Transport and elastic properties of planetary forming materials

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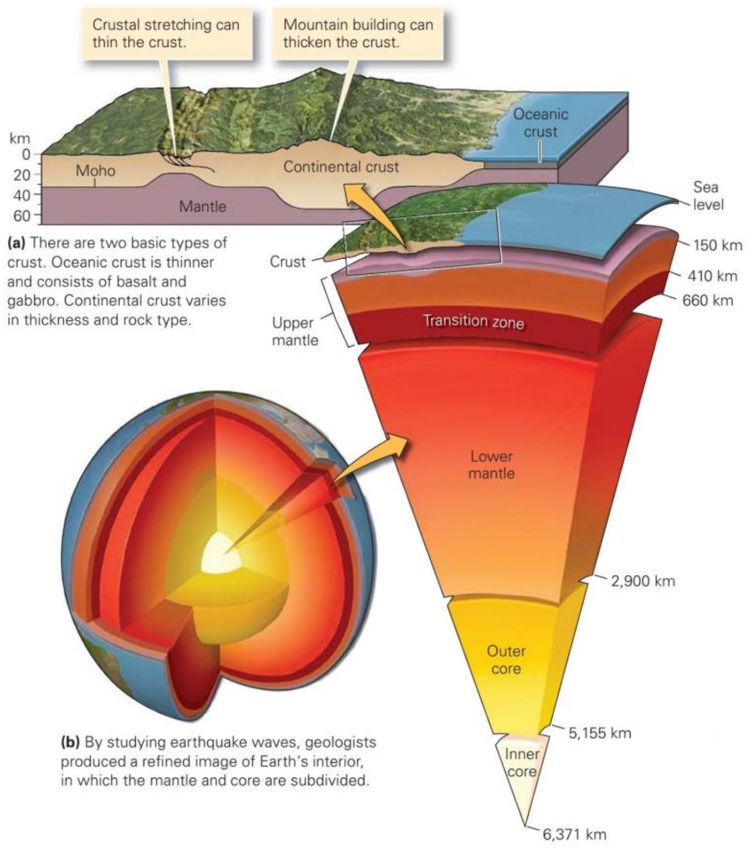
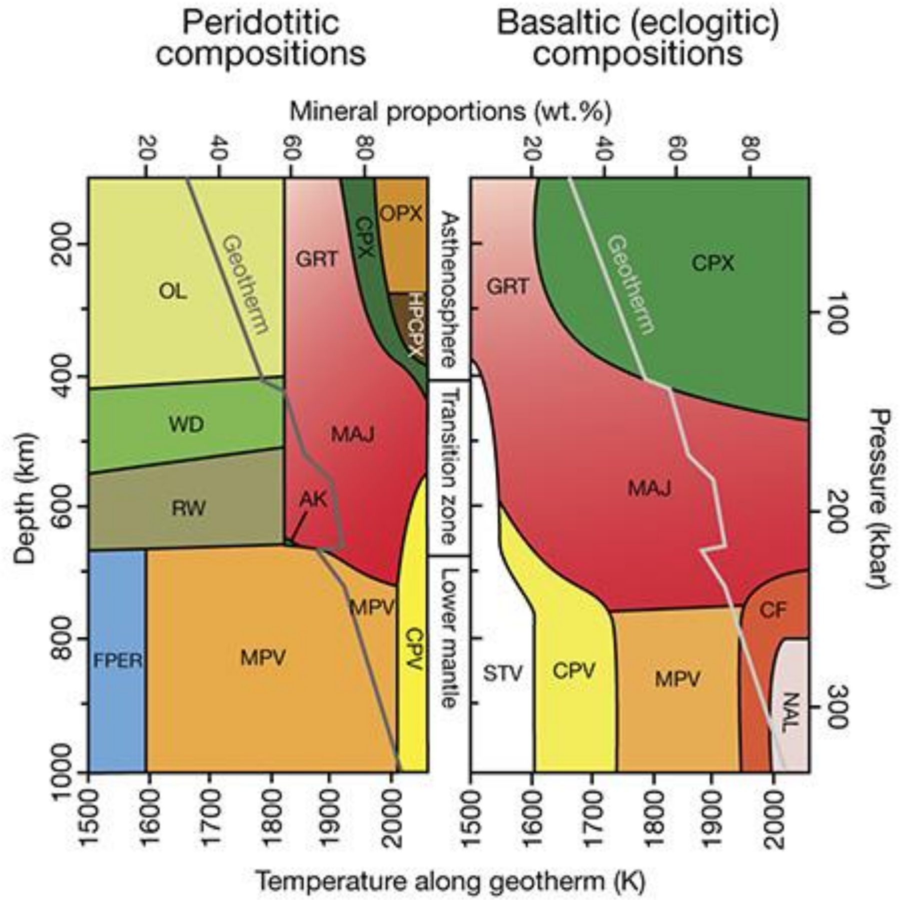
contents

- 1st talk (26th): **Transport and elastic properties of planetary forming materials**
- 2nd talk (27th): **Their applications to the Earth and planetary interiors**

Introduction – Earth's interior

- Layered structures

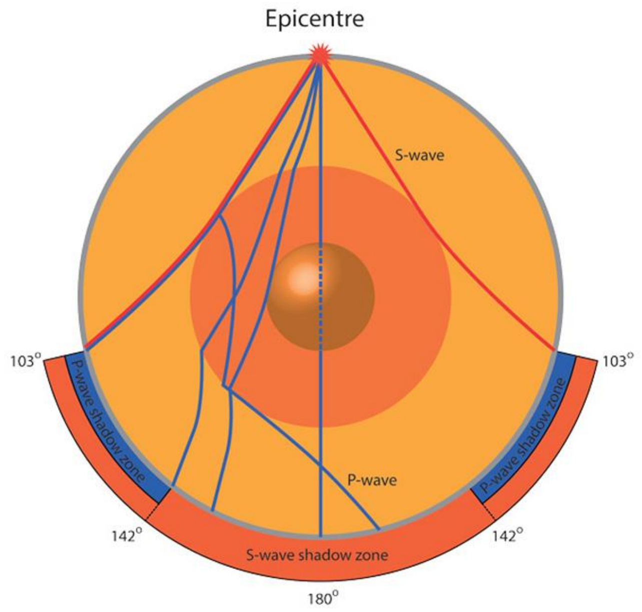


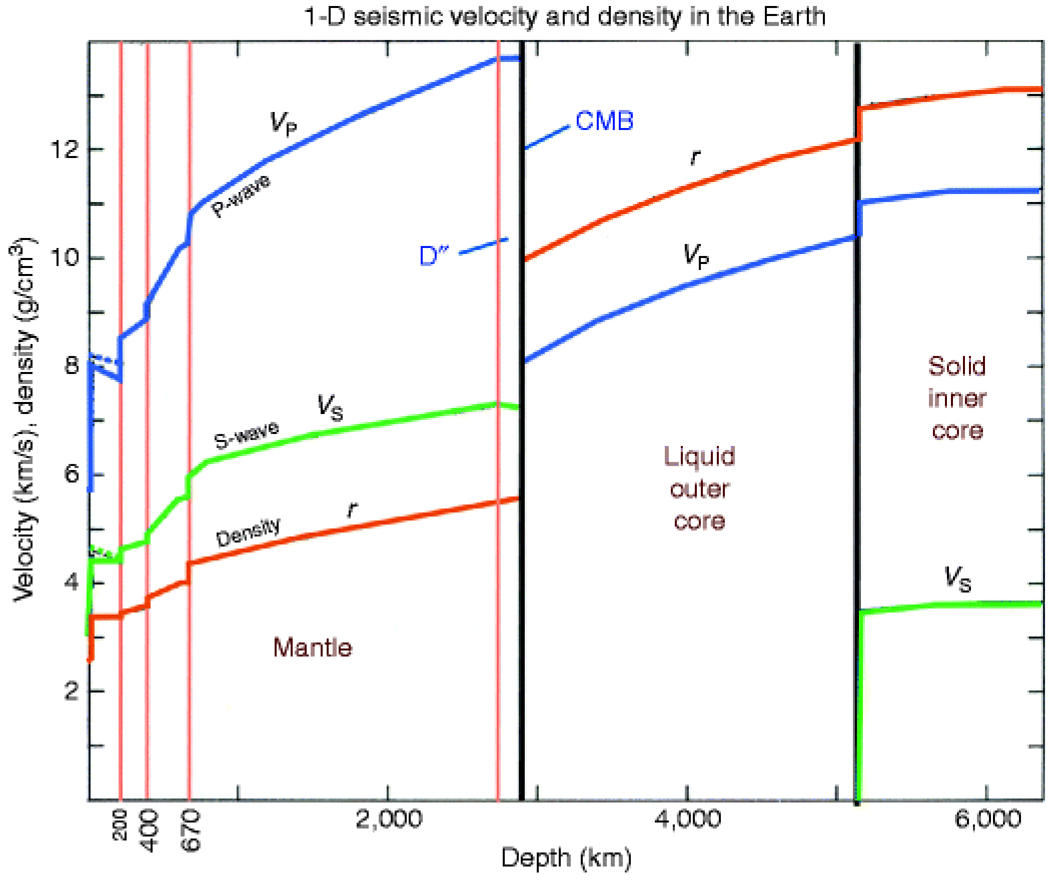


But, how do we know

Probing the Earth and planetary interiors

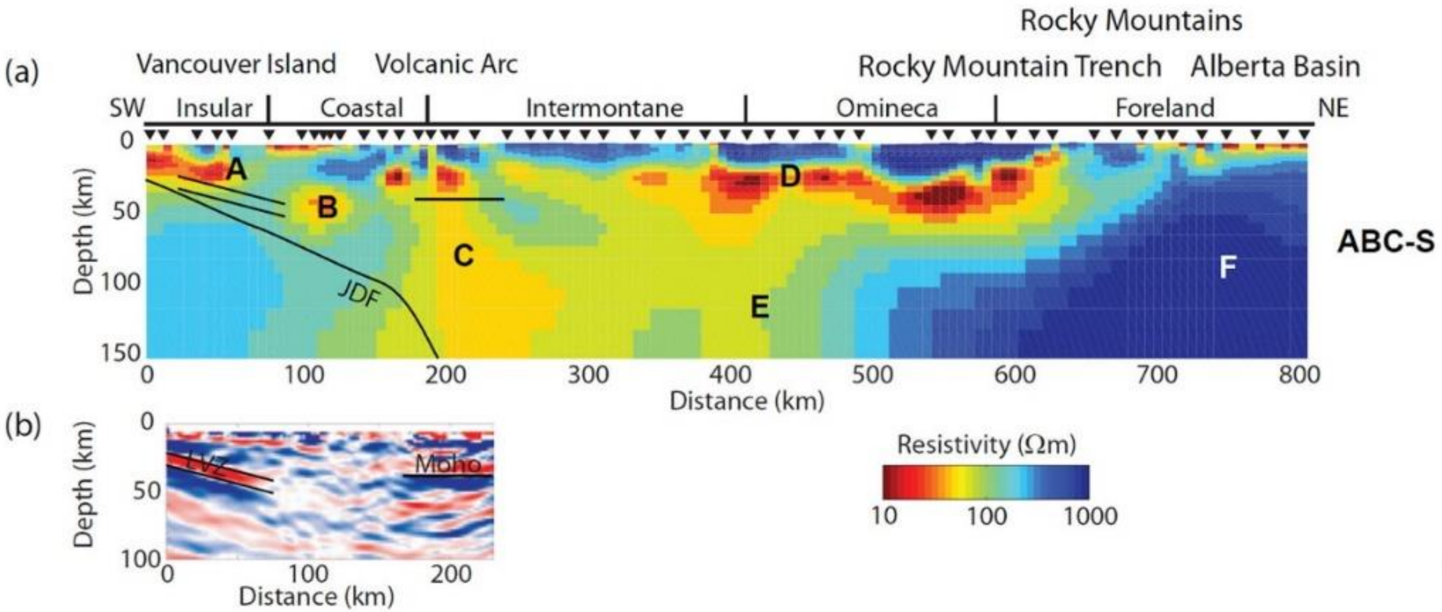
- Mainly through seismology

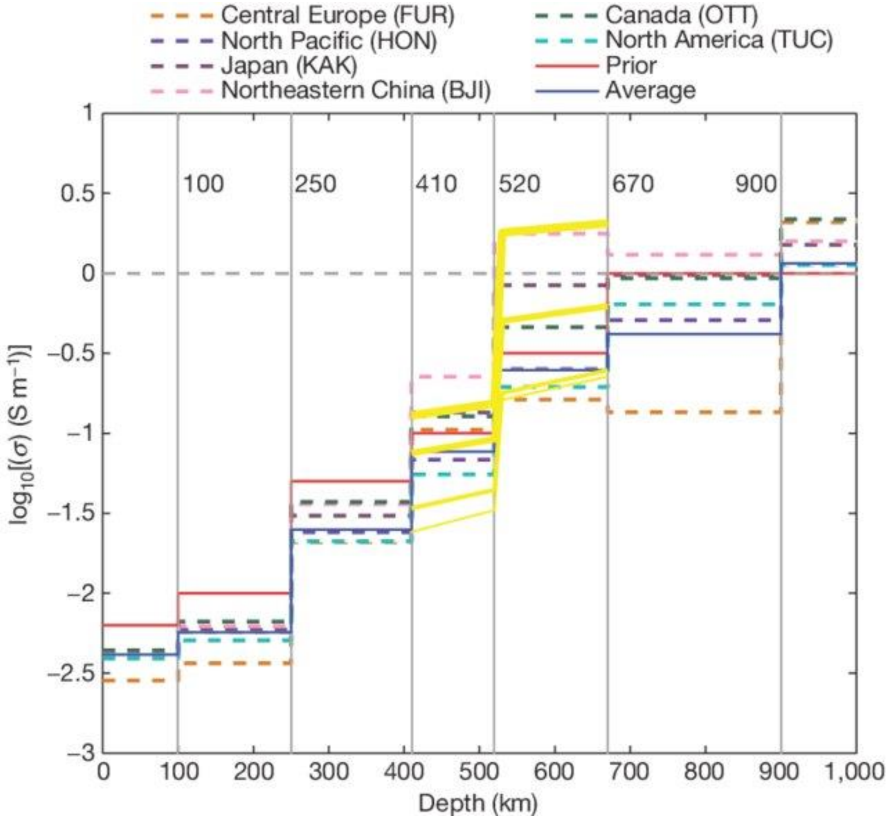




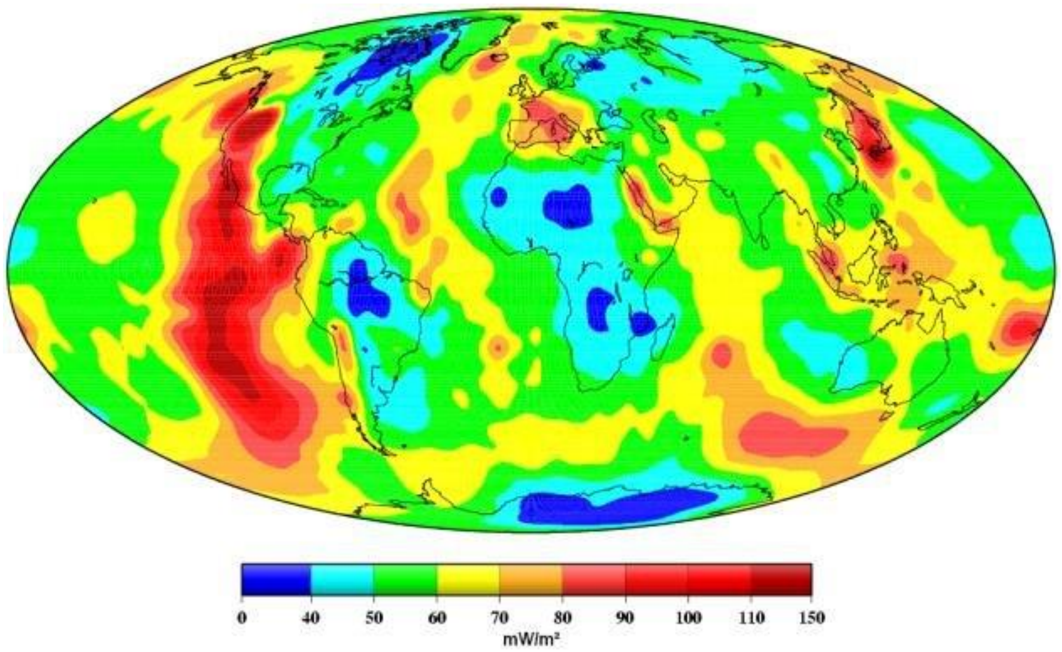
"PREM", Dziewonski and Anderson (1981)

