledgements:
This study is supported under a Department of Energy grant in conjuction with the Idaho National Laboratory and the National University Consortium. This work used the Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by National Science Foundation grant number OCI-1053575.