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Phonon considerations in the reduction of thermal conductivity in phononic crystals

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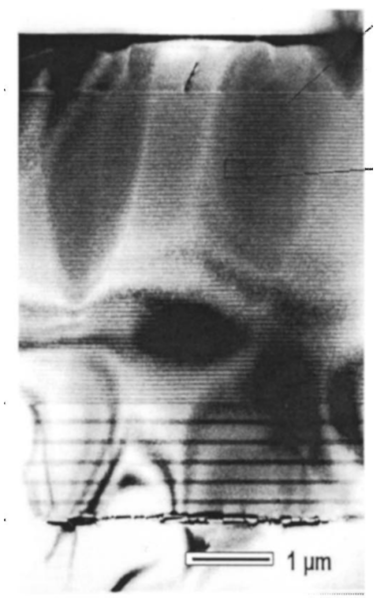
Controlling thermal conductivity through phonon transport

Phonon engineering for thermoelectric applications

Thermoelectric Figure of Merit

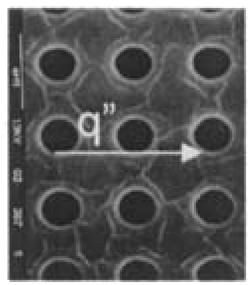
$$Z = \frac{S^2 \sigma}{\kappa}$$

Superlattices



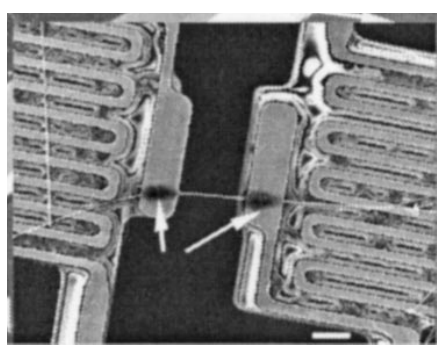
Cahill *et al*. Journal of Heat Trans. **124**, 233 (2002)

Microporous materials



Song and Chen, APL **84**, 687 (2004)

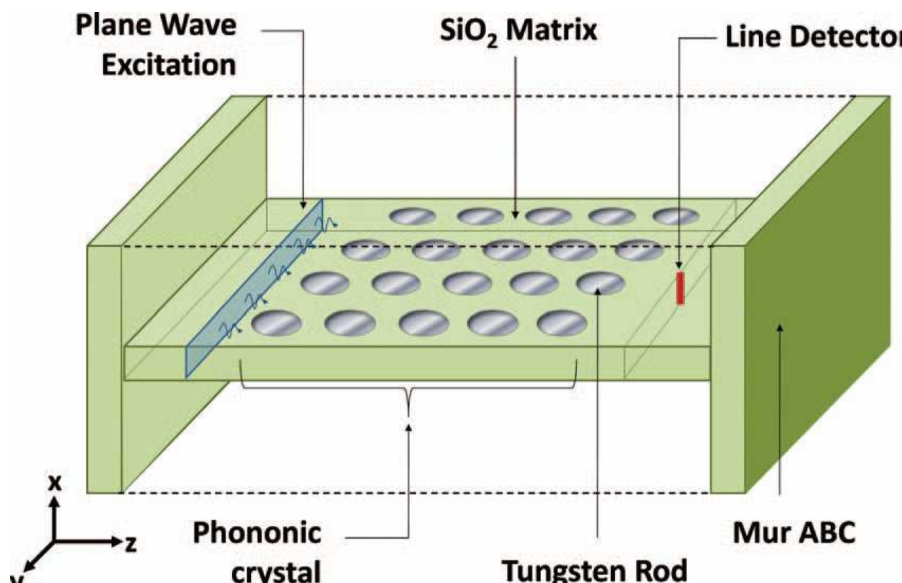
Nanowires



Li *et al*., APL **83**, 2934 (2003)

Recent realization of GHz PnC

Su, Olsson, Leseman, and El-Kady, APL **96**, 05311 (2010)



More details in this session at 15:10 (Roy H. Olsson III)