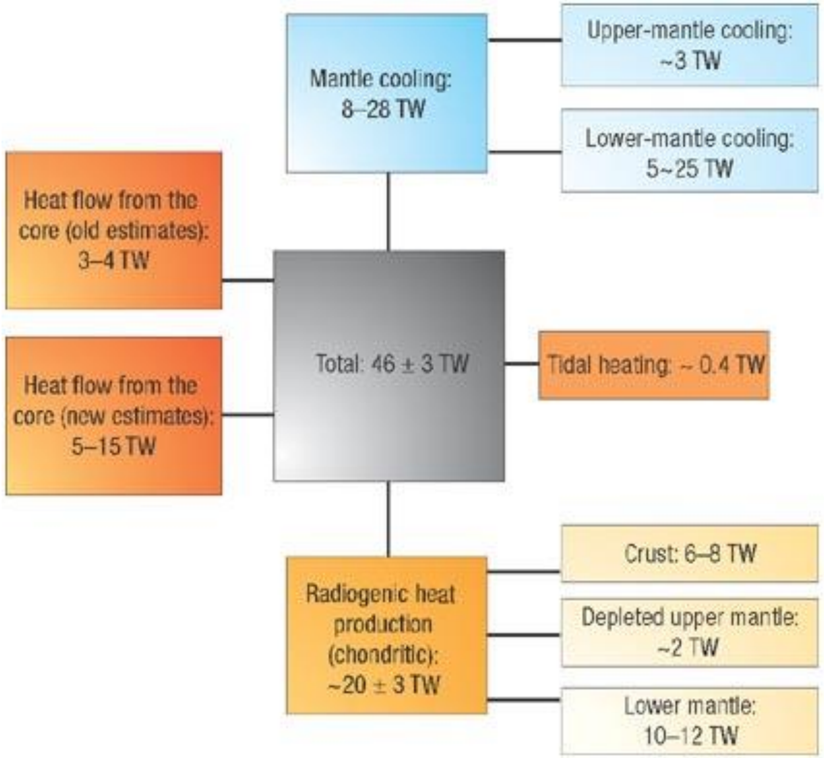
And electrical resistivity





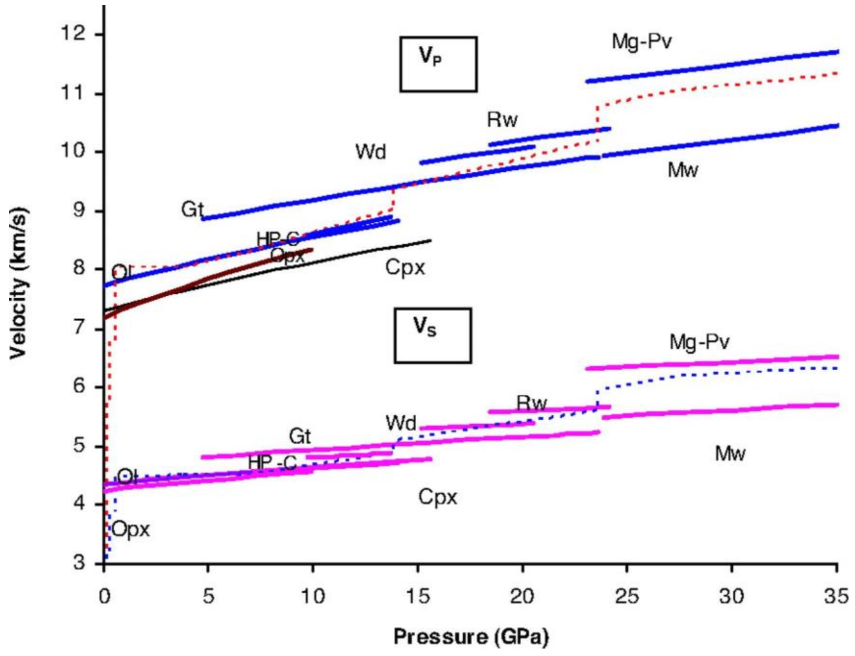
- The 3rd observation – heat flow measurements





- Seismic wave velocity, electrical resistance, heat flow provide first-hand information relevant to the planetary interiors

  - Geophysical profiles represent variations in
    - temperature
    - composition
    - density
    - physical state



Why do we need to study them

- The missing link
  - GEOPHYSICS PROVIDES BULK PROPERTY
- We need to define the source
  - Link lab models with the observations
- Model compositional variations, structures, and dynamic processes
- Understand the diverging paths of planetary evolution
- The fate of our planet

Physical properties of planetary forming materials

Thermo-elastic properties

- Elastic deformation when a force is applied
- reversible
- restores their form after deformation

Transport properties

- Driven by thermal, chemical or velocity gradient
- irreversible

Elastic properties

described by Hooke’s law -

stress is proportional to the strain

$$\sigma_{ij} = C_{ijkl}\epsilon_{kl}$$

proportionality constants – stiffness

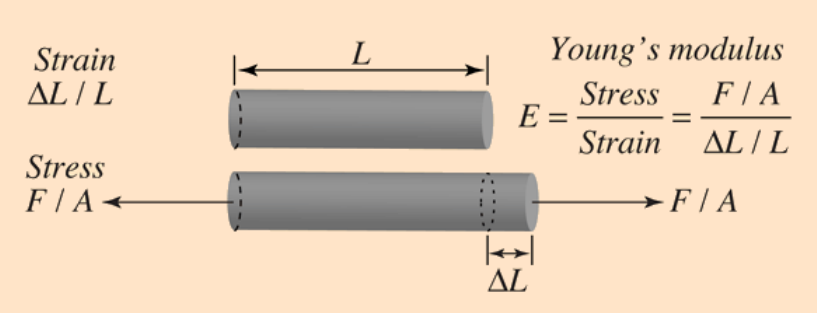
Bulk modulus, Young's modulus, Shear modulus

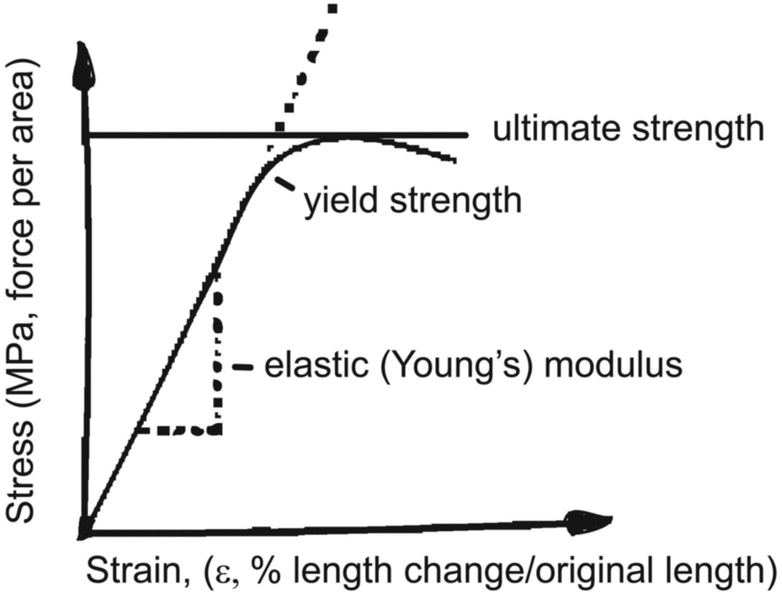
Poissons ratio

- elastic wave velocities (compressional and shear)

Elastic properties

- Young's modulus
  - material's strain response to uniaxial stress in the direction of the stress

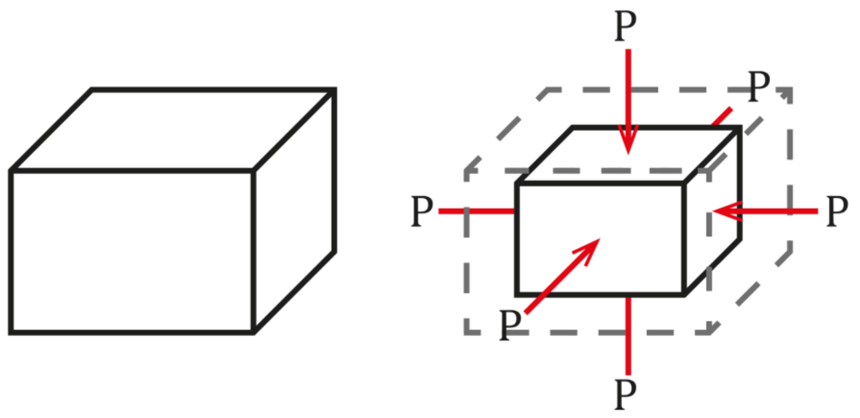




Elastic properties

- Bulk modulus (incompressibility)
  - measure of how resistant to compression
- elastic properties of a solid or fluid when subjected to uniform (hydrostatic) pressure
- returns to its original volume when the pressure is removed

$$K = -V\frac{dP}{dV},$$

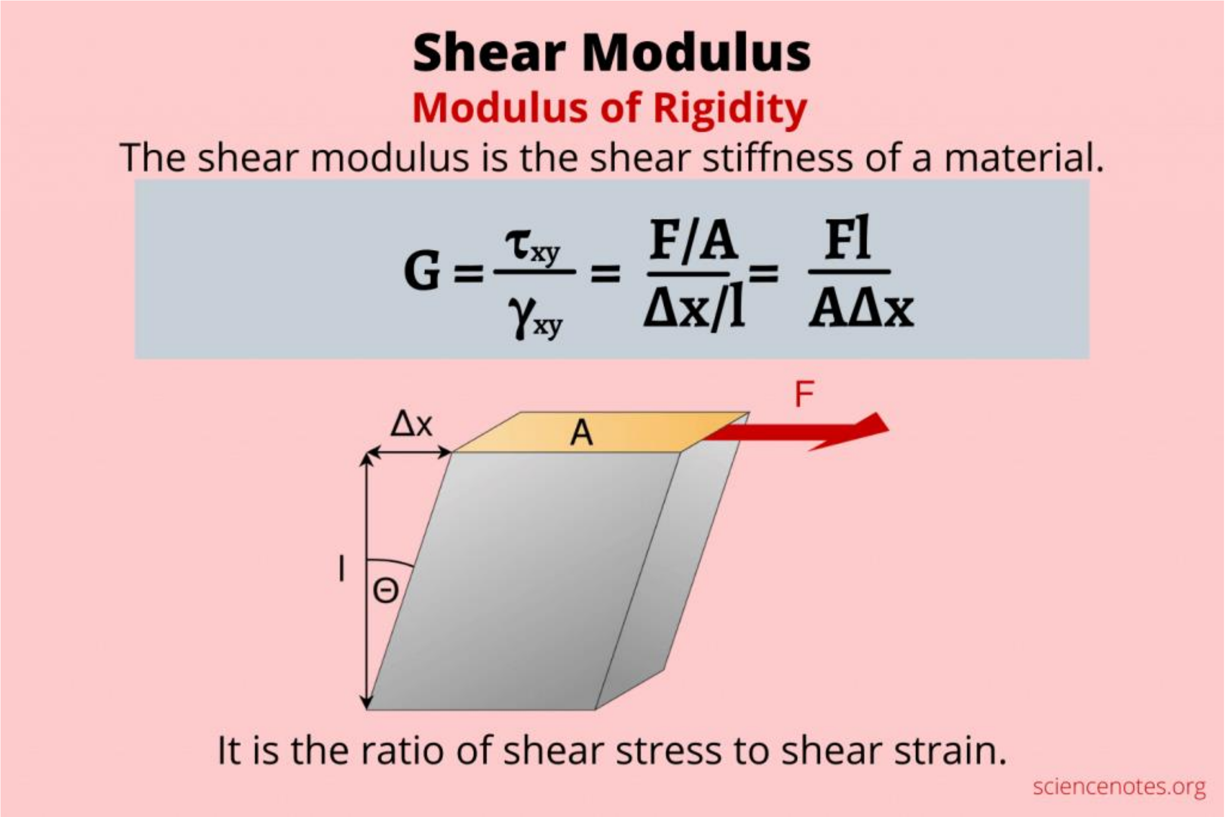


$$K = \rho\frac{dP}{d\rho},$$

isothermal bulk modulus – at constant T
adiabatic bulk modulus – at constant entropy (no heat exchange with surrounding)

