Thermal transport at high pressures

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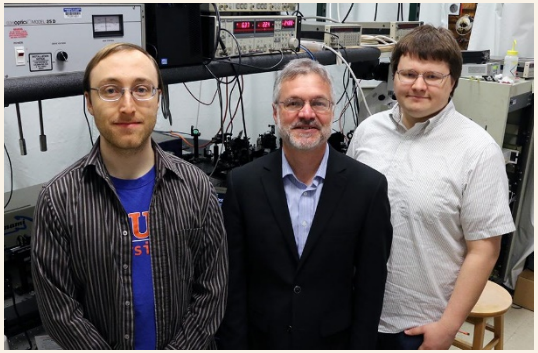

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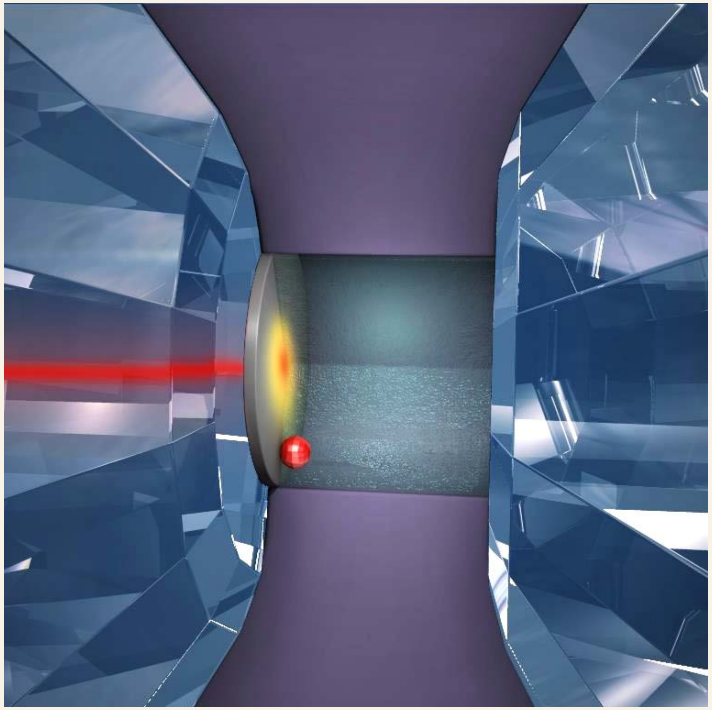
Thermal Transport at High Pressure
PI: David Cahill, U. Illinois



- Test theoretical models of thermal energy transport in materials and across interfaces.
- Pressure is used to systematically vary phonon and electron densities of states; and stiffness of interface bonding

People and Recent Publications

Greg Hohensee, Physics Ph.D. May 2015. placement: Western Digital Corporation.

May-Ling Li, 2nd year, Materials Science and Engineering

G. T. Hohensee, R. B. Wilson, and D. G. Cahill, "Thermal conductance of metal-diamond interfaces at high pressure," Nature Communications **6**, 6578 (2015).

G. T. Hohensee, M. R. Fellinger, D. R. Trinkle and D. G. Cahill, "Thermal transport across high pressure semiconductor-metal transition in Si and SiGe," Phys. Rev. B **91**, 5104 (2015).

Overview

- Background – thermal transport coefficients
- Methods – time-domain thermoreflectance, diamond anvil cell
- Thermal conductance of metal-diamond interfaces at high pressures.
- Thermal conductivity measurements of metallic Si without a transducer layer.

How we think about thermal conductivity

- Fourier's law defines a thermal conductivity:

$$\vec{J} = -\Lambda \vec{\nabla} T$$

- From Boltzmann transport equation to relaxation time approximation (RTA):

$$\Lambda_{\rm RTA} = \frac{1}{3}\int C(\omega) v^2(\omega)\tau(\omega) d\omega$$

$$C(\omega) = \text{heat capacity of phonon mode}$$
$$v(\omega) = \text{group velocity}$$
$$\tau(\omega) = \text{thermal relaxation time}$$

$$\tau_{\rm R}^{-1} = \tau_{\rm U}^{-1} + \tau_{\rm D}^{-1} + \tau_{\rm B}^{-1} + \ldots$$

- We measure the integral, Λ, to study the integrand, Λ(ω).
- Fit models for Λ(ω) to Λ(T), Λ(P) data.

How we think about interface thermal conductance

- Discrete form of Fourier's Law:

$$\vec{J} \cdot \hat{z} = G \Delta T$$

- Isotropic model:

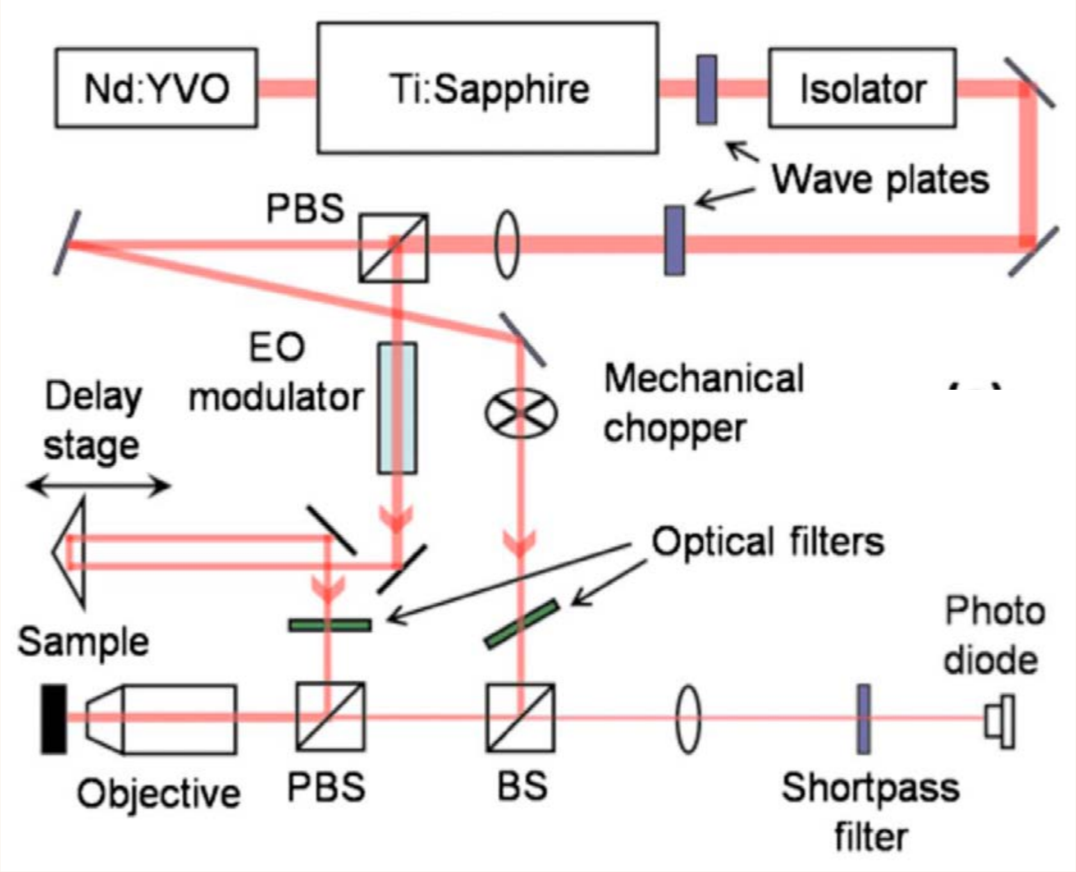
$$G = \frac{1}{4} \int C(\omega) v(\omega) T(\omega) d\omega$$

