EXCITE Workshop on Advanced X-ray and Electron Imaging in Geosciences

Sunday (04/09) evening
19:00 Icebreaker

Monday (05/09) morning - Electron Imaging 1
8:30 Welcome
8:45-10:15 **Paul Midgley** - Multi-Dimensional Electron Microscopy
10:15-10:35 Coffee/Tea break
10:35-12:05 **Dave Wallis** - High-angular resolution electron backscatter diffraction analysis of lattice distortion in geological materials

12:05-13:00 Lunch

Monday afternoon - Electron Imaging 2
13:00 - 14:30 **Michel Bestmann** - Correlative Microscopy: the NEW hype?
14:40 - 16:10 **Rich Taylor** - Quantitative geochemical mapping for petrology research
16:10-16:30 Coffee/Tea break
16:30-18:00 **Andrew Menzies** - Micro-XRF Imaging in Geological Sciences – Capabilities, Applications and Examples

Tuesday (06/09) morning - X-ray Imaging 1
8:30 - 10:00 **Christian Schlepütz** - Synchrotron X-ray tomographic microscopy: From high-resolution 3D structural information to observing material changes in situ
10:00 - 10:30 Coffee/Tea break
10:30 - 12:00 **Ian Butler/Florian Fusseis** - Experimental Environments for 4D X-RAY Microtomography

12:00 - 13:00 Lunch

Tuesday afternoon - X-ray Imaging 2
13:00 - 14:30 **Nicolas Piche/Mike Marsh** (online) - Advanced Segmentation and Image Analysis with Dragonfly
14:40 - 15:10 **Edward Andò** (online) - Measuring deformations in 4D image data
16:10 - 16:30 Coffee/Tea break
16:30 - 18:00 **Arne Jacob** (online) - Digital Core Analysis with GeoDict

19:30 Workshop dinner

Wednesday (07/07) - Attendant science & networking day
9:00 - 17:00 Attendees present and discuss their current and future research to their peers and the presenters
11:00 – 12:00 **Steffen Berg** (online) - Multiphase Flow in Porous Media - From 4D Imaging to a New Theory

Monday and Tuesday lectures will be live-streamed, also the keynote lecture of Steffen Berg on Wednesday. Zoom links will be sent by email to the registered participants.

Abstracts

Paul Midgley - Multi-Dimensional Electron Microscopy

Over the past decade or so there has been something of a revolution in transmission electron microscopy with the introduction of new hardware such as aberration correctors and monochromators, to enable routine sub-Angstrom imaging and high energy resolution spectroscopy. In addition, the introduction of new and faster detectors and spectrometers, coupled with a rapid rise in computational power has led to an increase in interest in using a combination of microscopy modes to yield 'multi-dimensional' (MD) data sets. Such MD data provides new insights into the properties and behaviour of materials. In this talk I will introduce multi- dimensional electron microscopy and discuss several case studies that use a number of techniques including electron tomography, analytical tomography (combining 3D real space with an energy / spectral dimension), time resolved microscopy and 4D-STEM methods to reveal heterogeneous crystallography of materials at the nanoscale.

Dave Wallis - High-angular resolution electron backscatter diffraction analysis of lattice distortion in geological materials

Microstructural analysis of deformed rocks is central to interpretation and modelling of deformation mechanisms, rheological properties, and associated geodynamic phenomena. Intragranular lattice distortions are a key part of this microstructural record and are most commonly analysed using electron backscatter diffraction (EBSD). Unfortunately, conventional analysis of EBSD patterns, employing Hough- transform-based indexing of each pattern, only reveals a fraction of the recorded information. Conventional EBSD only measures misorientations greater than a few tenths of a degree and cannot measure elastic strain. More information can be revealed using high-angular resolution electron backscatter diffraction (HR-EBSD), during which image processing of the diffraction patterns is used to probe very subtle variations in orientation and elastic strain. The HR-EBSD method has precision in misorientation angles on the order of 0.01 degrees and, critically, can also measure elastic strain with precision on the order of 0.0001. The precise misorientation angles are accompanied by improved determination of misorientation axes, relative to conventional EBSD, allowing reasonable estimates of densities of geometrically necessary dislocations. Similarly, the elastic strains can be used to calculate residual stress variations currently stored in the rock. These capabilities open a wealth of new opportunities for investigating wide-ranging deformation processes. Results from naturally and experimentally deformed rocks reveal complex distributions of multiple dislocation types and stresses that vary by hundreds of megapascals over length scales of a few micrometres.