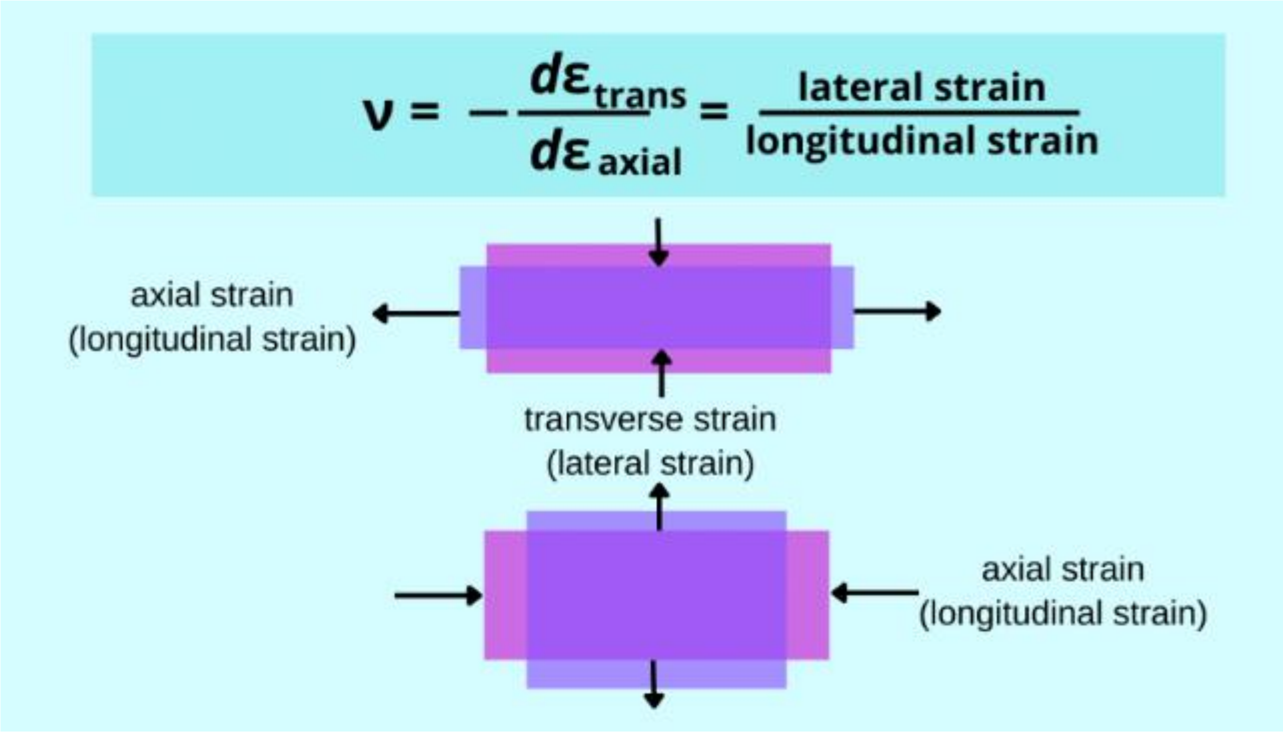
Elastic properties

- Shear modulus
- A measure of the ability of a material to resist transverse deformations



Elastic properties

- Poissons ratio
  - material's strain response perpendicular to the loading (stress)



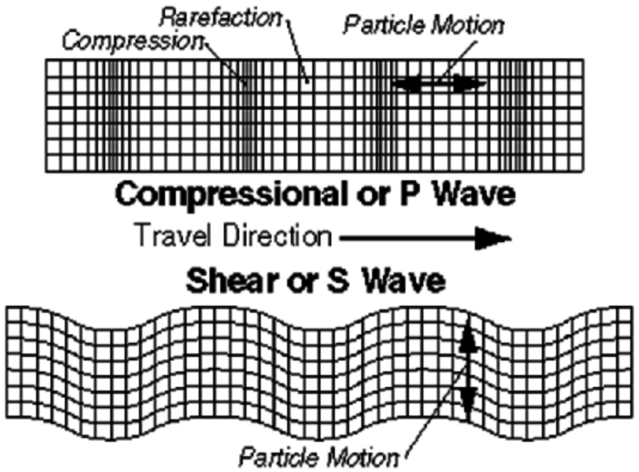
Elastic properties

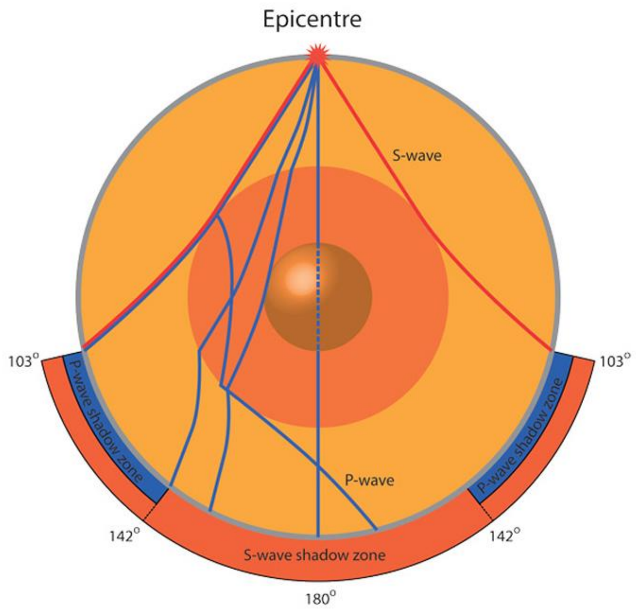
- elastic wave velocities

$$V = \sqrt{\frac{\text{stiffness}}{\text{density}}}$$

$$V_p = \sqrt{\frac{(k + 4\mu/3)}{\rho}}$$

$$V_s = \sqrt{\frac{\mu}{\rho}}$$





Elastic properties

- Elastic properties can be measured by various methods,
  - mechanical stress-strain measurements,
  - ultrasonic, resonant ultrasound spectroscopy
  - Brillouin spectroscopy
  - X-ray and neutron inelastic scattering
  - shock measurements

  - first-principles methods

Transport properties

- Transport properties
- The ability of a substance to transport matter, energy, or some other property along a gradient

A flux J produced by a driving force F, M is the mobility

$$J = MF$$

Irreversible process

- Transport of momentum:

transport of linear momentum along a velocity gradient

- Transport of energy:

transport of thermal energy along a temperature gradient

- Transport of particles :

transport of matter along a concentration gradient

Transport – in the planetary science context

- Momentum
  Viscosity
  deformation of the Earth
  mantle convection

- Energy
  Thermal conductivity
  Heat transfer

- Particles
  Diffusion
  phase transformation
  material circulation

Electrical conductivity
propagation of EM signals

Transfer of momentum - viscosity

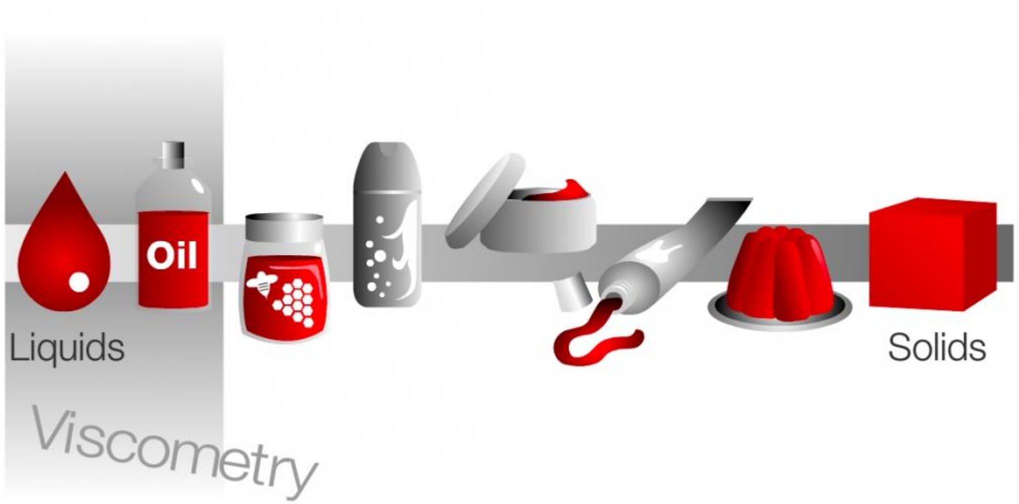
- The transfer of momentum across a velocity gradient
  - The magnitude of the corresponding momentum flux is determined by the viscosity

  - Dynamic viscosity $$\tau = \mu \frac{\partial u}{\partial y}$$

force needed to make the fluid flow at a certain rate,

  - Kinematic viscosity $$\nu = \frac{\mu}{\rho}$$

how fast the fluid is moving when a certain force is applied



Viscosity

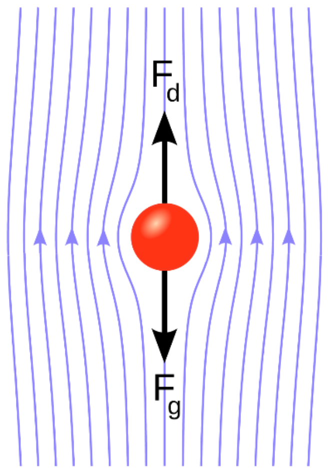
Factor (Pa·s)	Description	Examples	Values (Pa·s)	Ref.
10^{-6}	Lower range of gaseous viscosity	Butane	7.49×10^{-6}	[85]
		Hydrogen	8.8×10^{-6}	[86]
10^{-5}	Upper range of gaseous viscosity	Krypton	2.538×10^{-5}	[87]
		Neon	3.175×10^{-5}	
10^{-4}	Lower range of liquid viscosity	Pentane	2.24×10^{-4}	[78]
		Gasoline	6×10^{-4}	
		Water	8.90×10^{-4}	[78]
10^{-3}	Typical range for small-molecule Newtonian liquids	Ethanol	1.074×10^{-3}	
		Mercury	1.526×10^{-3}	
		Whole milk (20 °C)	2.12×10^{-3}	[81]
		Blood	3×10^{-3} to 6×10^{-3}	[88]
		Liquid steel (1550 °C)	6×10^{-3}	[89]
$10^{-2} – 10^{0}$	Oils and long-chain hydrocarbons	Linseed oil	0.028	
		Oleic acid	0.036	[90]
		Olive oil	0.084	[81]
		SAE 10 Motor oil	0.065 to 0.14	
		Castor oil	0.1	
		SAE 20 Motor oil	0.14 to 0.42	
		SAE 30 Motor oil	0.42 to 0.65	
		SAE 40 Motor oil	0.65 to 0.90	
		Glycerine	1.5	
		Pancake syrup	2.5	
$10^{1} – 10^{3}$	Pastes, gels, and other semisolids (generally non-Newtonian)	Ketchup	$\approx 10^{1}$	[83]
		Mustard		
		Sour cream	$\approx 10^{2}$	
		Peanut butter		[84]
		Lard	$\approx 10^{3}$	
$\approx 10^{8}$	Viscoelastic polymers	Pitch	2.3×10^{8}	[77]
$\approx 10^{21}$	Certain solids under a viscoelastic description	Mantle (geology)	$\approx 10^{19}$ to 10^{24}	[91]

Viscosity of liquids

- Based on Stokes' law

$$F_d = 6\pi\mu R v$$

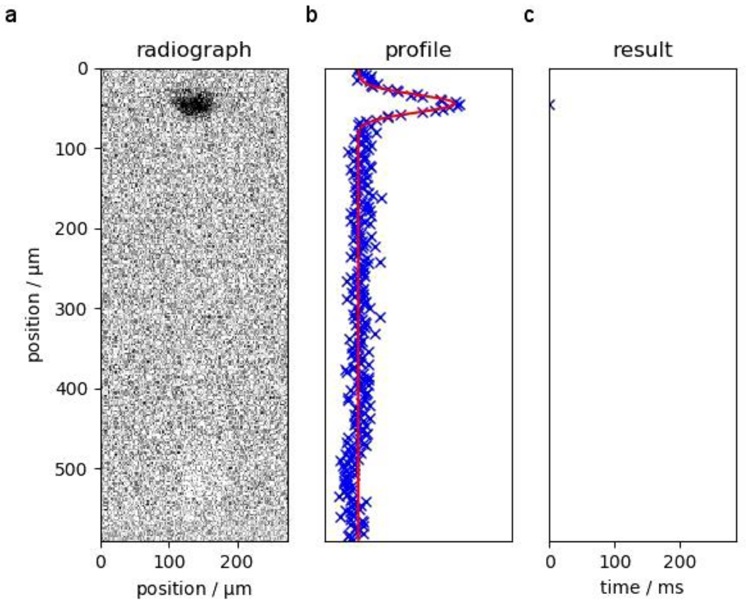
Fd is the frictional force
μ is the dynamic viscosity
R is radius v is the velocity



At the terminal velocity

$$F_g = (\rho_p - \rho_f)\, g\, \frac{4}{3}\pi R^3,$$

$$v = \frac{2}{9}\frac{(\rho_p - \rho_f)}{\mu} g\, R^2$$



Xie et al. 2020

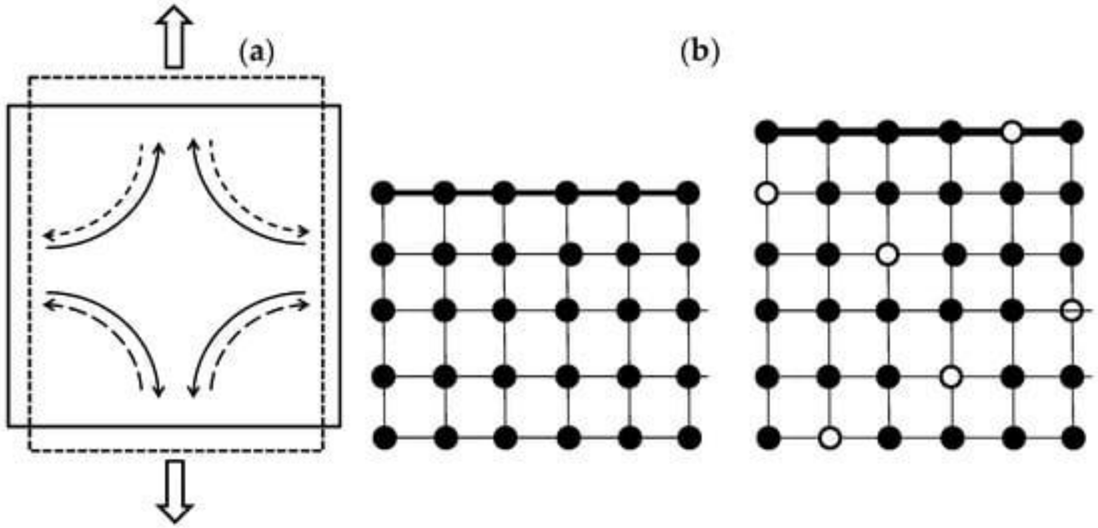
viscosity

- The viscosity of solids (rheology)

high temperature creep of crystal (plastic deformation)