$$C(\omega) = \text{heat capacity of phonon mode}$$
$$v(\omega) = \text{group velocity}$$
$$\rightarrow \quad T(\omega) = \text{transmission coefficient}$$

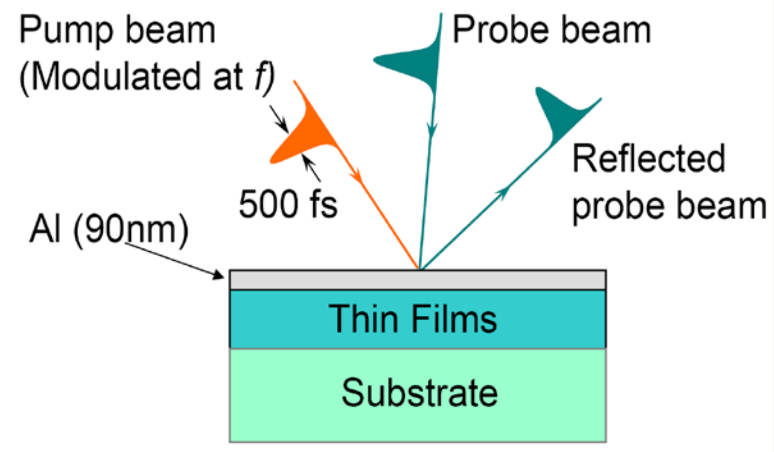
[weak bonding, non-equilibrium effects, …]

- We measure the integral, *G*, to study the integrand *G*(ω).
- Fit models for *G*(ω) to *G*(T), *G*(P) data.

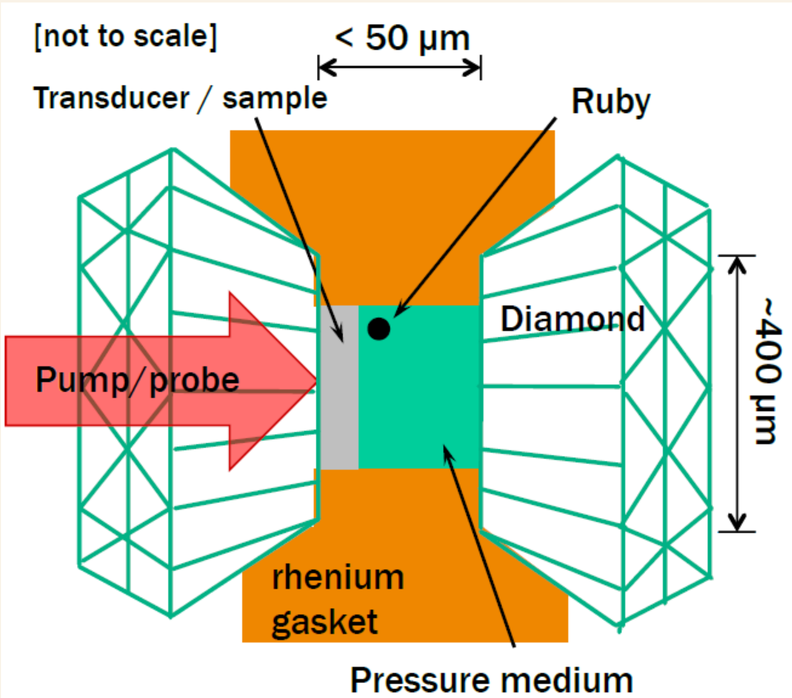
Time-domain thermoreflectance (TDTR)



- Pump-probe optical method for measuring heat transport at small length and time scales.

