Thermal conductivity: An example of structure-property relations in crystals

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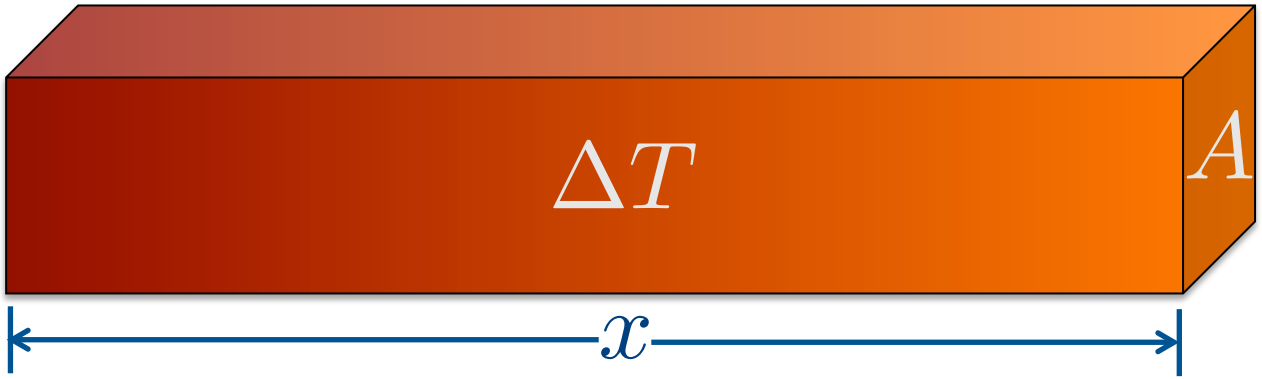
Thermal conductivity in 1D: Definitions



rate of heat flow

surface area

temperature gradient

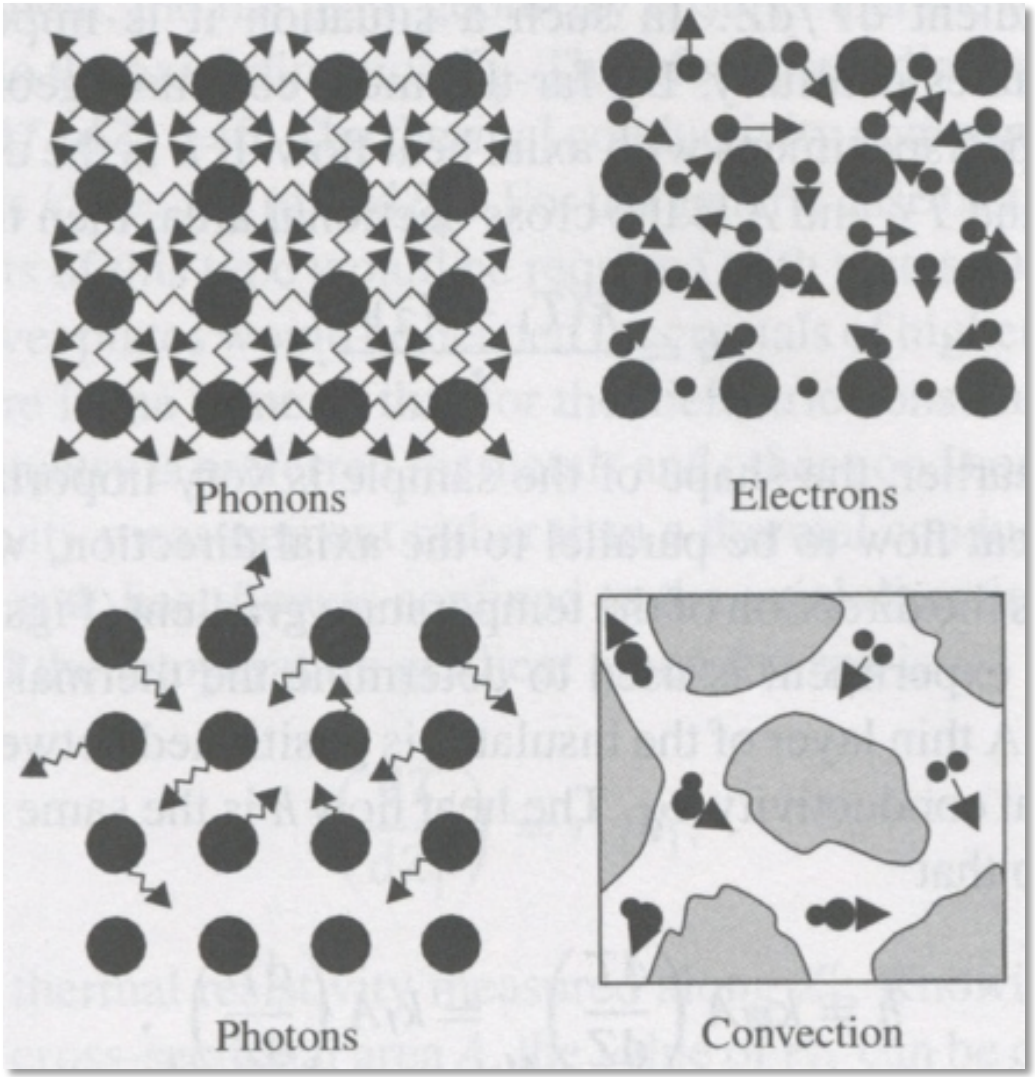
$$\dot{Q} = -\kappa A \frac{\mathrm{d}T}{\mathrm{d}x}$$

thermal conductivity (units of W $m^{-1}K^{-1}$)