$$\eta = \frac{\sigma}{\dot{\varepsilon}}$$

- Diffusion creep - diffusion of vacancies through the crystal lattice



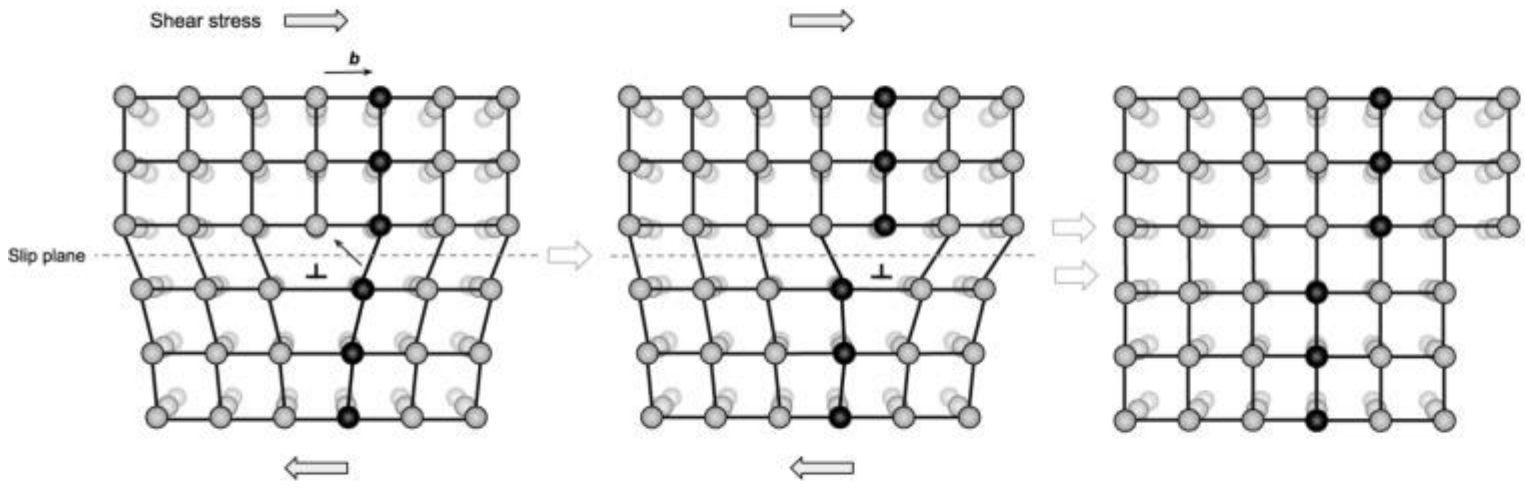
viscosity

- Viscosity of solids

$$\eta = \frac{\sigma}{\dot{\varepsilon}}$$

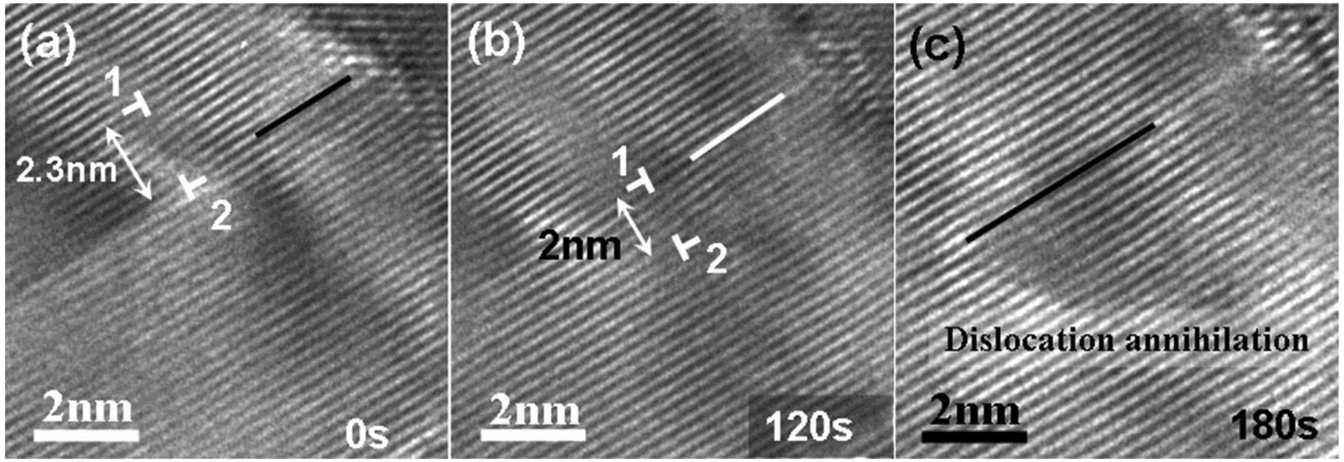
high temperature creep of crystal

- Dislocation creep- the movement of dislocations through the crystal lattice



Thermal conduction

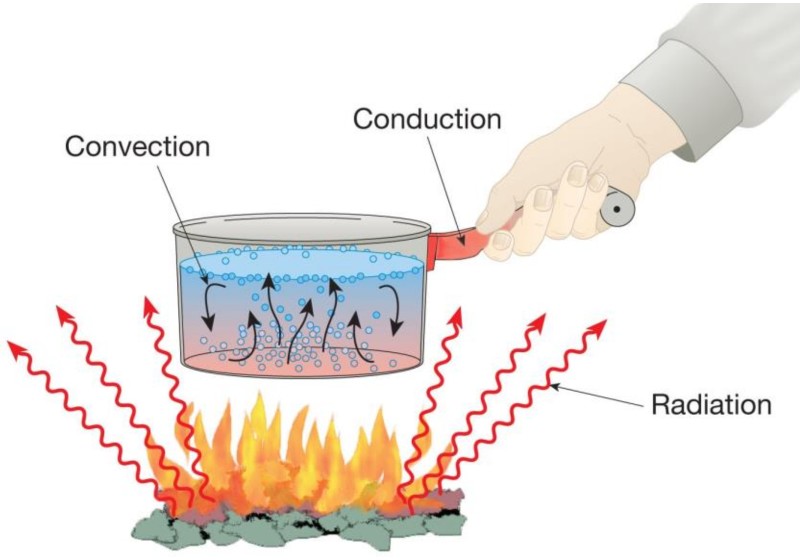
- *In situ observation of a pair of moving dislocations*



(Wang et al. 2011)

Heat transport

- Heat transfer mechanisms
- Conduction – the movement of kinetic energy
- Convection - Convection is heat transfer through fluid motion
- Radiation – energy transfer through EM radiation

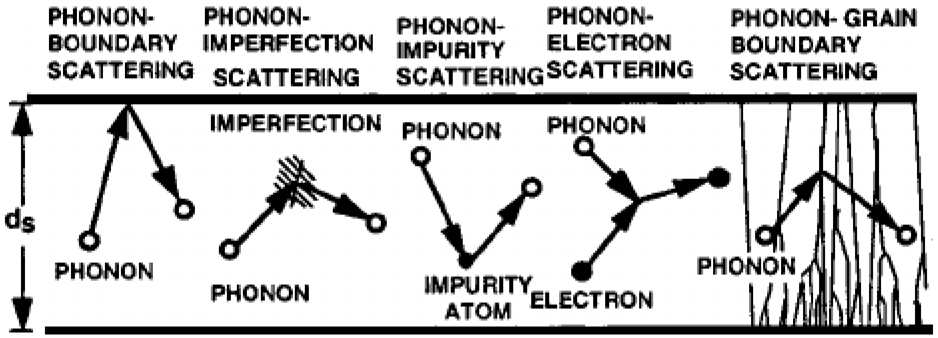


Thermal conduction

- Thermal conductivity κ is determined by lattice vibration (phonon conduction),

$$\kappa = \frac{1}{3} C_v v l$$

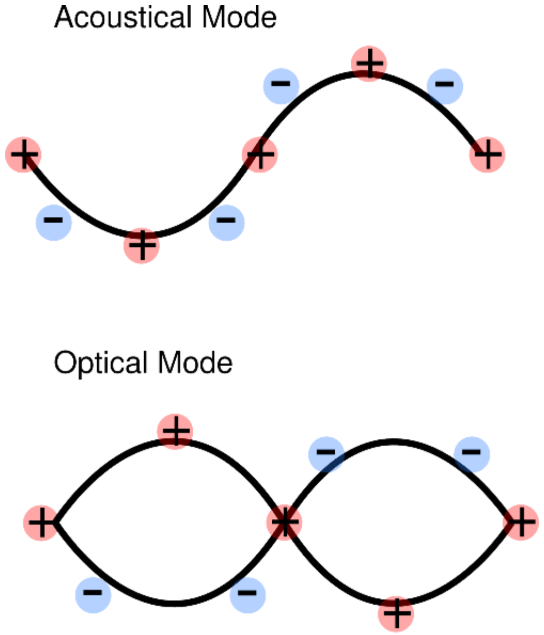
Phonon mean-free path – the distance between two scattering events

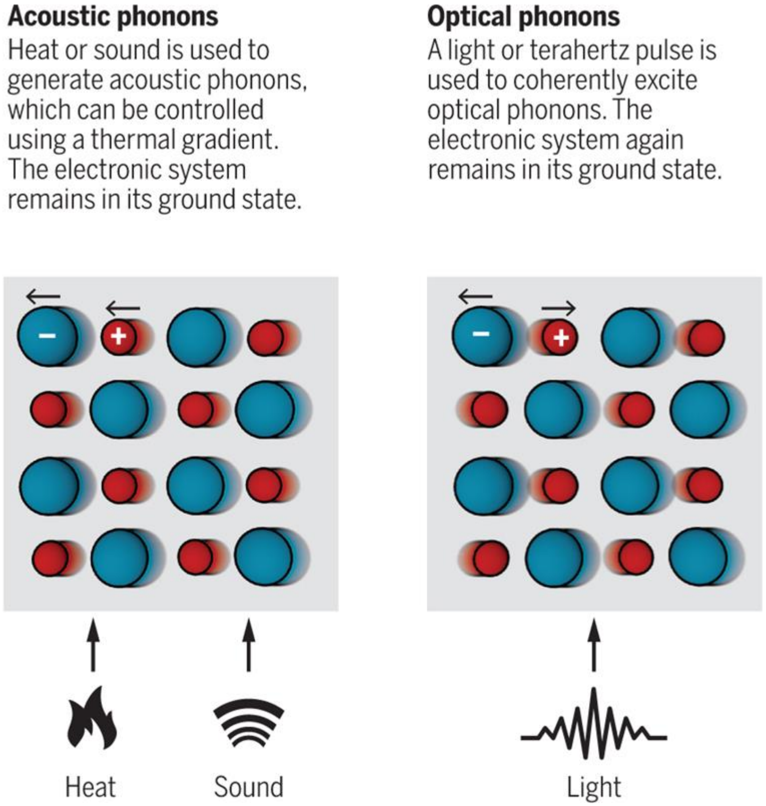


Higher the scattering lower the TC

Impurities (Fe, Al)
Grain boundaries

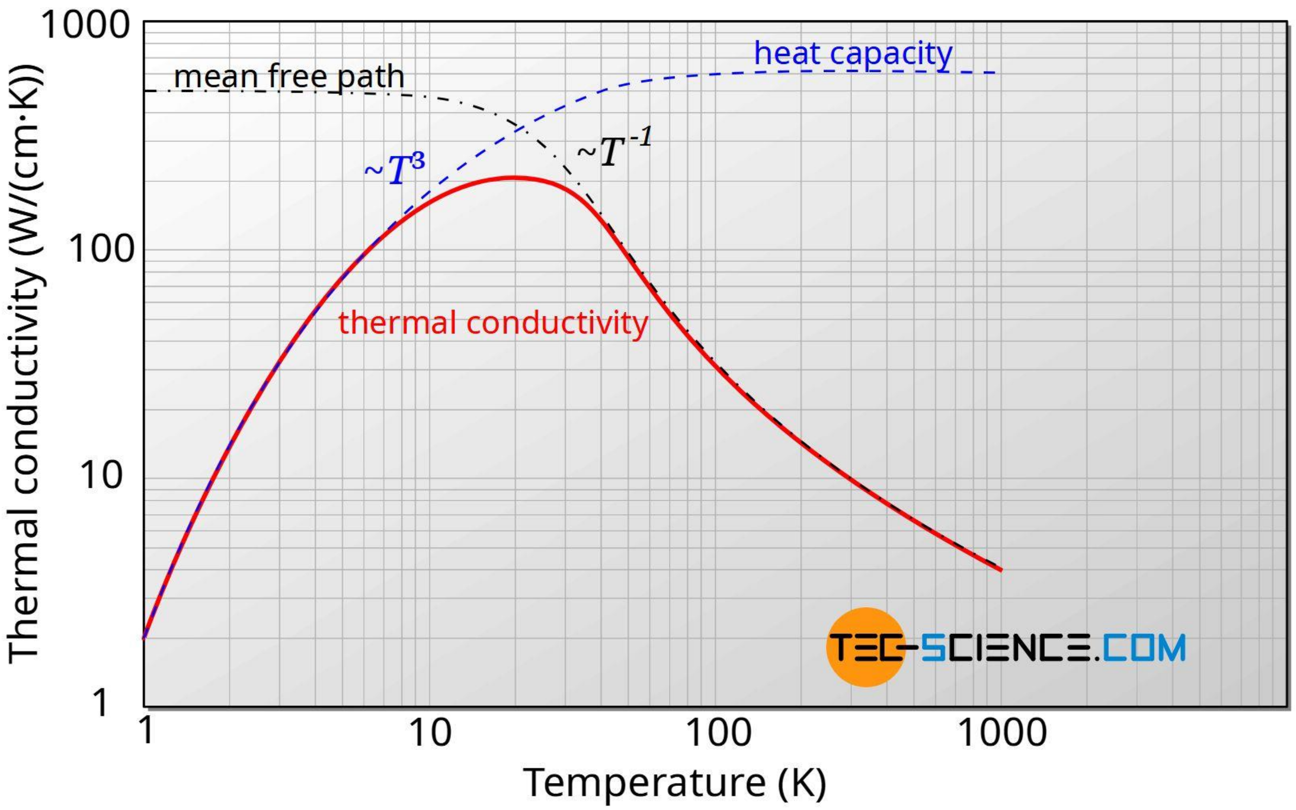
Thermal conduction





Thermal conduction

- phonon mean free path $\propto$ 1/T



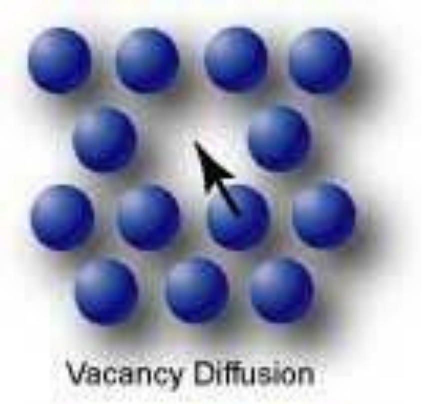
Diffusion (chemical)

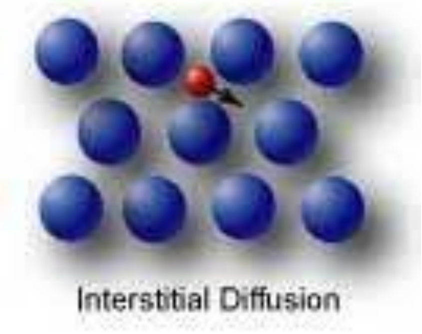
- diffusion in solids- Mass transport by atomic motion
- Fick's law (first) - steady state

$$F = -D\frac{dC}{dx}$$

F is the diffusion flux (Kg/m^2 s)
dC/dx, concentration gradient (Kg/m^4)
D diffusion coefficient (m^2/s)

