Element partitioning and diffusion in natural grains

P452 - Computational Physics Term Paper Project

By: Chandan Kumar Sahu
5th year Int. MSc., School of Physical Sciences, NISER Bhubaneswar

Supervised by:
Dr. Priyadarshi Chowdhury and
School of Earth and Planetary Sciences, NISER Bhubaneswar

Dr. Subhasish Basak
School of Physical Sciences, NISER Bhubaneswar

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The diffusion equation

Diffusion is the spontaneous movement of particles, atoms, or molecules from regions of higher concentration to regions of lower concentration, driven by random thermal motion.

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial x}\right)$$

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$

Discretization of 1-D diffusion equation

Diffusion is the spontaneous movement of particles, atoms, or molecules from regions of higher concentration to regions of lower concentration, driven by random thermal motion.

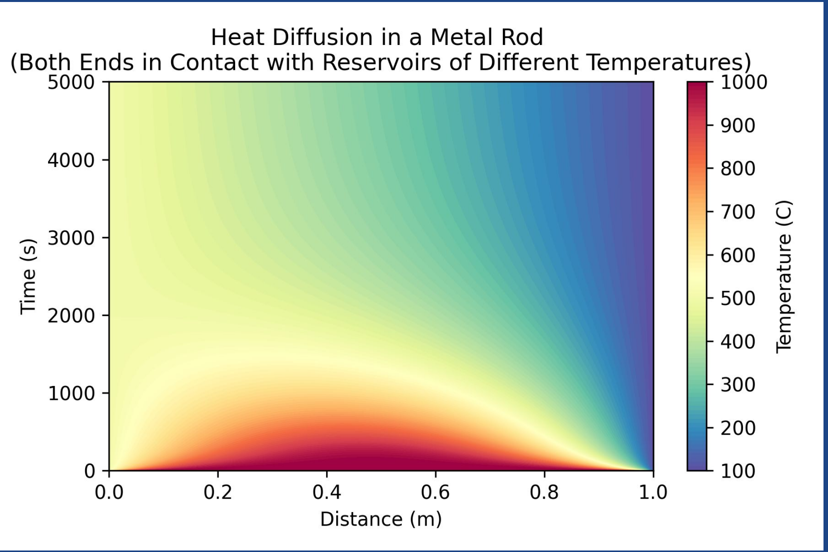
$$\frac{\partial T}{\partial t} \approx \frac{T^{j+1} - T^j}{dt}$$

$$\frac{\partial^2 T}{\partial x^2} \approx \frac{T_{i+1} - 2T_i + T_{i-1}}{dx^2}$$

$$\frac{T_i^{j+1} - T_i^j}{dt} = D\left(\frac{T_{i+1}^j - 2T_i^j + T_{i-1}^j}{dx^2}\right)$$

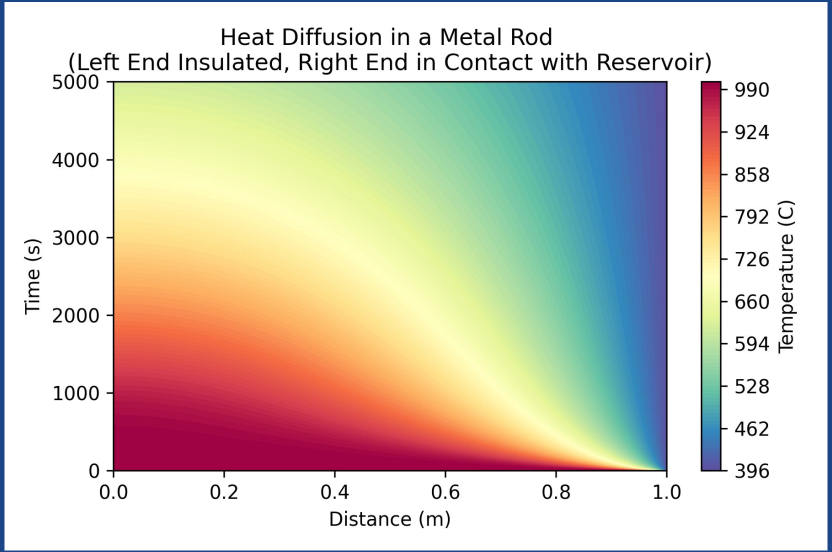
Heat diffusion in one metal rod

Case 1



Heat diffusion in metal rod with their left and right ends at fixed temperatures of 500 K and 100 K respectively.