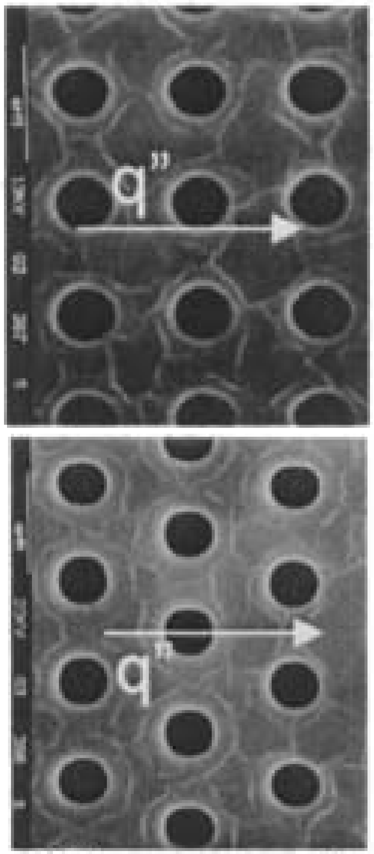
Outline

Goal: Study phonon scattering and thermal conductivity reduction in PnC

- Predicting the thermal conductivity in periodically arranged porous solids
- Thermal conductivity reduction in the PnC
- Thermal conductivity measurements of PnC with time-domain thermoreflectance

Thermal conductivity in periodic, porous Si

Aligned

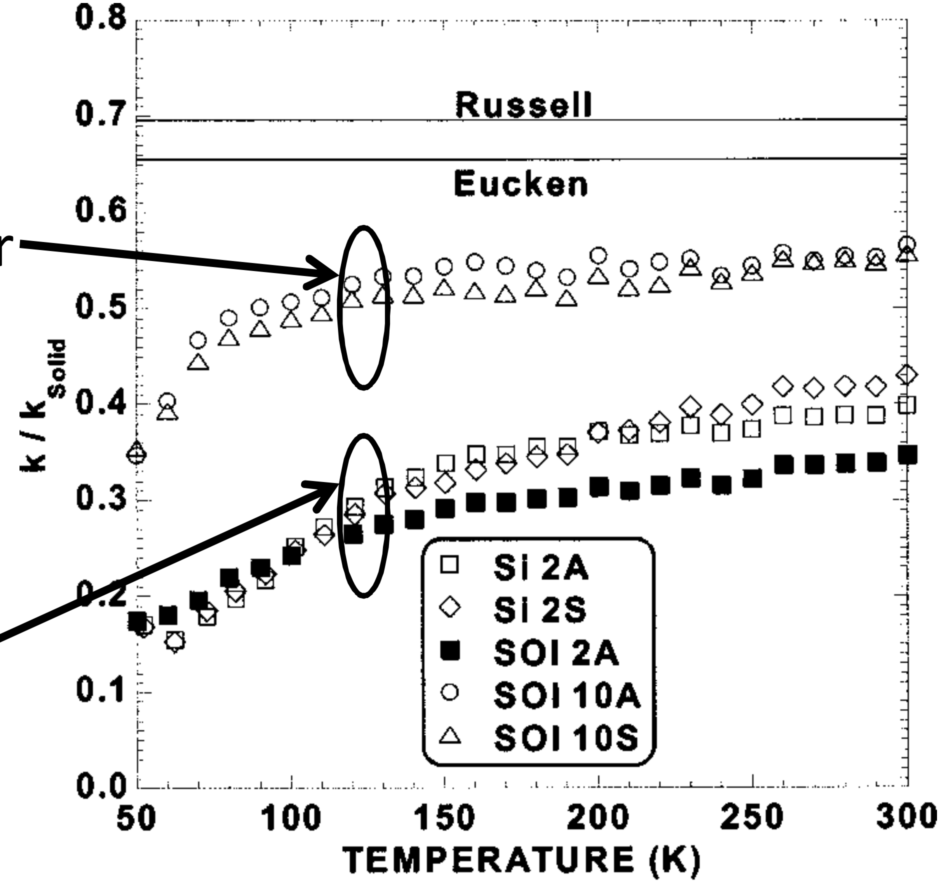


Staggered

10 μm diameter

2 μm diameter

Song and Chen, APL **84**, 687 (2004)



How can we model this thermal conductivity reduction?