Michel Bestmann - Correlative Microscopy: the NEW hype?

Correlative Microscopy correlates different data sets from light microscopes and/or electron microscopes (CLEM) acquired with different detectors and/or different magnifications. The power of CLEM is to gain a full range of different information from the same microstructure, which is essential for the interpretation and to understand for example deformation processes. CLEM was applied primary in life science, but in recent years, it is also popular in geoscience. In addition, the light- and electron-microscope companies develop automated systems for applying an easy to use CLEM workflow. In this talk I will present two examples from deformed quartz vein samples with the focus of the correlation of light and scanning electron microscopy (SEM), including EBSD and cathodoluminescence, and based on these data sets the integration of microstructural controlled geochemical analysis of Ti in quartz. These observations provide the basis for a new generation of models of deformation mechanisms and rheological properties.

Rich Taylor - Quantitative geochemical mapping for petrology research

Automated mineralogy on the scanning electron microscope (SEM) has a unique part to play in the future of geoscience research, enabling large datasets to be generated with a consistent approach. The combination of quantitative geochemical measurements alongside rapid, large area mapping provides a unique geochemistry and petrology solution. Flexible outputs of quantitative geochemical data. This allows the user to decide how and where to interrogate their samples, both within the new, user-friendly interface and with streamlined workflows into third party software. The use of quantitative chemistry as the basis for automated mineralogy provides unique capabilities for large area analysis such as thin sections. Quantitative textural information can be extracted from the sample such as grain sizes, shapes, and mineral associations, alongside quantitative geochemical data providing mineral classification, including mineral and whole rock/sample compositions. This provides a wealth of information for the petrologist to understand their sample and a one-stop-shop for many geoscience workflows.

Here we demonstrate the power of large area quantitative EDS mapping by combining ZEISS Mineralogic automated mineralogy with geoscience-oriented functions of XMapTools. By importing calibrated, quantitative EDS maps XMapTools can be used to rapidly perform a variety of petrological calculations without the need for a separate, long-winded calibration step using microprobe data. Here we use quantitative EDS from high grade metamorphic rocks to obtain mineral and bulk compositions alongside textural information such as modal abundances. These mapped data are imported directly into XMapTools and can be used to generate oxide values, cation per formula unit (cpfu), end member proportions, and perform thermodynamic calculations.

Andrew Menzies - Micro-XRF Imaging in Geological Sciences – Capabilities, Applications and Examples

Micro-X-ray fluorescence (micro-XRF) is a spatially-resolved version of traditional X-ray fluorescence analysis (XRF). The micro-XRF analytical technique was first described more than 50 years ago and since then it has remained mostly a niche technique, albeit quite common in several industrial application fields, but without becoming part of standard geoanalytical techniques. In recent years, however, a series of technological developments, from excitation sources, to enhanced detection possibilities and signal processing capabilities and algorithms, have allowed improvement in the performance of the technique, consequently making micro-XRF useful as a standard geological analytical tool. Specifically, these technological developments include improving (minimizing) beam size, improving X-ray source options and capabilities, applying numerous types of filters, and next generation SD detectors with high signal throughput and energy resolution. The small beam and localized measurement position can be used in single point mode, or in scanning mode for a line scan or area map. This position-tagged style of spectroscopy then allows for the creation of element distribution maps, as well as for other complex post-processing procedures, including mineralogical analysis. Some of the main advantages of micro-XRF analysis are the ability to perform large area maps on a variety of sample types, non-destructive analysis, minimal sample preparation (no carbon coating or polishing required), small spot analysis, fast measurements with major, minor and trace element sensitivity, and ability to process results for quantification and / or mineralogy. Examples of all these benefits will be shown from the geological and mining sciences.

