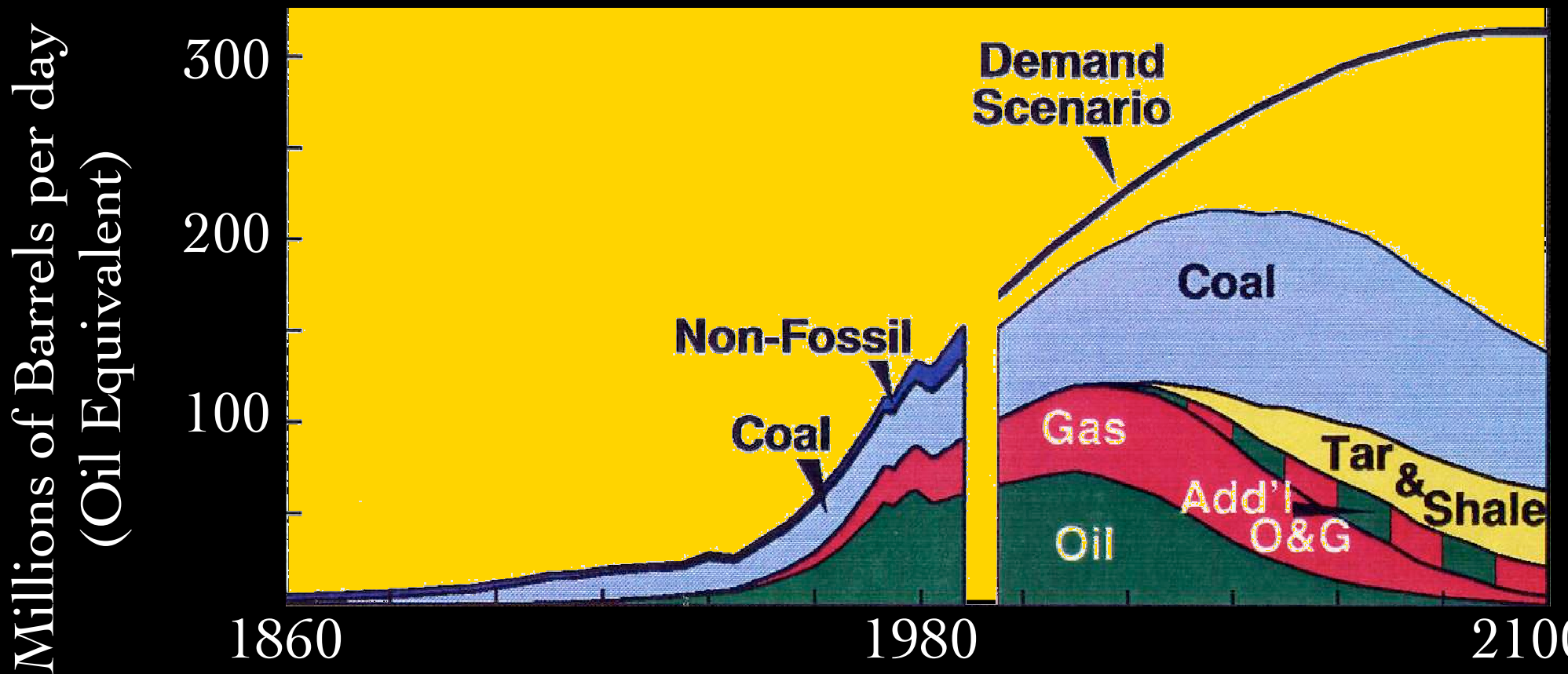
Microstructure Effects of Thermoelectric Nanowire Composites

8/24/2006

Mara Howell
Prof. R. Edwin García
Prof. Tim Sands

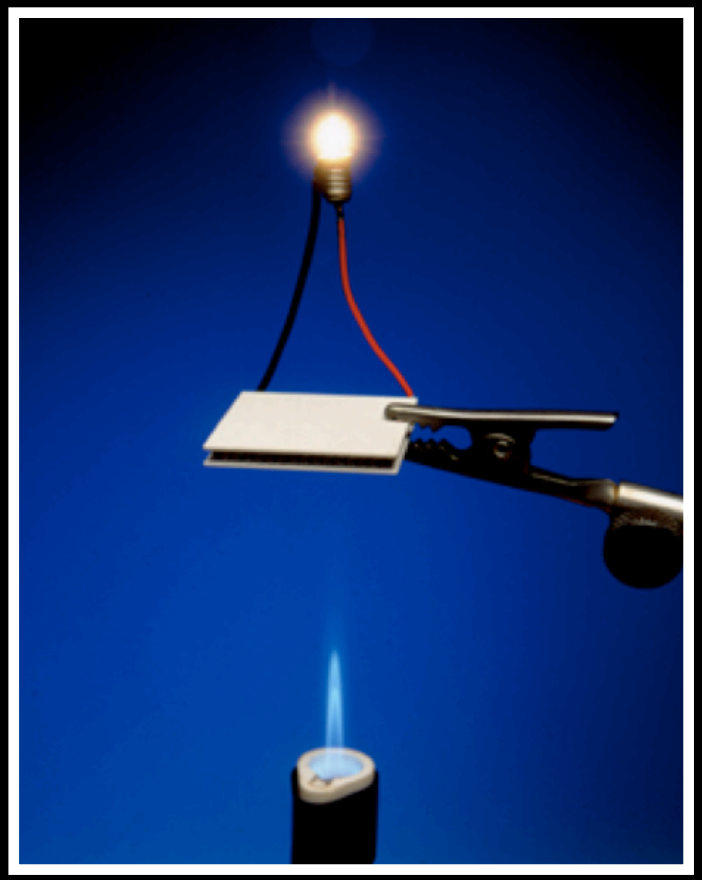
PURDUE
UNIVERSITY

Motivation



Bookout, John F. (President of Shell USA) ,"Two Centuries of Fossil Fuel Energy" International Geological Congress, Washington DC; July 10,1985.

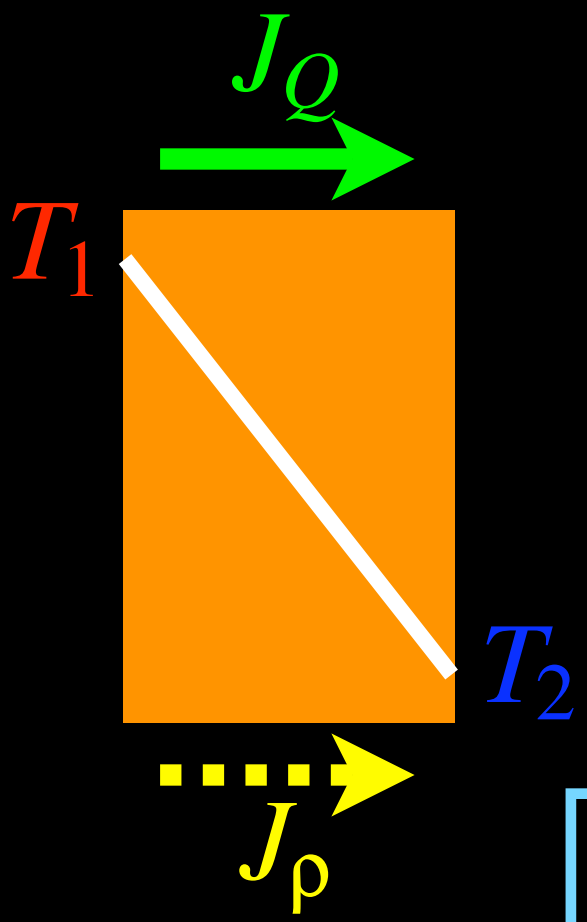
$$ZT = \frac{S^2\sigma}{\kappa_{el} + \kappa_{ph}}T$$



