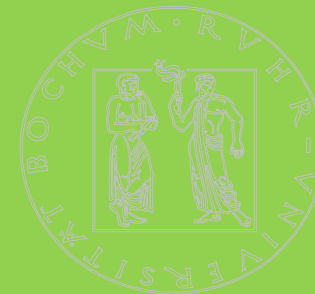


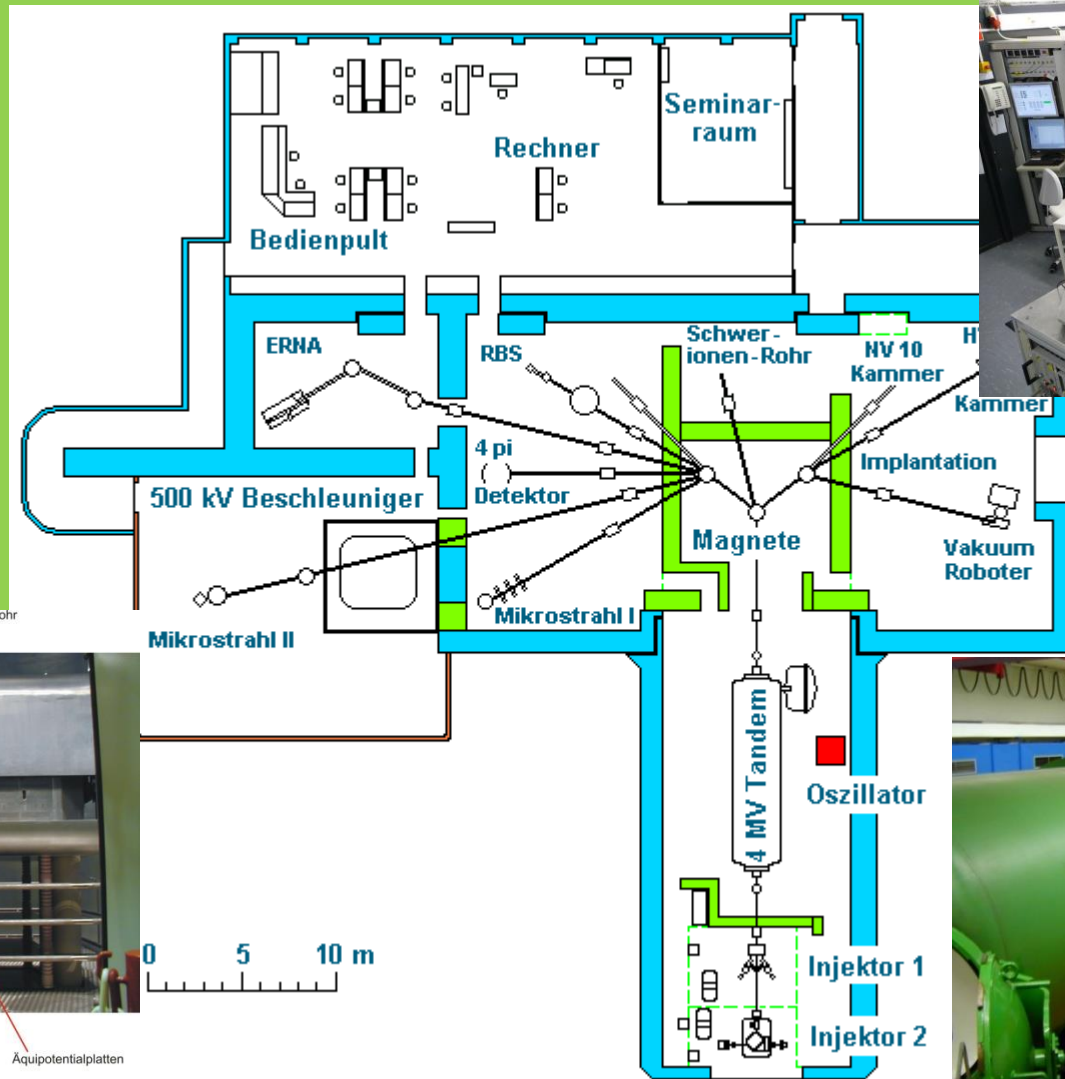
# Ion beam analysis of materials with MeV beams at the Ruhr University Bochum



Ruhr-Uni-Bochum

# Accelerators in Bochum

Ion Beams from a few keV up to some 20 MeV



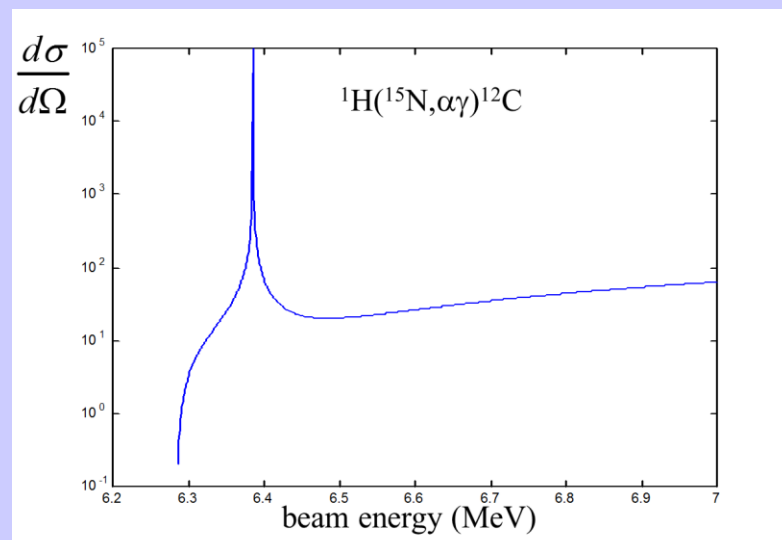
# Depth profiling with Nuclear Resonance Reaction Analysis