In tensor form (2nd rank):

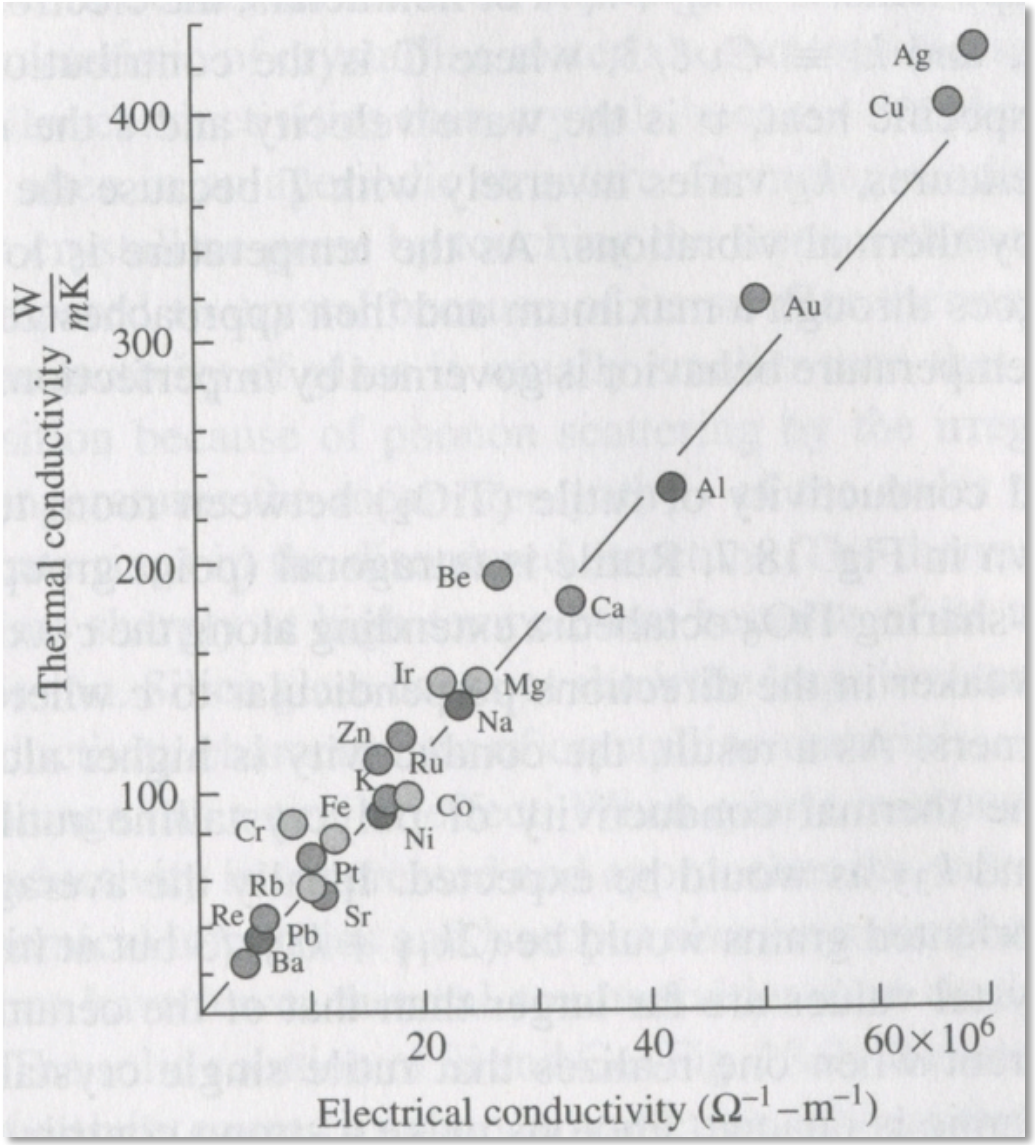
$$\dot{Q}_i = -\kappa_{ij} A \frac{\mathrm{d}T}{\mathrm{d}Z_j}$$

Mechanisms of thermal conductivity in materials



From R. E. Newnham, *Properties of Materials: Anisotropy, Symmetry, Structure*, Oxford University Press, 2005.