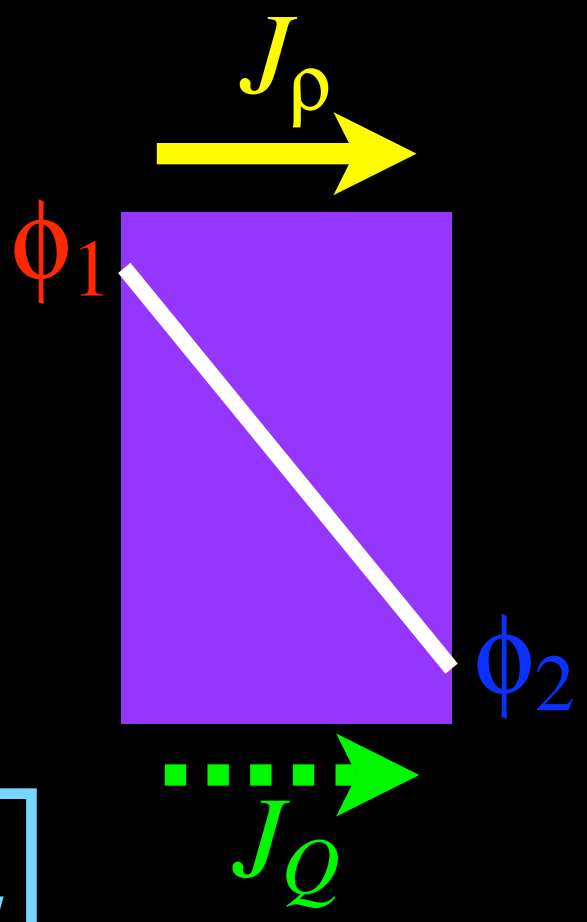
www.tellurex.com

Thermoelectricity

Seebeck ("Direct") Effect

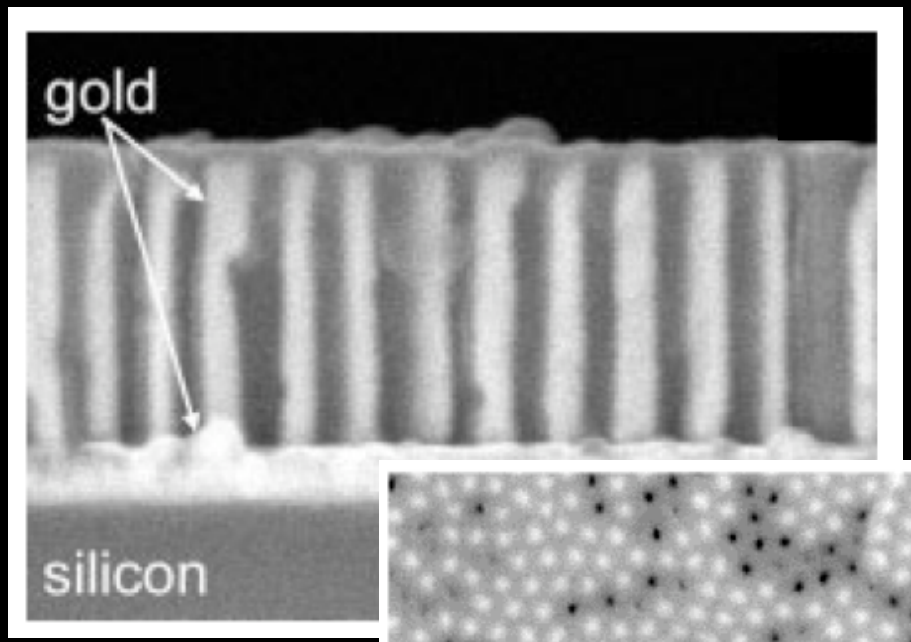


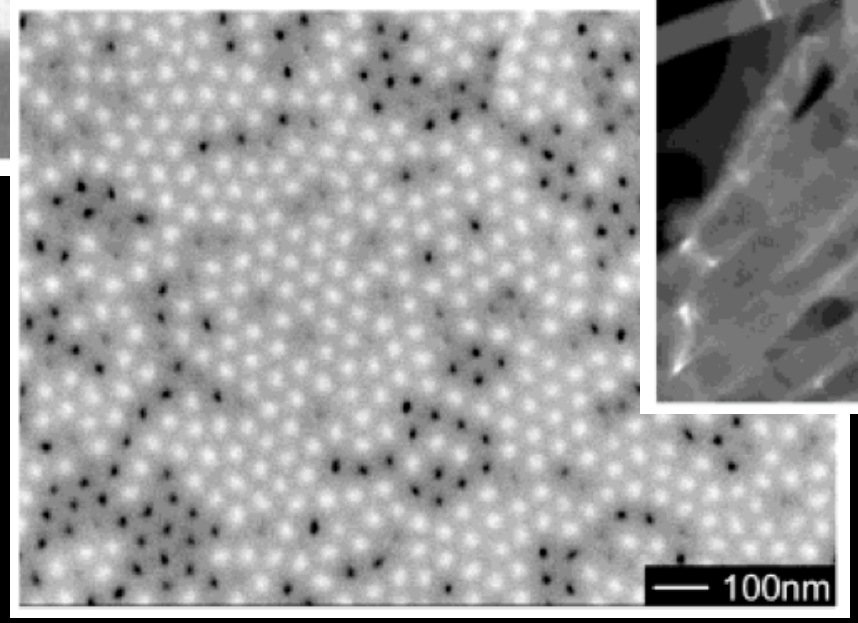
Peltier ("Converse") Effect

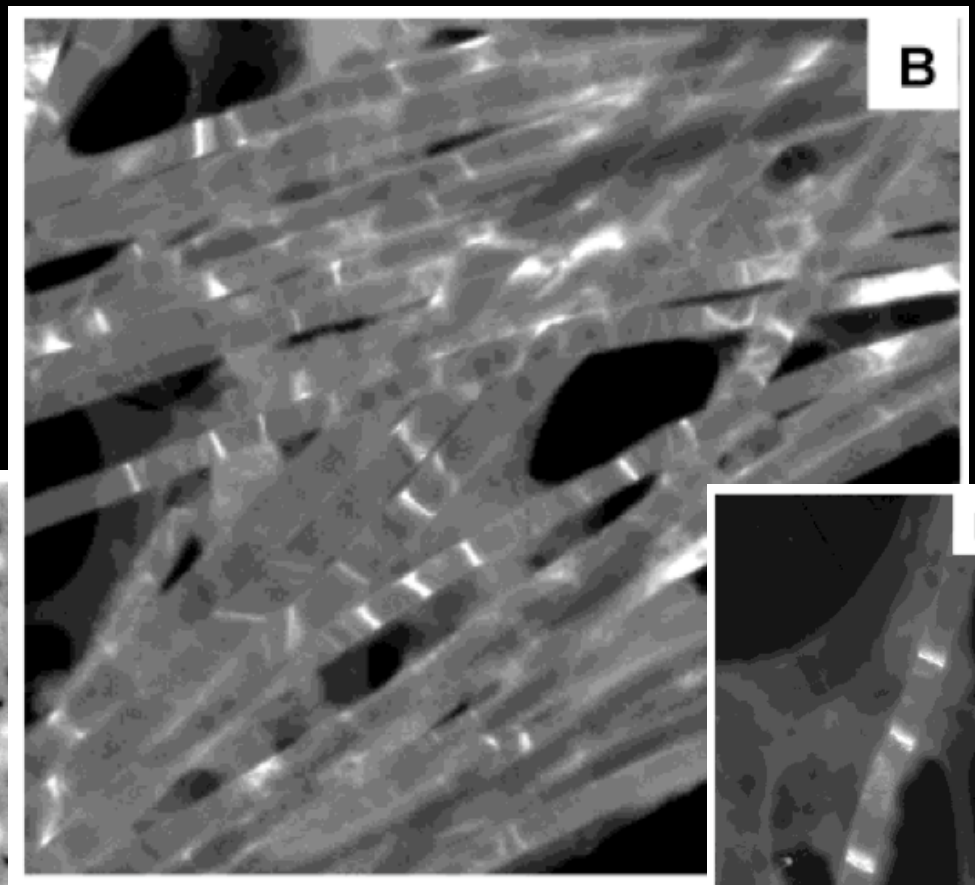


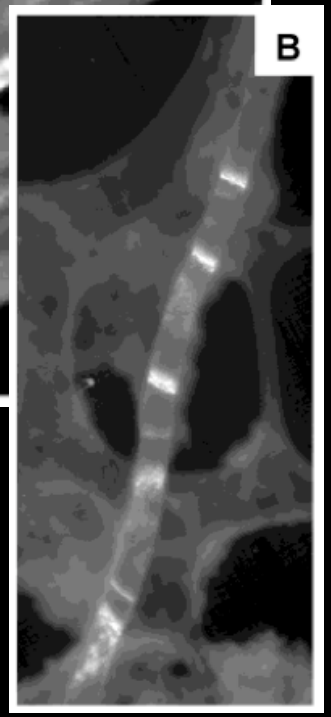
$$ZT = \frac{S^2\sigma}{\kappa_{el} + \kappa_{ph}}T$$

