# Kinetik Klausur – SS 2010
# (100 Punkte)

**20.7.2010**
**Abgabe bis: 17 Uhr, 26.7.2010**
**per email an: Sumit.Chakraborty@rub.de**

(1) Ordering of Fe and Mg between the two octahedral sites in pyroxene (M1 and M2) can be treated as a chemical reaction

Fe(M1) + Mg(M2) = Fe(M2) + Mg(M1)

Write down an expression for the stoichiometric change and the rate of this reaction and discuss what the order of such a reaction can be. Is this an elementary or a complex reaction? What is the simplest possible reactive intermediate for this reaction?

**(20 Punkte)**

(2) Write a function that measures the overall transformation of calcite to aragonite. Describe three possible scenarios of nucleation and growth that can occur for this transformation. Would you use an Avrami equation to describe the kinetics of this process? Discuss the advantages and disadvantage of such an equation.

**(20 Punkte)**

(3) Diffusion coefficients (and many other kinetic rate constants) depend on parameters such as temperature, pressure, composition and oxygen fugacity and the dependence is given by equations such as:

$$D = D_o 10^{nXA} fO2^m \exp\left(\frac{-Q - P\Delta V}{RT}\right)$$

where $D_o$ is a pre-exponential factor ($m^2/s$), n is a constant, XA is the mole fraction of component A in the solid / fluid / gaseous solution, m is a constant, Q is the activation energy (J/mol) and $\Delta V$ is the activation volume ($m^3$/mol). P, T and R have their usual meanings.

Calculate the self diffusion coefficient for Fe and Mg in an olivine of composition ($Fo_{0.8}Fa_{0.2}$) at the following condition: 1100 °C, 40 Kbar, $fO2 = 10^{-9}$ bar.
The values of the parameters for calculating diffusion coefficients are:

For $D^*_{Fe}$ :

$D_o$ = 1e-8, n = 3, m = 1/5, Q = 226000, $\Delta V$ = 5.5

For $D^*_{Mg}$ :

$D_o$ = 1e-10, n = 2, m = 1/6, Q = 220000, $\Delta V$ = 7

Calculate the chemical diffusivity, D(Fe-Mg) as well (assume olivine is thermodynamically ideal). Please make sure you pay attention to units and conversions in these calculations.

The time required to completely homogenize a spherical olivine once it is exposed to new compositions is given by: $Dt/a^2 = 0.4$, where a is the radius of the crystal. It is often argued that the composition of mantle olivines (grain sizes between 100 microns and 1 cm) that are carried by basalts to the surface are reset during the transport process (lasts about a month, maximum). Assume that the composition of olivine is similar to the one for which you have done the calculations above and that basalt has a temperature of 1100 °C. Discuss whether compositions of olivines would be reset or not. If you find that the result is variable, please indicate what kind of olivine crystals would you use to learn about the mantle and what kinds of crystals would you use to learn about processes that took place in the transporting basalt?

**(5 + 5 + 10 + 20)**

(4) “Diffusion cannot occur in a perfect crystal”. Discuss why this is true, what is necessary for diffusion to occur and how the situation may be different in metals vs. non-metals. **(20 Punkte)**