- Vacancy diffusion
- Interstitial diffusion



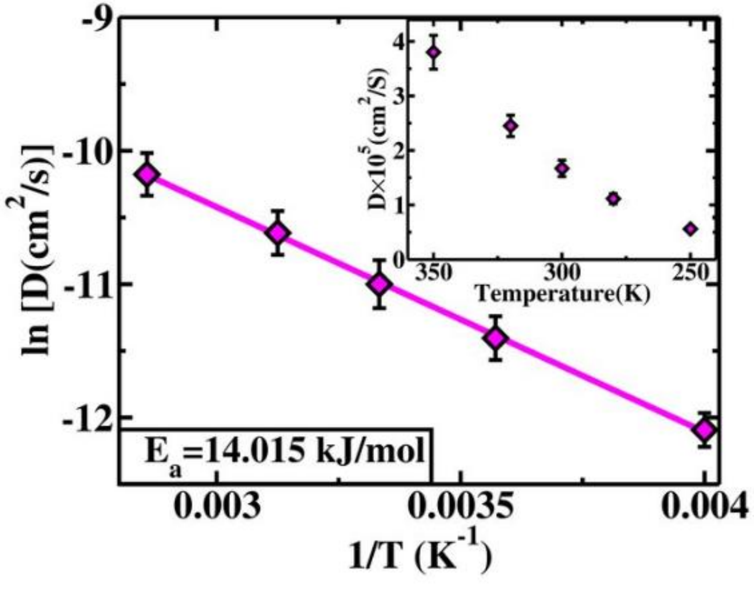


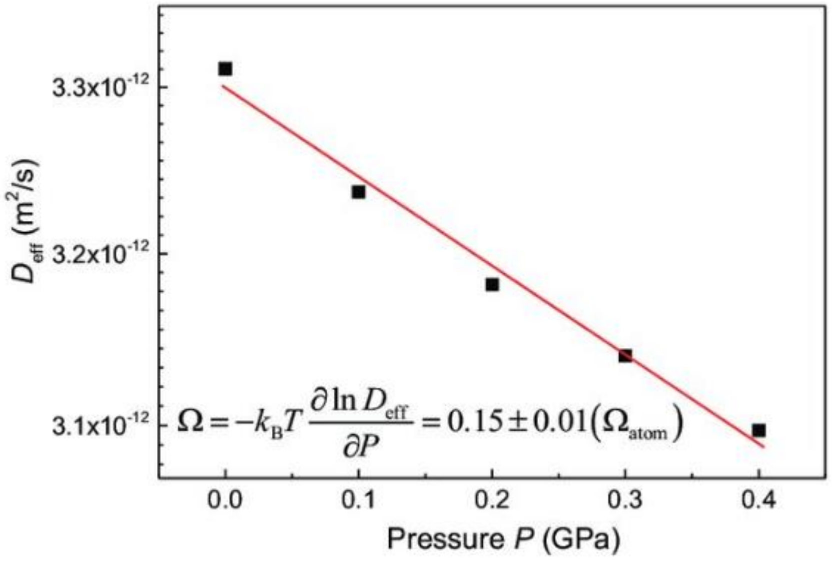
Diffusion (chemical)

$$D_{(P,T)} = D_0 exp\left(\frac{\Delta H - P\Delta V}{RT}\right)$$

$$\Delta H = -R\frac{\partial InD}{\partial(\frac{1}{T})}$$

$$\Delta V = RT\frac{\partial lnD}{\partial P}$$





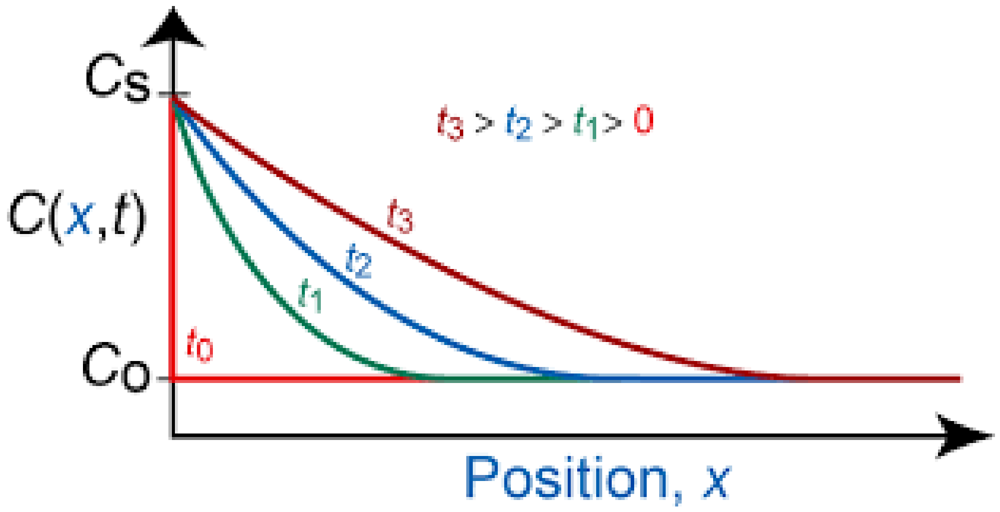
Diffusion (chemical)

Non-steady-state diffusion – Fick's second law

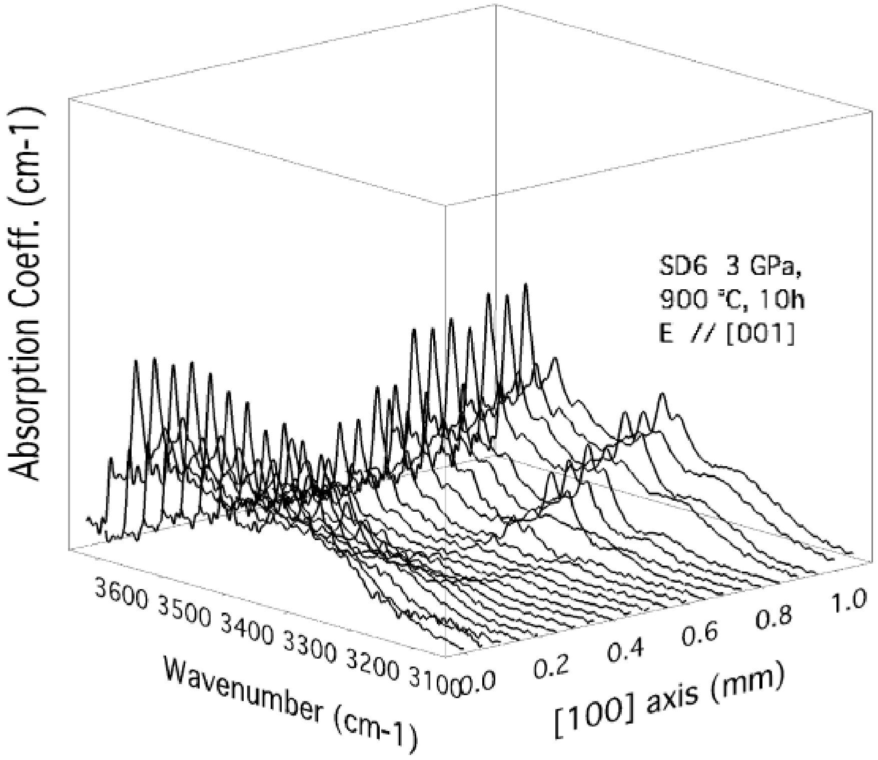
Concentration as a function of both time and position

$$\frac{c_x - c_0}{c_s - c_0} = 1 - \mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

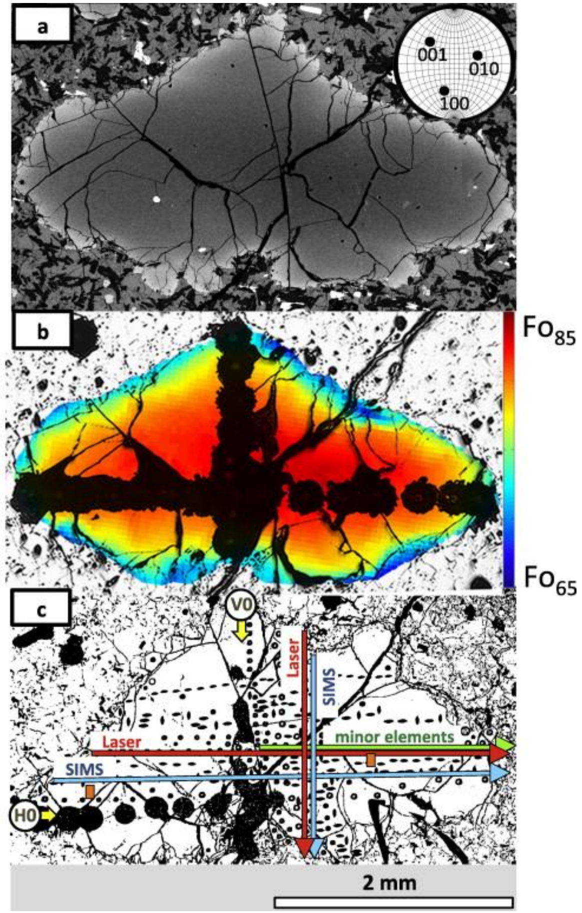
C_s = Concentration of source
C_x = Concentration at distance x
C_0 = Concentration of h0st



Diffusion (chemical)

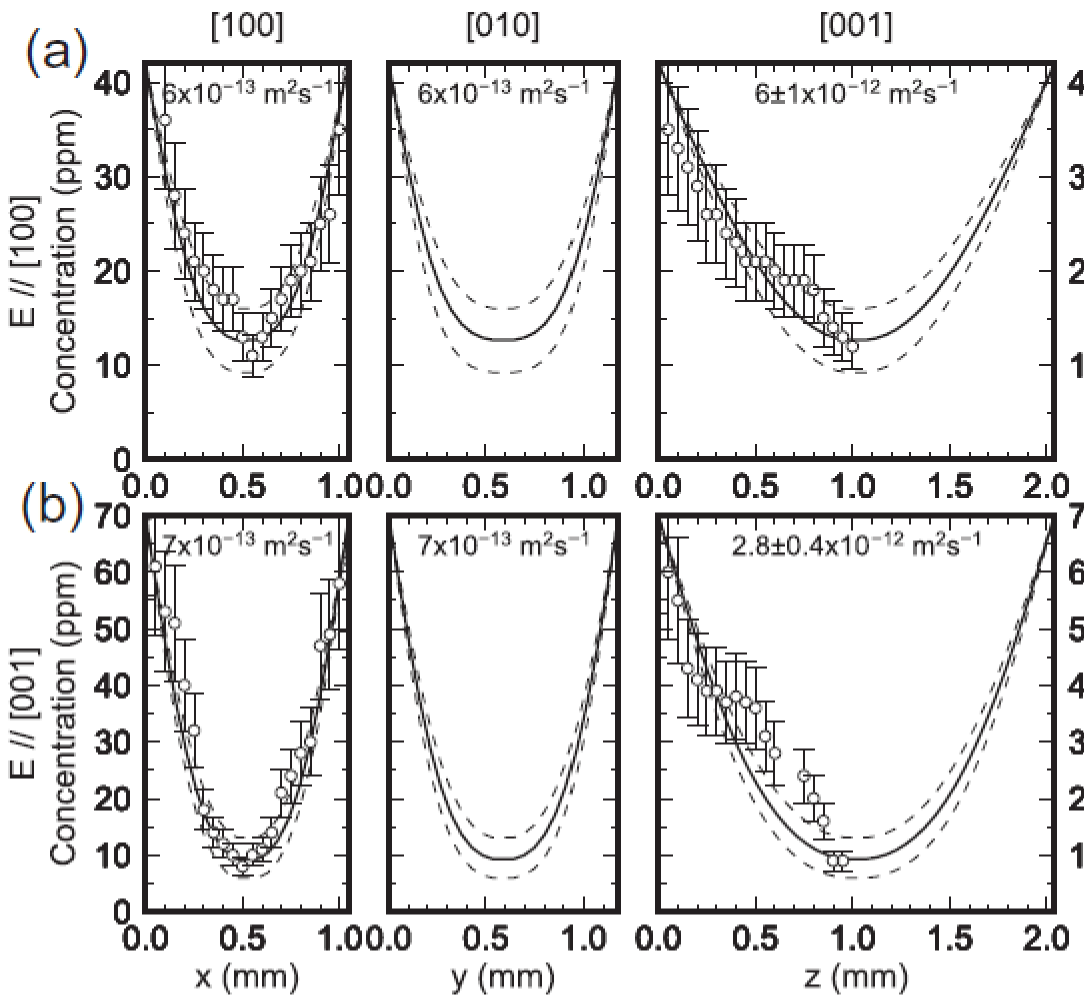


Demouchy et al. 2016



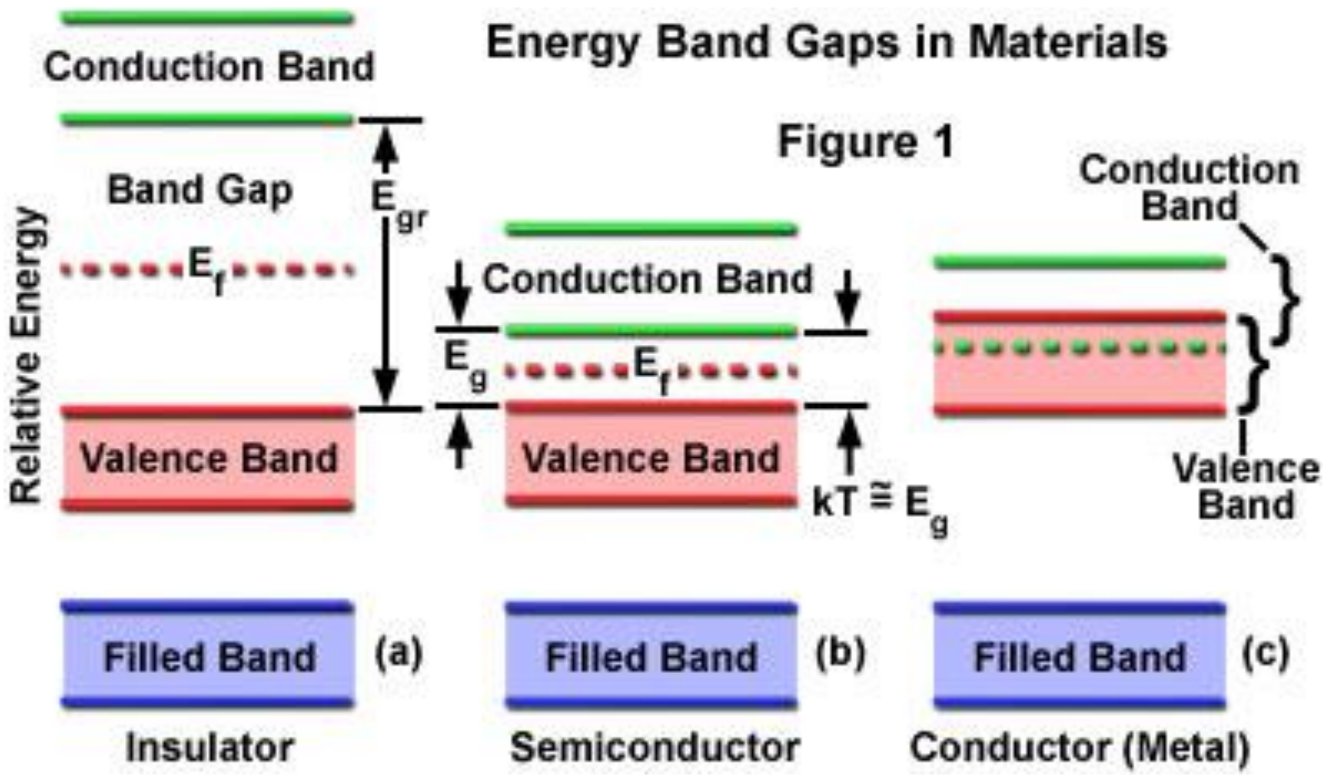
Kin et al. 2013

Diffusion (chemical)