Thermal conductivity by electrons in "good" metals



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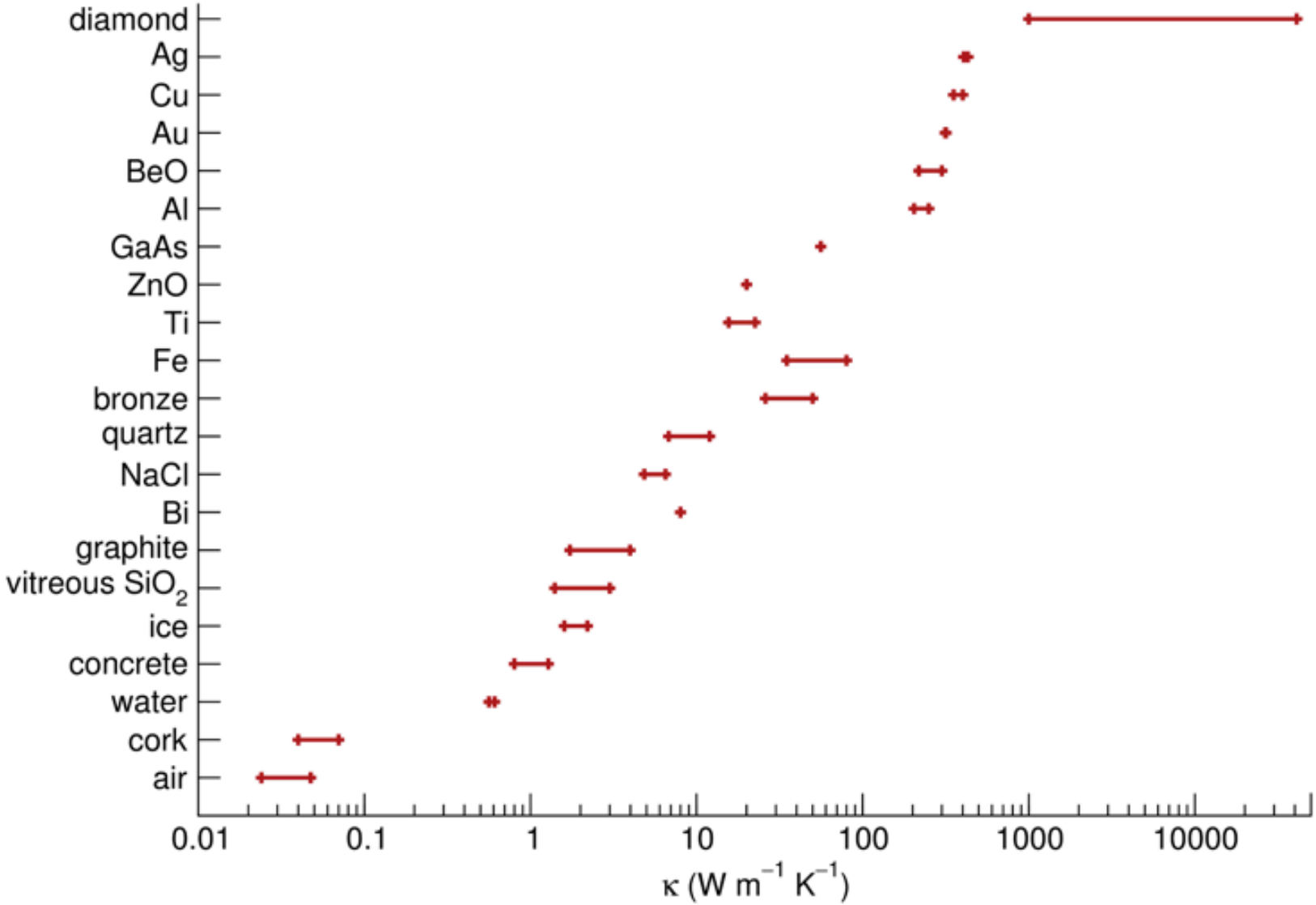
$$\kappa/\sigma = LT$$

Lorentz number
2.44×10^{-8} W Ω K^{-2}

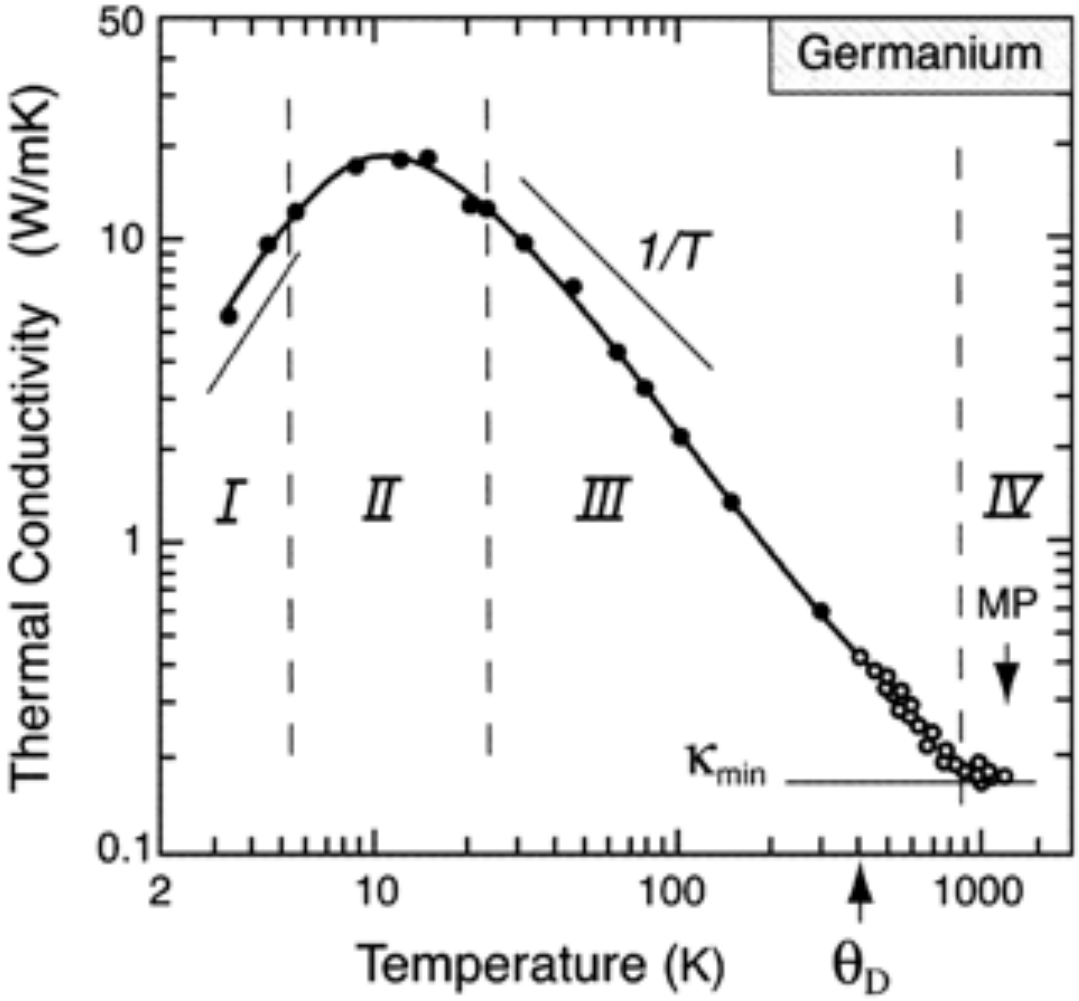
This is the (empirical) Wiedemann-Franz law, a consequence of free electrons in metal.