Motivation:

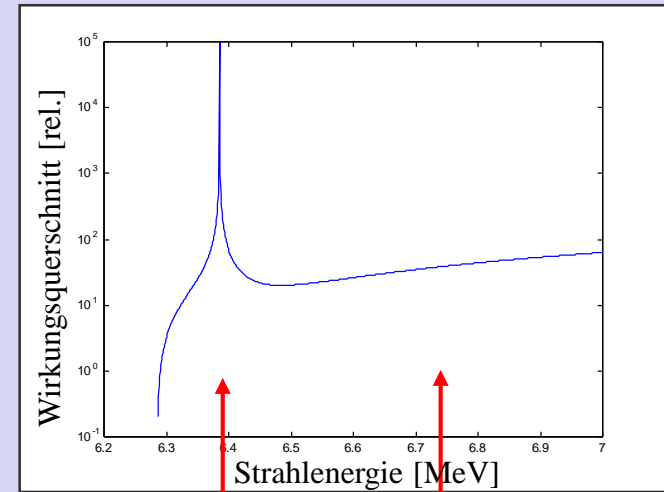
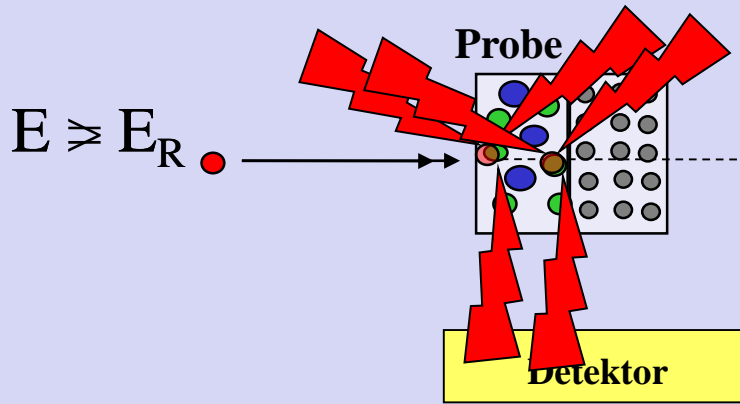
- **Detection of light elements (in particular Hydrogen)**
- **isotopic tracing**

Example:

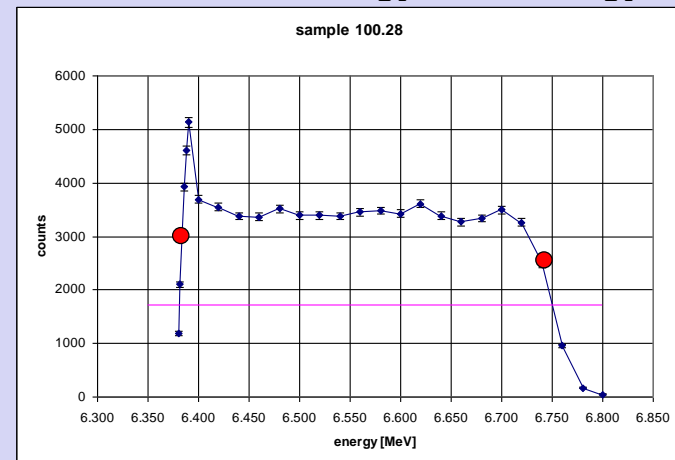
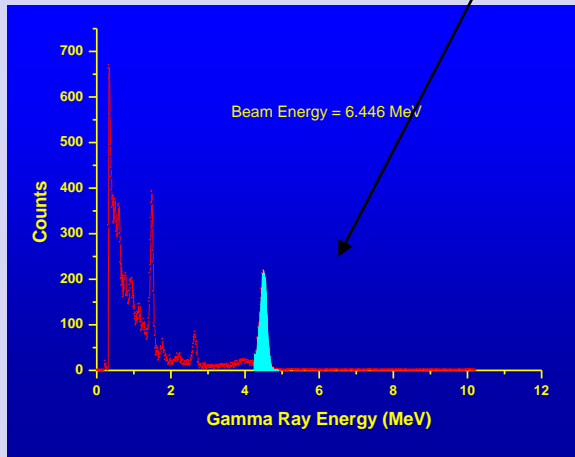
Hydrogen depth profiling  
with an  $^{15}\text{N}$  beam