Thermal conductivity in bulk Si

Thermal conductivity

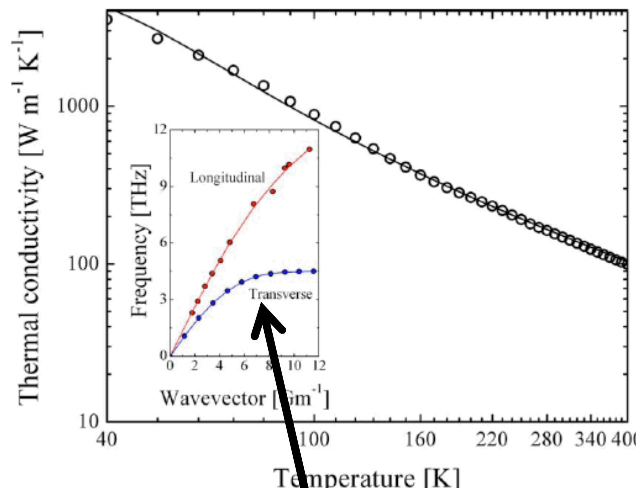
$$\kappa = \frac{1}{6\pi}\sum_j \int_q \frac{\hbar^2\omega_j^2(q)}{k_B T^2} \frac{\exp\left[\frac{\hbar\omega_j(q)}{k_B T}\right]}{\left(\exp\left[\frac{\hbar\omega_j(q)}{k_B T}\right]-1\right)^2} v_j^2(q)\tau_j(q)q^2 dq$$

Fit thermal conductivity model to experimentally measured κ on bulk Si to determine τ (A,B,C, and E)

Scattering time

$$\frac{1}{\tau_j(q)} = \frac{1}{\tau_{\mathrm{Umklapp},j}} + \frac{1}{\tau_{\mathrm{impurity},j}} + \frac{1}{\tau_{\mathrm{boundary},j}}$$

$$\frac{1}{\tau_{Umklapp,j}} = BT\omega_j^2(q)e^{\frac{C}{T}}$$



$$\frac{1}{\tau_{Impurity,j}} = A\omega_j^4(q) \qquad \frac{1}{\tau_{Boundary,j}} = \frac{\partial\omega_j(q)}{\partial q}\frac{1}{E}$$

Fit polynomial to measured dispersion in bulk Si

Similar approach to that described by Mingo, PRB **68** 113308 (2003)

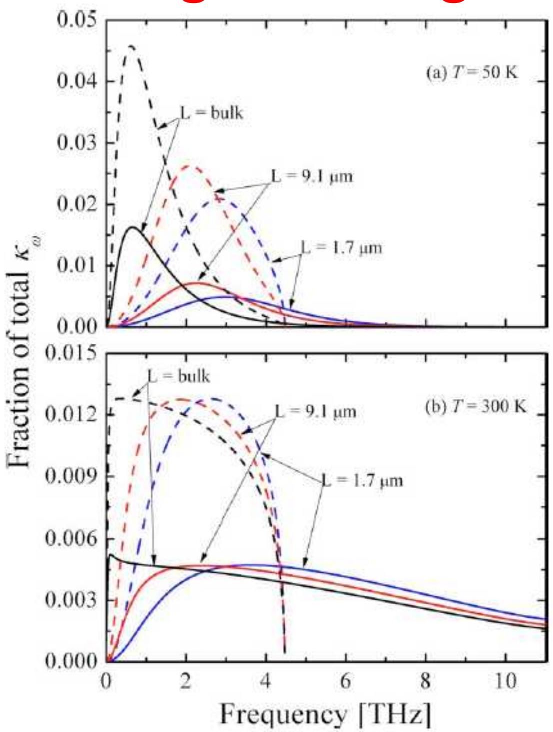
Origin of reduction of κ in microporous Si