Nanowire Composites





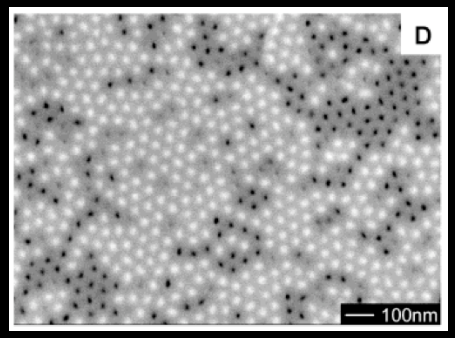


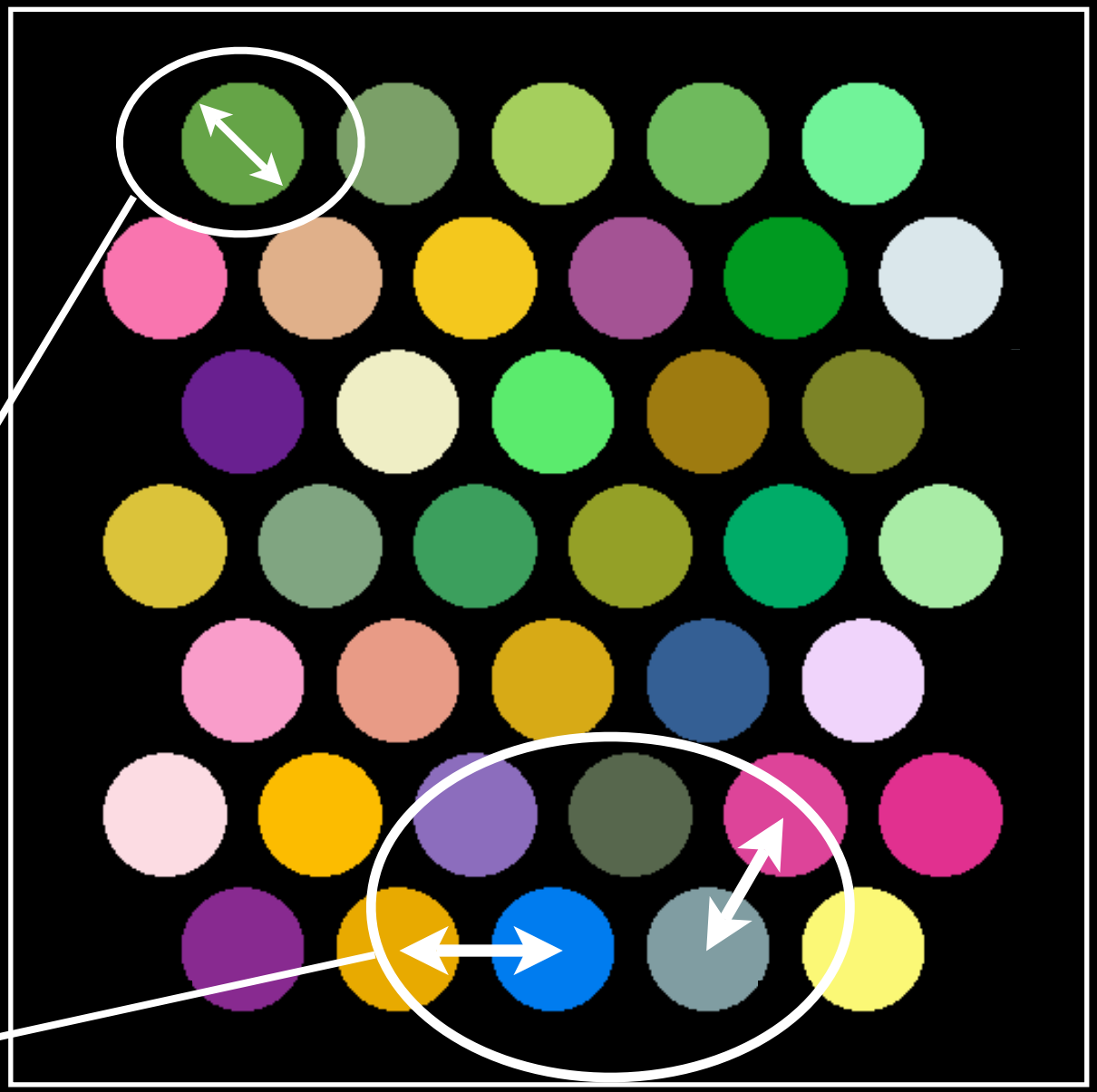


Sander et al., Chem. Mat., V. 15, 2002

Sander, M.S., Tan, L.-S., Advanced Functional Materials 13 (2003) p. 393.