# Nukleare Reaktions Analyse (NRA) am Beispiel $^{15}\text{N}(p, \alpha \gamma)^{12}\text{C}$

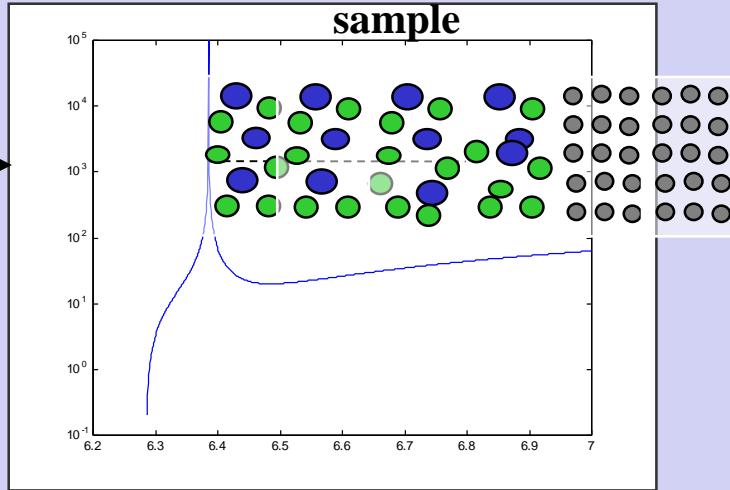


$E = E_R$     $E > E_R$

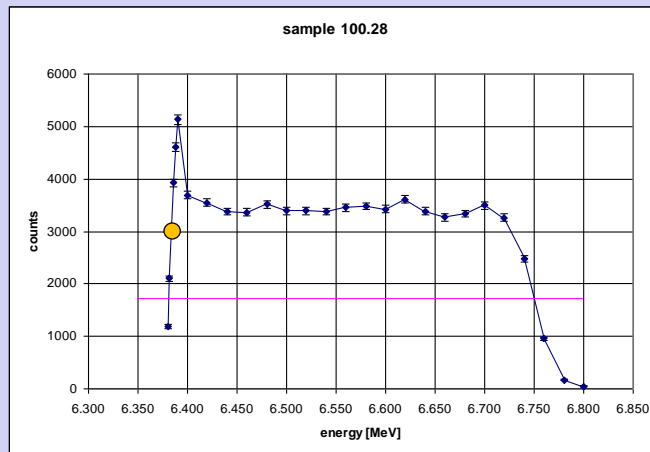


Wasserstoff in Silizium  
Ringversuch Bundesanstalt für Materialforschung

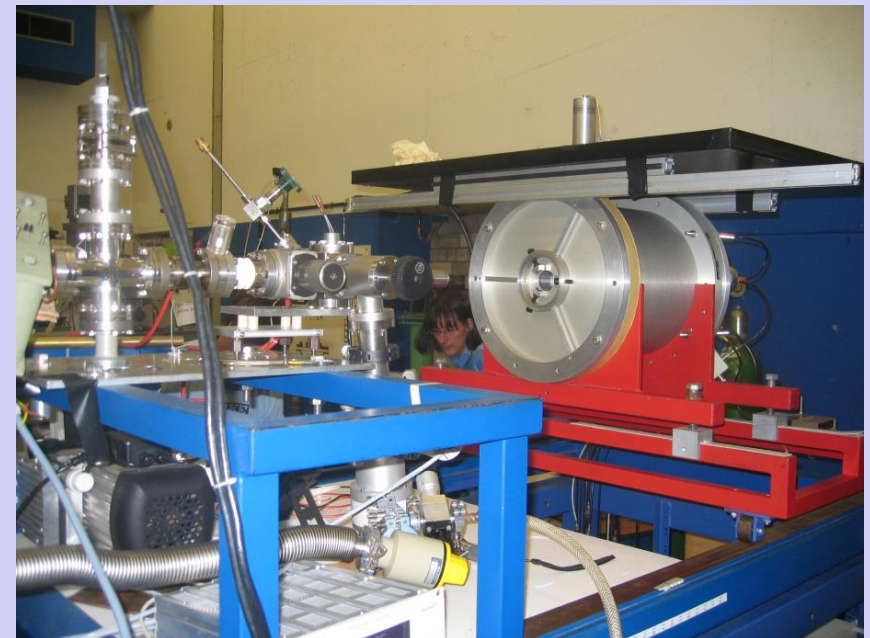
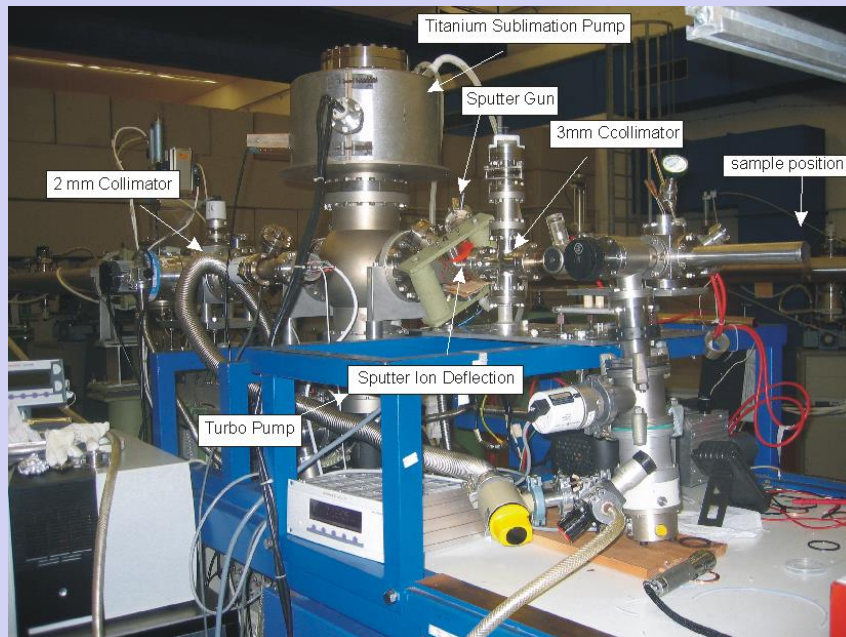
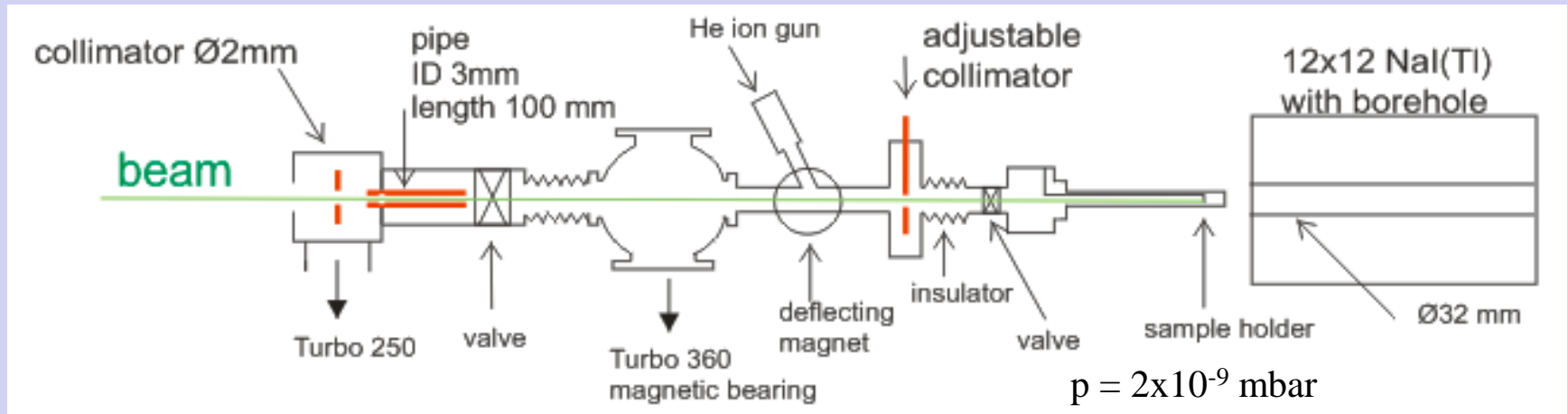
beam



