Doctoral School at the University of Vienna, Austria

Deformation of geological materials: Mechanical-chemical feedback and the coupling across scales

The geodynamic evolution of the Earth is controlled by internally and externally driven processes. Most of these processes are associated with deformation and chemical reactions, which affect minerals, rocks, fluids, and melts constituting the Earth. Recent advances in experimentation, instrumental analysis and numerical modeling have opened new perspectives for a comprehensive and quantitative approach in geological research. In this doctoral school research is focused on the materials aspects of rock deformation and its interplay with mineral reactions. We study rock deformation using natural examples and experiment combined with state of the art instrumental micro-chemical, micro-structural and textural analysis, and numerical modeling. This multidisciplinary research aims at developing reliable predictive capacity in geological modeling by identifying and parametrizing the feedback mechanisms between chemical reactions and deformation. We intimately combine scientific research and education. The research topic provides a wealth of demanding and challenging problems with multiple implications for applied research. Working on a common topic in a multi-methodological approach, the participating doctoral collegiates are in the position to develop this focus area further and integrate their expertise in internationally coordinated research initiatives.

This research initiative is hosted at University of Vienna offering 10 PhD positions funded for three years. It integrates infrastructure and expertise from the Department of Lithospheric Research, the Department of Geodynamics and Sedimentology and from the Institute of Mineralogy and Crystallography. Collegiates have access to state of the art instrumental analysis including electron and ion beam micro-analytical devices, TIMS, LA-ICP-MS, SIMS (U, Th, Pb, Hf, O isotope systematics, single crystal and powder X-ray diffraction, as well as spectroscopic devices. Short courses on topics relevant to the research focus are held at regular intervals by in house scientists as well as by guest lecturers. Collegiates are encouraged to spend part of their time at cooperating institutions such as ETH-Zürich, Deutsches GeoForschungsZentrum, and Center of Excellence on Physics of Geological Processes at University of Oslo.

The research projects are grouped into three broad topical fields.

Topical Field I Localization of deformation, chemo-mechanical feedback

Project I.1: Deformation mechanisms and chemical / mineralogical changes around porphyroblasts/clasts

PI's: B. Grasemann
Coop.: D. Schneider (University of Ottawa)
M. Bestmann (University of Erlangen)
Marcin Dabrowski (PGP, Oslo)
Nicole Hoymann (GFZ Potsdam)
Benjamin Huet (University of Vienna)

Rationale: Inclusions in a progressively deforming rock will influence the stress and strain field around these heterogeneities influencing the bulk rheology of the rock. We will combine high resolution analytical data from fault rocks with mechanical numerical models in order to study the stress and pressure distribution in rocks with inclusions and the possible influence of such heterogeneities on the deformation mechanisms in the surrounding matrix.

Methods: Light microscope, SEM/CL/FIB/STEM/EBSD/EDX, EPMA, whole-rock geochemistry

Personnel: Anna ROGOWITZ

Project I.2: Chemical vs. petrophysical control on strain localization in porous sediments

PI: U. Exner
Int. Coop.: P. Baud (EOST Strasbourg)

Rationale: Deformation bands are fault zones in high-porosity sediments, usually characterized by a reduction of porosity and permeability caused by grain rotation and fracturing. Analyzing natural samples from sediments with a wide range of mineralogical composition, but similar maximum displacement and burial depth, this project aims to quantify the influence of chemical composition, cementation and alterations on the petrophysical properties and deformation mechanisms. Complementary deformation experiments are performed to constrain mechanical properties of rock samples of different composition.

Methods: Light & CL microscopy, SEM/CL, EPMA, whole-rock geochemistry, XRD, experimental rock deformation (EOST Strasbourg)

Personnel: Marco LOMMATZSCH

Topical Field II Reaction induced stress deformation

Project II.1: Chemically induced stress and deformation in mineral single grains

PI's: R. Abart, G. Habler
Int. Coop.: S. Zaefferer (MPI Düsseldorf)
J. Schreuer (Ruhruniversität Bochum)

Rationale: In single crystals any compositional heterogeneity induces mechanical stress, which in turn feeds into the free energy of the material. By this mechanism the thermodynamic stability of the material as well as its kinetic behavior during reaction may be influenced. We do cation exchange experiments in rock forming minerals to produce single crystals with chemically distinct domains (domain single crystals) to investigate their thermodynamic properties and kinetic behavior with particular focus on diffusion in self stressed systems.

Methods: cation exchange experiments and material characterization using EPMA, FEG-SEM-FIB, and EBSD; numerical modeling of coupled elastic deformation and diffusion

Personnel:

Anne–Kathrin SCHÄFFER

Project II.2: Hydration reactions and reaction induced deformation

PI's: R. Abart, G. Habler

Int. Coop.: W. Heinrich , G. Dresen (GFZ Potsdam)

M. Soerenssen (Uni Oslo)

Rationale: The behavior of solid phase aggregates with domains that undergo expansion (swelling systems) is of interest to many fields in scientific (melt extraction, hydration) and applied (recovery of oil, corrosion) research. We design simple systems comprised of calcite and periclase by hot isostatic pressing and then expose the aggregates to a hydrating atmosphere at elevated pressures and temperatures. This leads to formation of brucite from periclase and associated swelling by about 100%. We study the kinetics of the hydration reaction and the mechanical behavior of the hot pressed aggregate to learn about the modes of mechanical response as a function of the periclase to calcite ratio and reaction overstepping.