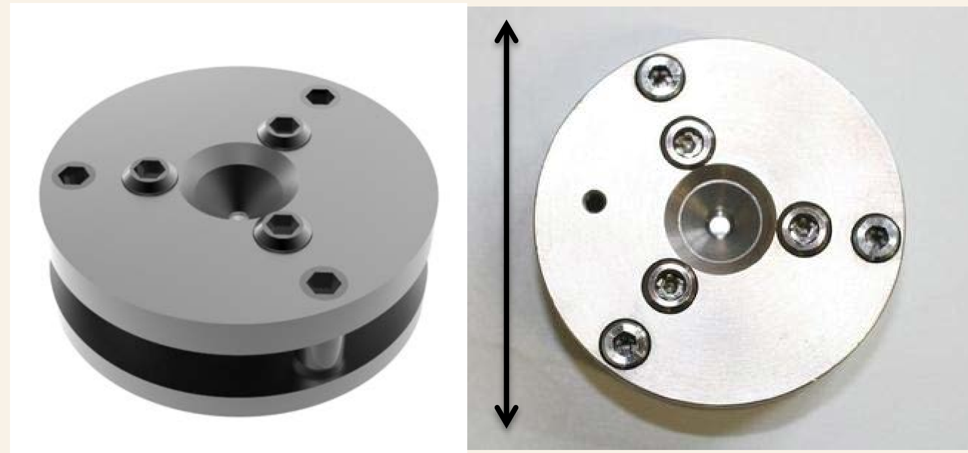


TDTR on diamond anvil cell (DAC) samples at high pressure



49 mm

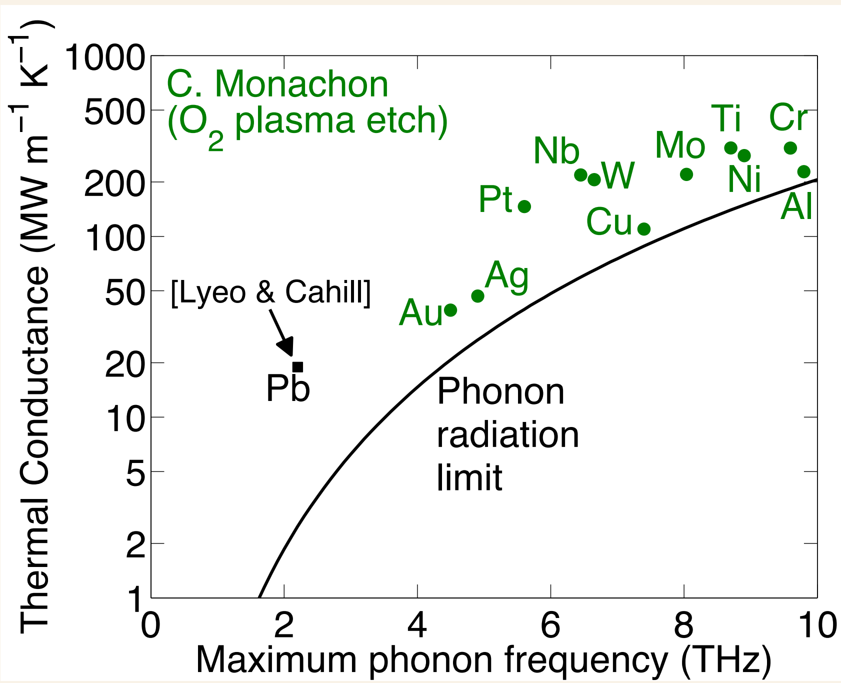
Boehler-Almax

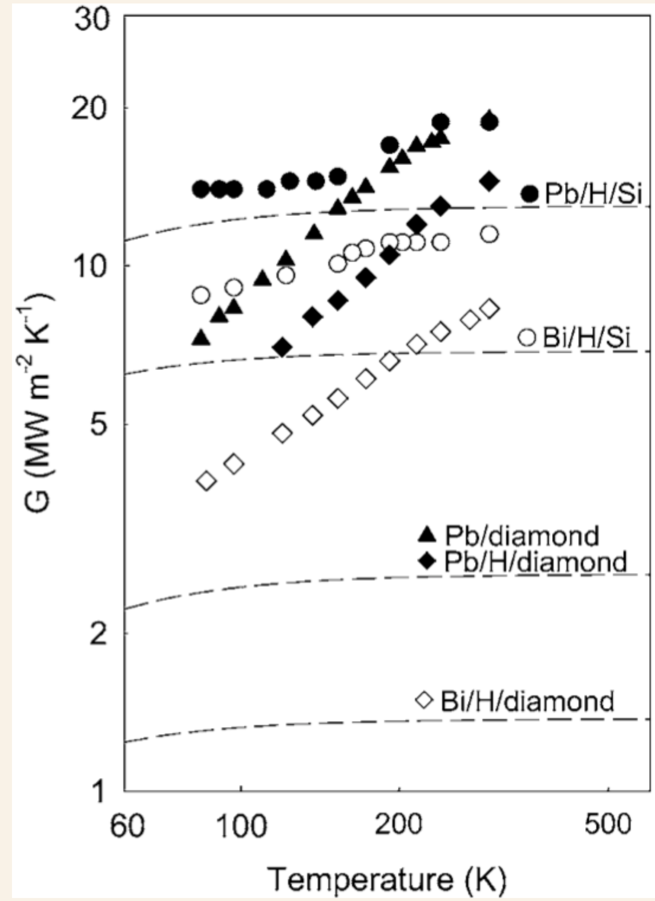


The question of thermal conductance between highly dissimilar materials

- Has roots in the Kapitza resistance problem for liquid He interfaces (1941-).
- Present incarnation, metals on diamond, Stoner and Maris in 1993.

Radiation limit: maximum two-phonon thermal conductance.

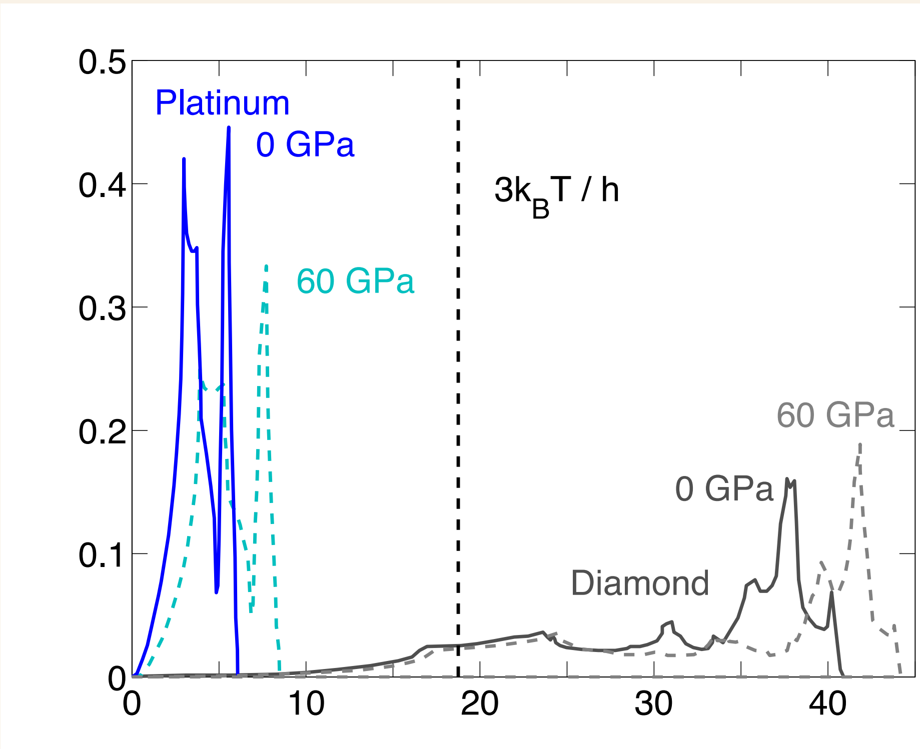




Lyeo and Cahill, *Phys. Rev. B.* **73** (2006)