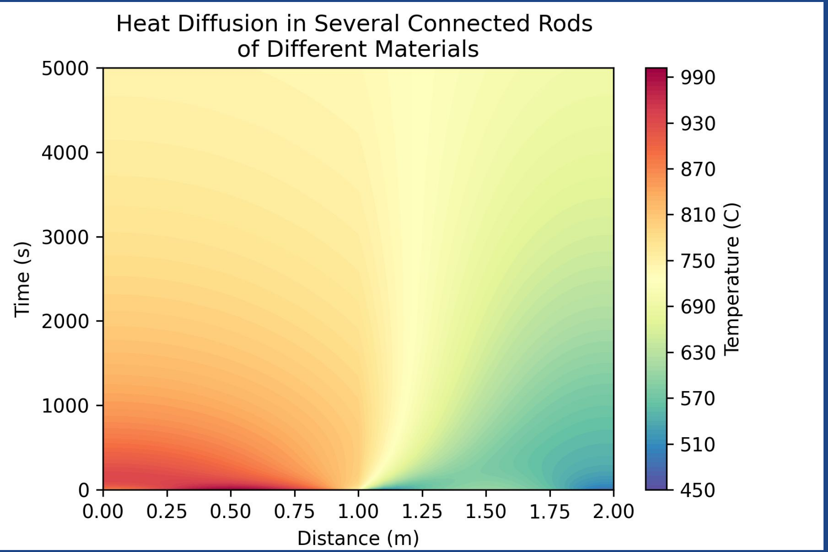
Case 2



Heat diffusion of a metal rod with insulated left end right end at fixed temperature of 400 K.

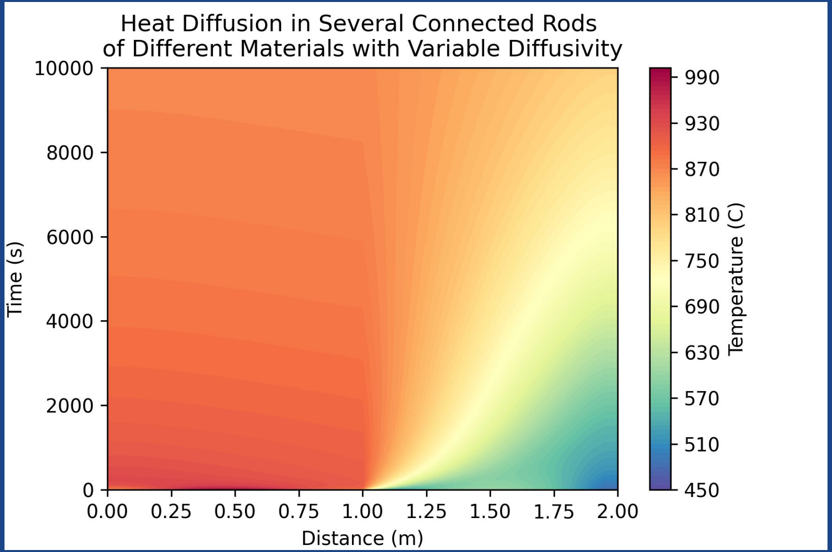
Heat diffusion in two joint metal rods

Case 3



Heat diffusion in two metal rods of different materials and diffusivities, heated to some arbitrary temperatures joint together in an isolated medium.

