

Using Atomistic Simulations to Study Thermal Conductivity

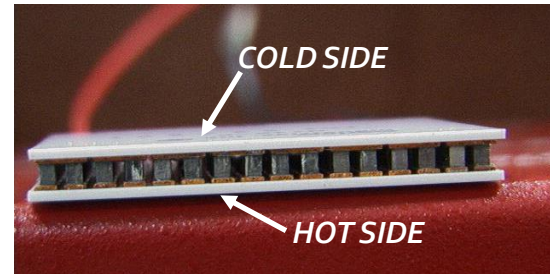
Asegun Henry

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Why Is Heat Important



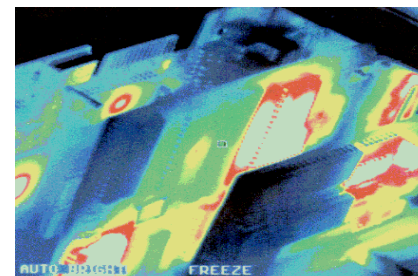
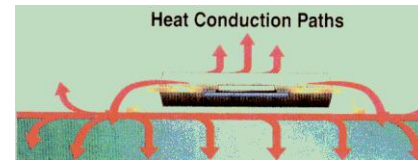
Heat Exchangers



Thermoelectrics

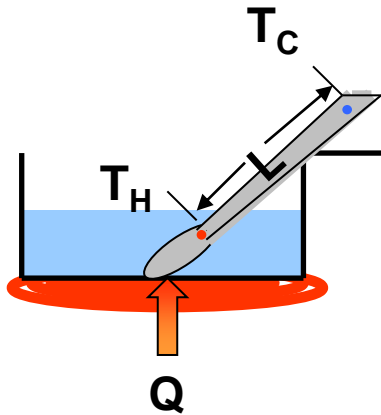


Over 90% of Energy Production
Comes From Heat!