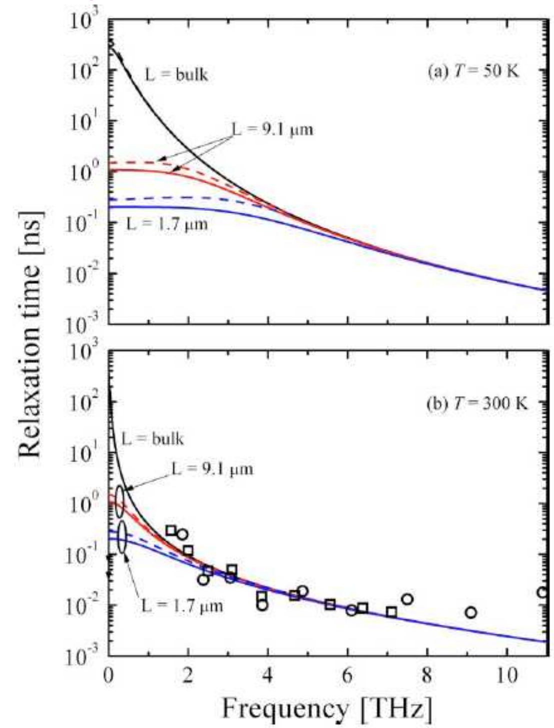
Scattering at pore boundaries

$$\frac{1}{\tau_{Boundary,j}} = \frac{\partial \omega_j(q)}{\partial q}\frac{1}{L}$$