Microstructural Effects



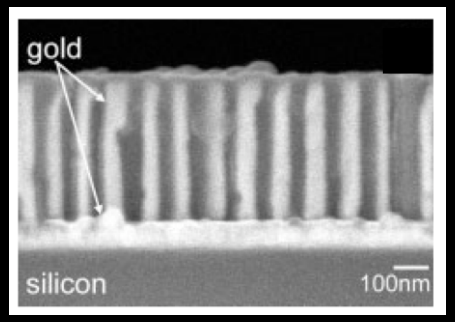


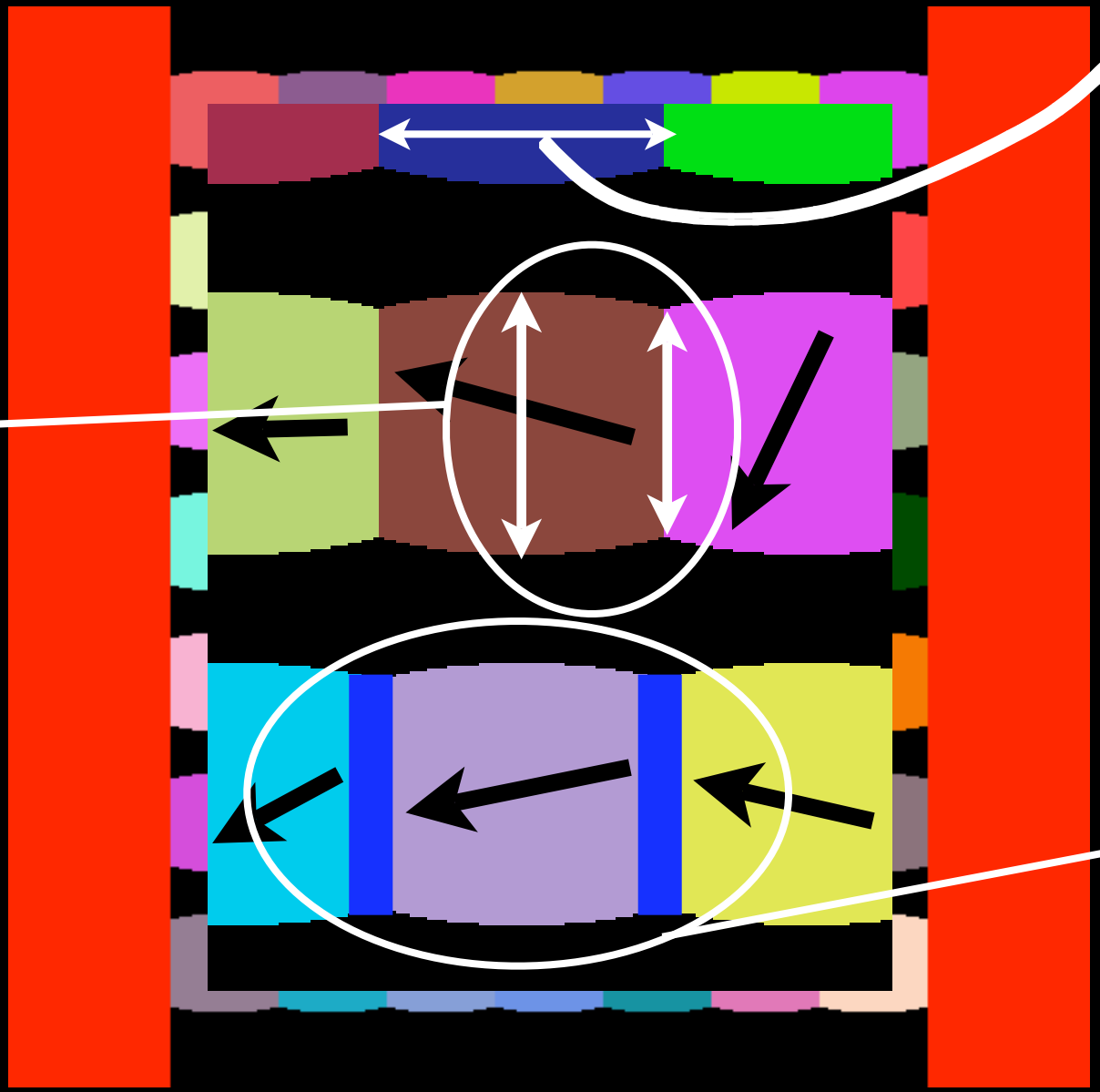
Wire diameter

Volume fraction of nanowire

Spacing between wires

Microstructural Effects





Length of grains

Wire diameter

Grain boundaries

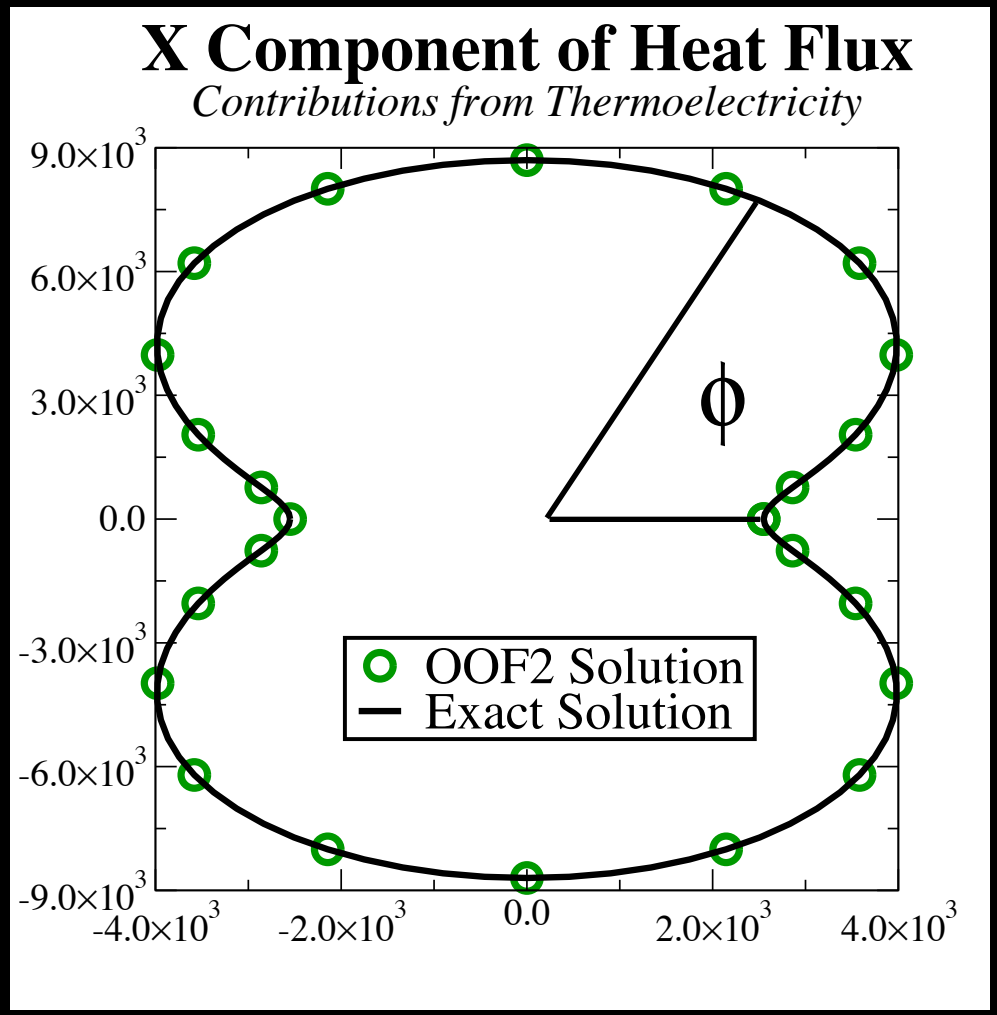
Extending OOF2

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

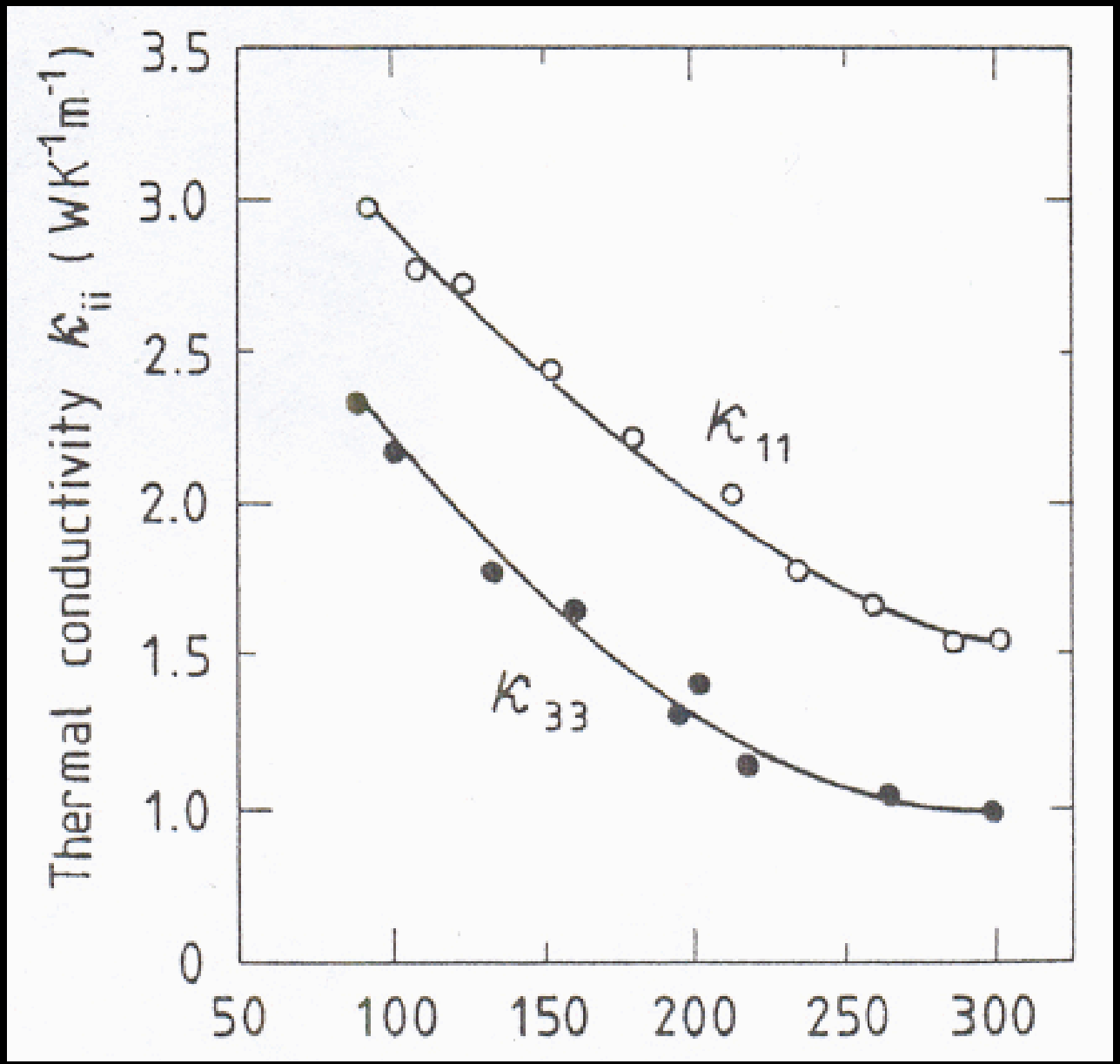
$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \vec{J}_\rho$$

$$\vec{J}_Q = -\overleftrightarrow{\kappa}\,\nabla T - T\,\overleftrightarrow{L}\,\nabla \phi$$

$$\vec{J}_\rho = -\overleftrightarrow{\sigma}\,\nabla \phi - \overleftrightarrow{L}\,\nabla T$$