Thermal conductivity across materials



Data from wikipedia

Temperature-dependence: 4 regimes



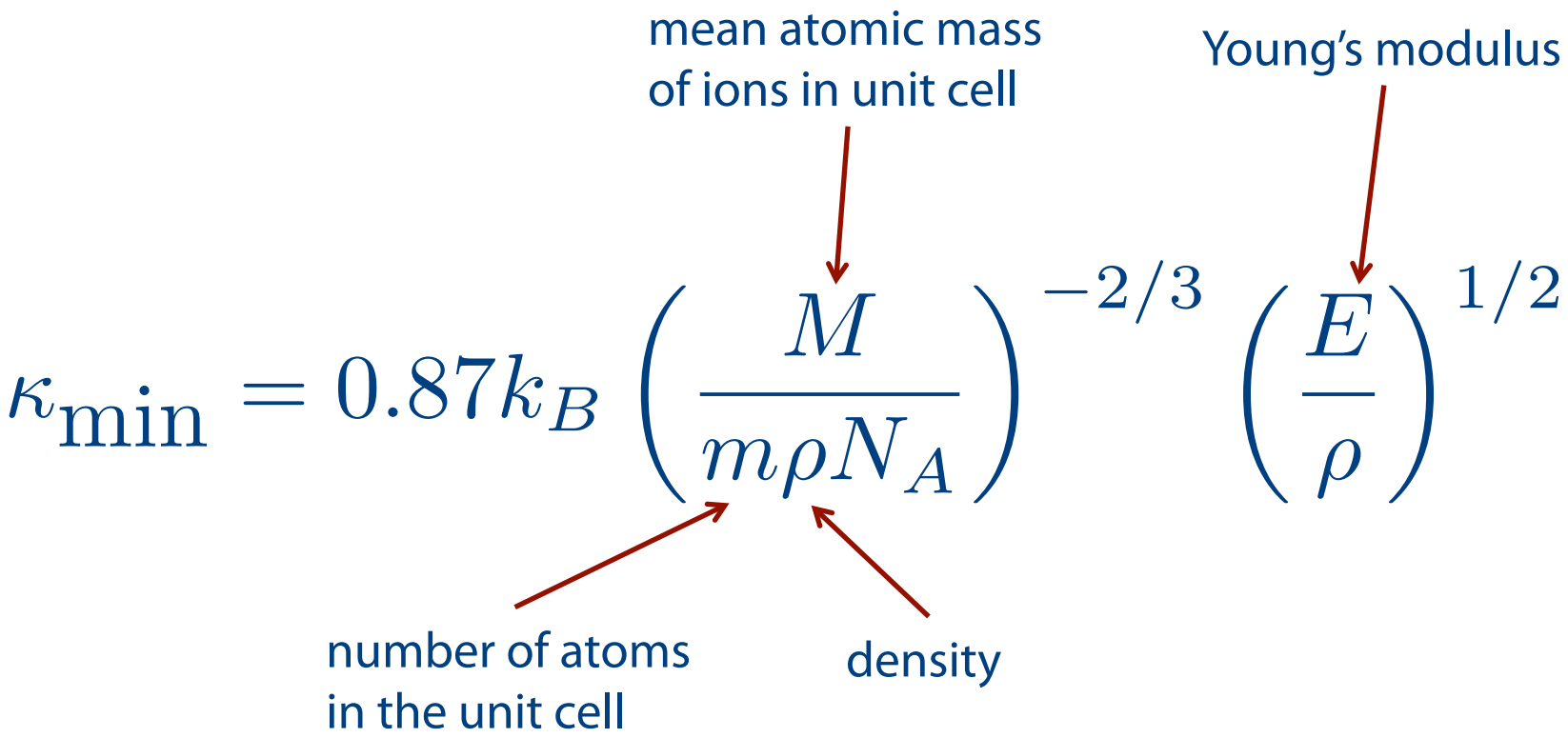
At low *T*, κ is determined by the physical size of the material, grain size and dislocation spacing.

In region III, κ (corrected for the thermal expansion) decreases as 1/*T* largely due to anharmonic phonon scattering, the umklapp processes.