Pore-edge to pore-edge spacing

Long wavelength modes scattered by boundaries

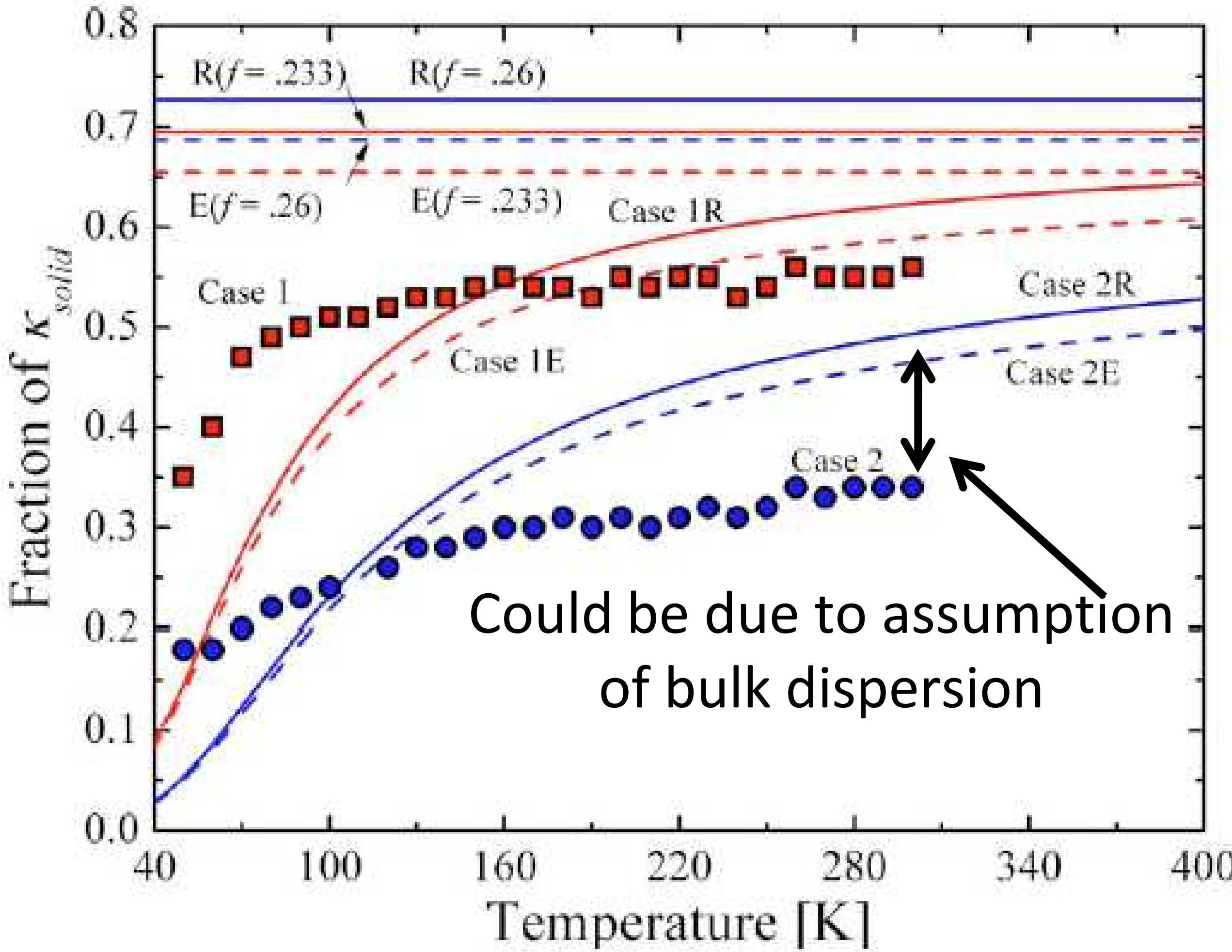




Hopkins, Rakich, Olsson, El-kady, and Phinney, APL **95**, 161902 (2009)

