

# *EUG XI*



Symposium PCM4

Quantitative Modelling of Diagenetic,  
Metamorphic, Deformational  
and Igneous Microstructures

Convenors

Paul Bons  
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# PCM4

## Quantitative Modelling of Microstructures

### Sunday PO Session

#### PCM4 : SUpo01 : PO Automated Fabric Analyser System for Quartz and Ice

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A new fully automated data acquisition system that can be used for the collection of c-axis crystallographic fabric data in hexagonal mineral systems has been developed. It collects a comprehensive set of crystallographic measurements, including digital images of a thin section. The c-axis measurement sites can be selected either interactively or in an automatic stepping mode.

This is a portable acquisition system that uses a modified Zeiss Axioskop microscope (the most compact in the range of Zeiss petrographic microscopes) and a PC laptop computer. The total system weighs less than 16 kg. The computer controls the microscope and a digital CCD camera system, and contains a software package that is responsible for the data acquisition with the whole system operating on a 12-volt power source.

The microscope stage can accommodate thin sections of up to 100 x 100 mm with motors controlling translations in the X and Y directions to 10 mm resolution. No tilting of the thin section is required for the analysis. The software system on the computer controls the microscope stage and captures images directly from the camera. The image and photometric information is analysed to determine the c-axis orientation. If the crystal element being tested is not sufficiently uniform (due to impurities, grain boundaries, or bubbles), a search is made close around the selected site for clear crystal material. The software incorporates a quality control system that tests for and rejects doubtful results.

The process yields spatial information describing individual grains and their orientation within a sample. Each c-axis is recorded with its XY position, orientation and relationship within the captured sequence. The results can then be analysed using a variety of discriminators to sort and select different collections of candidate grains to prepare fabric and AVA diagrams or analyse nearest neighbour grain relationships.

To ensure the system is producing optimum results and accuracy it has been assessed by comparing measured orientations with c-axes obtained using a conventional Universal Stage from single crystals of quartz. Currently the system is being applied to a set of experimentally deformed polycrystalline ice aggregates with highly deformed and recrystallised grains. It is proposed to establish a set of benchmark quartzite samples that can be made available to other researchers, who may purchase such a Fabric Analyser, so they can compare their results with known standards.

#### PCM4 : SUpo02 : PO Transport Property Predictions of Reservoir Rock by Quantitative Image Analysis: From the Pore-Scale Properties to Plug-Scale Properties

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Petrophysic property predictions of the reservoir rock has become a very important task for the quantitative modelling of fluid-rock processes in sedimentary rocks, the quantification of fluid flow, the quantitative modelling of diagenetic transformations and the microstructure/texture/fabric features. For many years, the Petrographic Image Analysis has been widely used as a rapid 2D technique for the quantitative measurement of the morphology and quantity of pores in reservoir rock and porous materials. Reservoir engineers, petrophysicists and exploration geologists are interested in discovering how the permeability and the porosity are related to the pore aperture size, the pore-aperture size distribution, the pore shape and pore geometry in order to evaluate the sealing capacity of cap rocks as well as to define the "rock-types" and "flow-units" in a reservoir model. This paper aims to describe a method of quantification of petrophysical prop-

erties in carbonated and chloritic sandstone pore systems from the Petrographic Image Analysis in more than four orders of magnitude, from a submicron to a centimeter scale. In this study we analysed two kinds of reservoirs rock in order to predict their transport properties: - carbonate pore system of oligocene limestone of North Aquitaine Basin, - chloritic sandstone pore system. We used the Back-scattered electrons grey level images and integrated two scales: the images with a 46<sup>x</sup> magnification which allowed us to characterize the macroporosity and the images with a 965<sup>x</sup> magnification which gave us information about microporosity. This technique enabled us to measure different classic petrophysic properties such as pore area, specific surface area, average pore diameter, distribution of pore size, pore shape factor, macroporosity and microporosity. We used image parameters in order to obtain the model of capillary pressure curve versus saturation. Using empirical equations of permeability derived from Carman-Kozeny expression and a bundle of capillary tubes model, we calculated the permeability of carbonate and chloritic silicoclastic pore systems from different image parameters. The same petrophysical parameters are directly measured on core through classic three-dimensional petrophysical techniques (3D), such as Hg-injection porosimetry, permeametry and the BET technique. Finally, we compared values of different petrophysical properties of carbonate and chloritic sandstones pore system, obtained from 2D image analysis and 3D classic petrophysical techniques. The best modelling of capillary pressure versus saturation is obtained when the gap between image porosity and mercury porosity is very low. The analysis of the relationship between mercury capillary pressure and image capillary pressure shows that the pore size / pore-throat size ratio varied from 1 to 100 and gradually increases from macroporosity to microporosity. Carman-Kozeny model gives the best values of permeability with a best fit of coefficient c. This model integrated better the pore space microgeometric parameters.