At very high *T* κ plateaus out and becomes independent of *T*.

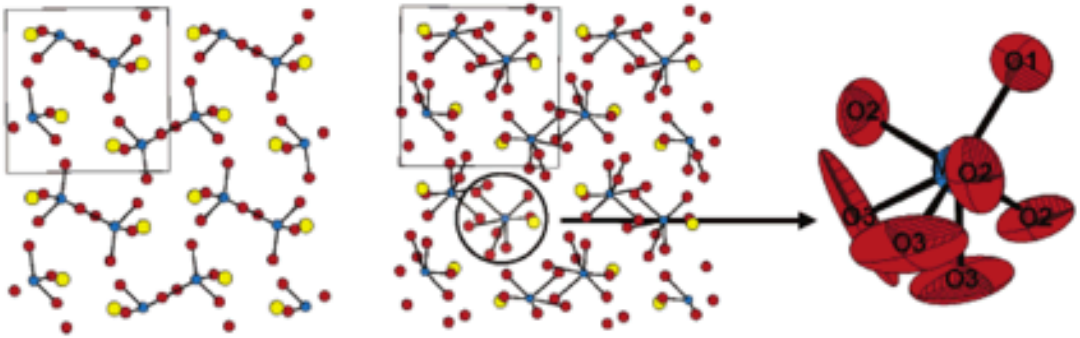
D. R. Clarke, *Surface Coatings Technol.* **163 – 164** (2003) 67–74.