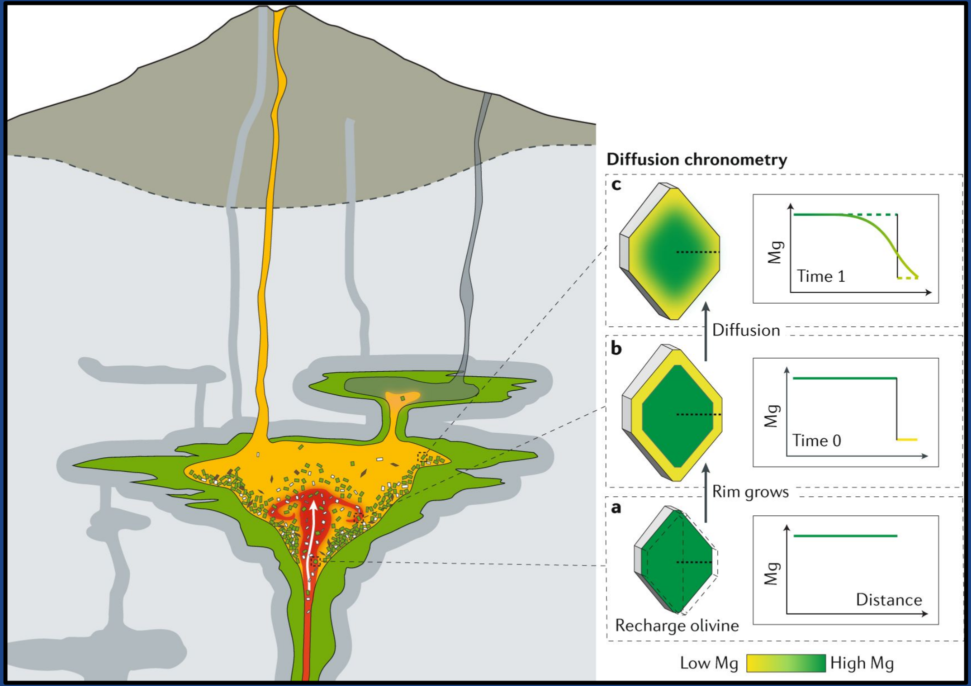
Case 4



Heat diffusion in two metal rods of different materials and diffusivities, heated to some arbitrary temperatures joint together in an isolated medium. The diffusivities of the rods vary with length.

Interdiffusion in Olivine

Olivine [$(Fe,Mg)_2O_4$] mineral contains two grain compartments of Mg and Fe.



At high temperature, Iron atoms, typically present in trace amounts in forsterite, diffuse into the lattice and replace magnesium atoms, forming solid solutions known as the series of olivine minerals.

Source: Costa et al. 2020

The Crank-Nicolson Scheme

Due to stability issues, using implicit or semi-implicit solver schemes is more convenient. Here, we use the Crank-Nicholson semi-implicit scheme to solve the diffusion equation numerically.

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

$$\frac{C_i^{j+1} - C_i^j}{dt} = \frac{D}{2} \left(\frac{C_{i+1}^{j+1} - 2C_i^{j+1} + C_{i-1}^{j+1}}{dz^2} \right) + \frac{D}{2} \left(\frac{C_{i+1}^{j} - 2C_i^{j} + C_{i-1}^{j}}{dz^2} \right)$$

$$C_i^{j+1} - \frac{D\,dt}{2\,dz^2} \left(C_{i+1}^{j+1} - 2C_i^{j+1} + C_{i-1}^{j+1} \right) = C_i^j + \frac{D\,dt}{2\,dz^2} \left(C_{i+1}^{j} - 2C_i^{j} + C_{i-1}^{j} \right)$$

Taking $\frac{D\,dt}{2\,dz^2} = \sigma$, we rewrite the equations as

$$(1+2\sigma)\, C_i^{j+1} - \sigma C_{i+1}^{j+1} - \sigma C_{i-1}^{j+1} = (1-2\sigma)\, C_i^j + \sigma C_{i+1}^j + \sigma C_{i-1}^j$$

$$MC^{j+1} = NC^j$$

The Crank-Nicolson Scheme

$$MC^{j+1} = NC^{j}$$

$$M = \begin{bmatrix} 1+2\sigma & -\sigma & 0 & \cdots & 0 \\ -\sigma & 1+2\sigma & -\sigma & \ddots & \vdots \\ 0 & -\sigma & 1+2\sigma & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -\sigma \\ 0 & \cdots & 0 & -\sigma & 1+2\sigma \end{bmatrix}$$

$$N = \begin{bmatrix} 1-2\sigma & \sigma & 0 & \cdots & 0 \\ \sigma & 1-2\sigma & \sigma & \ddots & \vdots \\ 0 & \sigma & 1-2\sigma & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \sigma \\ 0 & \cdots & 0 & \sigma & 1-2\sigma \end{bmatrix}$$

$$C^{j+1} = M^{-1}NC^{j}$$

We used isolated boundary conditions in our code to make the grain concentration uniform away from the diffusion zone.

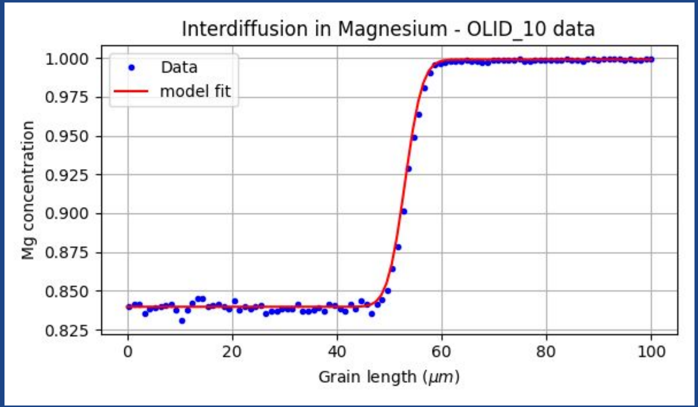
Crank-Nicolson method provides a fast and efficient method to solve the diffusion equation in natural grains without going into the instability regime.