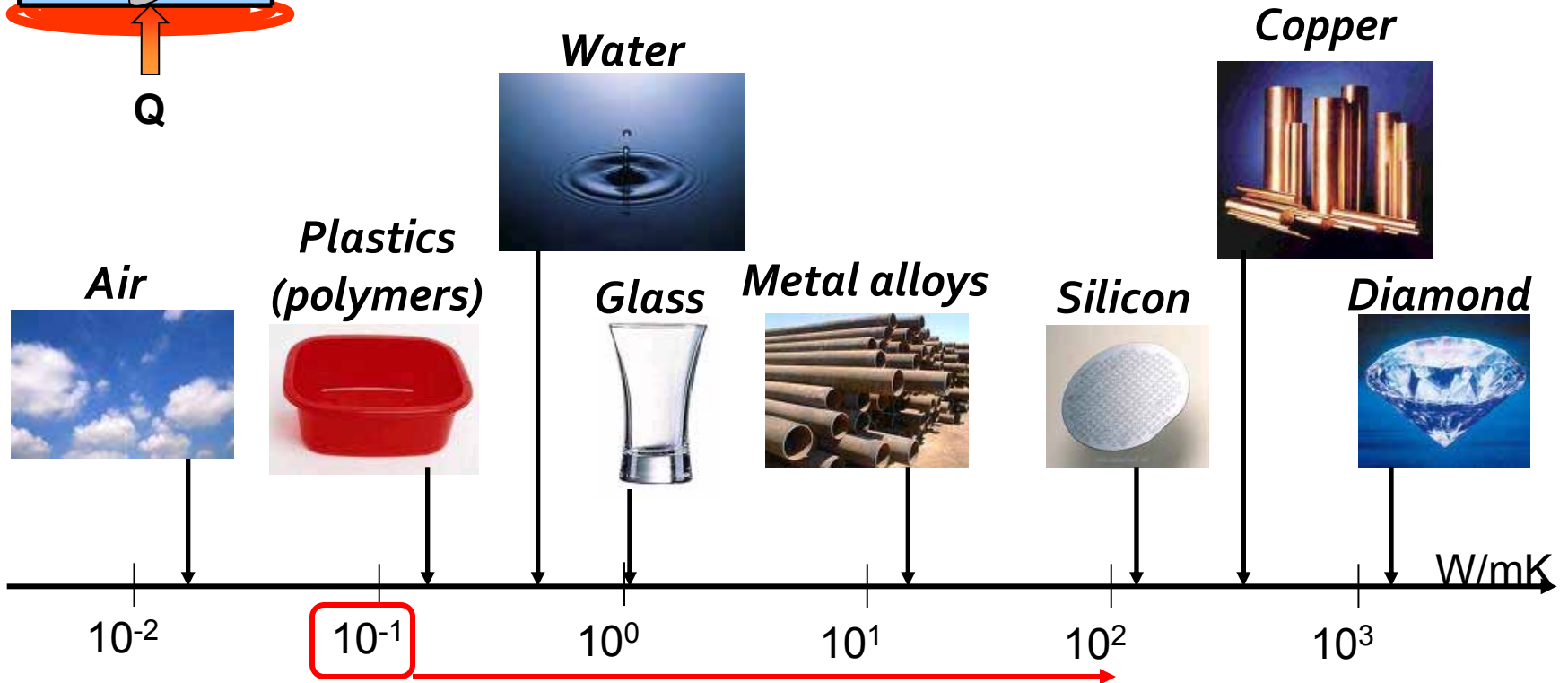
Computer Chips

Thermal Conductivity

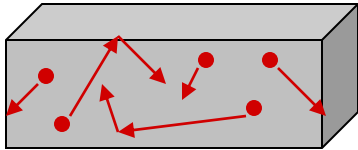


$$K =$$

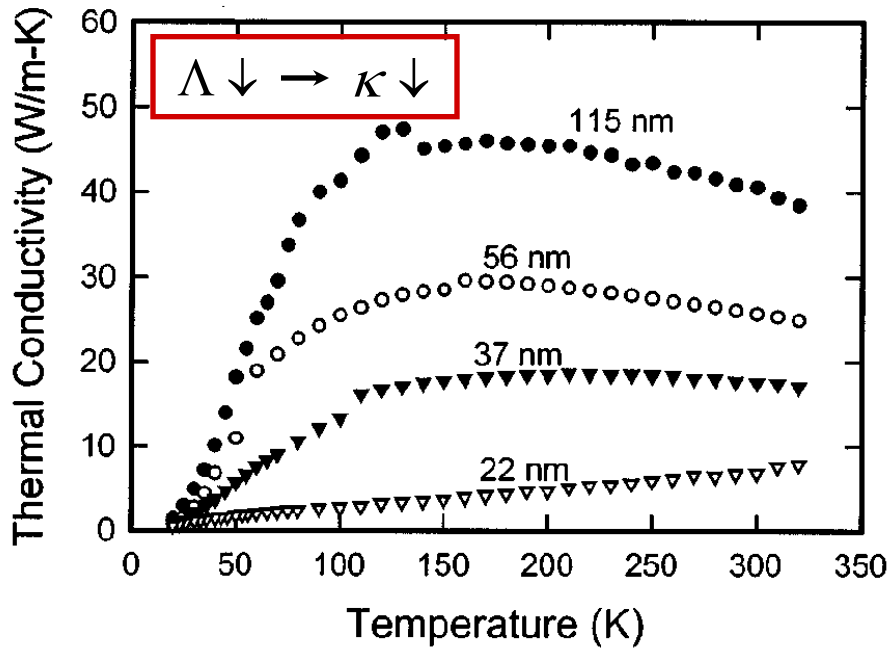
- How well a material can conduct heat/energy
- How strongly the atomic motions are coupled