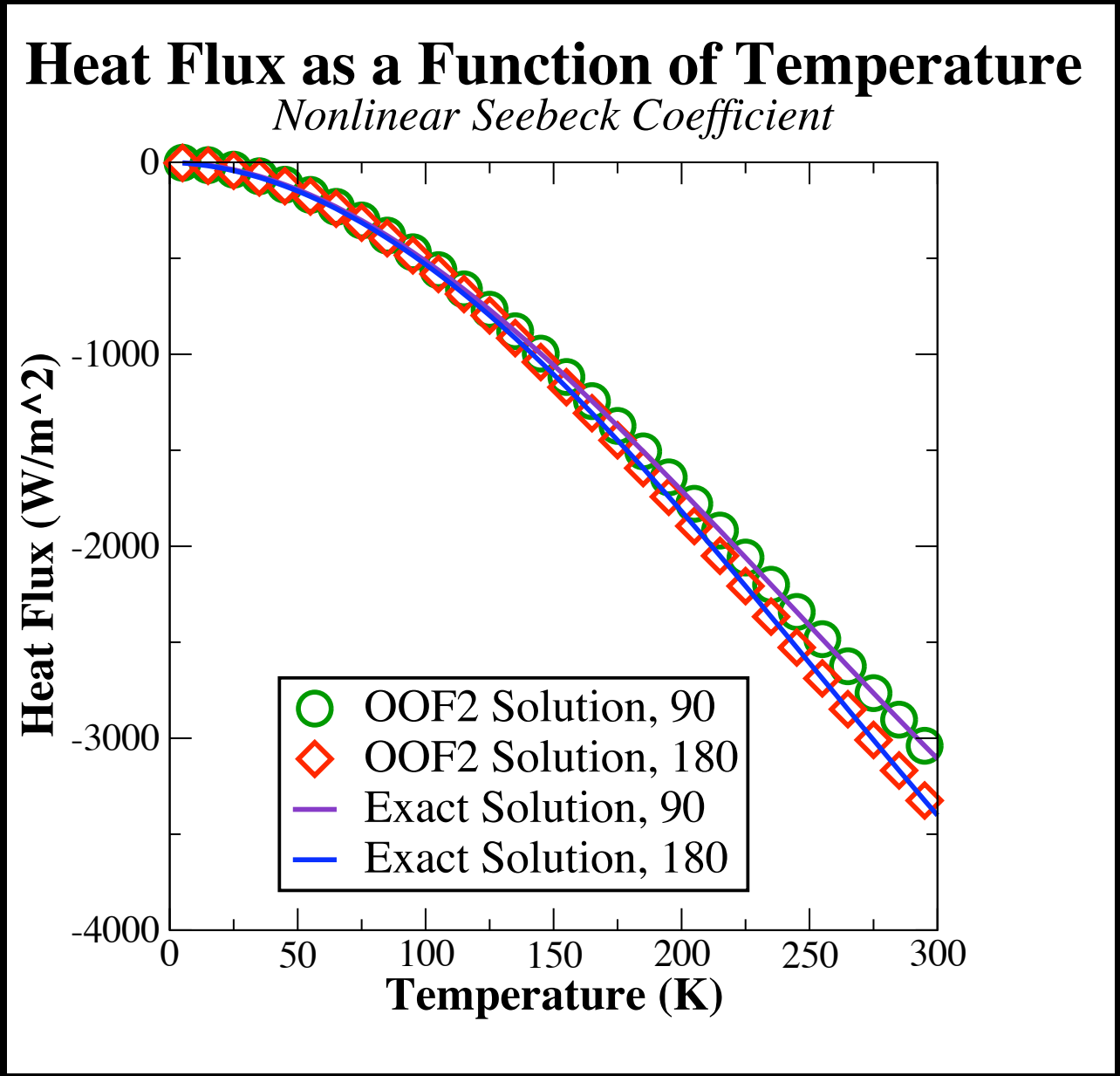
Validation of Model



Non-Linear Properties for Bismuth Telluride

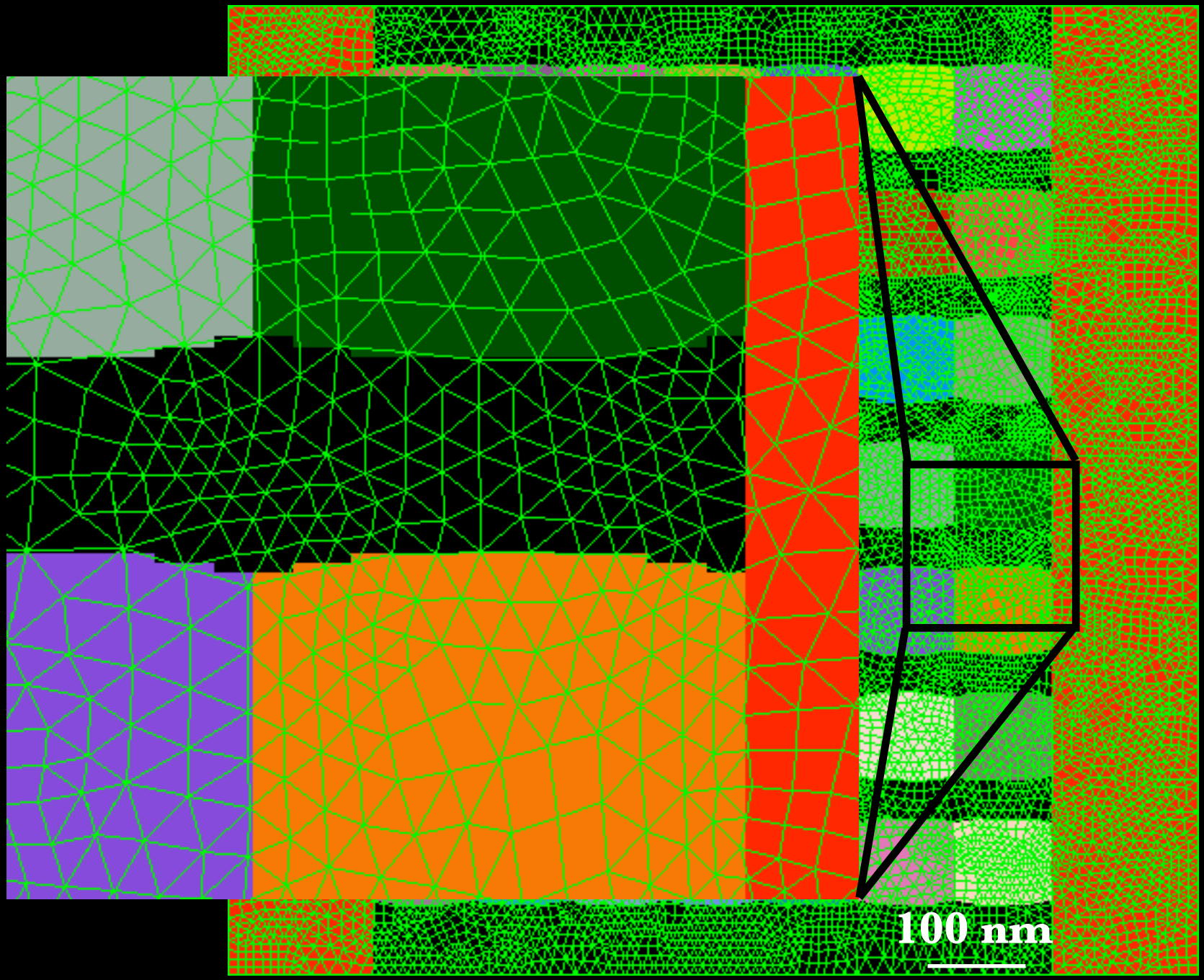
Kaibe, H. et al., J. Phys. Chem. Solids, V. 50, 1989