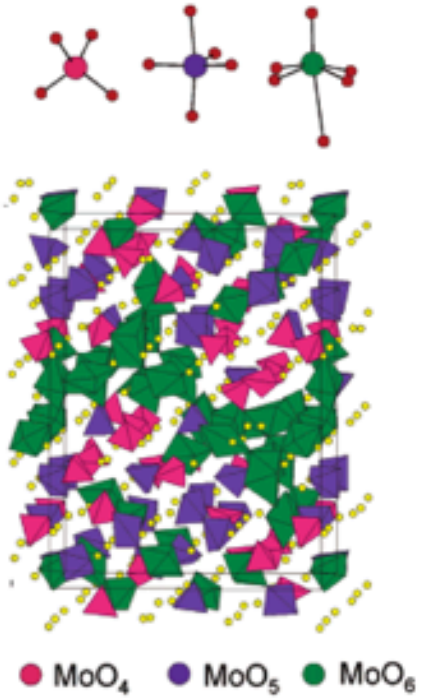
An approximate expression for κ_{min}

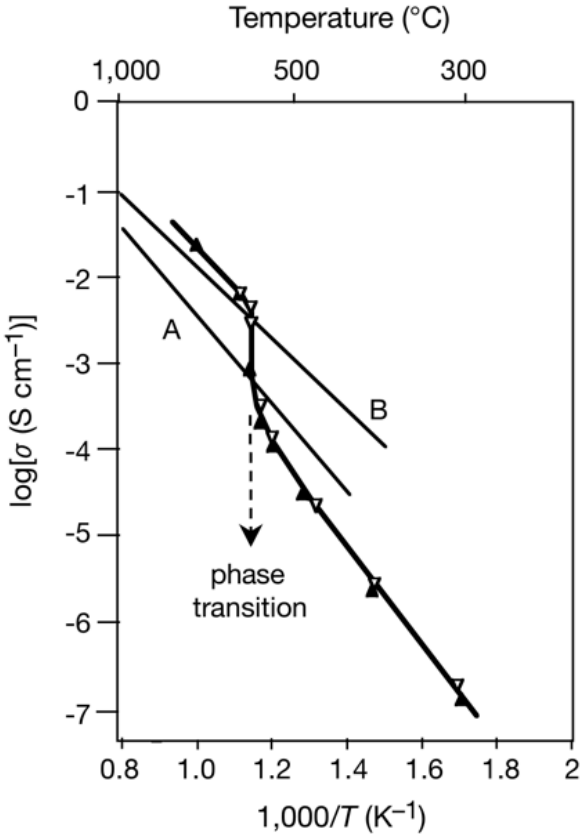


M. Winters and D. R. Clarke, *J. Am. Ceram. Soc.* **90** (2007) 533–540.

Some interesting materials: $La_2Mo_2O_9$





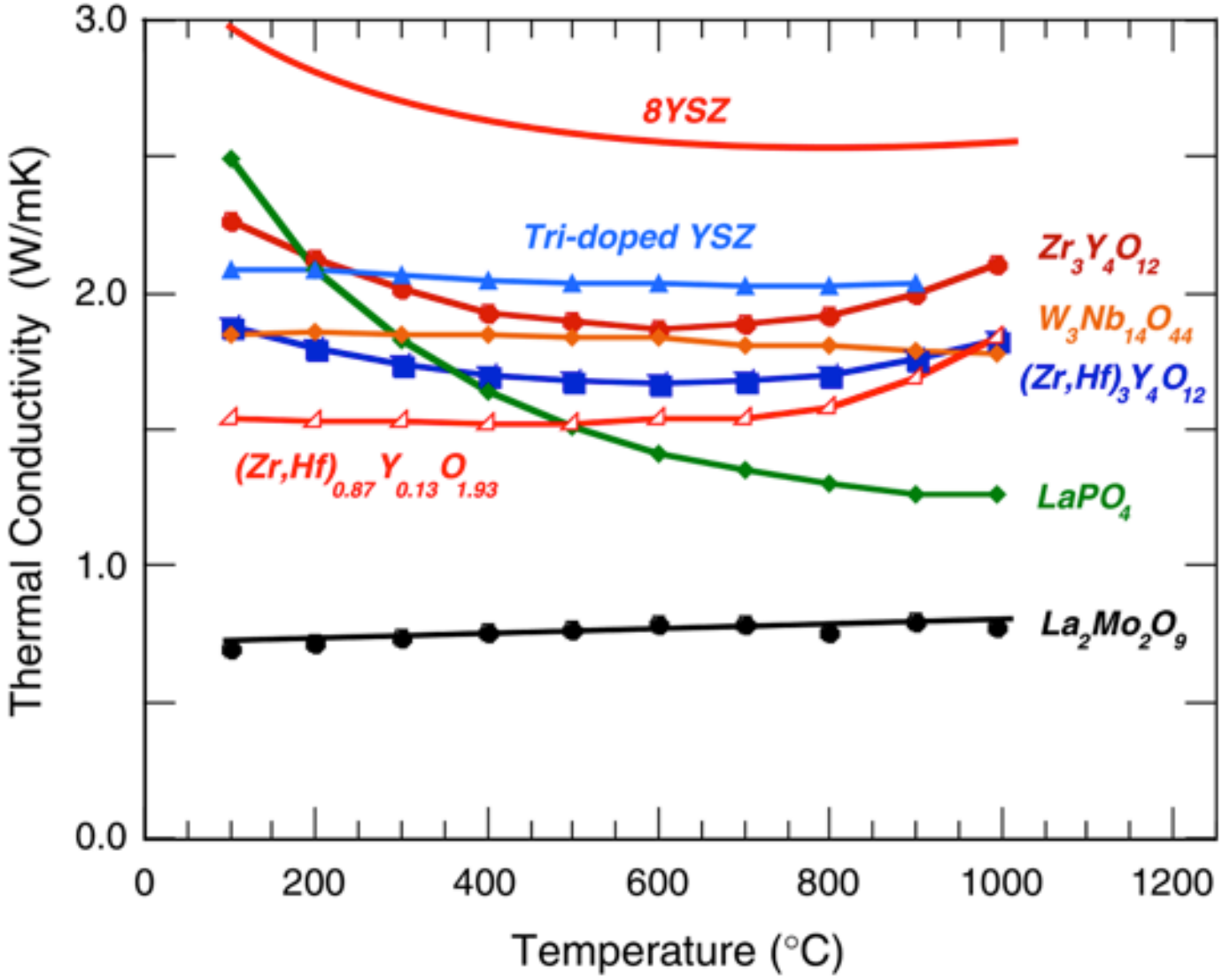


Material with a very high oxide-ion conductivity at elevated temperatures.

The low–*T* structure is extremely complex.

Lacorre *et al. Nature* **40** (2000) 856–858; Radosavljevic Evans, Howard, Evans, *Chem. Mater.* **17** (2005) 4074–4077.

Some interesting materials: $La_2Mo_2O_9$ has a record low κ for an oxide



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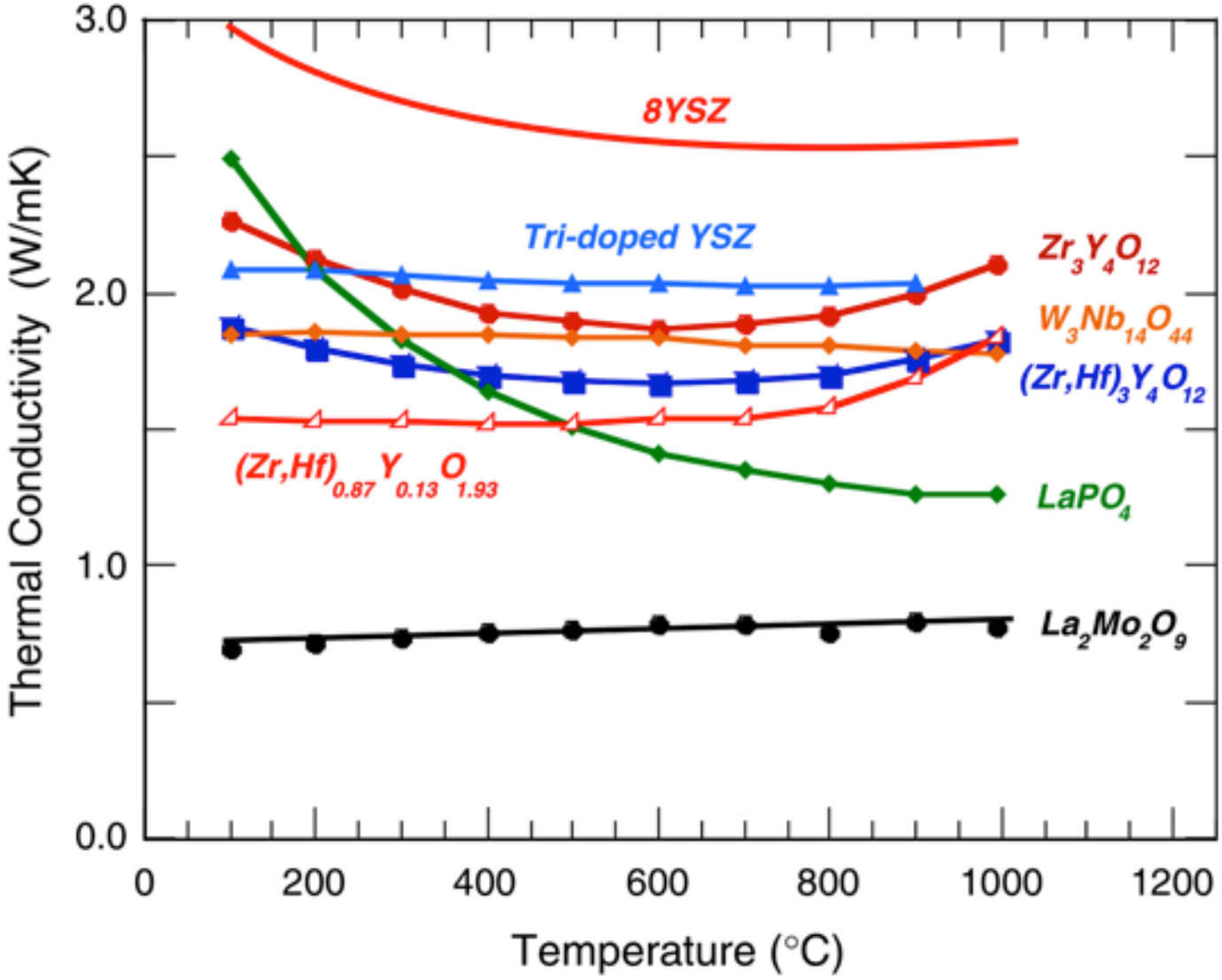

