

universität
wien**center for earth sciences**

geodynamik&sedimentologie - lithosphärenforschung - umweltgeowissenschaften

DMG - Short Course on

“KINETICS OF GEOLOGICAL MATERIALS”

Date: August 30th to September 3rd 2010
Location: University Centre Althanstrasse, 1090 Wien
Organizer: R. Abart, University of Vienna
e-mail: rainer.abart@univie.ac.at
Web: <http://lithosphere.univie.ac.at/petrology/news/>

ORGANIZATION

This five days short course is organized within the framework of “DMG Doktorandenkurse” of the German Mineralogical Society. It is meant to give a broad perspective on the processes that underlay the kinetics of mineral reactions such as breaking and establishing bonds at reaction sites, nucleation, growth, and chemical mass transfer. It primarily addresses graduate students and researchers. Undergrads with a particular interest in reaction kinetics are very welcome as well. The course will be comprised of a series of lectures, practical exercises on the PC and informal discussions.

Lectures and practical exercises will be held at University Centre Althanstrasse (UZA II), Althanstrasse 14, A-1040 Wien. The course will start Monday August 30th at 10:00 am, and it will end on Friday September 3rd at 15:00 pm. A detailed program is given below.

We envisage a maximum of 30 participants. Successful participation will be acknowledged with three European credit points.

SCIENTIFIC PROGRAM

Based on major topical fields the course will be divided into four parts:

Part A: Empirical rate laws

To begin with, the concept of rate laws, rate limiting steps, elementary reactions and order of reactions will be introduced. Then empirical rate laws will be discussed, which provide relations between reaction progress and time without considering geometrical aspects (zero-dimensional models). To work with such rate laws PC exercises will be done using MATLAB software.

Part B: Diffusion in geological materials

The mechanisms of diffusion in single crystals, in polycrystals, and in polyphase materials will be discussed. The mathematical formulation to describe diffusion in one-dimensional settings will be introduced and finite difference schemes will be programmed in MATLAB to simulate 1-D diffusion. Tracer diffusion, binary interdiffusion, and multicomponent diffusion will be addressed. Finally we will assess the role of grain- and inter-phase boundaries during diffusion in polycrystals and in multiphase aggregates. Diffusion modelling will be applied to work out examples of geospeedometry and geochronology (concept of closing temperature).

Part C: Grain- and phase boundaries

At first, grain boundaries will be classified based on a discussion of the five macroscopic degrees of freedom of a grain boundary and their implications for the microscopic grain-boundary structure (coincidence site lattice model). A macroscopic thermodynamic description of grain- and phase boundaries is introduced (interface thermodynamics) and implications of interfacial energy for equilibrium shape (Wulff diagrams) and capillary forces (Gibbs-Thomson relation) will be investigated. Transient phenomena such as capillary force driven grain boundary movement, normal grain growth and coarsening, and Zener drag will be discussed. Exercises will be done to derive general rules for the topology of grain boundary networks, analytical expressions will be evaluated to simulate capillary force driven grain-boundary movement.

Part D: Nucleation

The classical nucleation theory is will be introduced for polymorphic phase transformation. The concept is then extended to nucleation in binary systems. Homogeneous and heterogeneous nucleation including the controls on epitactic nucleation and growth will be addressed. The implications of nucleation kinetics for the evolution of grain-size distribution will be discussed.

AIMS AND OBJECTIVES

The aim of this course is to build a basic understanding of the processes controlling reaction kinetics in mineral systems and to establish competence in analyzing reaction microstructures. The participants should learn to identify the features, which are diagnostic for distinct processes. The students will acquire the ability to develop physical models that describe the observed phenomena adequately. It is beyond the scope of this course to educate experts in the field, but still hope to transport crucial information to such an extent that participants can critically read and evaluate literature on reaction kinetics and are able to cope with related problems independently.

REGISTRATION

Registration can be done by e-mail to rainer.abart@univie.ac.at or by fax using the form on the last page of this course release. Registration should be completed no later than June 30th.

FEES

Each participant will be charged 30 € on site for lecture notes and catering during the short course.

Provisional Programme**Kinetics of Geological Materials**

Lecturers:	R. Abart	University of Vienna
	F. Gaidies	Carleton University, Ottawa
	R. Milke	Free University Berlin
	E. Petrishcheva	Free University Berlin

Part A: Empirical Rate Laws

Unit 0	Refresher on thermodynamic principles
Unit 1	Rate limiting steps
	Reaction order
	Rate equations

Part B: Diffusion

Unit 2:	Basics of diffusion
	Macroscopic view of diffusion
	Microscopic view on diffusion
	Mathematics of diffusion problems
Unit 3:	Diffusion in crystals, defect chemistry
Unit 4:	Grain boundary diffusion
Unit 5:	Application of diffusion, geospeedometry, closing temperature

Part C: Grain- and phase-Boundaries

Unit 6:	Interface free energy, capillary forces
Unit 7:	Capillary force driven coarsening
	Normal grain growth
	Zener drag

Part D: Nucleation and growth

Unit 8:	Classical nucleation theory for polymorphic phase transformation
Unit 9:	Nucleation theory for binary systems – interface control versus diffusion control
Unit 10:	Heterogeneous nucleation and epitactic growth

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August 30th to September 3 2010

REGISTRATION FORM

Registration deadline: 30. 06. 2010

Name:
Affiliation:
Address:
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Telephone:
FAX:
E-Mail:

I pertain to the following group (please check)

- undergraduate student
- graduate student
- postdoc
- senior researcher
- other, please specify

Please send to: Univ.-Prof. Dr. Rainer Abart
Department of Lithospheric Research
University of Vienna
Althanstrasse 14, UZA 2, 2B325
A – 1090 Wien
Tel. ++43(1)4277- 53319,
Fax: ++43(1)4277-9534

e-mail : rainer.abart@univie.ac.at