Electrical conduction

- Electrical band gap



smaller the band gap higher the mobility of charge-carrying electrons or holes

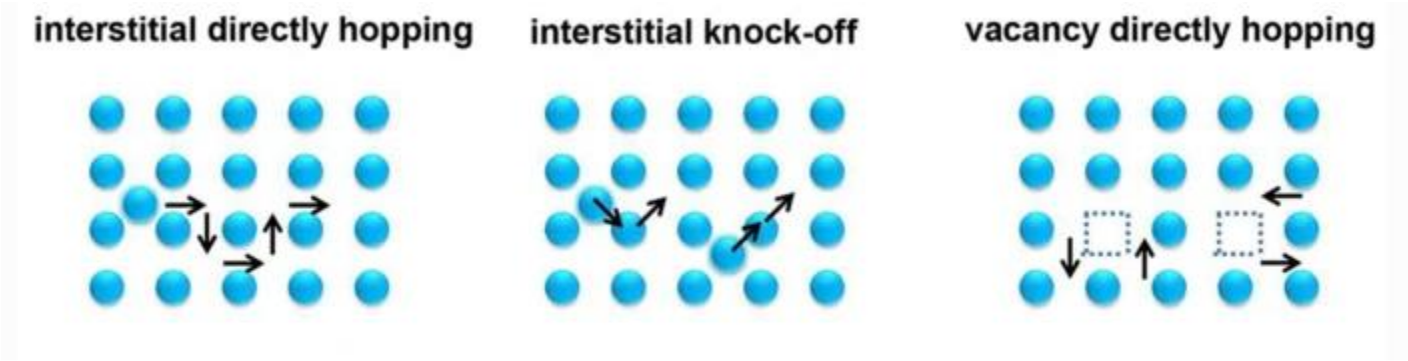
Electrical conduction –conduction mechanisms

- **Ionic conduction**

In ionic conduction, ions diffuse from one site to another aided by the migration of atomic vacancies in the lattice. The ionic exchange and diffusion can be illustrated using

$$A_A^{\times}\,(site\ 1) + V_A(site\ 2) \Leftrightarrow A_A^{\times}\,(site\ 2) + V_A(site\ 1)$$

where $A_A^{\times}$ is the regular charge-balanced site of the element (e.g. Mg, Fe, Si and O), and V_A is the corresponding vacant site.



Electrical conduction –conduction mechanisms

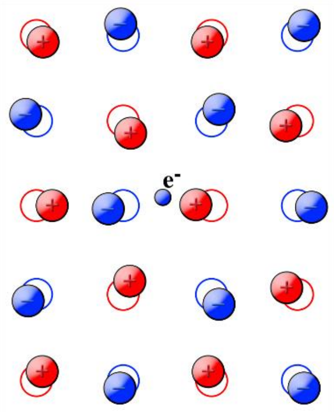
- **Hopping (small polaron) conduction**

hopping of electron holes between neighboring ions with different valence states

For example, the transfer of electron holes between ferric (Fe^{3+}) and ferrous (Fe^{2+}) ions controls the hopping conduction in Fe-bearing mantle minerals.

$$Fe^{3+} \Leftrightarrow Fe^{2+} + \dot{h}$$

where $\dot{h}$ is an electron hole.



Electrical conduction

- Activation energies

For a single conduction mechanism, a material's electrical conductivity pressure- (P) and temperature- (T) dependence can be expressed by the Arrhenius law as follows,

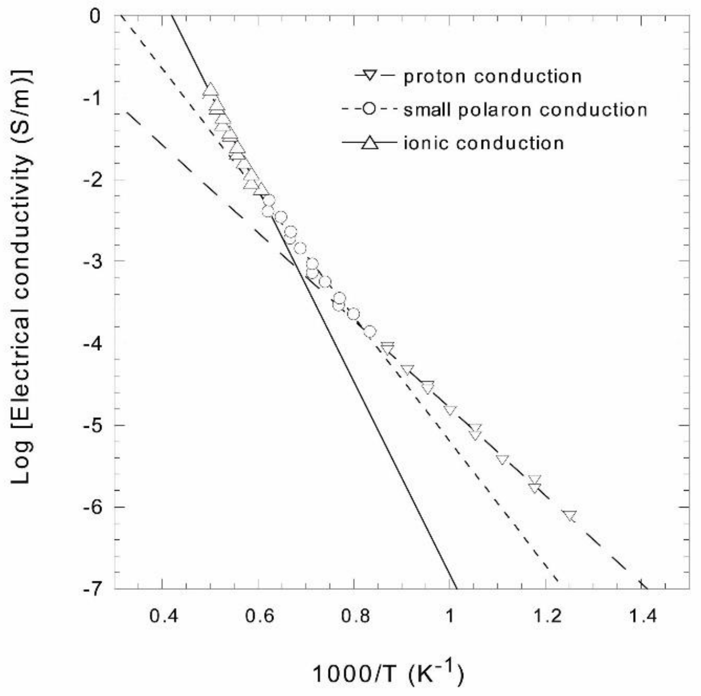
$$\sigma(P,T) = \sigma_0 exp\left(-\frac{\Delta H + P\Delta V}{RT}\right)$$

σ_0 is the pre-exponential factor,

ΔH is the activation energy,

ΔV is the activation volume,

R is the gas constant



Electrical conduction

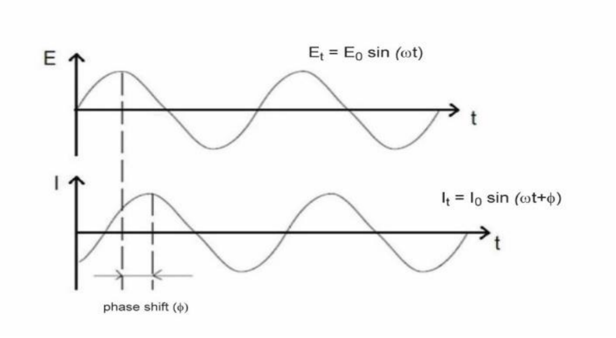
EC of a material is proportional to the number of charged particles and their mobility,

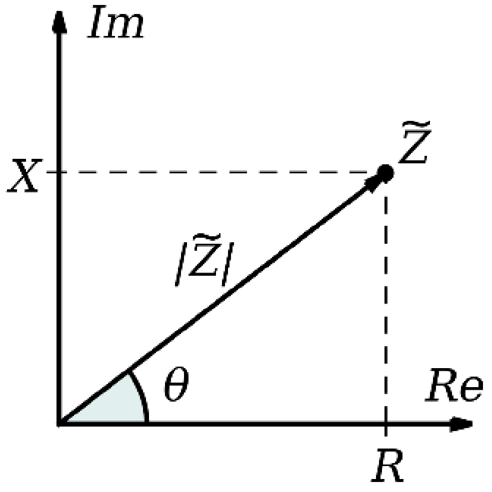
$$\sigma = |q|n\mu \text{ or } \sigma = \sum_i |q_i| n_i \, \mu_i$$

- Conduction in a material is described by Ohm's Law $I = V/R$,
- ideal resistor (R) is independent of frequency - current and voltage signals are in phase with each other $I = V/R$
- When a resistor behaves as an impedance,

  the current flow is out of phase with the voltage

  voltage-to-current ratio becomes frequency-dependent





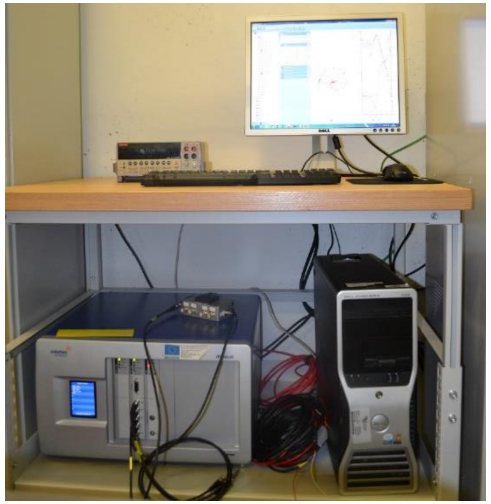
$$Z = R + JX$$

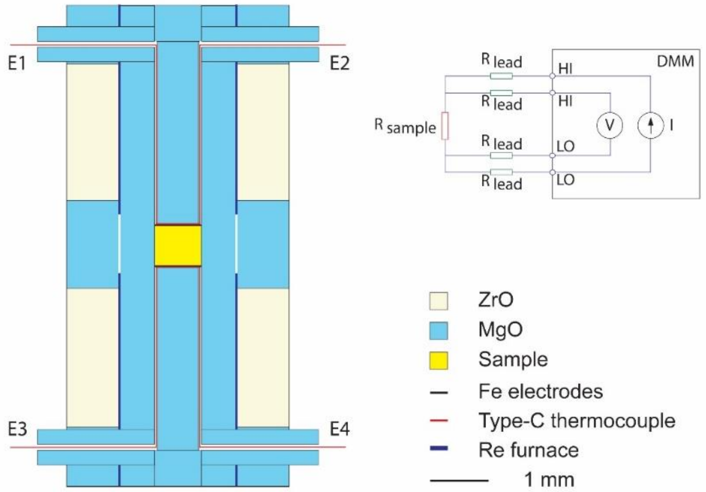
$$Z = \sqrt{R^2 + (X_L - X_C)^2}$$

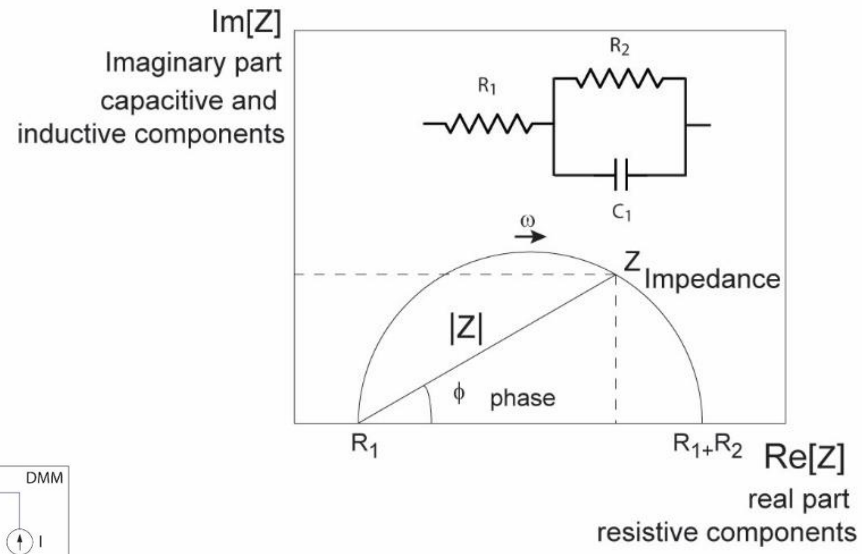
$$Z = \frac{E_t}{I_t} = \frac{E_0 \sin(\omega t)}{I_0 \sin(\omega t + \phi)} = Z_0 \frac{\sin(\omega t)}{\sin(\omega t + \phi)}$$

Experimental procedures and protocols

- Impedance spectroscopy method

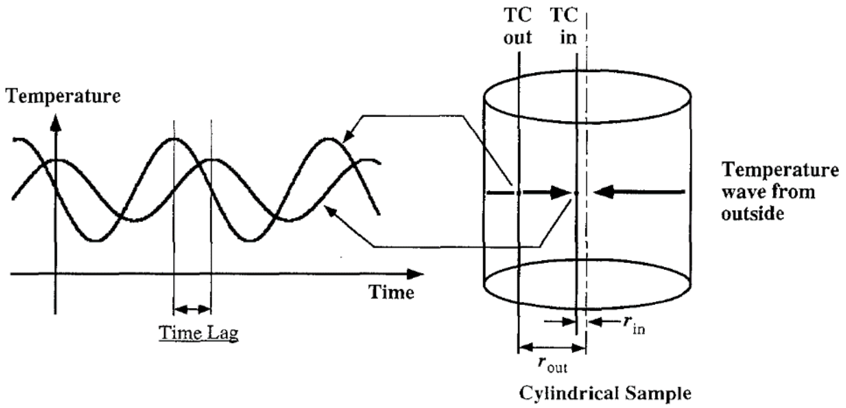


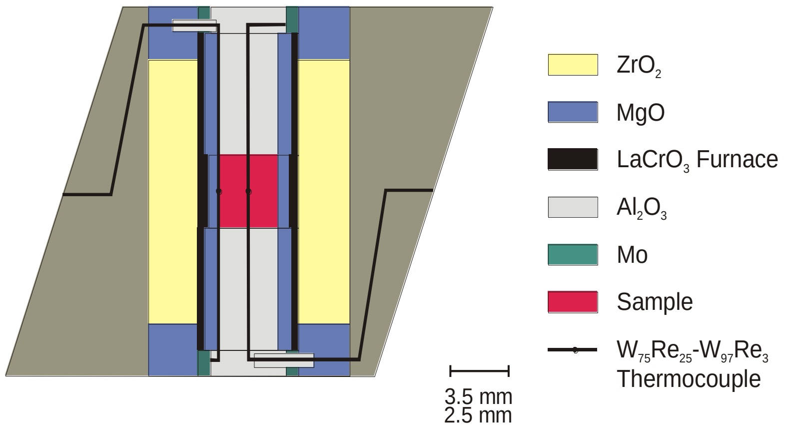


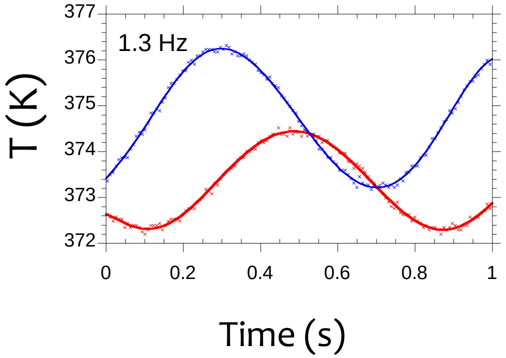


Thermal conductivity - experimental procedures

- Ångström method







$$\Phi = \Phi_{r_1} - \Phi_{r_2} = \tan^{-1}\left[bei(u)/ber(u)\right]$$

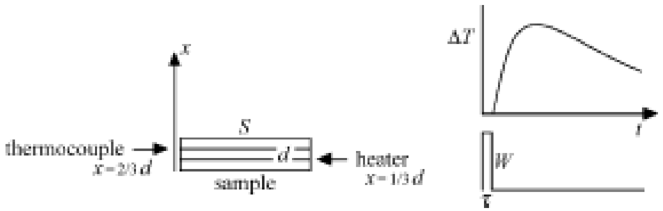
$$\Theta = \frac{\Theta_{r_1}}{\Theta_{r_2}} = \frac{1}{\sqrt{bei^2(u) + ber^2(u)}}$$