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Some interesting materials: The "gold" standard

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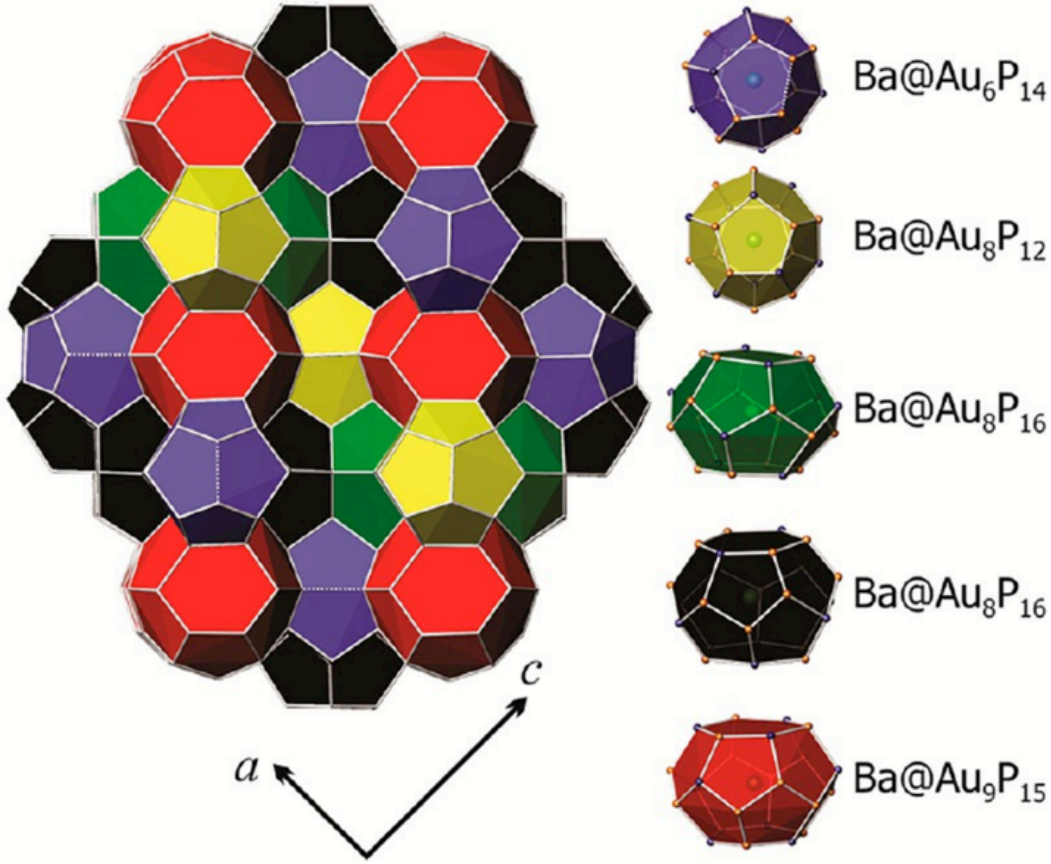
Clathrate $Ba_8Au_{16}P_{30}$: The "Gold Standard" for Lattice Thermal Conductivity

James Fulmer,[†] Oleg I. Lebedev,[§] Vladimir V. Roddatis,[∥] Derrick C. Kaseman,[‡] Sabyasachi Sen,[‡] Juli-Anna Dolyniuk,[†] Kathleen Lee,[†] Andrei V. Olenev,[†] and Kirill Kovnir*[,†]