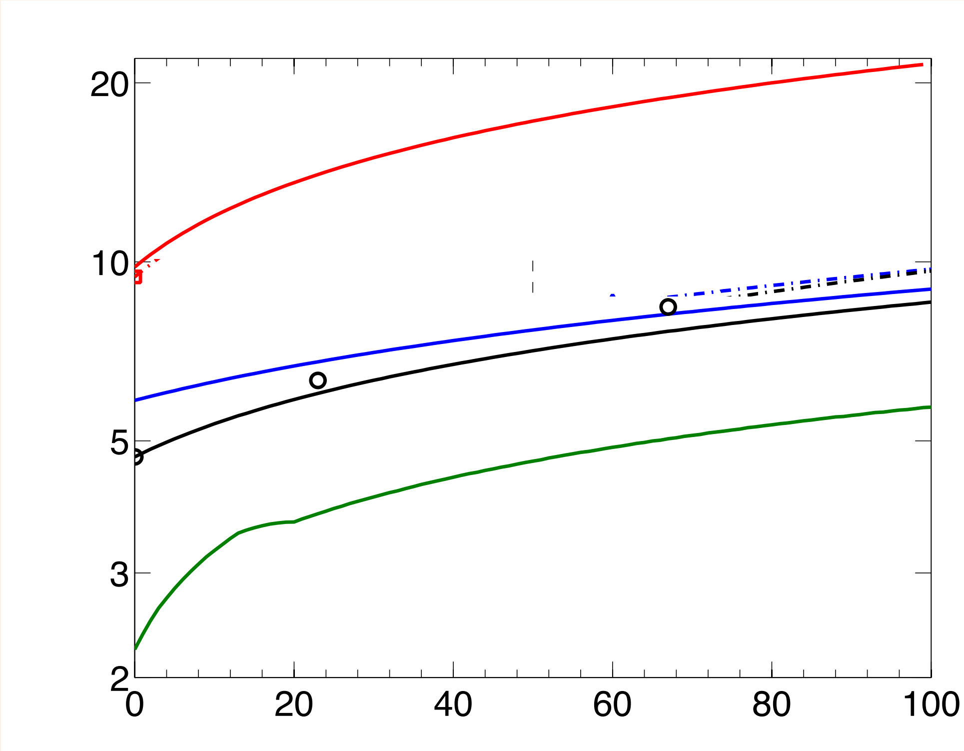
New information from a new control: high pressure

Pressure tuning of mismatched phonon densities of states (DOS)



Xie et al., PRB **60** (1999)
Menendez-Proupin, PRB **76** (2007)

Can explore wide stiffness range with different metals



Tambe et al., PRB **77** (2008)
Menendez-Proupin et al., PRB **76** (2007)
Greef & Graf, PRB **69** (2004)

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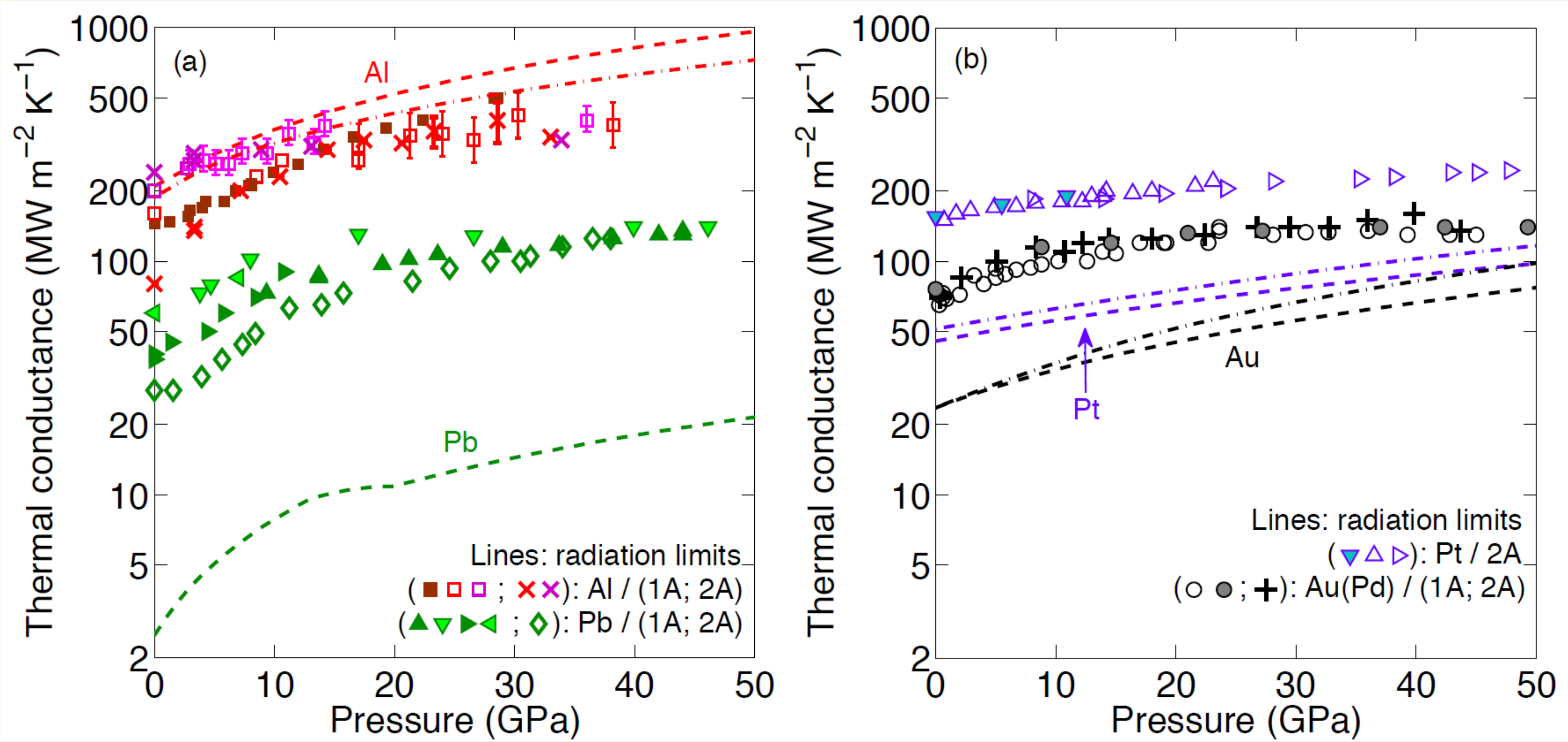
Data for 4 metals on 1A and 2A diamond as a function of pressure up to 50 GPa



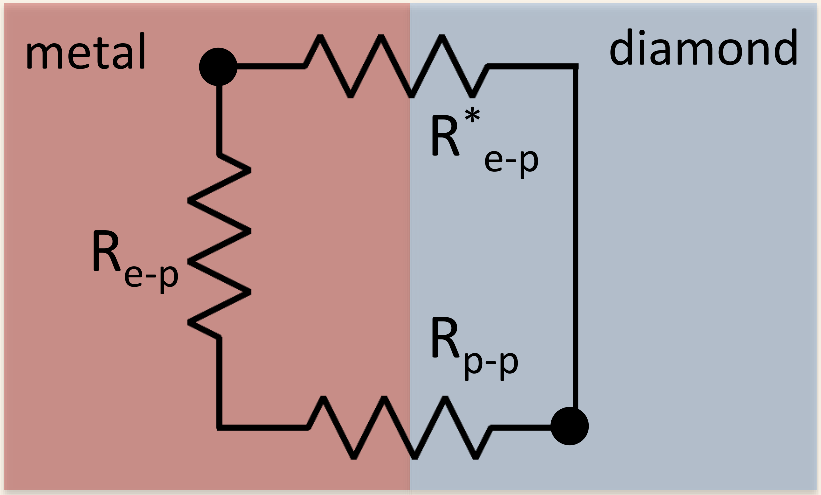
Hohensee, Wilson, Cahill, *Nat. Comm.* **6**, 6578, (2015)

Observation A: no measurable dependence on defect density of the diamond anvils

- We have previously seen an anomalous dependence of interface conductance on dilute Ge additions to Si
- Attributed to non-equilibrium phonon distributions near the interface.
- Type 1A and 2A diamonds show the same thermal conductance
- Our type 1A diamonds have a thermal conductivity only 1/3 of pure diamond (700 W m^{-1} K^{-1}) due to high nitrogen concentration (1500 ppm by our analysis)
- Null result suggests non-equilibrium phonon distributions are not important in these experiments.