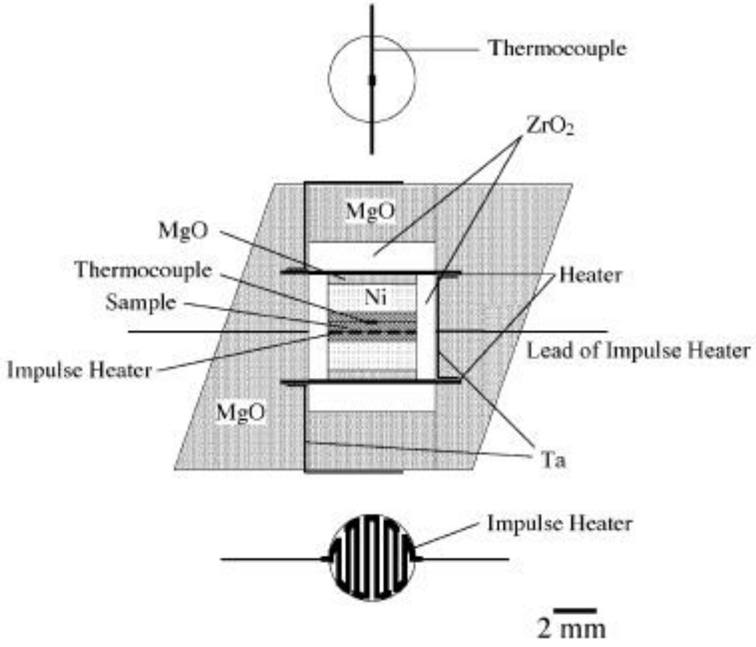
$$D = \omega\left(\frac{r_2 - r_1}{u}\right)^2$$

$$\kappa = D\rho Cp$$

Thermal conductivity - experimental procedures

- Ångström method



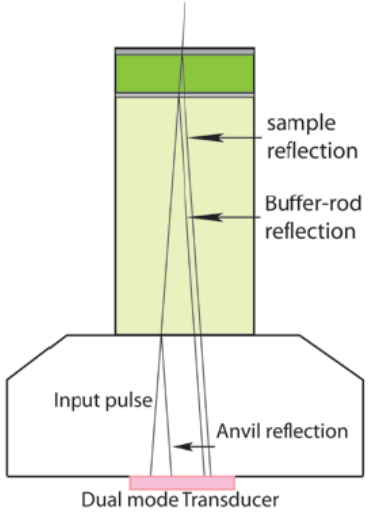


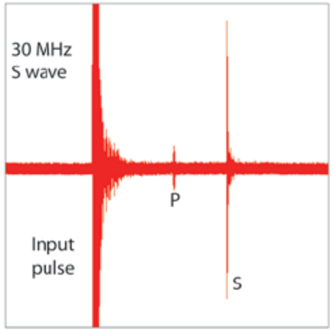
$$\Delta T = A \sum_{n=1}^{\infty} \frac{1}{n^2} sin \frac{n\pi}{3} sin \frac{n\pi x}{d} \exp(-n^2 Bt)\,[\exp(n^2 B\tau) - 1]: \;\; t > \tau$$

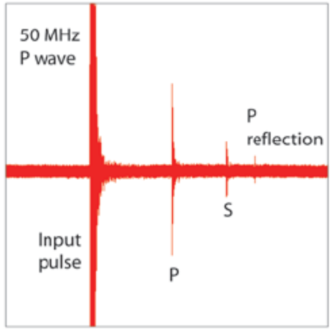
$$A = \frac{2Wd}{\pi^2 \mathrm{K} S}\,, \qquad B = \frac{\pi^2 \lambda}{d^2}$$

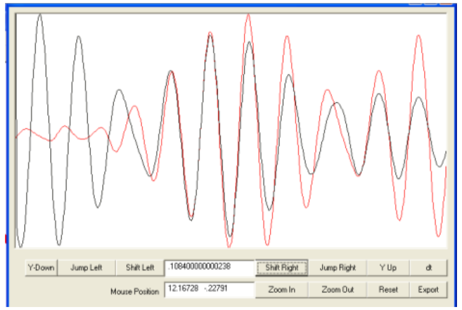
Elastic properties - experimental procedures

- Ultrasonic Interferometry method





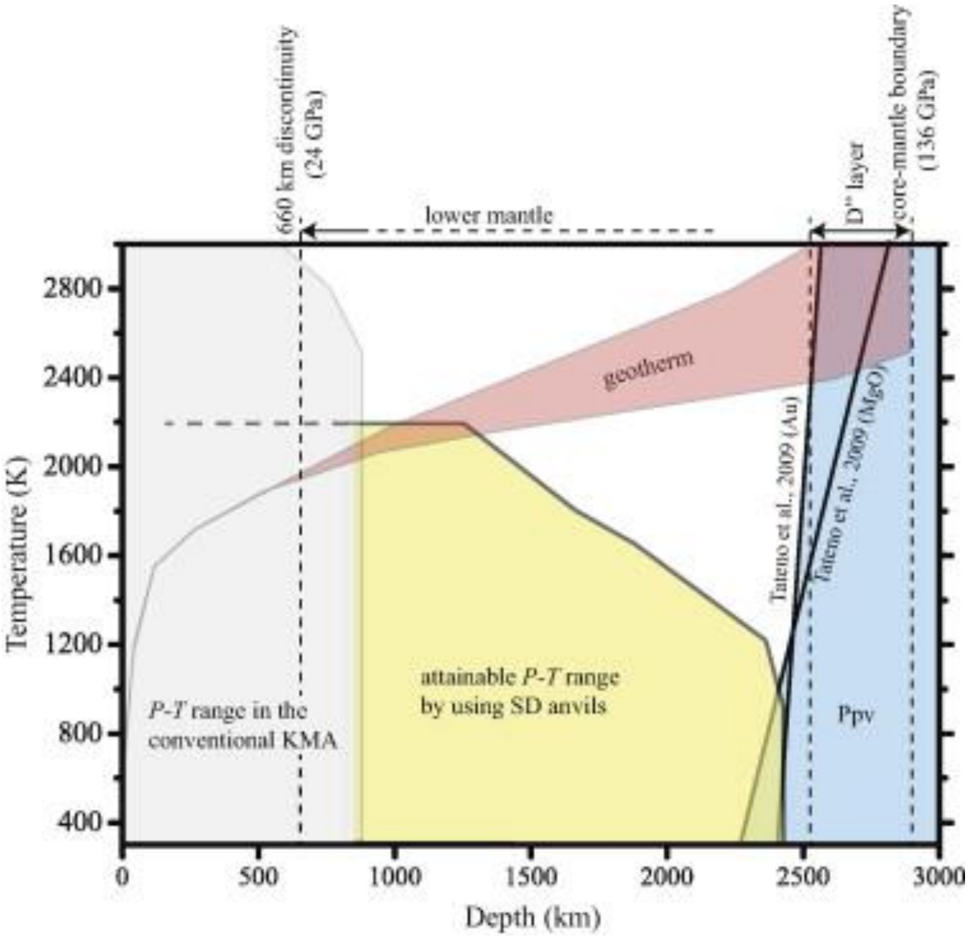




Pulse-echo overlap method gives
a 2-way travel time

Velocity = sample length/one-way travel time

Multi-anvil apparatus for Earth, planetary, and materials sciences

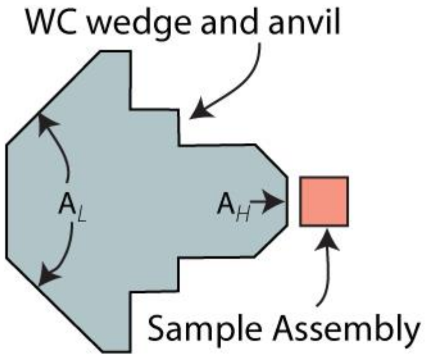


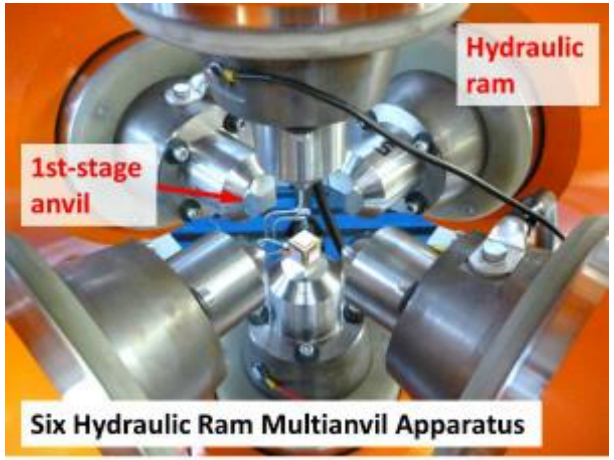
Yamazaki et al. 2014

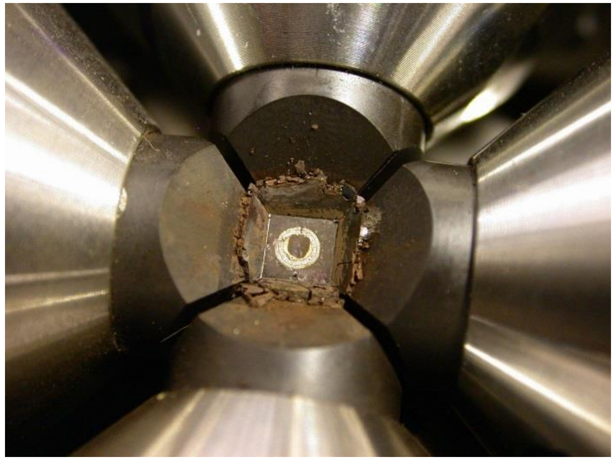
Depth-temperature diagram showing the attainable pressure and temperature range in multi-anvil apparatus

Types of Multi-Anvil systems in use

- Single-stage (individual rams)
  - *D-DIA*
  - *6-ram presses (IPM Misasa, BGI Bayreuth)*



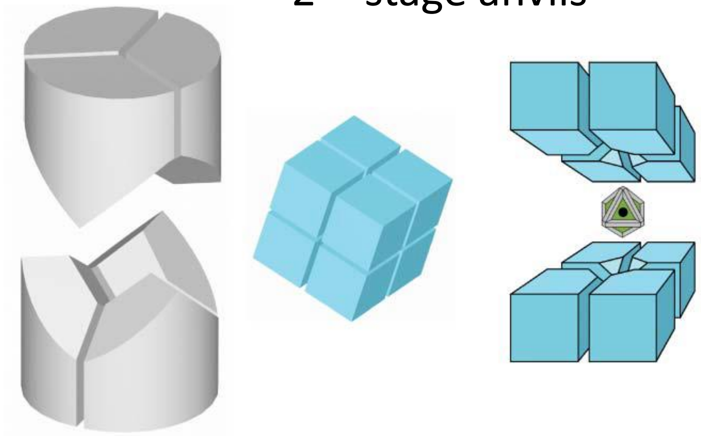




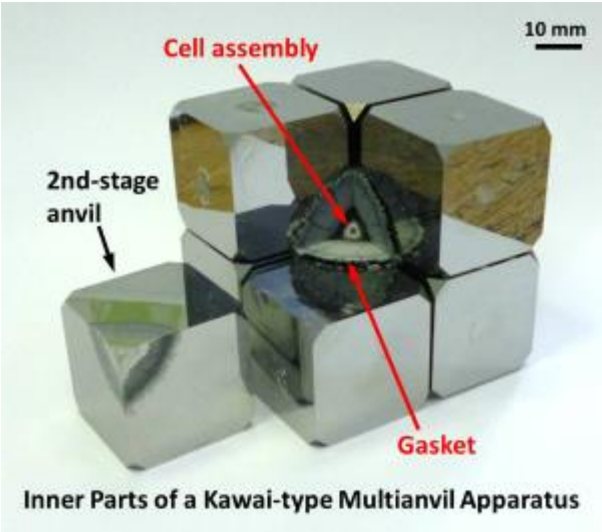
Types of Multi-Anvil systems in use

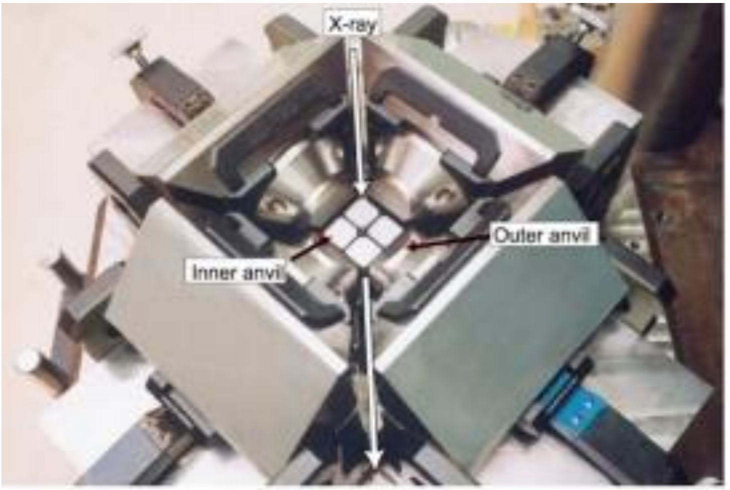
- Multi-stage (sliding system/guide blocks)
  - *DIA*
  - *6-ram press*
  - *split-sphere*
  - *cylindrical (Walker mdoule)*
  - *split cylinder (Tcup, T-25)*