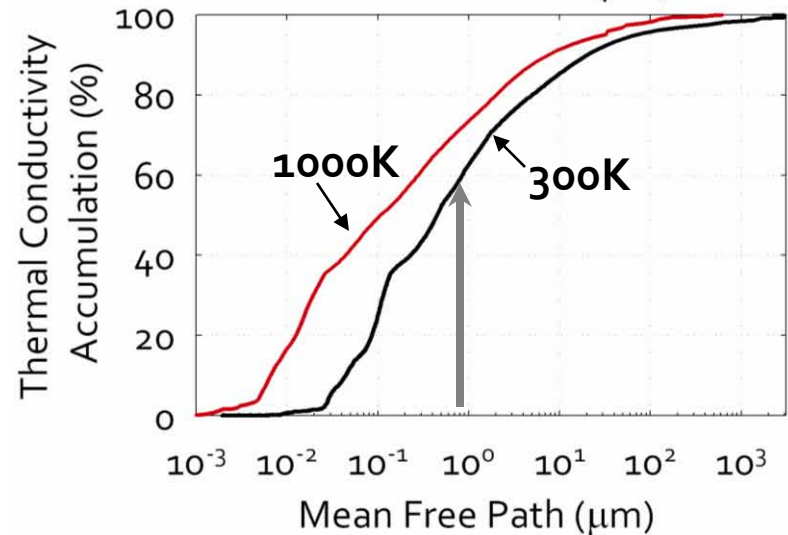
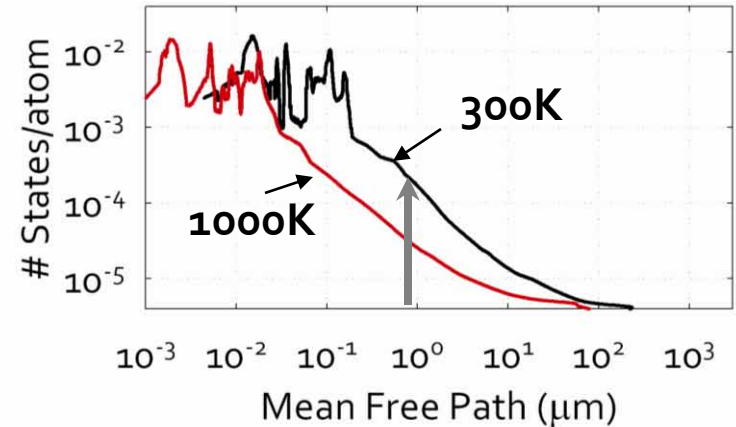
Classical Size Effects



$$\kappa = \frac{1}{3} \sum_p \int_0^{v_{\max}} C \cdot v \cdot \Lambda \cdot dv$$