Methods: hot isostatic pressing and hydrothermal experiments (3 months stay @ GFZ Potsdam); in house material characterization - FEG-SEM-FIB, EBSD, EPMA; continuum mechanical modelling of fracturing (3 months stay @ Uni Oslo),

Personnel: Hakan KULECI

Project II.3: Irradiation damage induced by MeV heavy-ion irradiation

PI: L. Nasdala

Rationale: Stress in minerals as induced by irradiation damage involves two major phenomena. First, larger-scale stress occurs among growth zones: Zones withelevated U and/or Th concentrations may suffer elevated radiation damage, which results in enhanced volume expansion and eventually in the formation of fractures in adjacent zones. Second, nanometre-scale stress is induced by partial irradiation-induced amorphisation: The volume expansion of nm-sized, amorphous clusters causes dilative stress in the neighbouring crystalline remnants. These effects are planned to be studied in heavy-ion irradiation experiments on FIB lamellae of selected minerals. The main objective is to quantify irradiation effects, and to use the stress (affecting the short-range order around anionic molecular units) to estimate the degree of the self-irradiation damage in unknown geological samples.

Methods: Sample preparation in house using FEG-SEM-FIB; material characterization in house using EPMA, EBSD, PL, and Raman spectroscopy; mineral syntheses at the Memorial University of Newfoundland; Tandem accelerator irradiation at the Forschungszentrum Dresden-Rossendorf

Personnel: Andreas ARTAČ

Topical Field III Deformation assisted re-equilibration phenomena

Project III.1: The mechanical and chemical behavior of solid inclusions during host mineral deformation

PI's: G. Habler, B. Grasemann, R. Abart
Int. Coop.: -

Rationale: Inclusion domains in porphyroblasts may preserve assemblages of relatively early evolutionary stages of natural metamorphic rocks. We intend to study the interplay between mineral reactions in inclusion domains and host mineral deformation during metamorphic overprinting of pre-existing phase assemblages in polymetamorphic or polyphase metamorphic metapegmatites, metapelites or eclogites. Comparison of the compositional, microstructural and textural behavior of natural host-inclusion systems with results from thermodynamic, mechanical and diffusion modeling is expected to provide information on the chemo-mechanical feedback during metamorphism.

Methods: optical microscopy, EPMA, EBSD, CL, SEM, FIB, 3D reconstruction of microstructures, thermodynamic modelling, mechanical finite element modelling

Personnel: Thomas GRIFFITHS

Project III.2: The effect of strain heterogeneities on Rb-Sr and Sm-Nd isotopic re-equilibration in minerals and rocks

PI's: G. Habler, B. Grasemann, R. Abart

Rationale: Understanding the influence of deformation on isotopic rejuvenation is of utmost importance for the proper interpretation of age information from bulk sample isotopic analysis. Rb-Sr and Sm-Nd characteristics of minerals and rocks across outcrop scale strain gradients will be studied upon the Vinschgau Shear Zone in the Southern Ötztal-Stubai Complex (Italy). The Rb-Sr isotopic record of muscovite, biotite, apatite and feldspar as well as the Sm-Nd isotopic record of garnet, apatite and feldspar from samples with differing strain intensity will be investigated. In combination with major element mineral compositions and microstructures, possibly combined with (LA-)ICP-MS trace element data we intend to obtain information on the influence of the deformation intensity and prevailing deformation mechanisms on the extent of chemical and isotopic equilibration.

Methods: Microscopy; EPMA; TIMS (Rb-Sr & Sm-Nd isotope analysis); ICP-MS; SEM-FIB

Personnel: Tobias EBERLEI

Project III.3: Rejuvenation effects during plastic deformation/Microchemistry and microstructure/texture of accessory minerals and the effect of deformation on the retention of radiogenic isotopes

PI's: U. Klötzli, B. Grasemann, R. Abart

Rationale: Plastic deformation is able to induce isotope exchange processes which result in unpredictable changes in the radiogenic and stable isotope content of minerals. This unambiguously hampers our ability to reliably interpret absolute age data derived from deformed minerals. Therefore, knowledge, in both a qualitative and quantitative way, of the role of plastic deformation in this respect is vital for a geologically meaningful interpretation of the age data. We will investigate the influence of plastic deformation on rejuvenation and alteration effects on high-temperature geochronometers (U-Th-Pb) and stable isotopes (O, Hf) in accessory minerals (zircon, xenotime, monazite) in relation to the respective host minerals, degree of plastic deformation, strain amount, and primary age systematics. The results will allow us to obtain a better understanding of the underlying isotope exchange processes in accessory minerals during plastic deformation. This in turn will allow us to more directly identify individual crystals and crystal domains which should deliver reliable absolute age data.

Methods: Quantitative microstructures, in-situ and mineral separates: EBSD; Quantitative microchemistry, in-situ and mineral separates: EPMA (crystal chemistry), LA-MC-ICP-MS, SIMS (U, Th, Pb, Hf, O isotope systematics); integrated chemical stability: chemical abrasion (only mineral separates)

Personnel: Elizaveta KOVALEVA