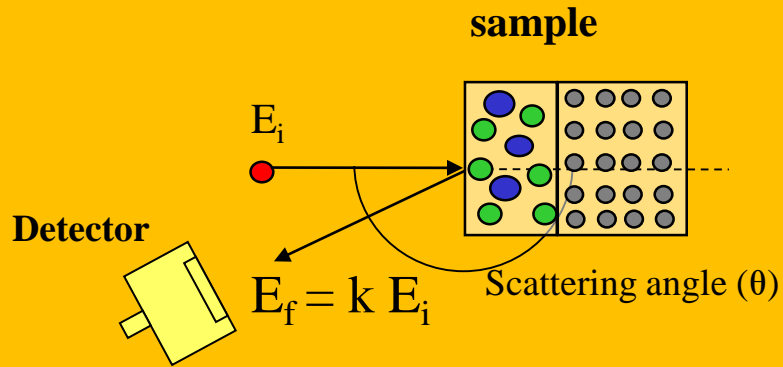
Depth resolution: a few nm



# The set-up in Bochum



# Rutherford Backscattering Spectroscopy

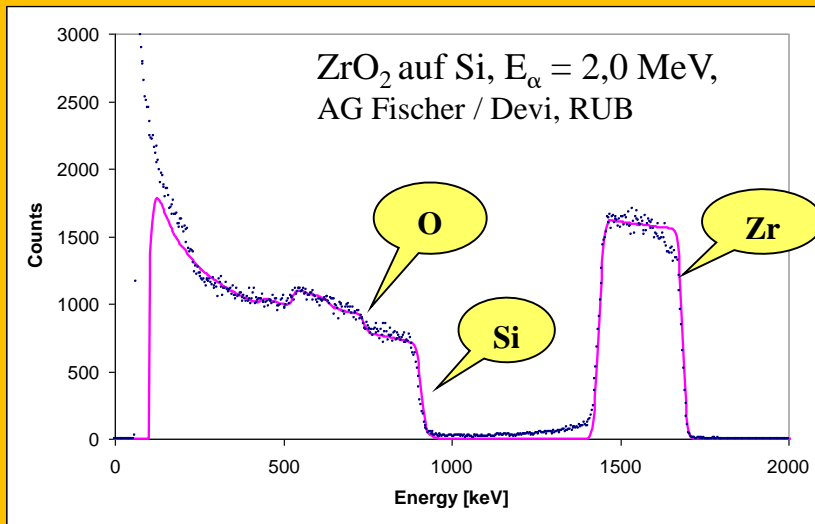


Probability  
for scattering:

$$\frac{d\sigma}{d\Omega} \propto \left[ \frac{Z_{Ion} Z_{Probe}}{E_{Ion}} \right]^2$$

Energy of scattered particle:

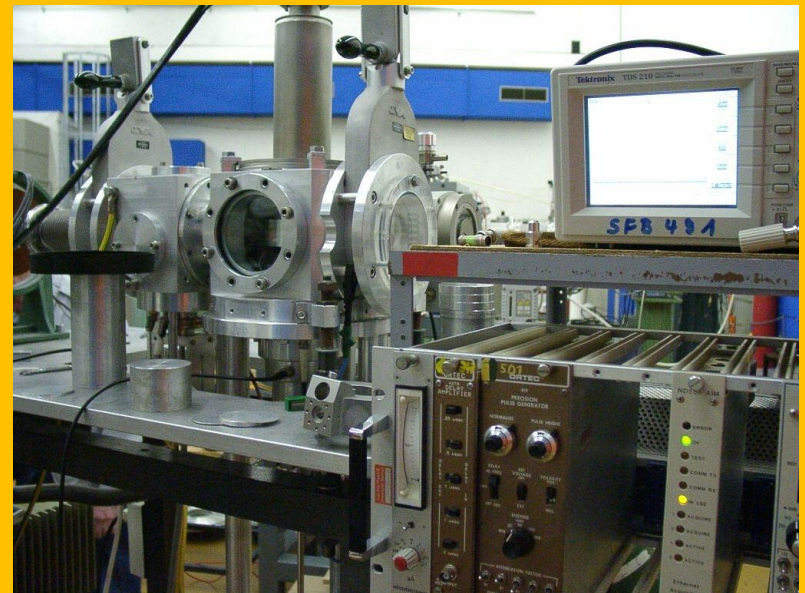
$$k = \left[ \frac{\sqrt{M_{Probe}^2 - M_{Ion}^2 (\sin \theta)^2} + M_{Ion} \cos(\theta)}{M_{Ion} + M_{Probe}} \right]^2$$