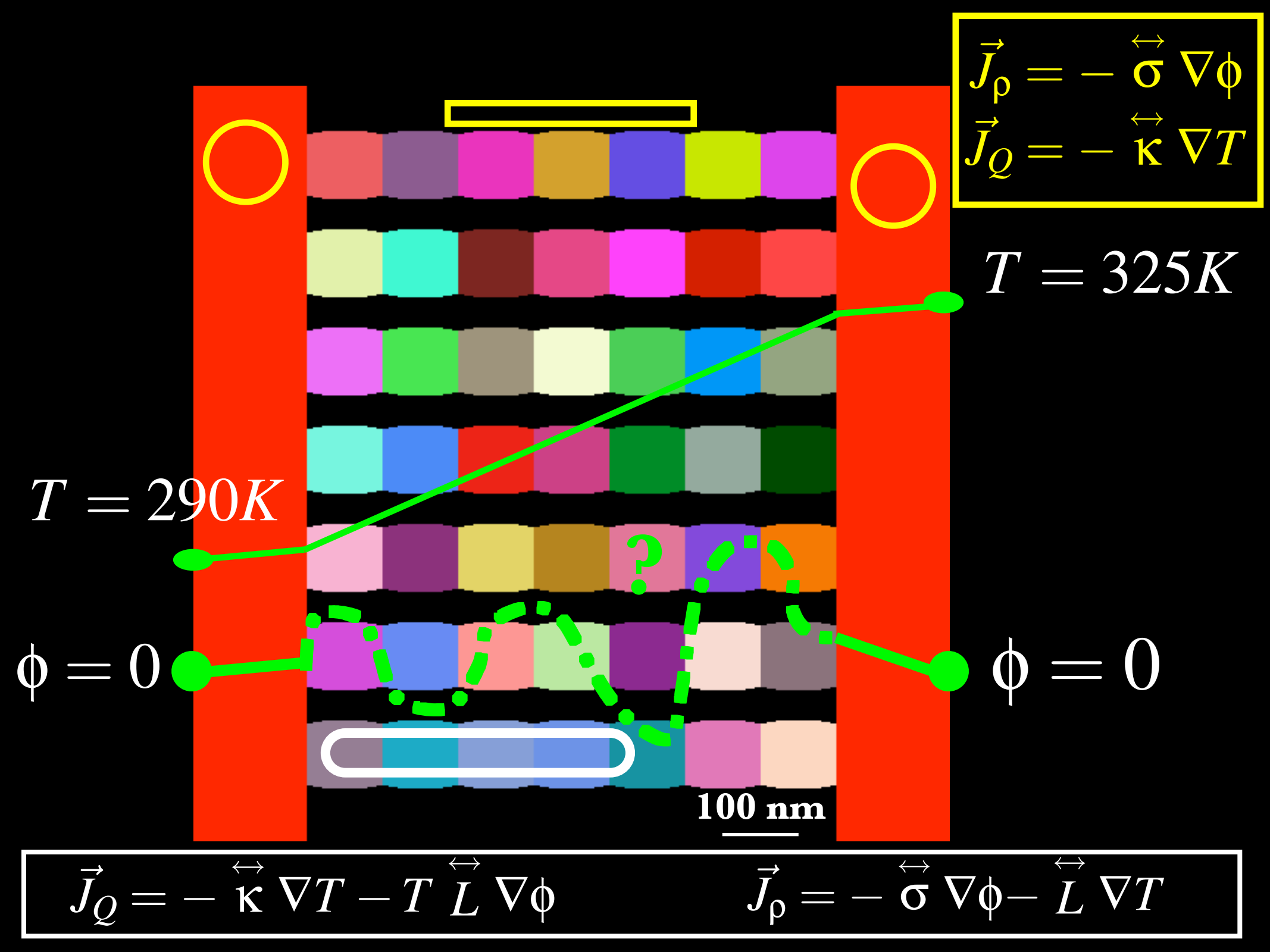
Validation of Model



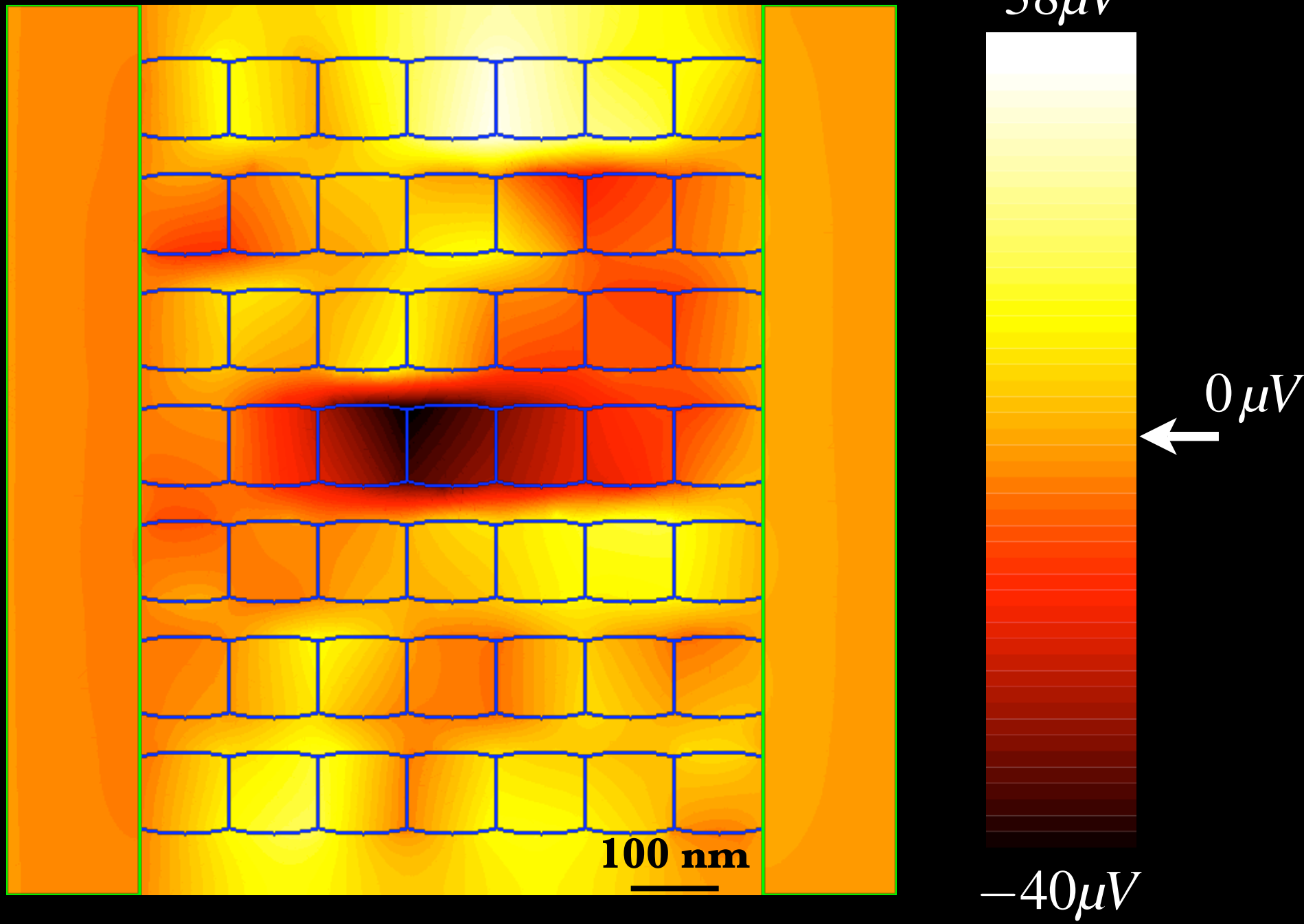
$$J_Q = -\kappa \nabla T - T \cdot L \nabla V$$