Christian Schlepütz - Synchrotron X-ray tomographic microscopy: From high-resolution 3D structural information to observing material changes in situ

Synchrotron X-ray tomography has initiated a new paradigm in structural investigations over the past decades and finds applications in virtually all disciplines where microscopic information on the internal structure of materials is key to understanding their properties. Meanwhile, these developments have paved the way for ever more powerful tomography devices on the lab scale which are readily accessible to the scientific communities. In this talk, I will cover some of the basic principles of tomography and the particular benefits (and drawbacks) of using synchrotron radiation for tomographic studies. Various examples of current research performed at the TOMCAT beamline of the Swiss Light Source will demonstrate the versatility and applicability of the method to different disciplines and give a sense for the current state of the art. With the advent of 4th generation synchrotron sources, the field will doubtlessly continue to evolve rapidly, and I will try to give a glimpse of what new opportunities the future may hold.

Ian Butler/Florian Fusseis - Experimental Environments for 4D X-RAY Microtomography

Time resolved (4D) X-ray microtomography experiments that replicate the pressure and temperature conditions of the Earth's subsurface require the use of specialist experimental equipment. While some equipment can be obtained from commercial manufacturers, equipment dedicated to investigation of geological processes is often bespoke and built by individual research laboratories to meet their specific needs. Using the range of experimental environments developed at the University of Edinburgh as examples, this talk will, in a first part, explore approaches to the design and construction of X-ray transparent experimental equipment for use at elevated pressure and temperature. The choice of suitable materials and their mechanical properties will be considered as well as solutions to problems like cell and sample sealing. The experimental equipment considered is suitable for investigations of multiphase fluid flow in porous and fractured media, mechanical deformation of geological materials and coupled thermal, mechanical, chemical, and hydraulic processes, and the equipment is relevant to investigations related to both the natural and engineered subsurface. A second part of this talk will concern the deployment of these experimental environments at laboratory- and synchrotron light sources, and use a number of case studies to illustrate possible analytical workflows to turn images into quantitative analyses.

Nicolas Piche/Mike Marsh - Advanced Segmentation and Image Analysis with Dragonfly

Dragonfly is currently the fastest growing image processing and analysis software in the areas of X-ray tomography and FIB-SEM acquisition in geosciences. It is also free for non-commercial use and cost effective for commercial use. In this talk we will present a range of advanced image segmentation capabilities in Dragonfly including histographic segmentation, segmentation wizard with artificial intelligence based segmentation and deep learning tools. These tools allow to segment challenging phases and features in geoscience samples, easily and with accessible and simple tools. In addition to segmentation, advanced analysis functionality will be discussed, including the porous microstructure analysis (PuMA) plugin from NASA. PuMA allows the calculation of fluid flow permeability, tortuosity and more. The presentation will start with an overview and examples of achievable results, followed by a practical demonstration with a range of suitable geoscience datasets to showcase the capabilities live.

Edward Ando - Workshop on measuring deformations

Quantifying deformations is a key topic in geosciences. In this workshop practical examples of the use of open source python-based software (https://pypi.org/project/spam/) will be presented with the appropriate background for the measurement of displacements (and thus strains) from 2D and 3D images so that attendants will be ready to get their hands dirty on their own data! The workshop will cover basics in Digital Image and Volume Correlation as well as Particle Image Velocimetry with SPAM that will allow users to quantify strains in time-resolved image data.

Arne Jacob - Digital Core Analysis with GeoDict

Math2Market's GeoDict is the best Digital Rock Physics and Digital Core Analysis software for material analysis and property simulation, with unmatched fast run times, low hardware requirements, and automation of workflows. The digital rock physics-digital core analysis (DRP-DCA) suite of GeoDict is built for the specific needs of the E&P sector. Including imaging analysis and processing capabilities, GeoDict enables performing the entire workflow in-house as an alternative to service providers solutions. The workshop presents the introduction to Digital Core Analysis and Digital Rock Physics with GeoDict 2022.