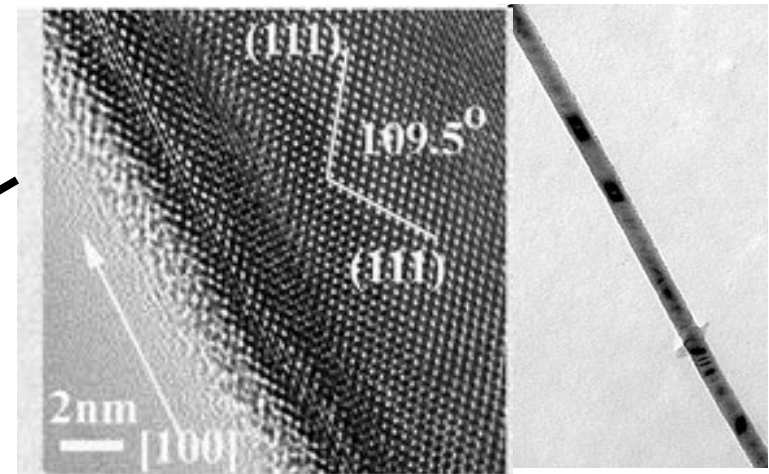
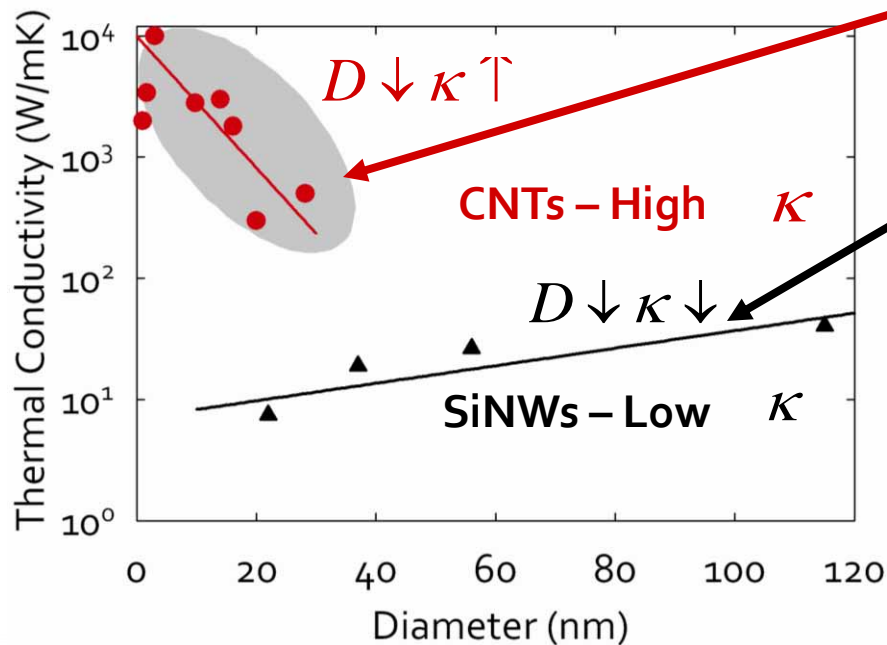
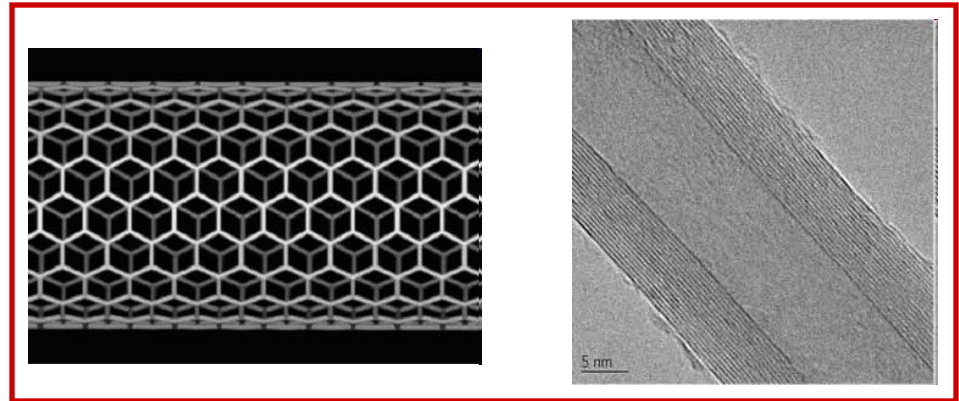
D. Li et al., Appl. Phys. Lett. **83**, 14, 2934-2936 (2003)



A. Henry and G. Chen, J. Comput. Theor. Nanosci., **5**, 2, 141-152 (2008)

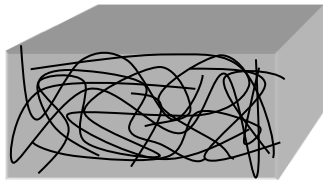
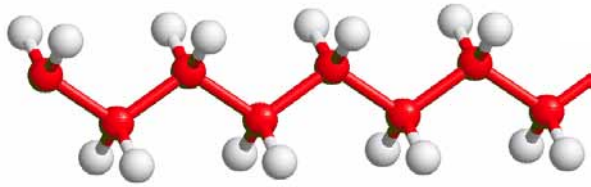
1D Nanostructures

- SiNW $D \downarrow \kappa \downarrow$
- CNTs $D \downarrow \kappa \uparrow$
- Why CNTs?
- What about Polymers?