2^{nd}-stage anvils

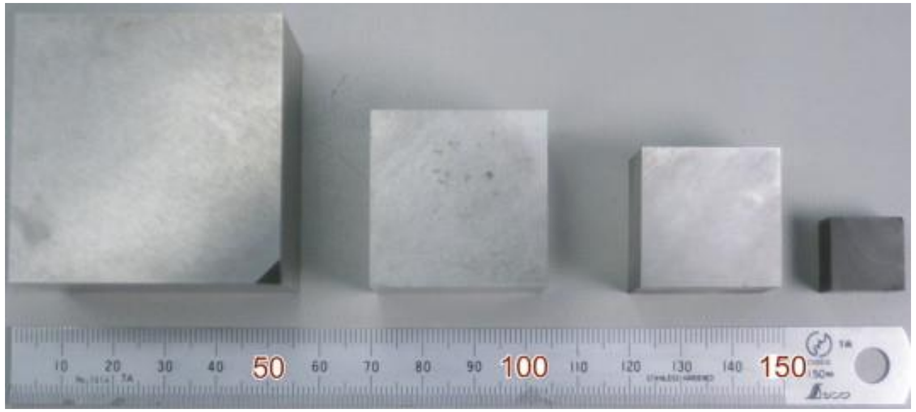


1^{st}-stage anvils

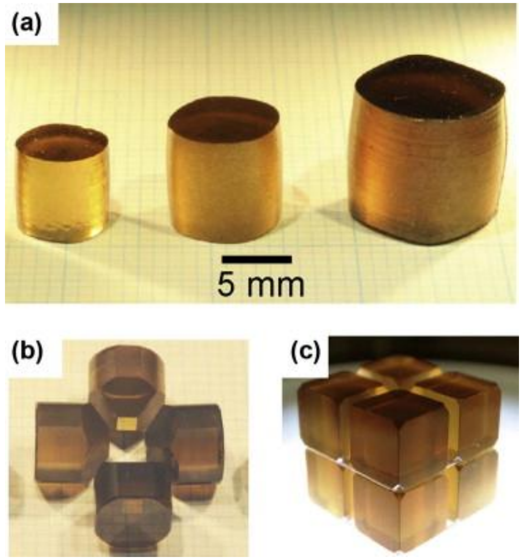




Types of anvils



Sintered diamond



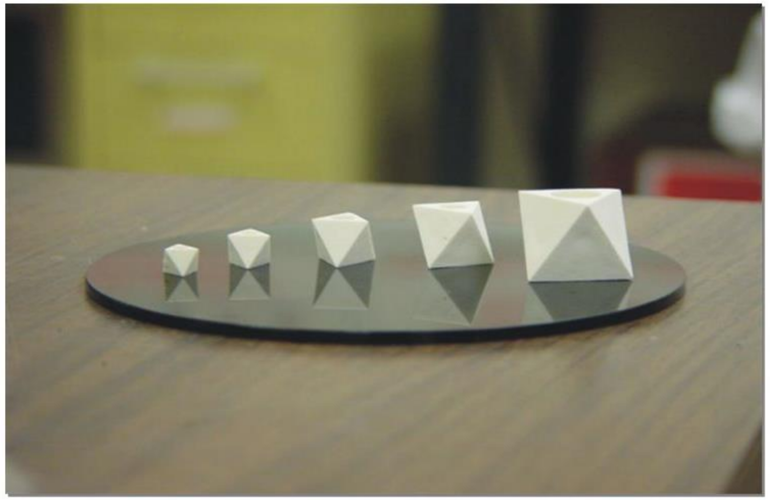
tungsten carbide anvils (from left to right: 46 mm, 32 mm and 26 mm) and a sintered diamond anvil (14 mm)

WC anvils : up to ~ 35 GPa (60 GPa using ultra hard version)
SD anvils : up to ~120 GPa

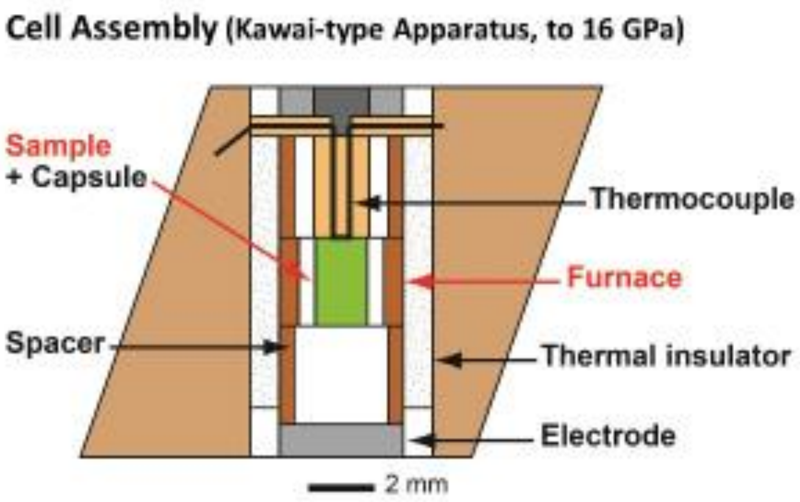
Ultra-hard Nano Polycrystalline Diamond (NPD) – HIME-DIA

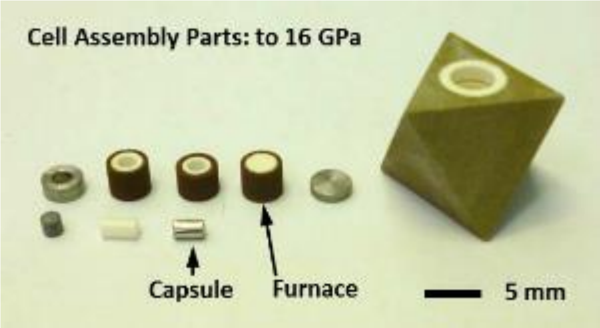
Assembly types for high P-T generation

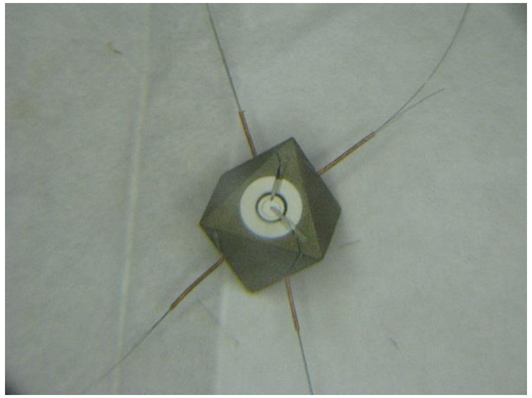
Octahedral cell assembly

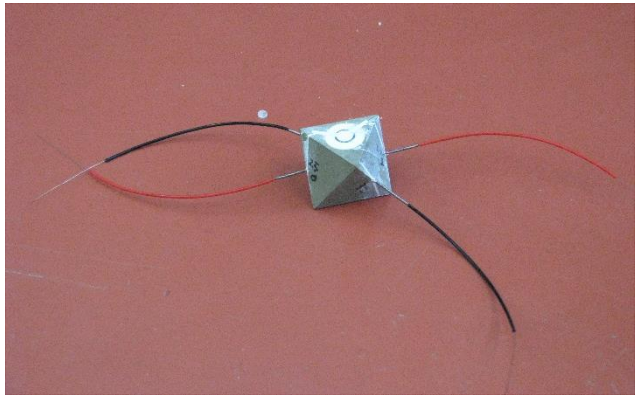


Five sizes of octahedra - 8 mm, 10 mm, 14 mm, 18 mm and 25 mm - used in the COMPRES assemblies.





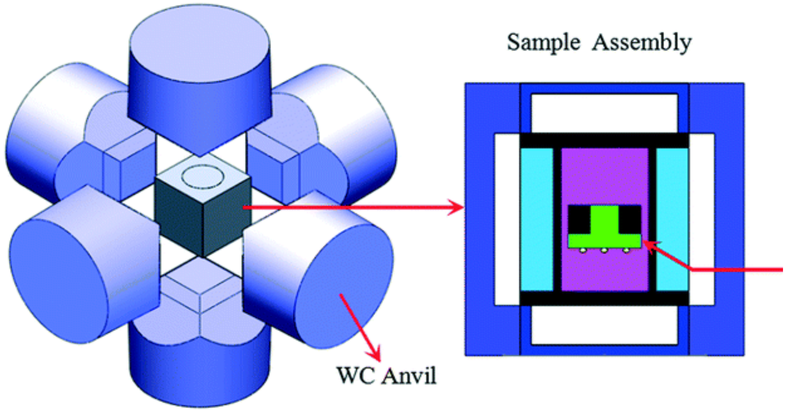




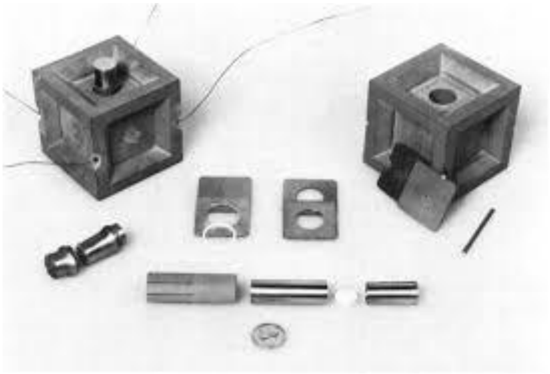
Assembly types for high P-T generation

Cubic cell assembly

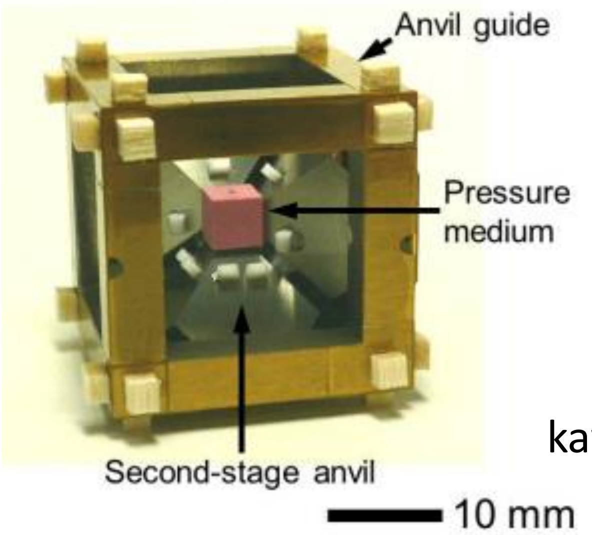
Commonly use in single stage MA devices (DDIA)



Li et al. 2017

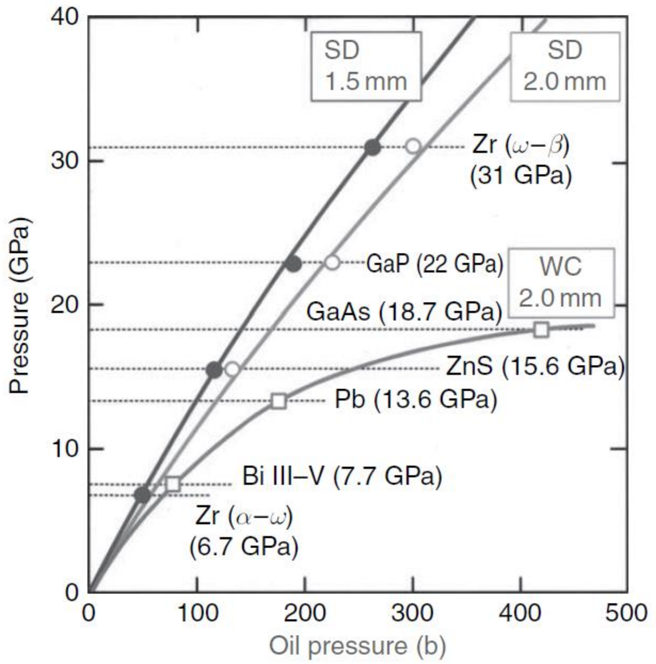


Graham 1987

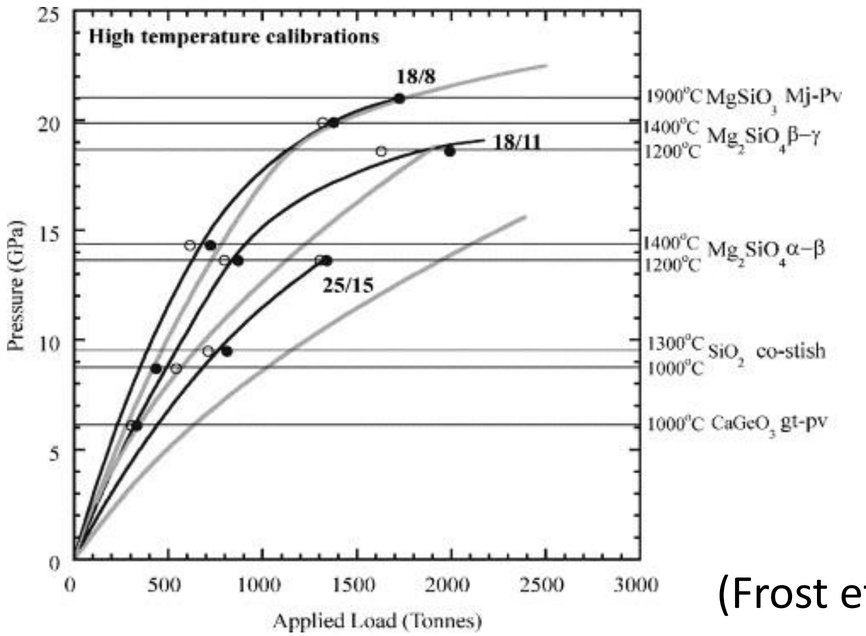


kawazoe et al. 2010

Pressure calibration in multi-anvil



(Ito 2007)



(Frost et al. 2004)

Room temperature pressure calibration based on pressure fixed points

High-temperature pressure calibration curves (black lines) for different MA assemblies. Room temperature calibrations are shown in grey

Heat generation in multi-anvil

- **Available furnace types**
  - Graphite (< diamond stability) - X-ray transparent
  - LaCrO3 (semiconductor)
  - Re
  - Graphite–boron composite heater (~2400 C) - X-ray transparent
  - TiB2 (<1600 C) - X-ray transparent
  - TiC+MgO (~ 2000 C) - X-ray transparent

Thermocouple Configurations

Radial

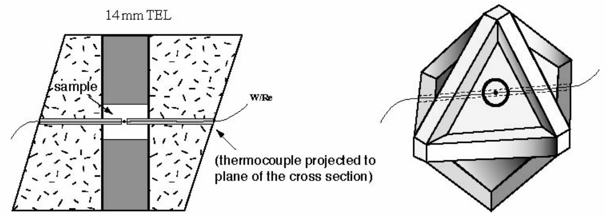


Figure 1. Cross-section and perspective view of assembly with thermocouple wire passed directly through sample in center of assembly.

Axial

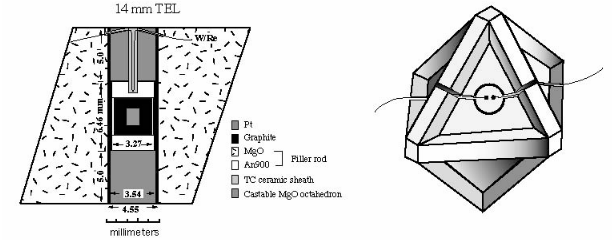
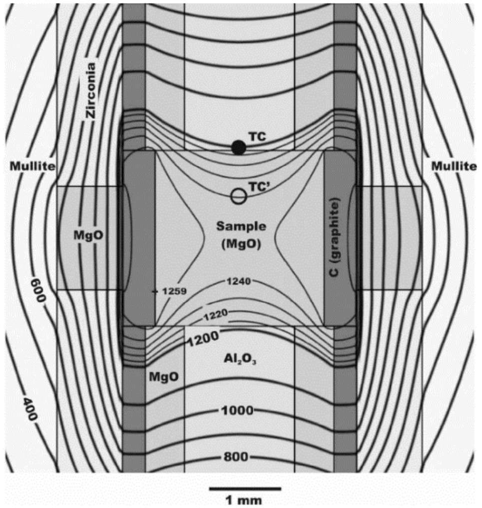


Figure 2. Cross-section and perspective view of assembly with thermocouple wire brought down through top of furnace. Wires are passed through channels cut into octahedra that are filled with alumina cement.



Temperature gradient in MA cell