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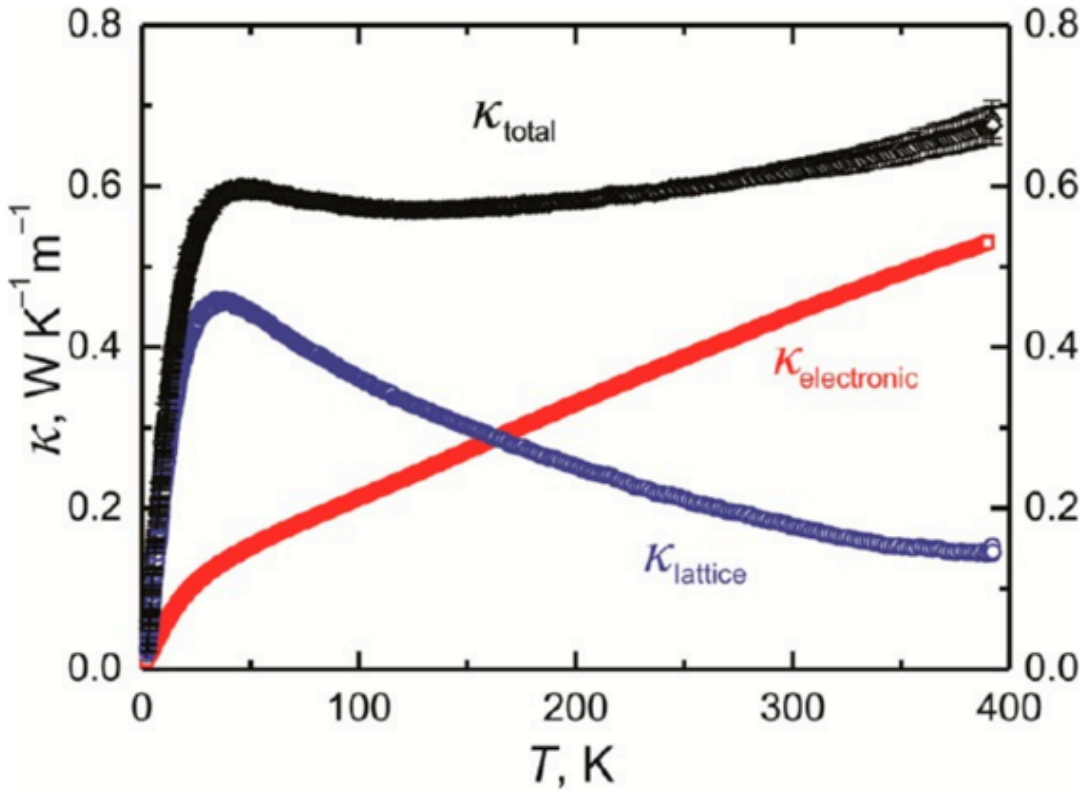

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WHY?

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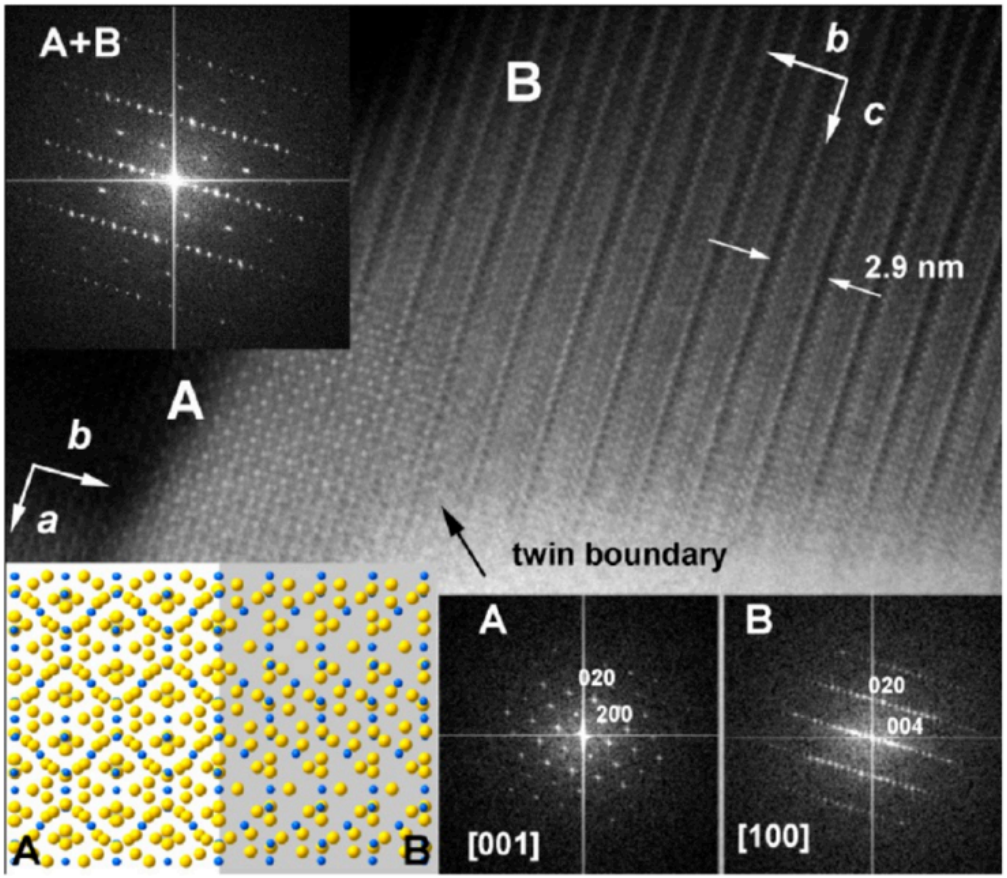

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