energy scale →

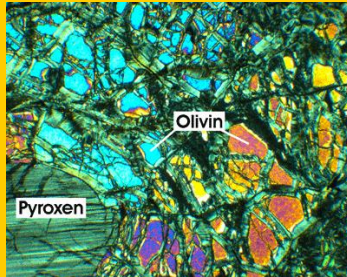
mass scale →

depth scale ←

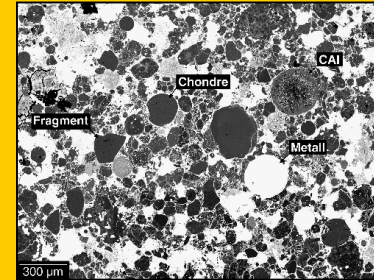


# Study of Diffusion in Minerals – why?

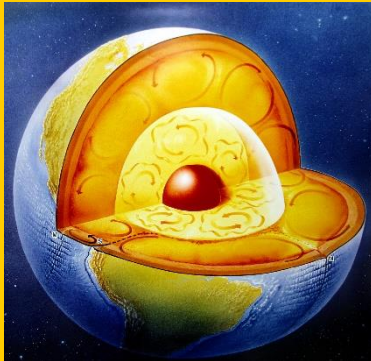
1. Diffusion is observed in samples  
e.g. from subduction zones



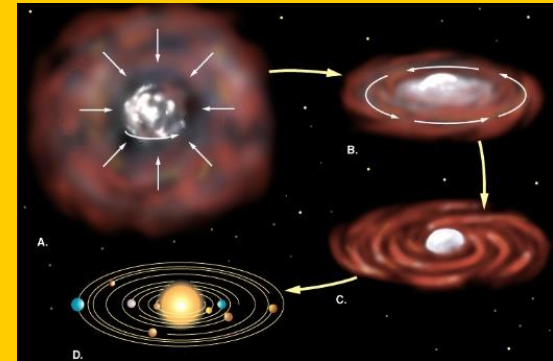
or meteorites...



...and one can learn something about  
processes in the interior of the Earth



or during the origin of the solar system



(time- temperature- and pressure scales)

when diffusion parameters are known!

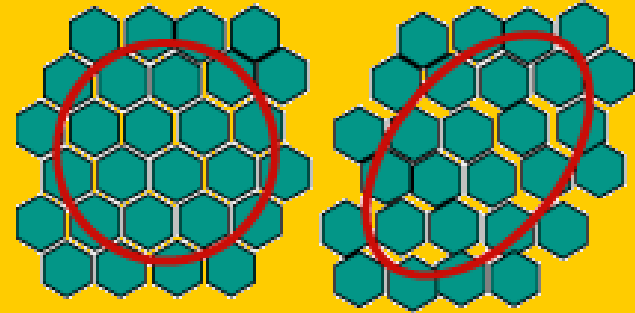


# Study of Diffusion in Minerals – why?

2. There is a close connection between diffusion and creep



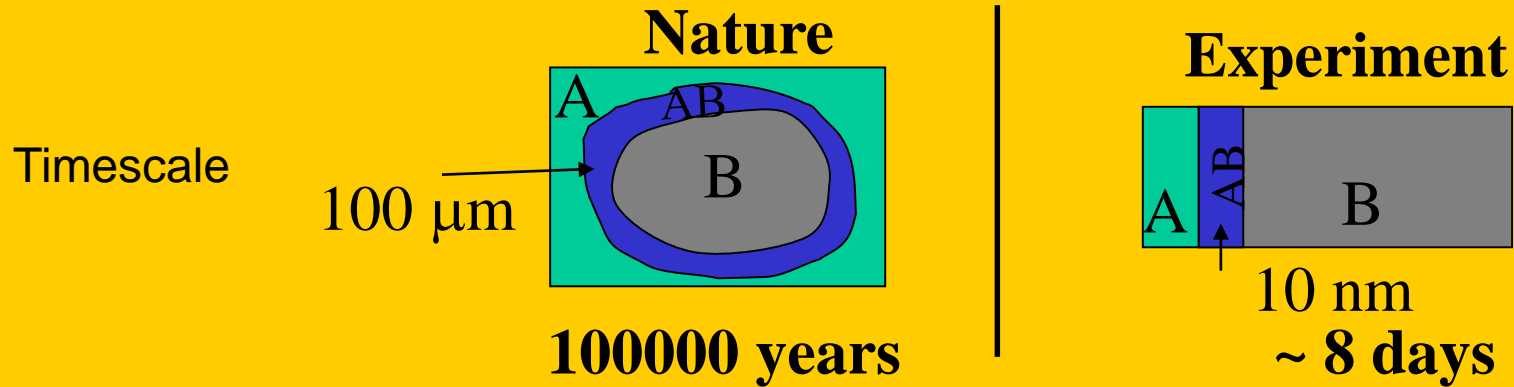
mechanical properties



microscopic properties

and it all depends on defects in crystals !