We will now apply the model to actual datasets.

Interdiffusion in Lab Grown Forsterite

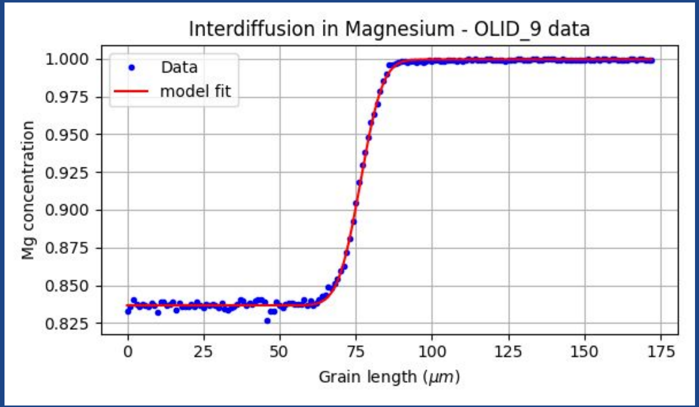
OLID 10

T = 1000 °C



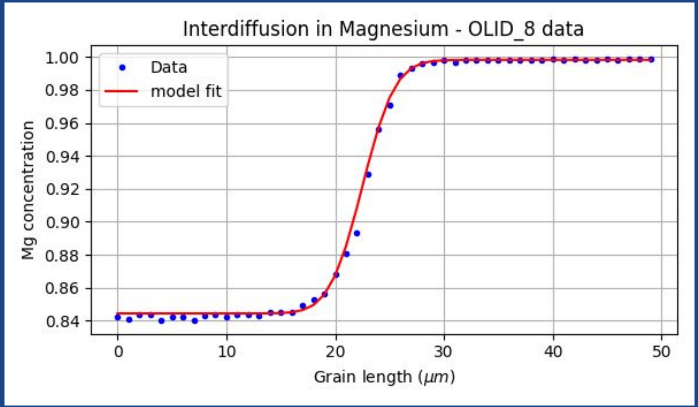
OLID 9

T = 1200 °C



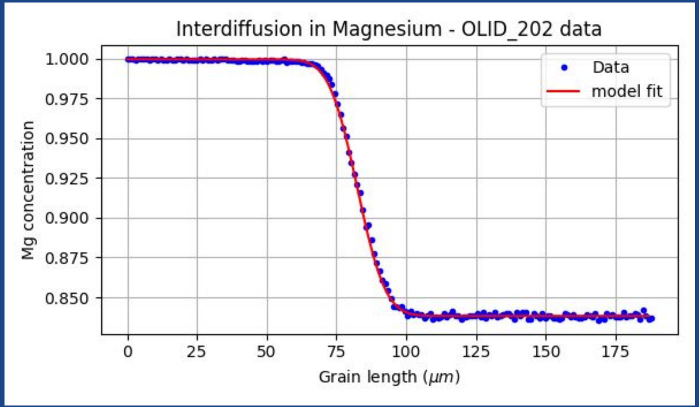
OLID 8

T = 1100 °C



OLID 202

T = 1300 °C



Fitting to Arrhenius equation

We fit the obtained diffusivity coefficients with the Arrhenius relation

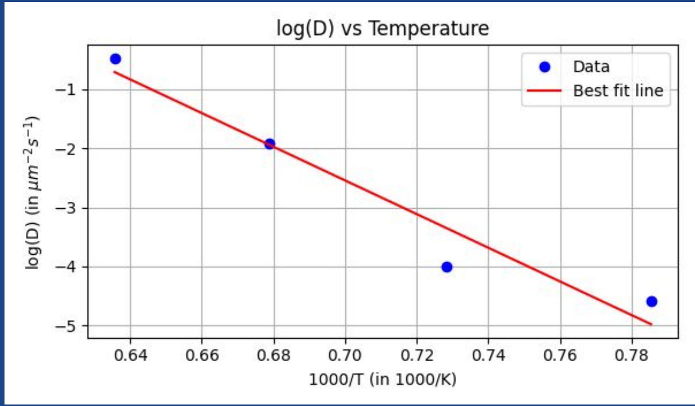
$$D = D_0 \exp\left(-\frac{Q}{RT}\right)$$