M. Shao et al., Chem. Commun., 2007, 793 (2006)

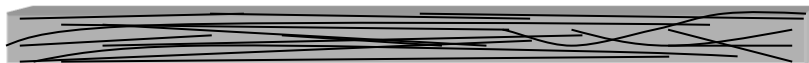
Bulk Polymer Stretching



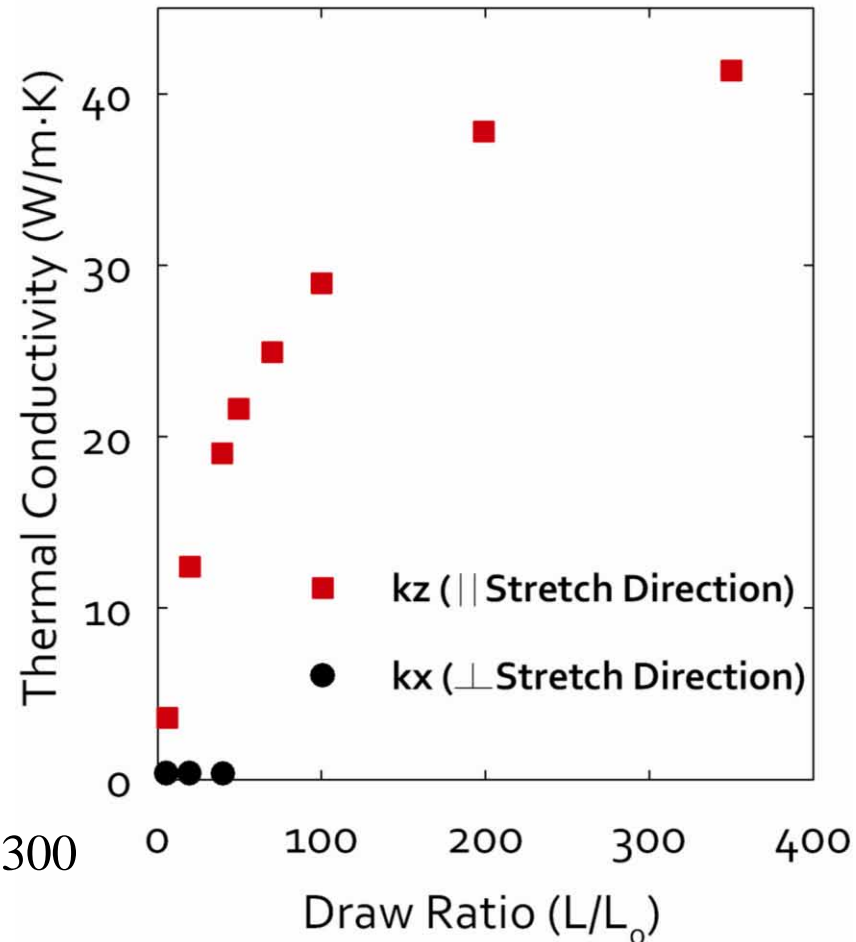
$$\frac{L}{L_0} = 1 \quad \kappa_{BULK} \sim 0.35 \frac{W}{m \cdot K}$$