Predicting κ in microporous Si

Porosity accounted for by “Eucken” and “Russel” models



“E” model

$$\frac{\kappa_{porous}}{\kappa_{solid}} = \frac{1-p}{1+\frac{p}{2}}$$

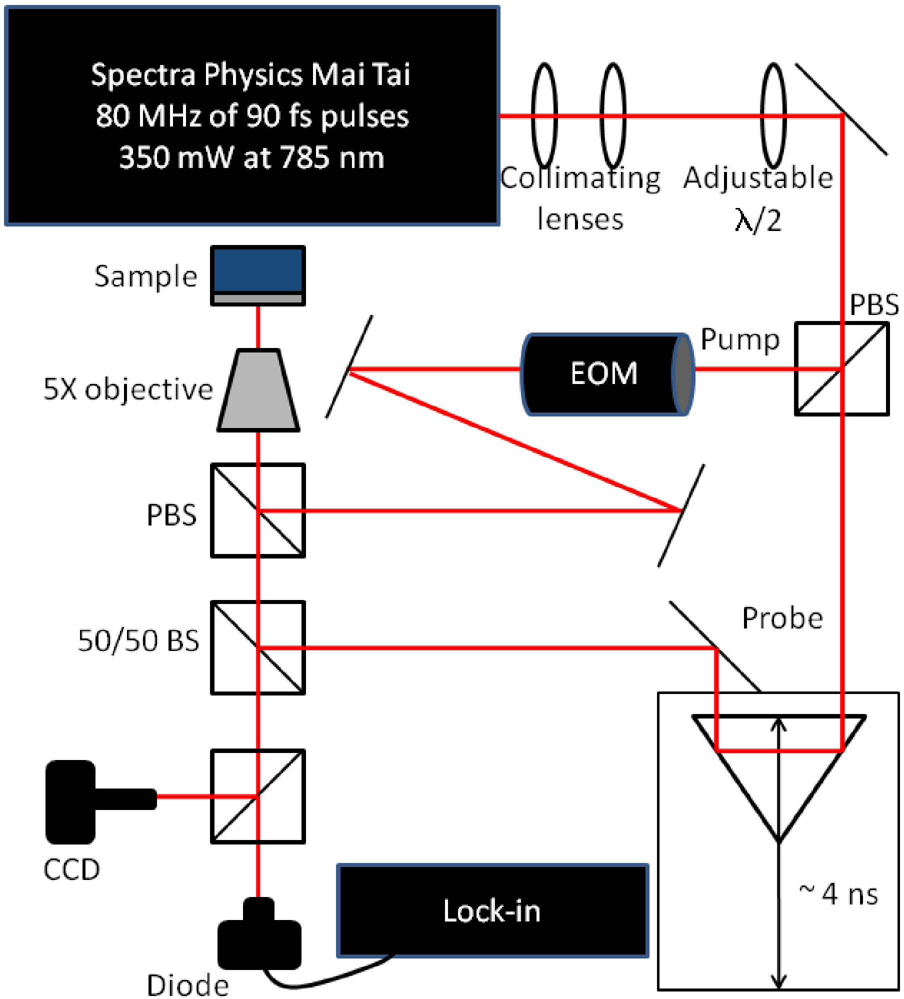
“R” model

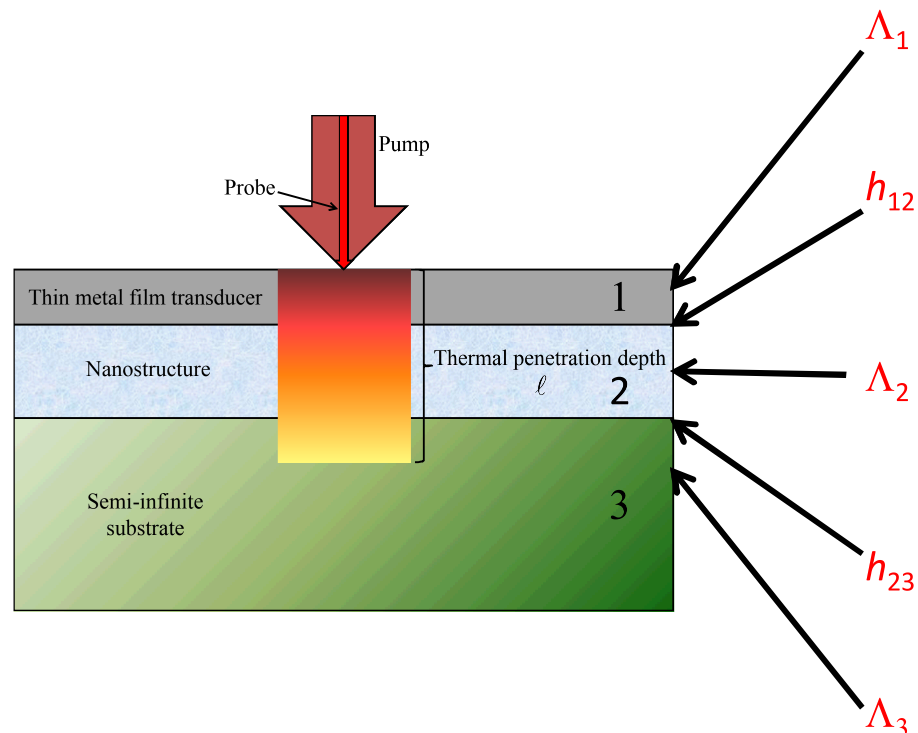
$$\frac{\kappa_{porous}}{\kappa_{solid}} = \frac{1-p^{\frac{2}{3}}}{1-p^{\frac{2}{3}}+p}$$

Consider bulk approach as “maximum” κ, or smallest reduction in κ

Hopkins, Rakich, Olsson, El-kady, and Phinney, APL **95**, 161902 (2009)