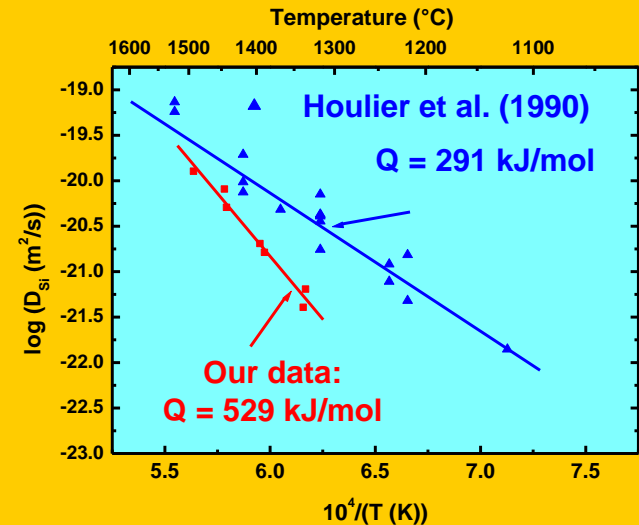
# Measurement of diffusion processes in the laboratory



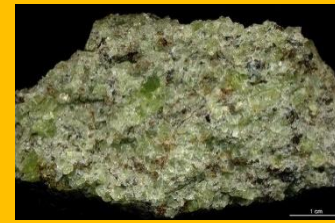
Temperature scale

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

$Q =$  activation energy



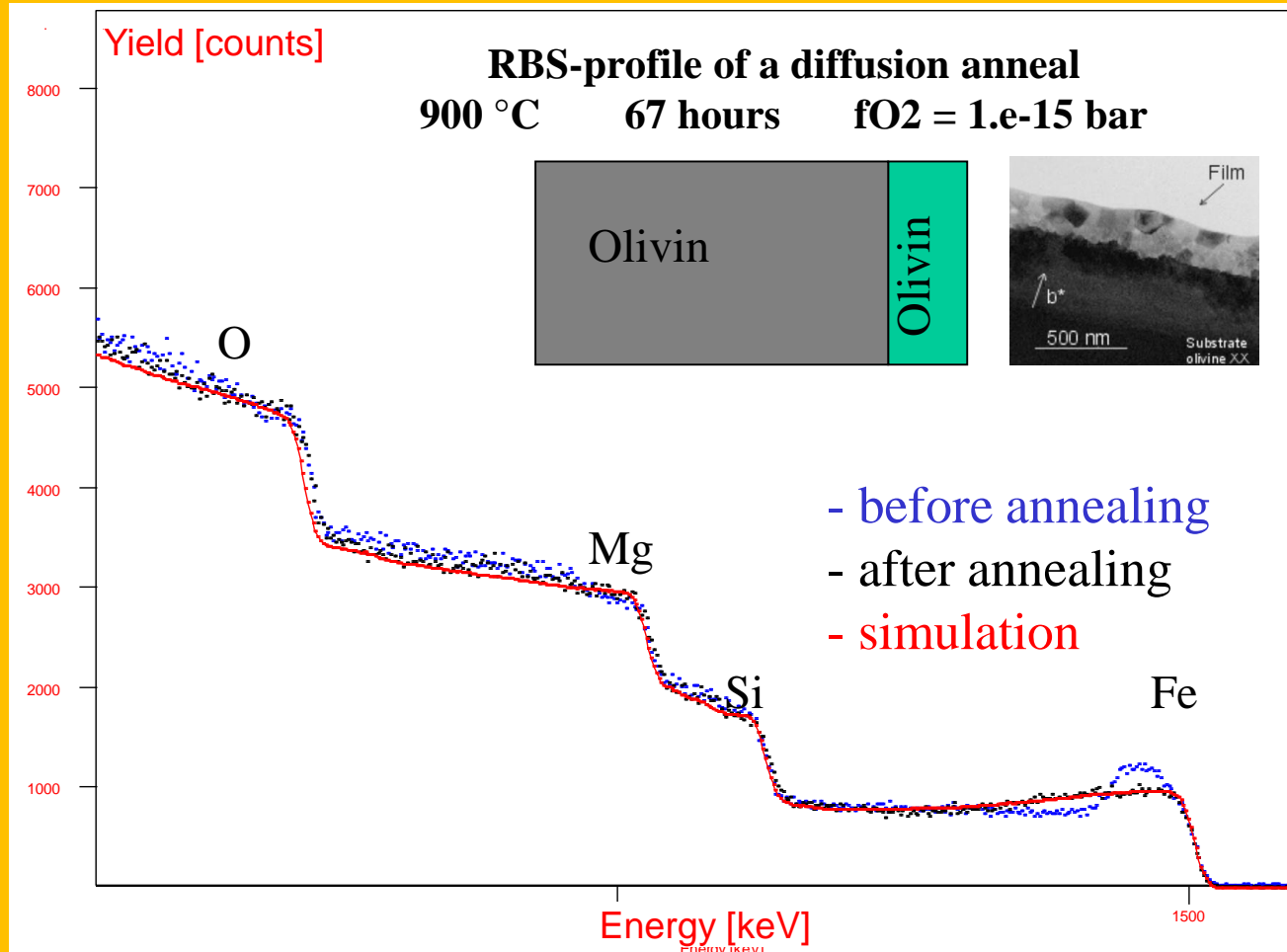
# Example: Fe-Mg diffusion in olivine:



Fayalite  
 $\text{Fe}_2\text{SiO}_4$

Olivine:  
 $(\text{Fe}_x\text{Mg}_{1-x})_2\text{SiO}_4$

Forsterite  
 $\text{Mg}_2\text{SiO}_4$



It would be very interesting for the understanding of diffusion studies to know more about amount and type of defects



**PAC ?**

There is only very little literature about PAC studies in minerals  
e.g. Miami University Oxford, Ohio 2005  
H. Jaeger, M. P. Rambo, R. E. Klueg, S. McBride...