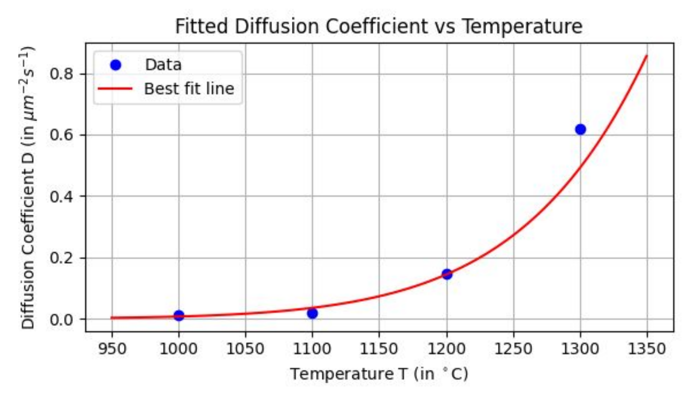
$$Q = 236.641 \text{ kJ/mol}$$

$$D_0 = 9.81 \times 10^{-9} m^2/s$$

Where Q is the activation energy and DO is the absolute diffusion coefficient.

We applied a linear fit on the obtained data points to determine the values of Q and DO.



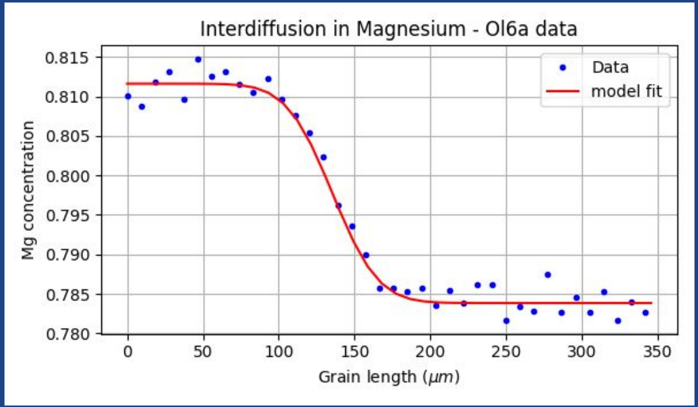


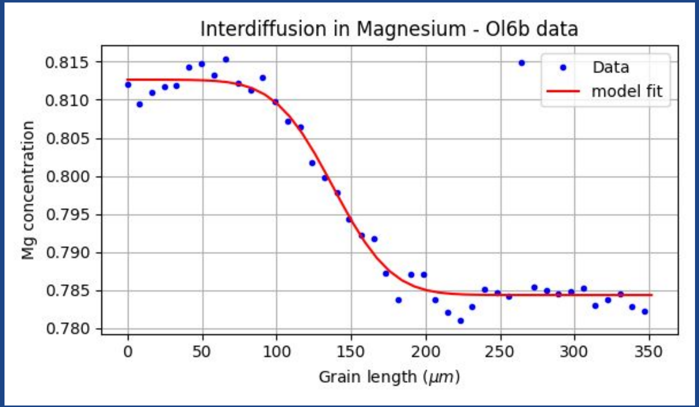
Interdiffusion in Forsterite Grains from Volcanic Eruptions

Ol6a

T = 1083 °C

Time = 56.5 days





Ol6b

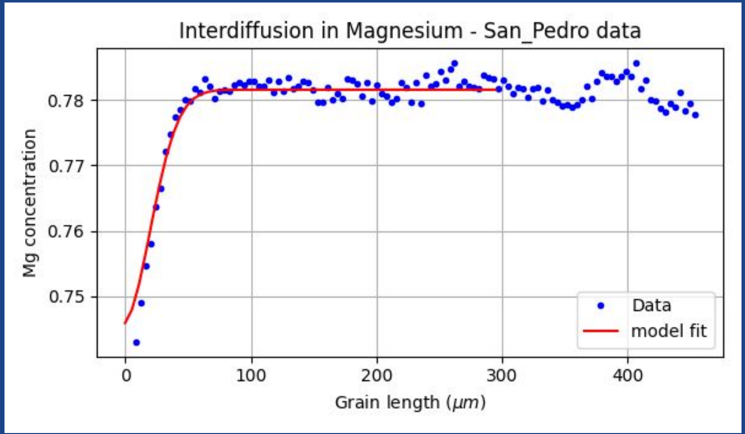
T = 1083 °C

Time = 91 days

San Pedro

T = 1083 °C

Time = 57 days



Conclusion

We modeled the diffusion equation using the forward euler for heat diffusion in metal rods and Crank-Nicolson method for grain interdiffusion.

Our interdiffusion model is in good agreement with the lab grown samples. We use this model to validate the diffusion of grain interdiffusion and partitioning for lab grown samples.

We then applied this model to natural grains to estimate the time period of natural grains collected from volcano Mt. Etna and San Pedro. Our results predict that the grains were active since 56 days, 91 days and 57 days for the two samples of Mt. Etna and San Pedro volcanoes respectively, before they actually erupted.

Thank you