$$\frac{L}{L_0} \sim 20$$



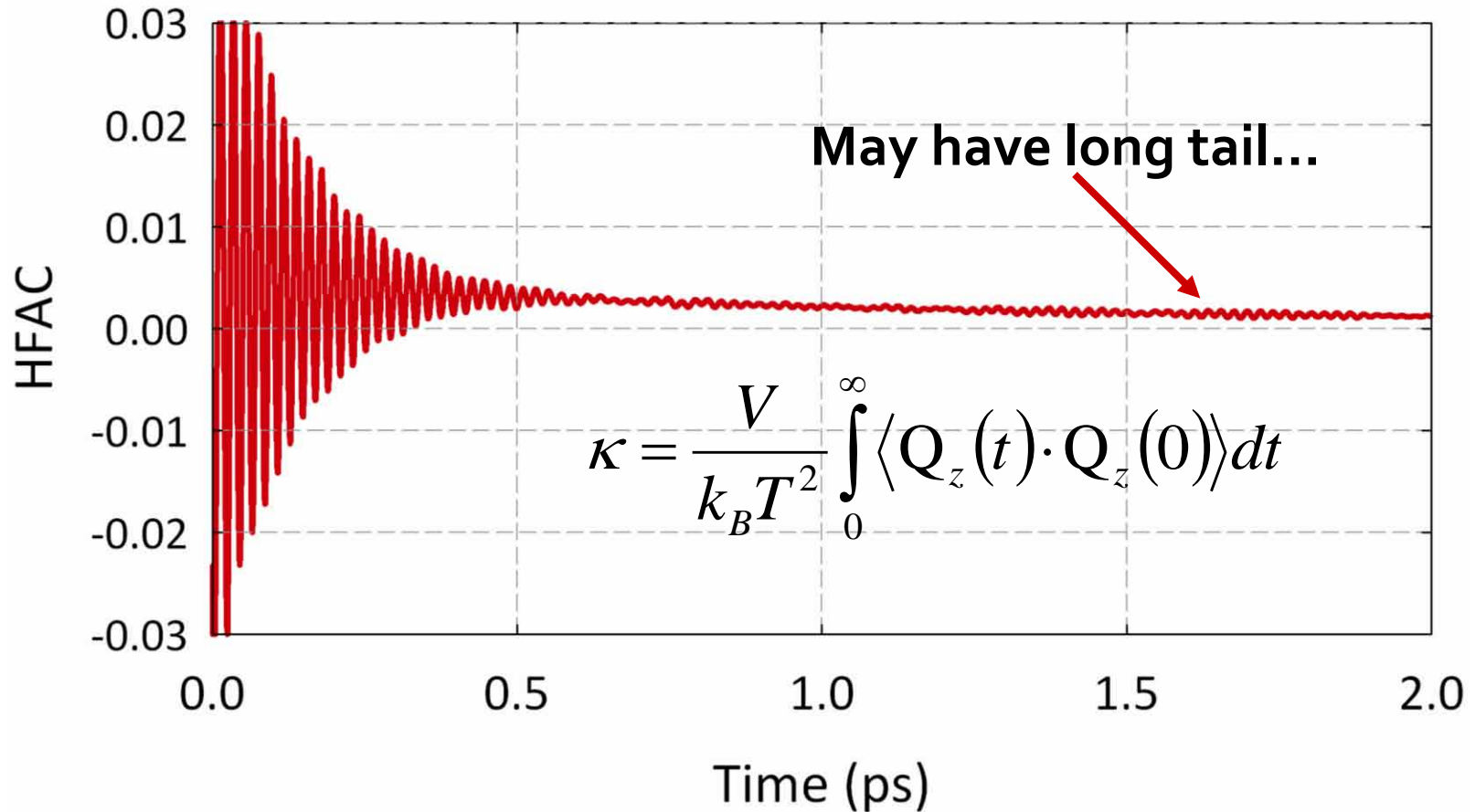
$$\frac{L}{L_0} > 300$$



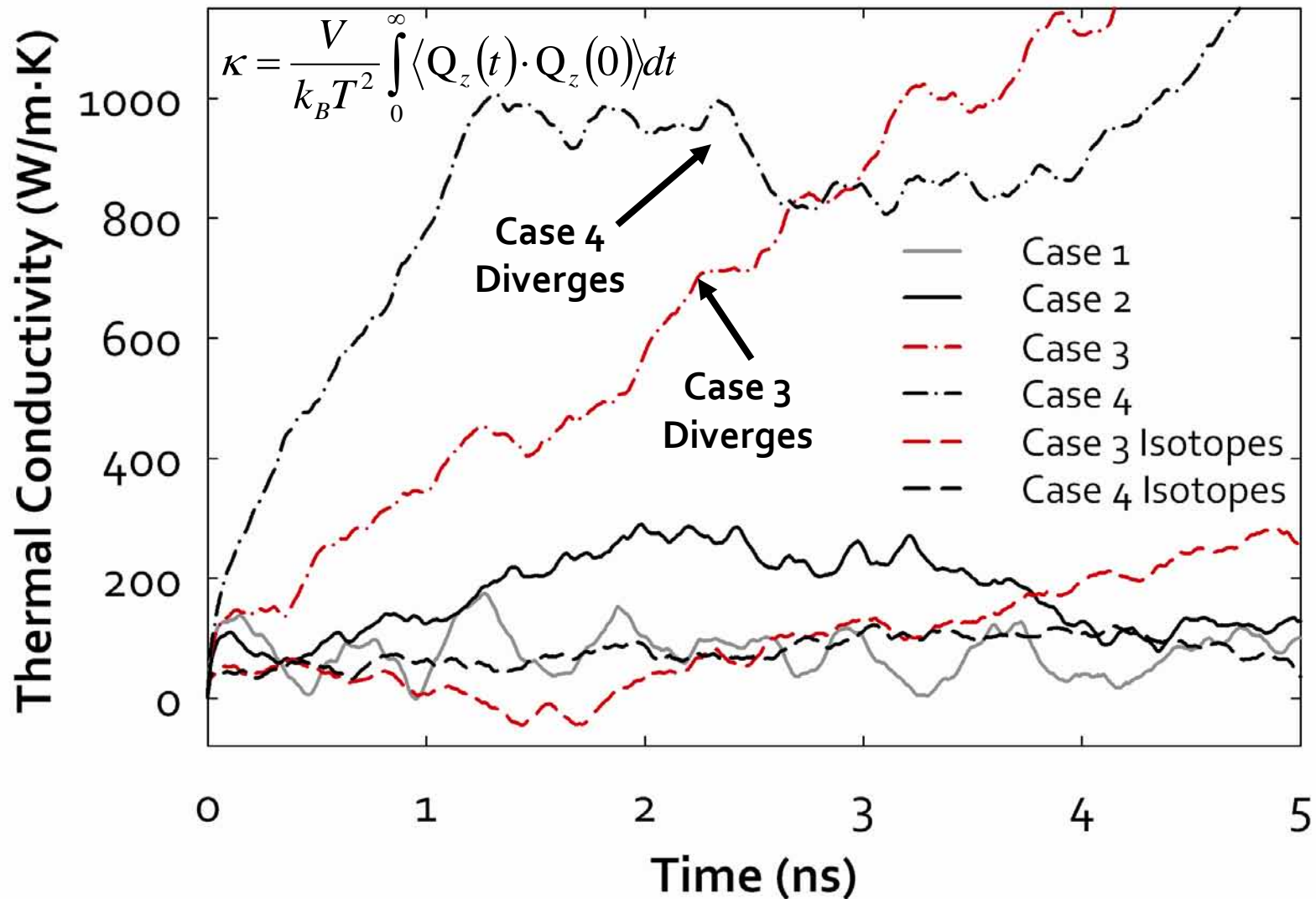
C. L. Choy *et al.*, Journal of Polymer Science: Part B: Polymer Physics, 37, 3359-3367 (1999).