Observation B: conductance of Pt/diamond and Au/diamond interfaces are similar

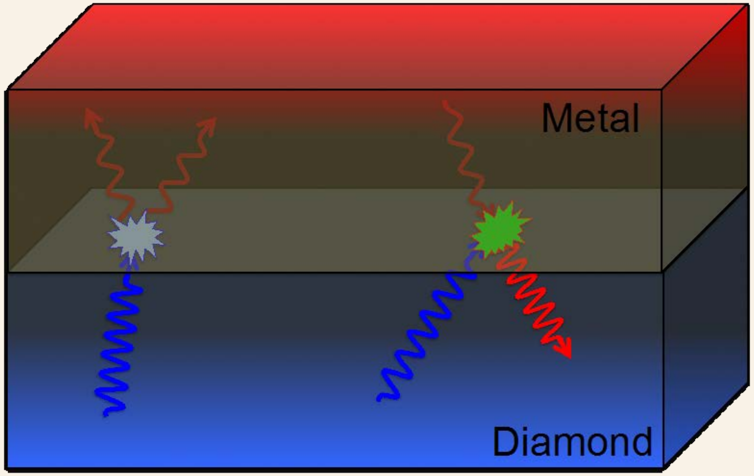
- Electron-phonon coupling within the metal contributes a series resistance Majumdar et al., *APL* (2004)
- Electron-phonon coupling from metal to diamond contributes a parallel conductance. Mahan, *PRB* (2009)



- Pt and Au have very different electron-phonon coupling strengths (Pt is larger by a factor of 20 by our measurements)
- Pt and Au have very different electronic heat capacities (Pt is larger by a factor of 11)
- Null result suggest electron-phonon coupling is not important

Observation C: pressure dependence of the data is much weaker than the pressure dependence of the radiation limit

- Excess conductance beyond the two-phonon, one phonon in diamond (d) and one phonon in metal (m) is attributed to three phonon interactions
- But which phonons?



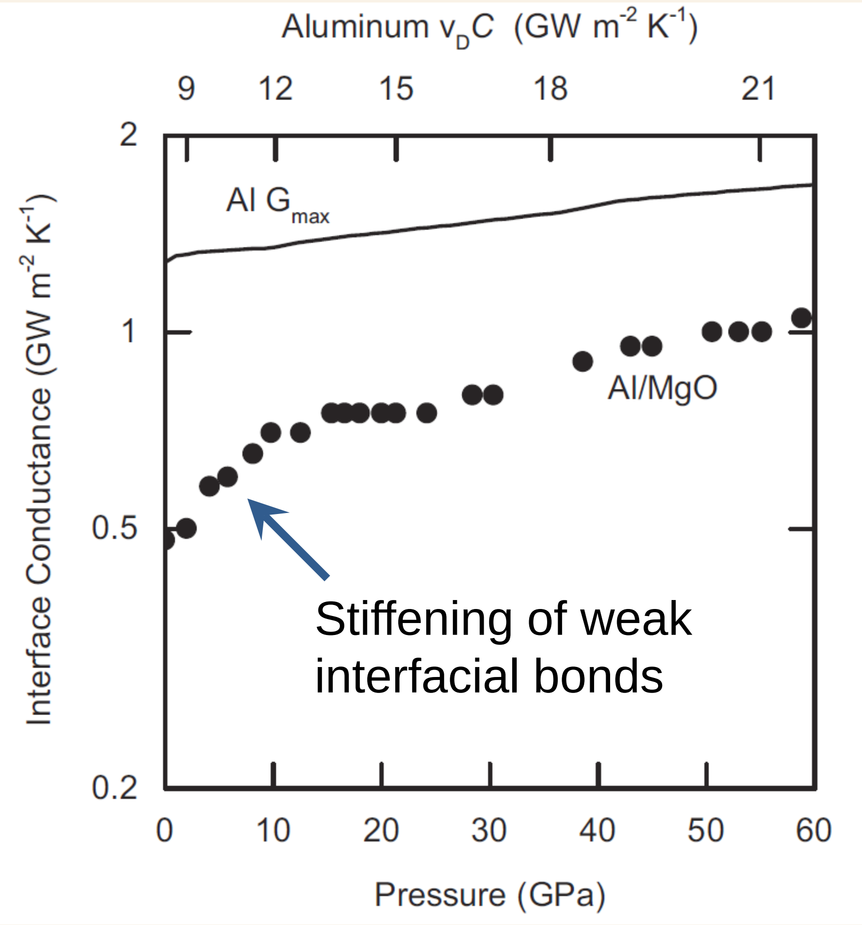
- Metal phonons change significant with pressure so two metal phonons interacting with one diamond phonon should be strongly pressure dependent