#### PCM4 : SUpo03 : PO Displacement Textures (Cleavage Domes) and Sector-Zoning as Hydrostatic Stress Indicators in Contact and Regional Metamorphic Terranes

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Although rarely recognised and reported, displacement of insoluble matrix grains, particularly graphite, is a rather common microstructure associated with porphyroblasts growing in C-rich rocks, in both contact and regional metamorphic terranes. Evidence for textural sector-zoning is also usually found associated with displacement. Of the common porphyroblastic phases, andalusite (var. chiastolite), garnet and staurolite all regularly show sector-zoning patterns (with up to 16 sectors possible in sections through icositetrahedra garnets) with associated displacement of insoluble material. Similar behaviour has been observed in cordierite and kyanite. In thin-section, evidence of displacement takes the form of accumulated insoluble material at the crystal faces; often this material forms small domes containing a weakly developed cleavage (cleavage domes) but in other instances only a massive accumulation of graphite, sometimes with a domal outer profile, forms. Previous work has shown that a bulk hydrostatic stress is required to form cleavage domes. Thus cleavage domes (and perhaps also massive displaced material) are a textural criteria of a bulk hydrostatic stress condition, indicating a non syn-deformation growth event. This would be the case for contact metamorphism around pre- or post-collision intrusions, with high fluid pressures forming during dehydration reactions; chiastolite, typical of contact metamorphism, invariably displaces graphite and is by definition sector-zoned. In regional metamorphic terranes, porphyroblast growth may be pre-, inter- or post-deformation. The most likely of these to show sector-zoning/displacement is pre-deformation; progressive burial in the footwall of the developing nappe pile would result in prograde dehydration reactions, providing a high fluid pressure, whilst relatively little or no deformation was occurring, allowing sector-zoned porphyroblast growth and associated matrix displacement. Propagation of the basal thrust/ductile shear zone under the rocks, incorporating them into the orogenic wedge, would result in a deviatoric stress developing, with high internal deformation during thrust translation, whilst at broadly the same time causing a drop in P and T conditions. Thus displacement (and textural sector-zoning) is often found in the early (core) stages of the growth of peak metamorphic porphyroblasts, with a poikiloblastic or syntectonic fabric towards the rim; areas with spiral garnets often have texturally sector-zoned garnet cores with displacement textures (e.g. Morar, Vermont, Finnmark,

Västerbotten). Unless cleavage-domes are overgrown by further porphyroblast growth, displaced material will be stripped from porphyroblast faces and destroyed, at the onset of deformation. However, if the strain is very small, the pattern of movement of cleavage domes around the porphyroblast could be used to give the shear sense.

#### PCM4 : SUpo04 : PO A Front-Tracking Program to Model Fibrous Microstructures in Strain Fringes

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Fibrous crystals in veins and strain fringes are of special importance to geologists, since they are thought to record part of the progressive deformation history of the host-rock. Therefore it is essential to study the development of these structures in detail. We developed a two-dimensional computer model (Fringe Growth) to simulate the incremental growth of crystal fibres in antitaxial strain fringes. The user can define the shape and roughness of a core-object (e.g. a pyrite crystal), the growth velocity and anisotropy of growing fibres, the opening velocity of fringes and the translation and rotation of a fringe relative to its core-object. Growth of fibres is simulated by movement of nodes connecting straight line segments that define the crystal boundaries. The program "Fringe Growth" is able to reproduce complex fibre patterns that are observed in natural strain fringes from Lourdes (France) and from the Yilgarn Craton (Australia). The similarity between simulated and natural examples suggests that the assumptions used in the computer program are realistic and that displacement-controlled fibres follow points on the core-object surface. Most fibres in the natural and simulated examples grow displacement-controlled but face-controlled and intermediate fibres are commonly found on the rims of fringes, within fibre bands and next to suture lines. No single displacement-controlled fibre in the modelled or natural fringes represents the whole movement path of a fringe away from its core-object since fibres usually end on suture lines, on the rims of fringes or are affected by relative rotation of core-object and fringe. This has major implications for the use of fibres for structural analysis. A single fibre analysis is prone to produce large errors. Therefore we suggest the use of all fibres in a fringe using an "object-centre path analysis". The program "Fringe Growth" is an excellent tool for research as well as teaching since movies of progressive fibre growth can be easily generated and are available together with the program (for Macintosh computers) at: ["http://www.uni-mainz.de/FB/Geo/Geologie/Students/Koehn/FringeGrowthHome.html"](http://www.uni-mainz.de/FB/Geo/Geologie/Students/Koehn/FringeGrowthHome.html).