Our first challenge is now  
to understand what we can learn  
from PAC results  
„finding a common language  
between geoscientists and PAC  
people“



e.g. the investigations of zircon ( $\text{ZrSiO}_4$ )  
Thesis McBride 2005

Measurement fitted with the perturbation function...

$$G_2(t) \doteq s_{20}(\eta) + \sum_{i=1}^3 s_{2i}(\eta) \cos(g_i(\eta)v_Q t) \exp(-g_i(\eta)\delta t)$$

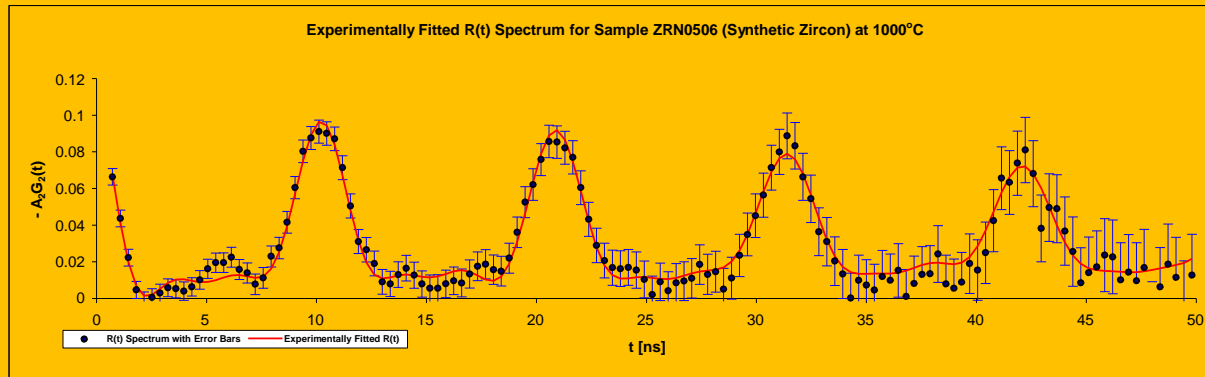


Figure G.1- Experimentally Fitted R(t) Spectrum for Sample ZRN0506 (Synthetic Zircon) at 1000 Degrees

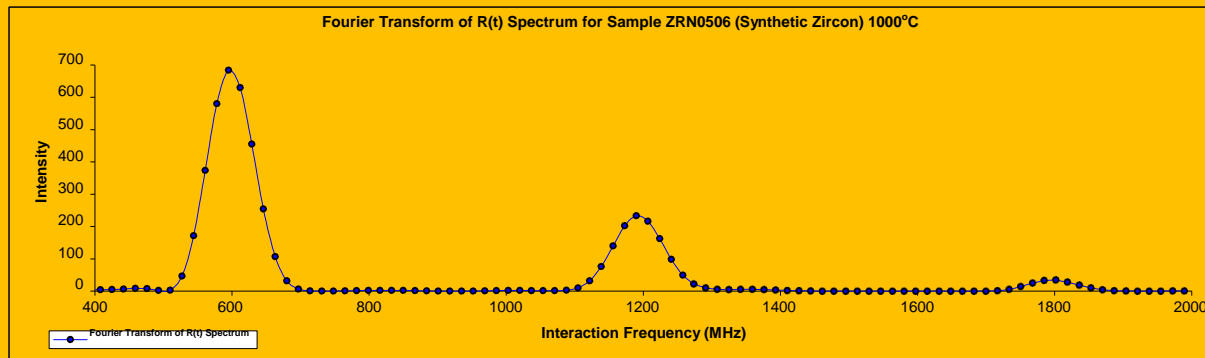
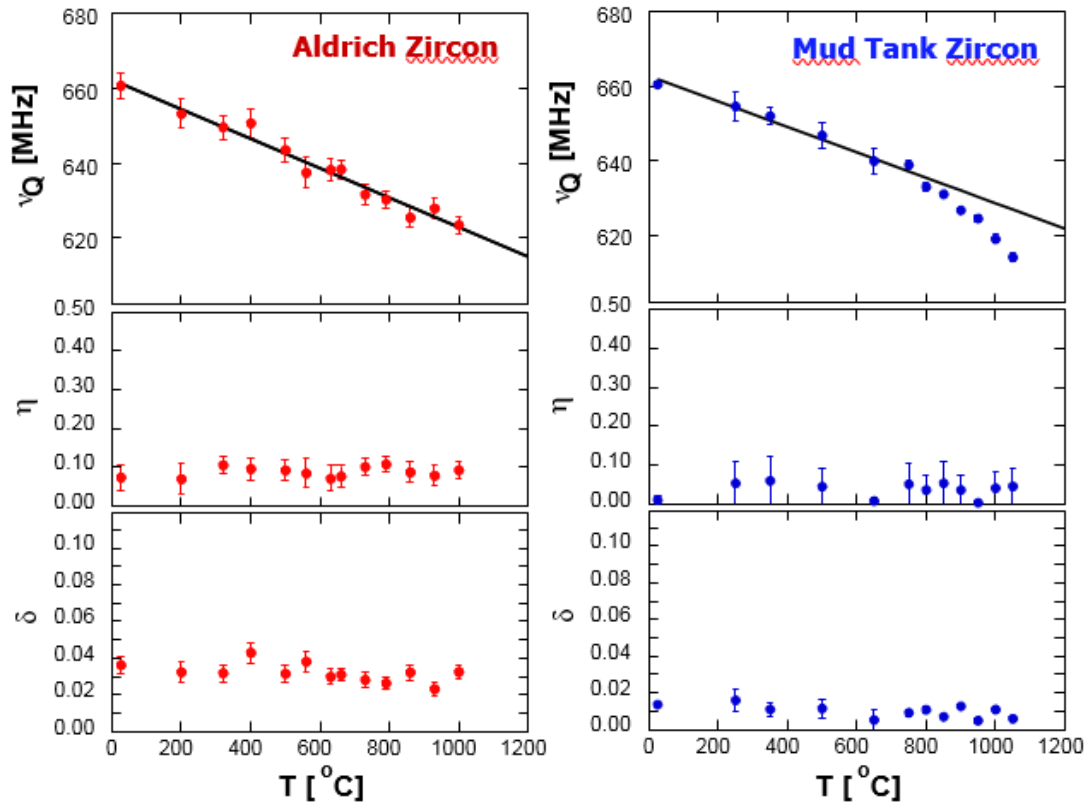