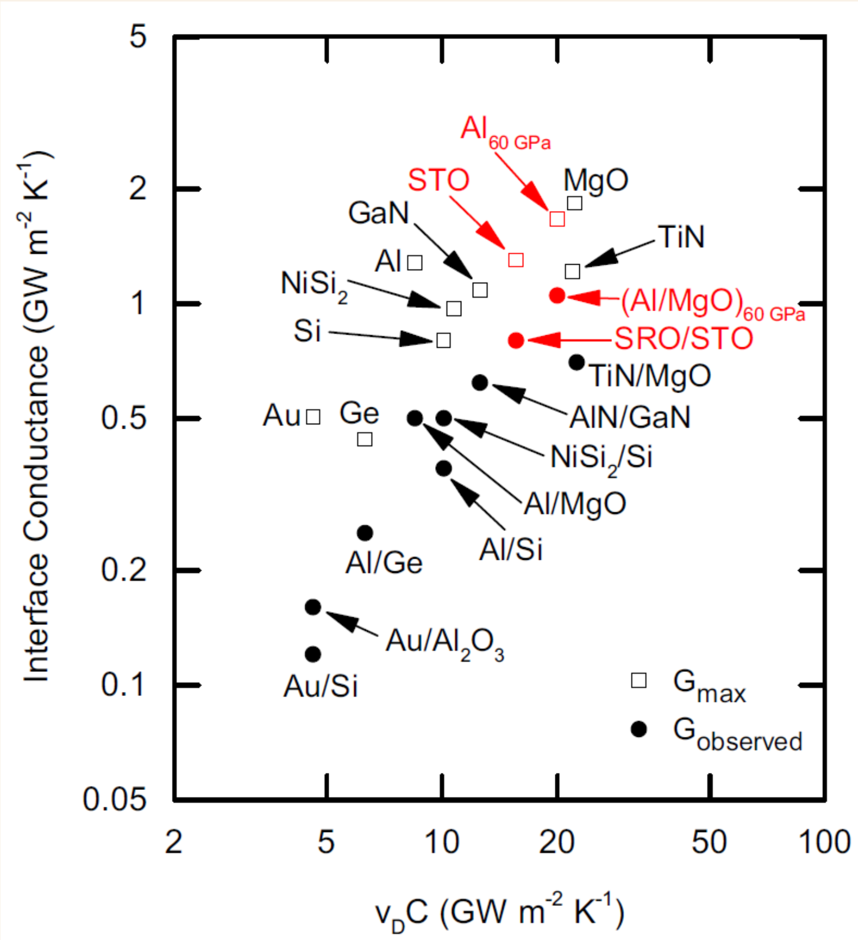
$$m_1 + m_2 \Leftrightarrow d$$

- Data are consistent (pressure dependence and magnitude) with a "partial transmission" mechanism

$$d_1 + d_2 \Leftrightarrow m$$

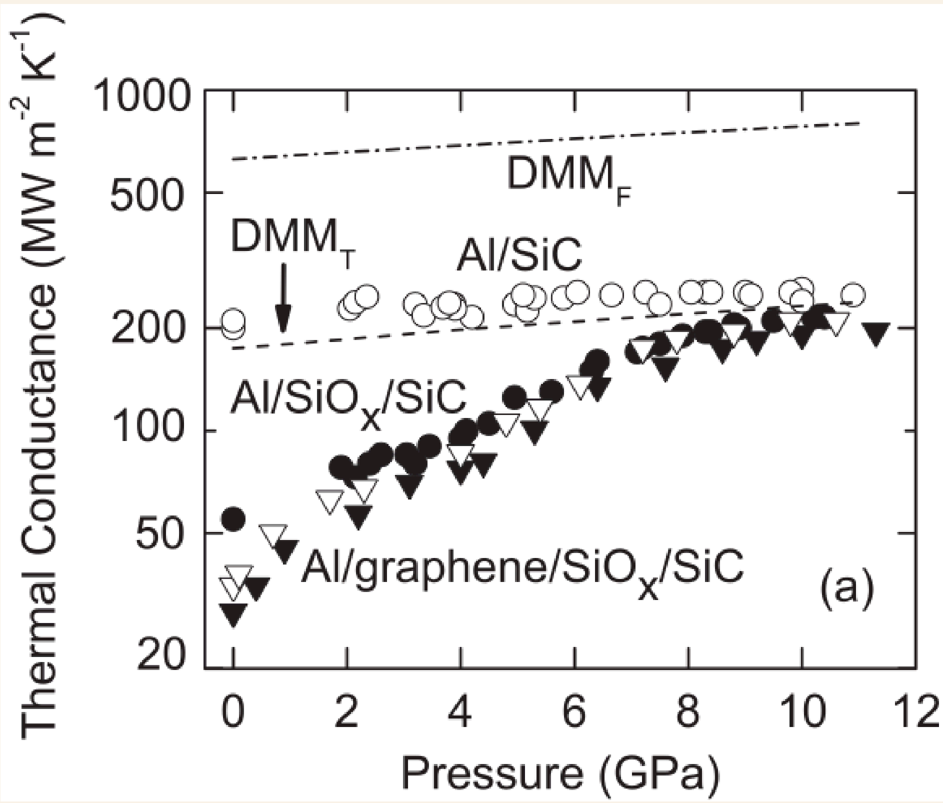
Digression: Highest thermal conductance ever observed is for Al/MgO at high pressure, G>1 GW m^{-2} K^{-1}

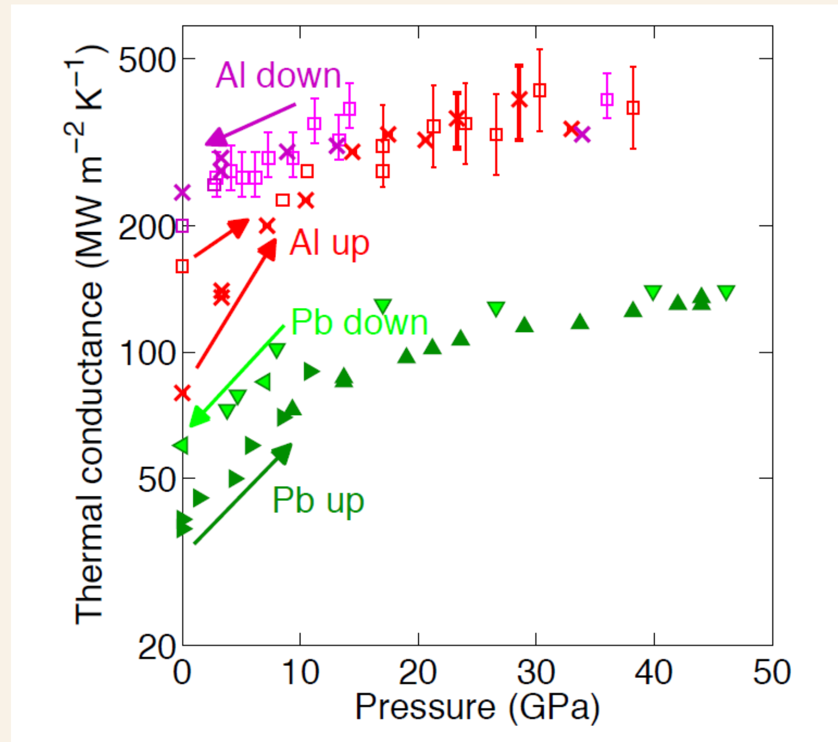




Stiffening of weak interfacial bonding was reversible in our prior work; at higher pressure, changes are not irreversible

- Example of pressure driven chemistry at interfaces?