Green-Kubo Analysis

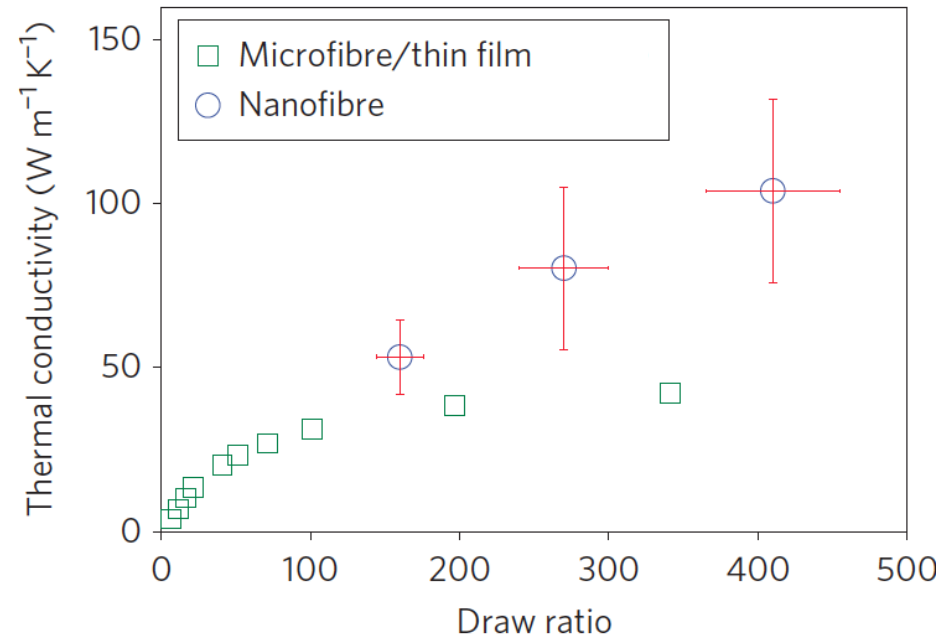
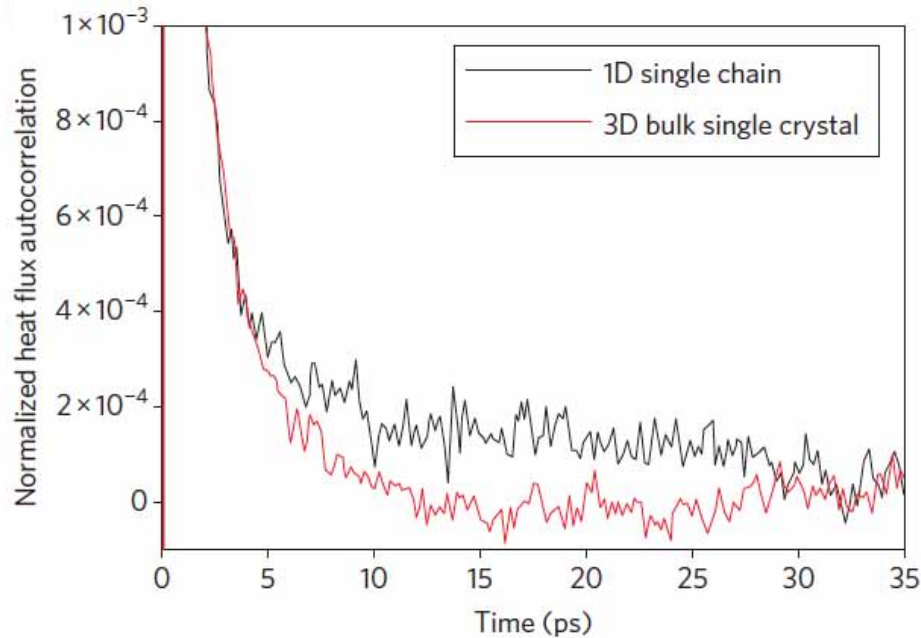
Heat Flux Autocorrelation



Single Polyethylene Chains



Polyethylene Nanofibers



S. Shen, A. Henry, J. Tong, R. Zheng and G. Chen, *Nature Nanotechnology* **5**, 251 - 255 (2010)

Acknowledgements

- Prof. Gang Chen, MIT
- Prof. Millie Dresselhaus, MIT
- Prof. John Lienhard, MIT
- Dr. Steven Plimpton, Sandia National Laboratories
- Dr. Aidan Thompson, Sandia National Laboratories
- NanoEngineering Group, MIT
- DOE – Computational Science Graduate Fellowship