Analytical and numerical solutions differ by 1 part per 10 million

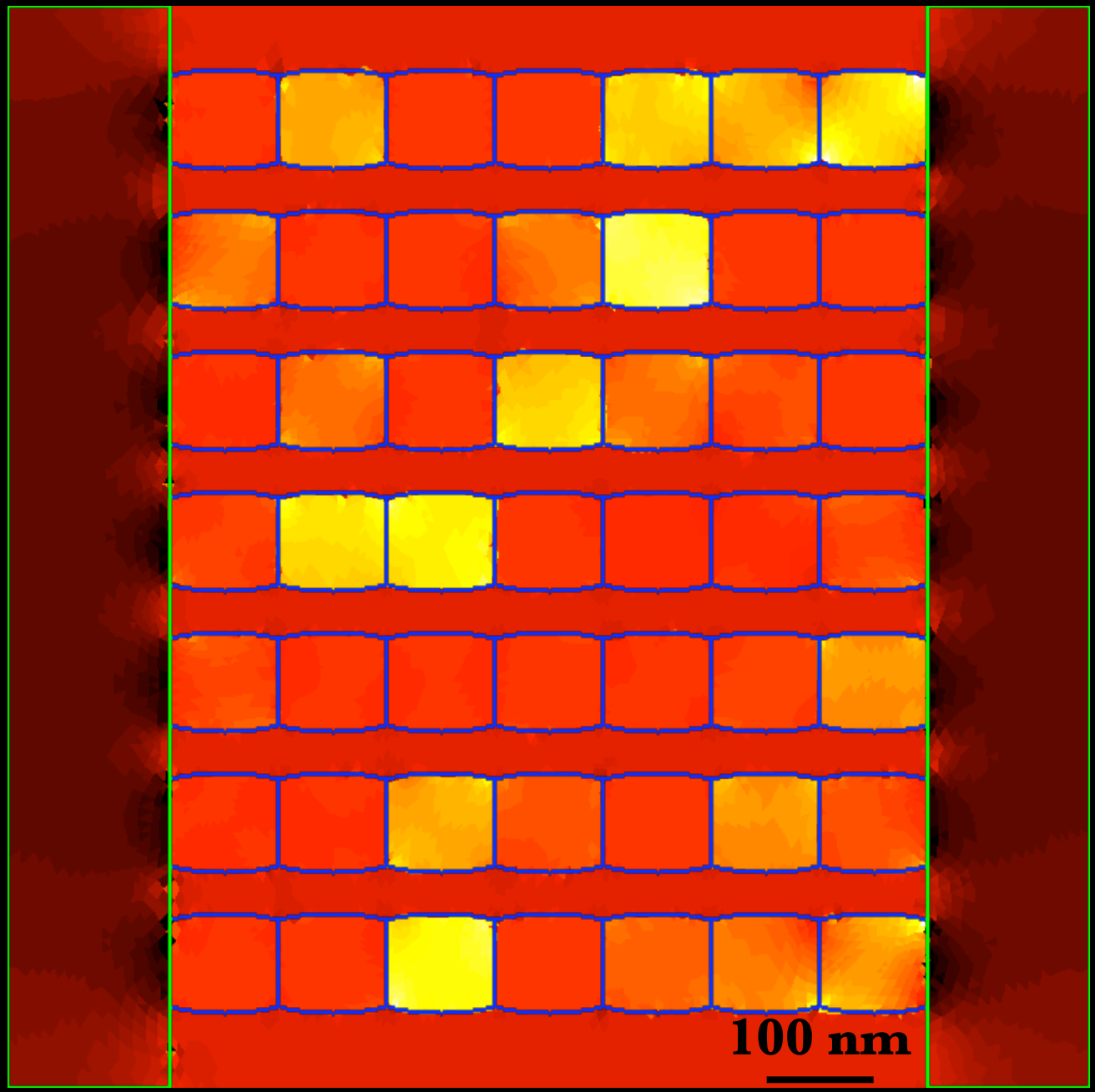

100 nm

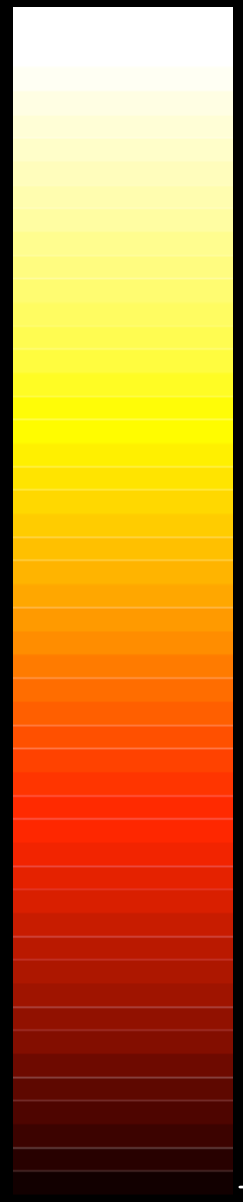

$\vec{J}_\rho = -\overleftrightarrow{\sigma}\,\nabla\phi$
$\vec{J}_Q = -\overleftrightarrow{\kappa}\,\nabla T$
$T = 325K$
$T = 290K$
?
$\phi = 0$
$\phi = 0$
100 nm
$\vec{J}_Q = -\overleftrightarrow{\kappa}\,\nabla T - T\,\overleftrightarrow{L}\,\nabla\phi$
$\vec{J}_\rho = -\overleftrightarrow{\sigma}\,\nabla\phi - \overleftrightarrow{L}\,\nabla T$