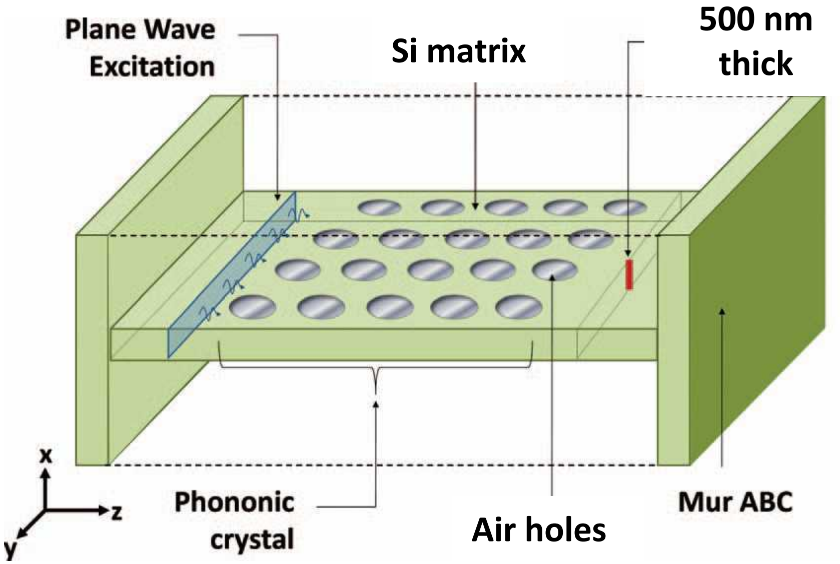
Time-domain thermoreflectance

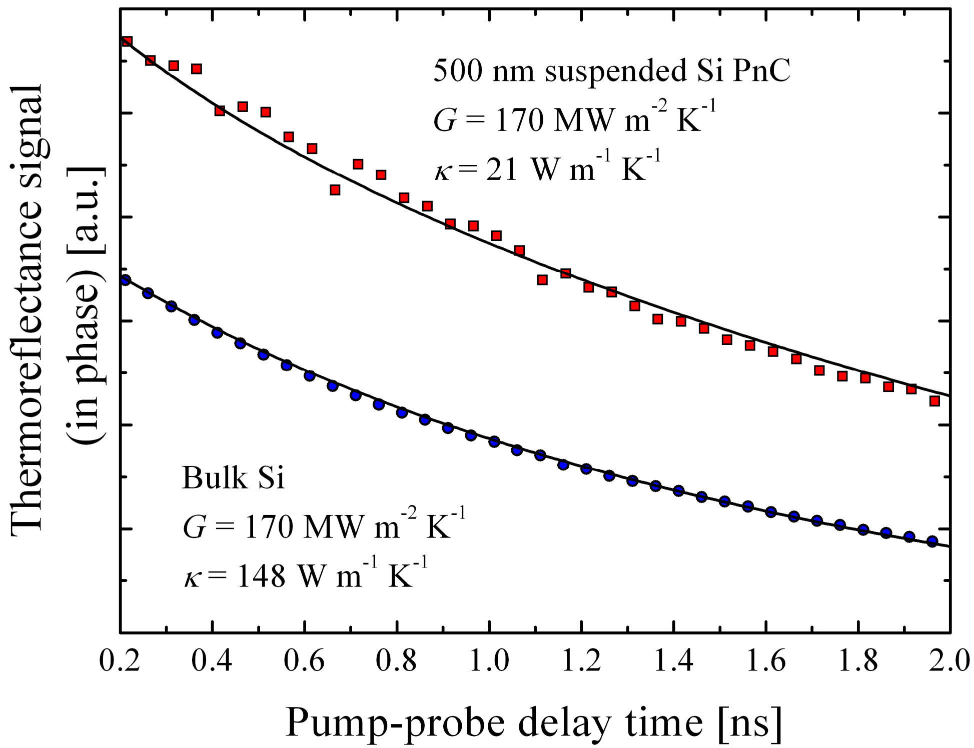




Measurement of κ of the Pnc

Thermal conductivity measurements on a 500 nm thick suspended PnC structure

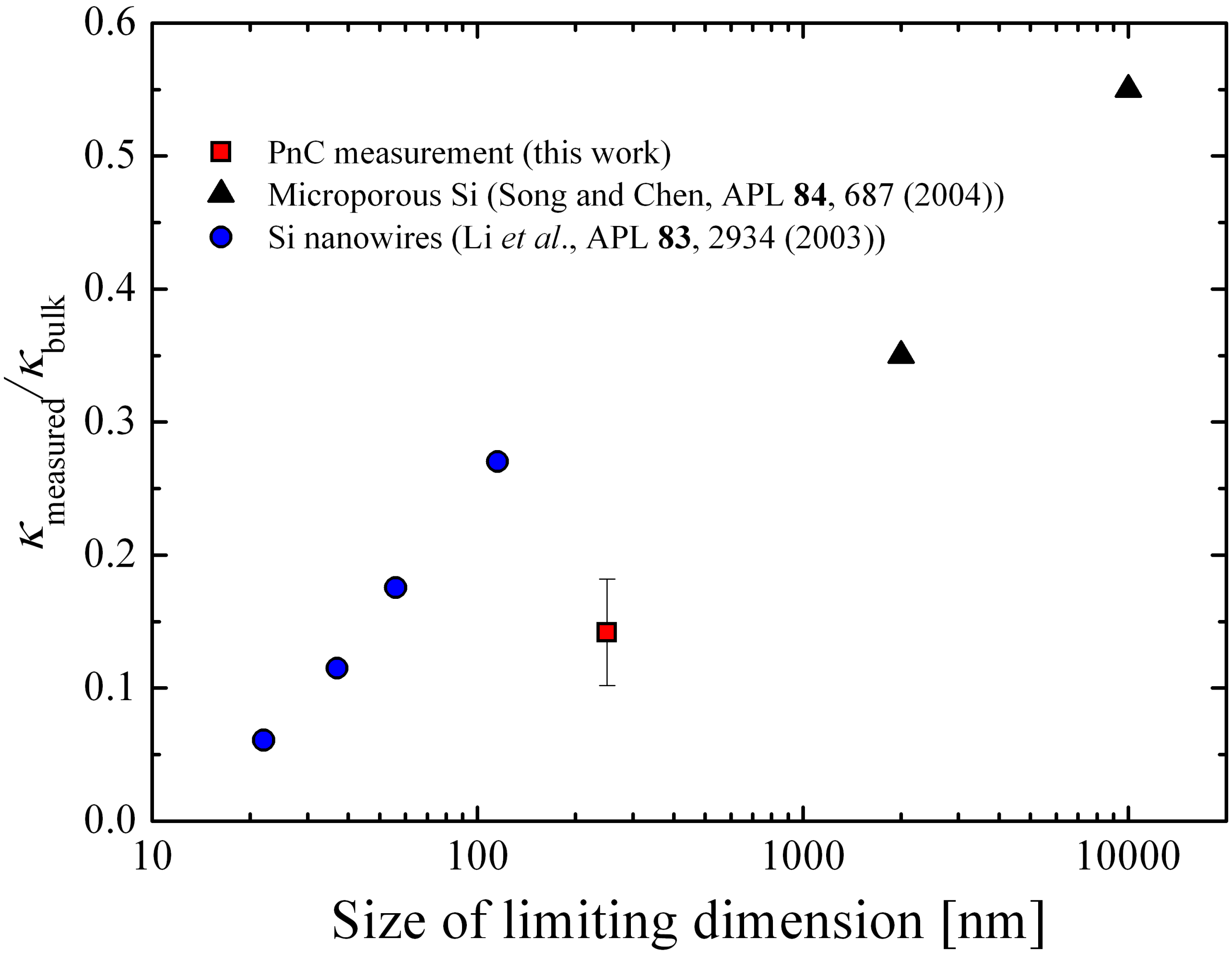




$$\frac{r}{a} = 0.32 \qquad a = 700\,nm$$

$$L = 250\,nm$$

Phonon engineering of κ in nanostuctures



Conclusions

Goal: Study phonon scattering and thermal conductivity reduction in PnC

- Reduction in thermal conductivity of microporous, periodic solids due to long wavelength phonon scattering
- PnC further reduces thermal conductivity through wave interference of phonon modes in periodic lattice
- TDTR experiments show reduced thermal conductivity in PnC beyond that from boundary scattering considerations

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