Hsieh et al, PRB (2011)

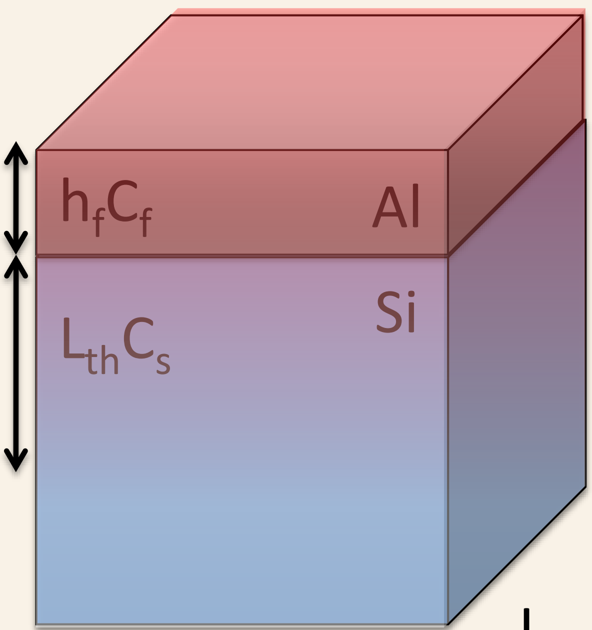
Hohensee, Ph.D. thesis, U. Illinois (2015)

Conclusions for interface conductance

- For dissimilar interfaces (metal/diamond), a partial transmission processes where two diamond phonons interact with one metal phonon provides a significant channel for heat transport
- Pressure strengthens weak interfacial bonding and enables experiments on the intrinsic thermal conductance of interfaces.

Measuring anisotropic thermal conductivity of metals

TDTR with transducer
(cross-plane thermal effusivity)

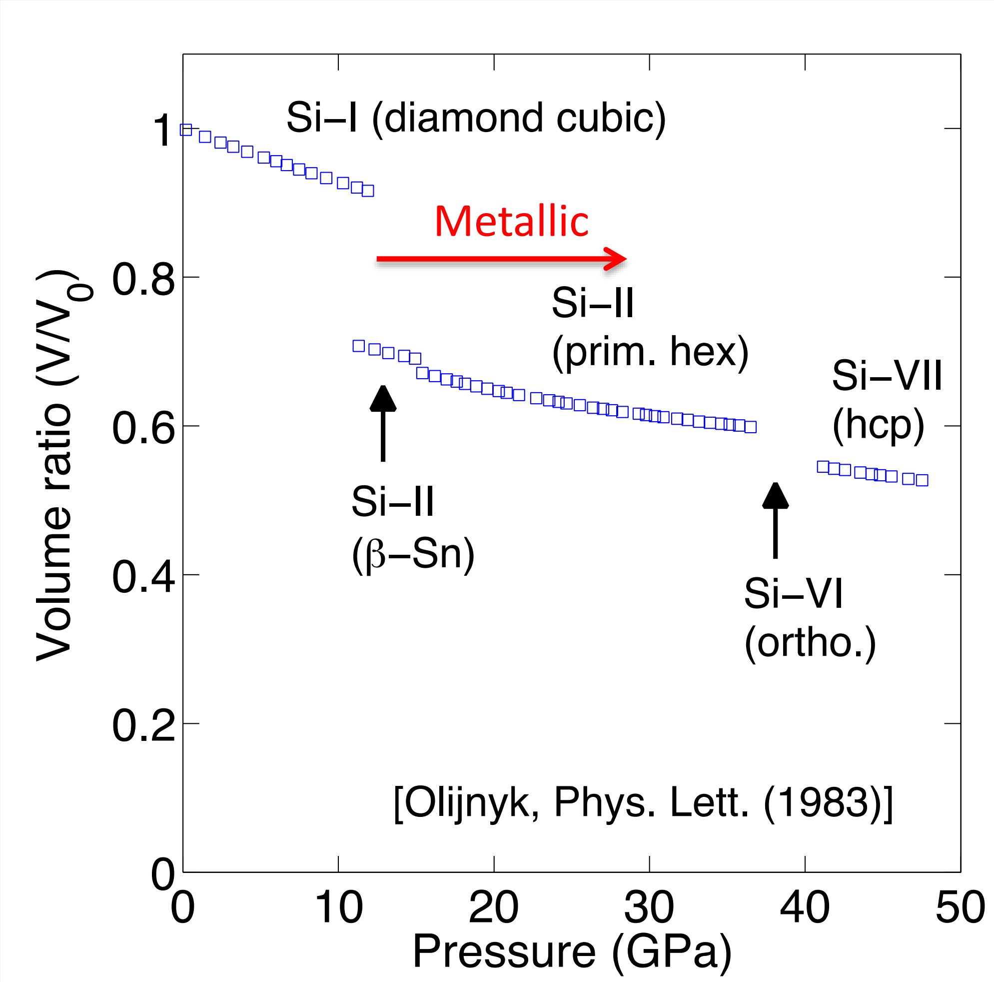


Side View

$$L_{th} = [\Lambda_s/(\pi f C_s)]^{1/2}$$

Feser and Cahill, *Rev. Sci. Instrum.* **84** (2013)