Voltage Field



Heat flux in the x direction



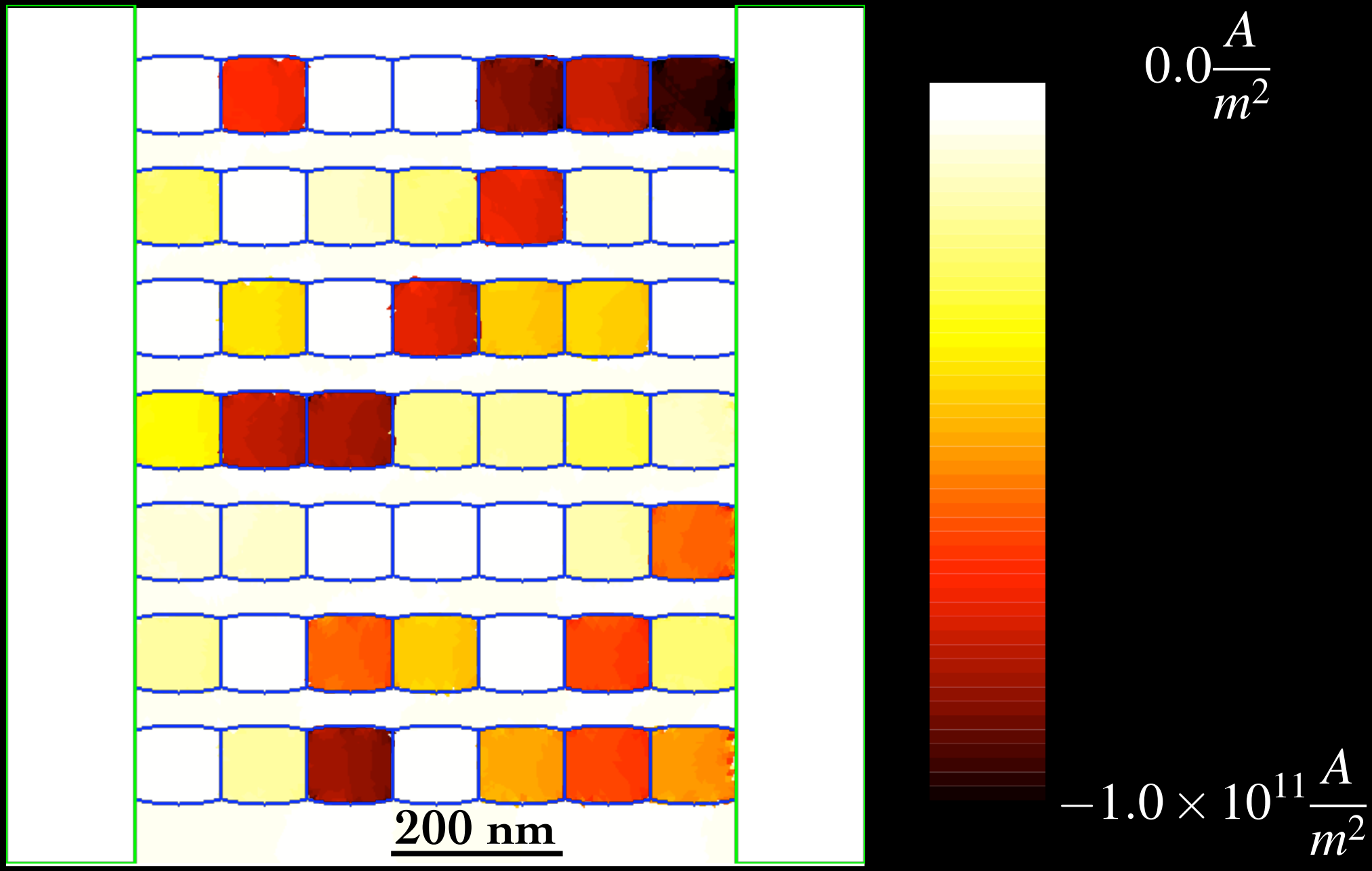


$100 \frac{MW}{m^2}$

$0 \frac{MW}{m^2}$

$-100 \frac{MW}{m^2}$

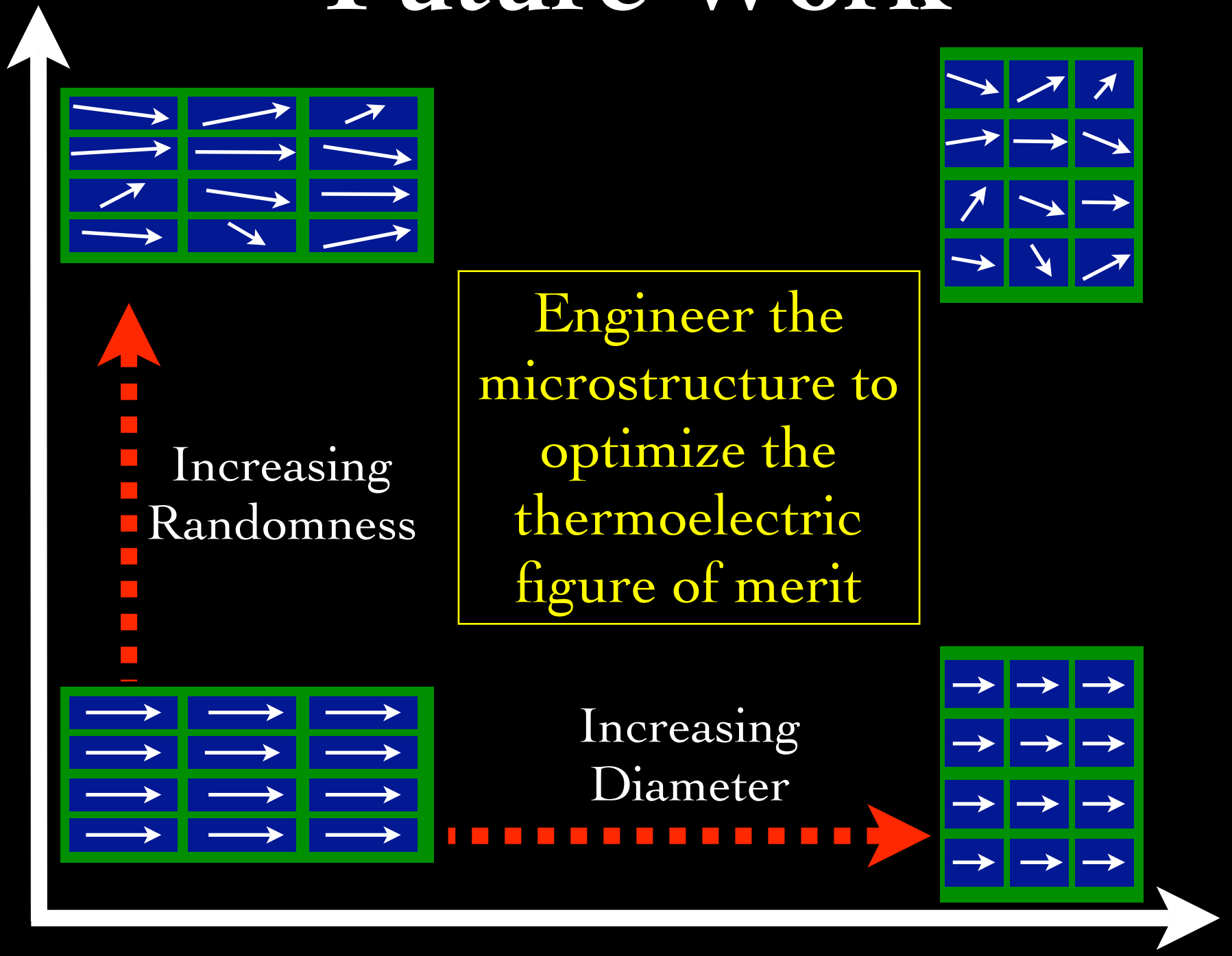
Charge flux in the x direction



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

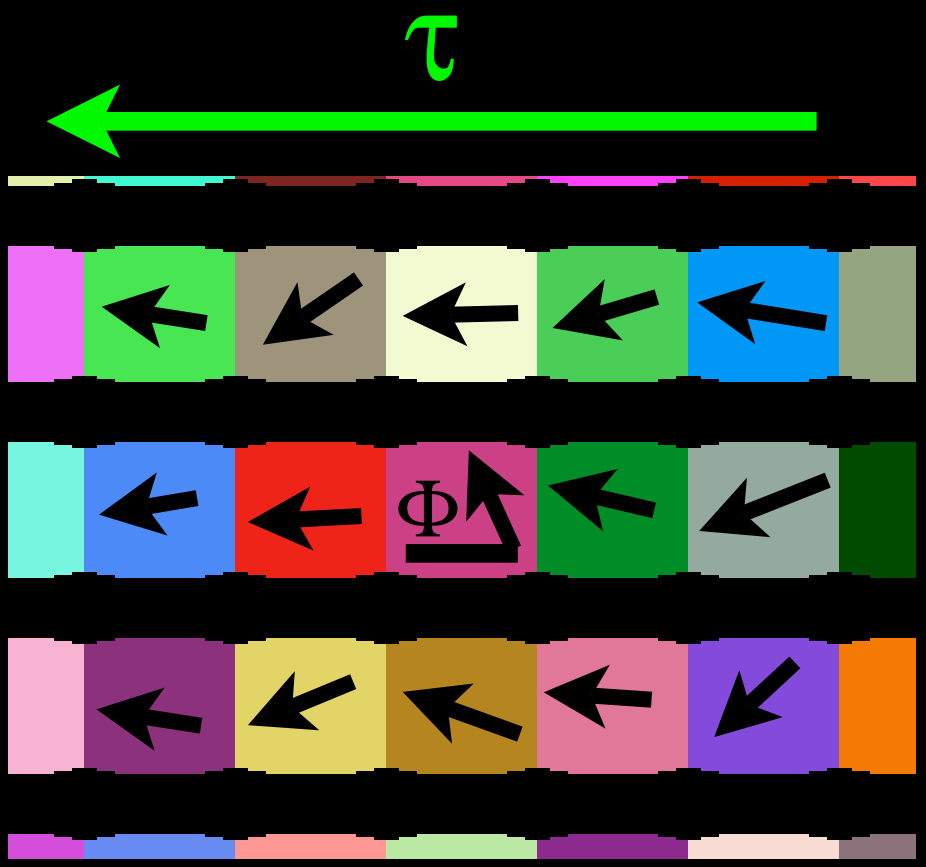
Future Work

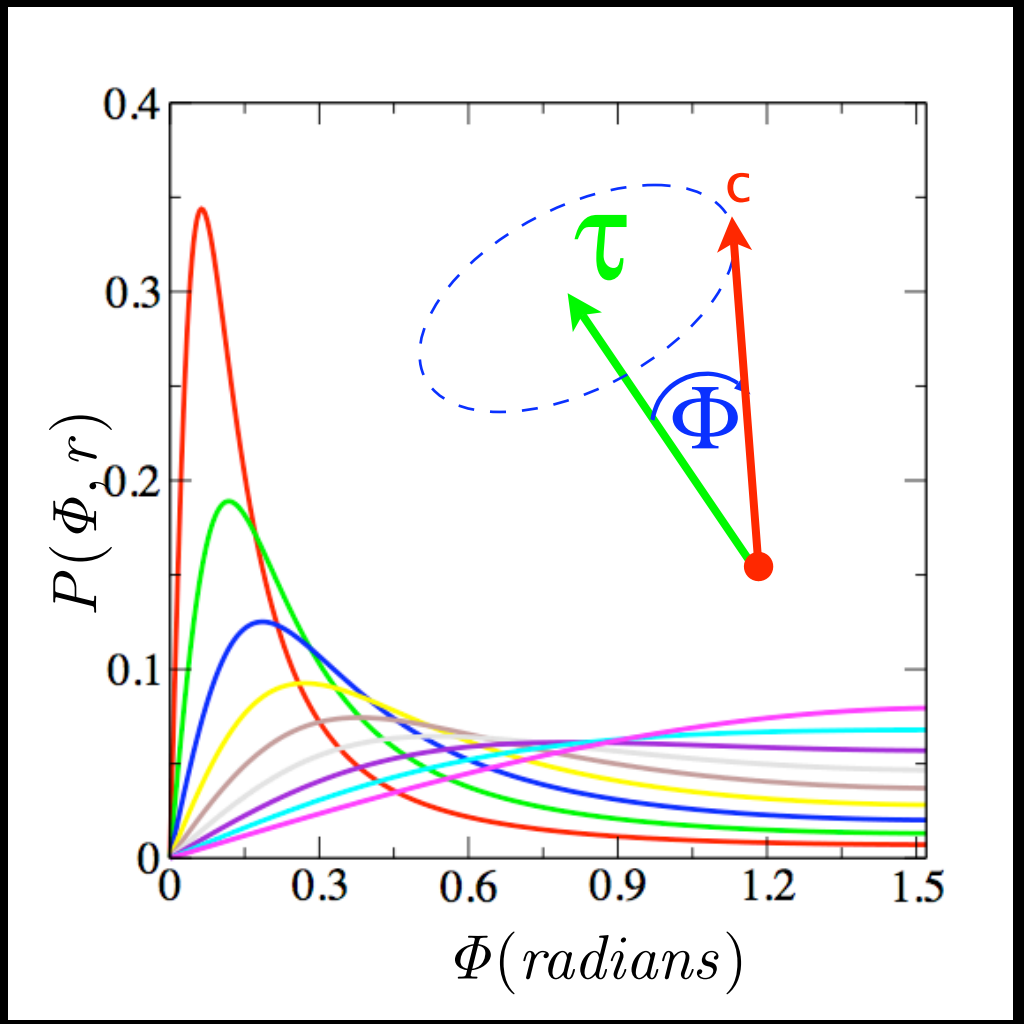

Increasing Randomness
Engineer the microstructure to optimize the thermoelectric figure of merit
Increasing Diameter

Questions??

Mara Howell
mhowell@purdue.edu

Texture Analysis





March Dollase Texture
Probability Distribution

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