Figure G.2- Experimentally Fitted Fourier Transform Spectrum for Sample ZRN0506 (Synthetic Zircon) at 1000 Degrees

...to deduce  
the EFG parameters:

$\eta$  (asymmetry parameter)  
 $\nu_Q$  (quadrupole frequency)  
 $\delta$  (damping parameter)

# The EFG parameters



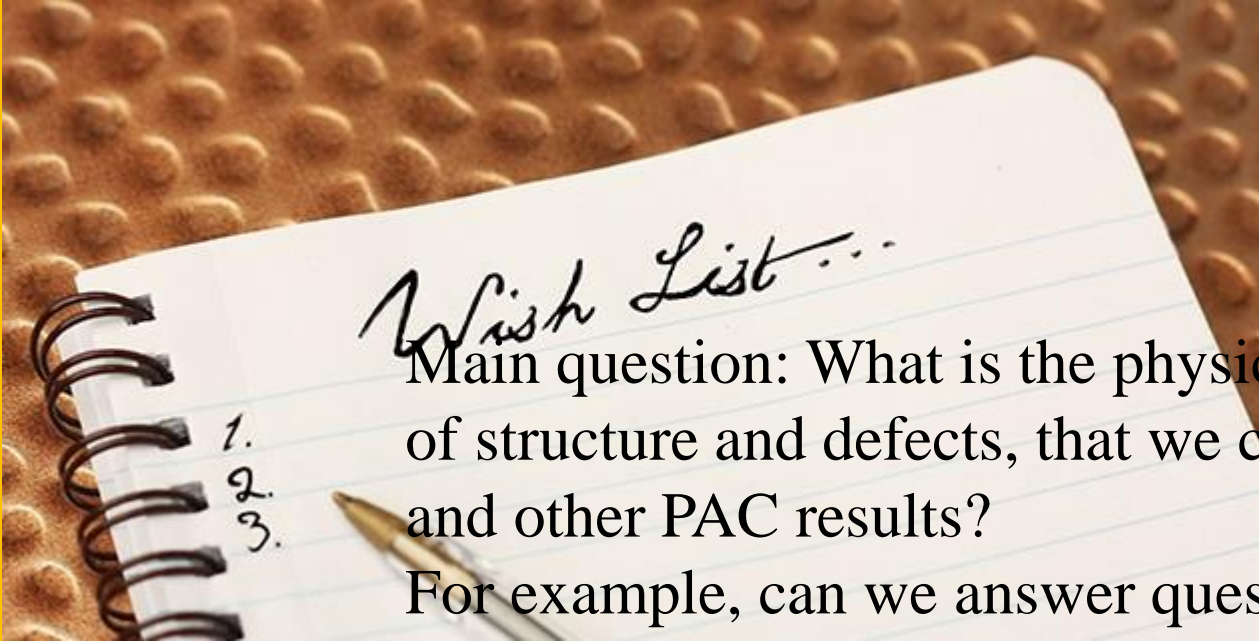
**Figure 7.3 - EFG Parameters for Commercial and Natural Zircon Sample-** The data was collected on runs that were made from room temperature up to 1000°C. Note the phase change occurs at roughly 700°C for the natural zircon while the commercially obtained zircon exhibits no phase change.

Change in slope of temperature dependence  
 > displacive phase transition ?

$\eta = 0$  no radiation damage  
 $\eta > 0$  radiation damage and impurities ?

what to learn from the damping parameter

from the geoscientist



## Wish List...

Main question: What is the physical picture, in terms of structure and defects, that we can learn from these and other PAC results?

For example, can we answer questions such as:

What is the concentration of a certain kind of defect at a given condition e.g. T, P,...

What is the geometry of the atoms around the defect site?

How much energy is required to form a certain kind of defect?

What are the different kinds of defects that are present in a crystal, and in what concentrations?  
etc. etc.



... is needed