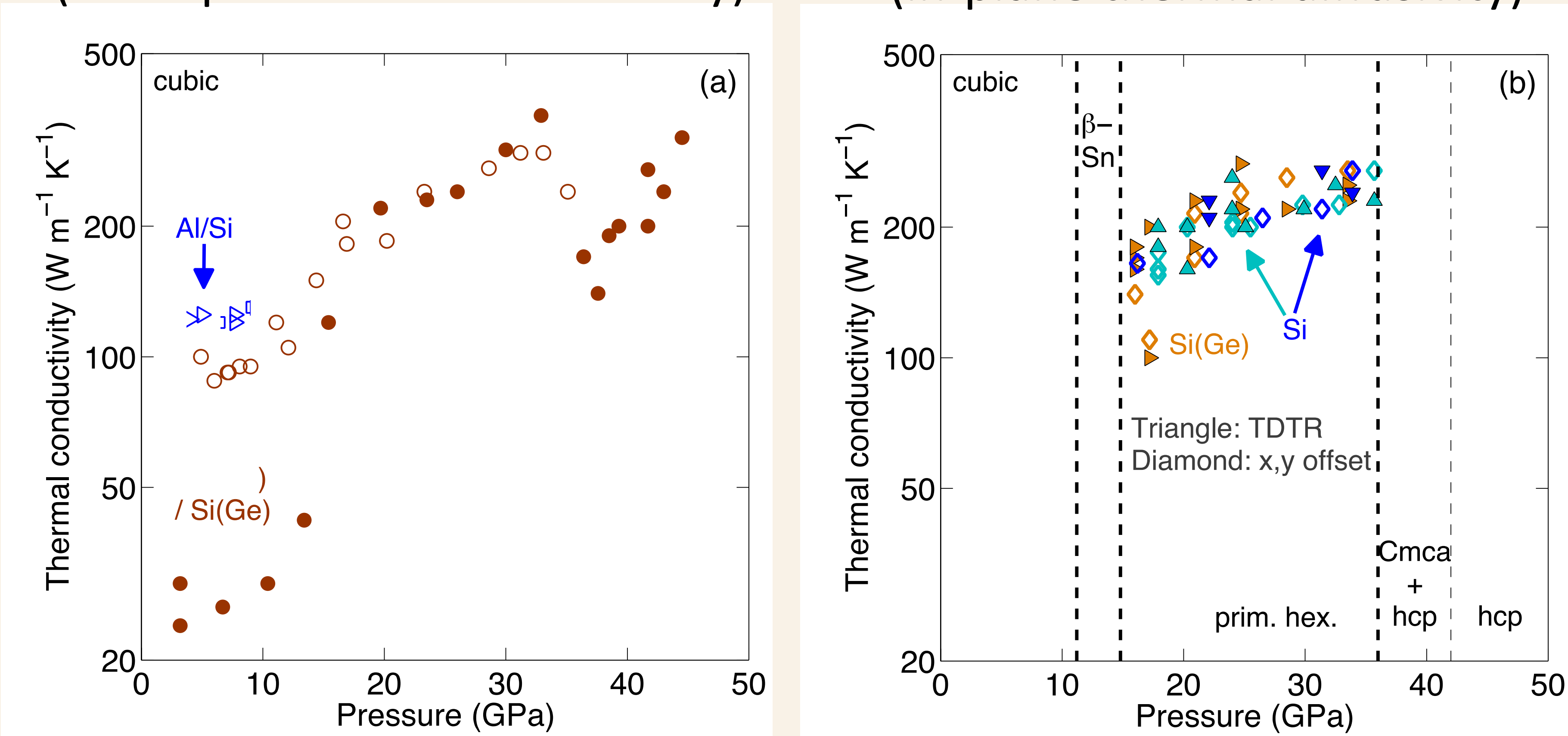
Si becomes metallic at high pressure



Thermal conductivity of metallic Si

TDTR with transducer
(cross-plane thermal effusivity)

TDTR *without* transducer
(in-plane thermal diffusivity)



Hohensee, Fellinger, Trinkle, Cahill, *PRB* (2015).

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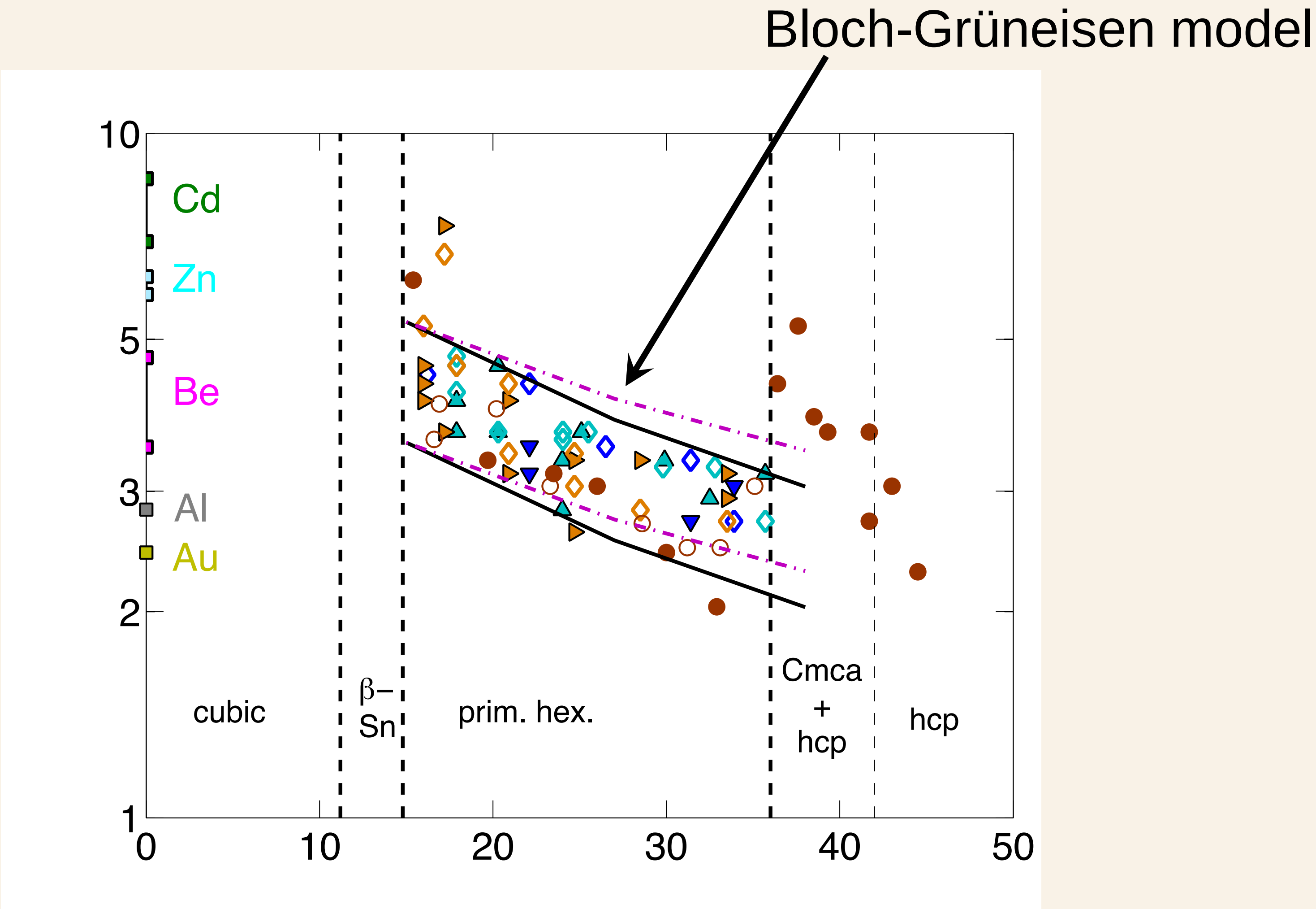
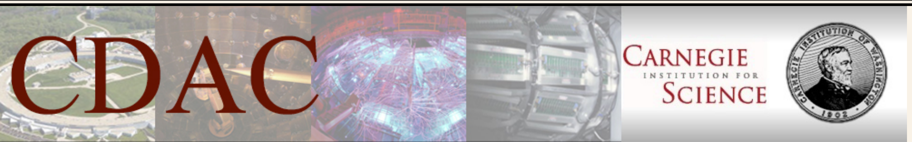
Use Wiedemann Franz Law to convert to electrical resistivity

$$\rho = \frac{L_0 T}{\Lambda}$$





Summary for metallic Si and future directions

- Measurements of metallic samples do not require a transducer film if the thermal diffusivity is not too small.
- High pressure will aid in the search for a reversible thermal switch that changes from semiconductor (or semi-metal) to metal abruptly at a designed temperature.
- Anticipate that magneto-optic Kerr effect (MOKE) transducers could replace thermoreflectance as the ultrafast thermometer in pump probe experiments. Less sensitive to d*n*/dT of the pressure medium; less sensitive to surface roughness.