#### PCM4 : SUpo05 : PO Interaction between Lava Flows: Crystallization Induced by Cooling and Re-Heating of Pahoehoe from Kilauea, Hawaii

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Re-heating of basalt lava in the lab suggests a relation between crystallization, oxidation and diffusion (Burkhard, 2001a) and the kinetics of crystallization, e.g., growth rates G, were demonstrated to decrease exponentially with time. High G is found for high cooling rates (small residence time ( $\tau$ ) in the temperature interval of crystallization), and G decreases from an air-quenched lava surface to its interior (Burkhard, 2001b). We here investigate the interaction between lava flows from active Pu'u O'o, Kilauea, Hawaii and selected a profile through two flows, an upper and a lower flow with a thickness of 6.6 and 3 cm, respectively. While the surface of the top flow is glassy, the entire bottom flow is crystallized. Growth rates of crystallization may be derived by use of the crystal size distribution method, if  $\tau$  is known (Marsh, 1988; Cashman & Marsh, 1988). We therefore adopted a cooling model: (1) cooling of the bottom flow due to atmospheric convection, (2) cooling of the upper part of the top flow due to atmospheric convection, and of the lower part of the top flow due to conduction and contact with the bottom flow, (3) re-heating of the bottom flow by conduction at the emplacement of the top flow and (4) cooling of both flows. The simple model suggests that the bottom flow effects the cooling process of the lower 3 cm of the top flow. This distance from the contact is relatively independent of the

# PCM4

## Quantitative Modelling of Microstructures

temperature of the bottom flow at the time of emplacement of the top flow. The presence of plagioclase which requires a minimum temperature of 920°C to crystallize within the glass (Burkhard, 2001a), sets the minimum temperature of the bottom flow around 700°C, if the top flow was at about 1160°C (e.g., [1]). Hence, a dominant part of cooling and re-heating took place above minimal temperatures for nucleation and growth which are above 850°C for pyroxene and Fe-Ti oxides (Burkhard, 2001a,b). Therefore, G decreases with depth, and variations in  $\tau$  induced by faster cooling of the lower top and re-heating of the bottom flow, are dominated by an increasing  $\tau$  with depth. Crystal sizes are more sensitive, they oscillate in the top and in the bottom flow with increasing distance from the surface. This oscillation correlates with an oscillation of number of nuclei. This correlation is a consequence of the time dependence of G and the overlap of nucleation and growth temperatures for the minerals discussed.

Burkhard DJM, *J. Petrol.*, **34**, (2001).  
Burkhard DJM, *Contrib. Mineral. Petrol. (subm.)*, (2001).  
Marsh BD, *Contrib. Mineral. Petrol.*, **99**, 277-291, (1988).  
Cashman KV & Marsh BD, *Contrib. Mineral. Petrol.*, **99**, 292-305, (1988).  
Brandeis G & Jaupart C, *Contrib. Mineral. Petrol.*, **96**, 24-34, (1987).  
Keszthelyi L, *Geophys. Res. Lett.*, **22**, 2195-2198, (1995).

### PCM4 : SUpo06 : PO The Metamorphism in the Eastern Part of Montagne Noire (Massif Central, France) P-T-t Path. Geothermobarometry

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Metamorphic rocks in the Eastern part of the Montagne Noire (Rosis syncline) display the succession of five isometamorphic zones: Zchl, Zbi-crd, Zst-crd, Zand-bi, Zsill, Zst- which define a typical Low Pressure High Temperature metamorphism prograde from the outside towards inside anatectic gneiss core of the Montagne Noire thermal dome (Thompson and Bard, 1982). Two cross sections C1, C2 located respectively in northern and southern parts of the studied area have been investigated in detail from microtectonic and petrologic point of view.

The tectonic study at all scales shows a generalized eastward syn-metamorphic extension evidenced by  $\delta$ ,  $\sigma$ , C/S criteria and normal fault shear zones (phyllonites) observed in each of the mapped metamorphic zones.

Bulk rock compositions vary from north to south. The northern gresopelitic series are Mg-rich whereas the southern ones, are Fe-rich inducing the widespread growth of garnet instead of cordierite and also different reactional sequence well documented in an isobaric (4 kbars) T-Fe/Mg section. In contrast to Demange descriptions (Demange, 1979), kyanite relicts have never been observed in the metamorphosed "schists X". So, an early decompression before the metamorphic climax is not evidenced. The P-T-time path in each metamorphic zone could be isobaric at approximately 4 kbars as the deduced metamorphic gradient (locus of T<sub>max</sub> in each zone).

The calibration of a thermometer based on the Fe-Mg exchange between garnet and biotite allowed us to calculate the metamorphic gradient along the C1 and C2 erosion surfaces. C1 gradient lies between 190°C and 80°C / km whereas C2 gradient is lower or equal to 50°C / km. These two metamorphic gradients are thus strongly different in relation with the intensity of post-metamorphism peak shearing. The relationships between isogrades, foliation and normal shear zones are also quite different when observed along C1 and C2. For example, in the north of the Rosis synclinorium, shearing of isogrades is stronger than in the southern part. From place to place, metamorphic zones are more or less wide, some of them (e.g. Zcrd-st) are discontinuous, wrapped around by shear zones, others (e.g. Zchl-grt) have even completely disappeared. Post-peak shearing is also responsible for the thinning of the metamorphosed series.

In conclusion, the LP-HT metamorphism in the Eastern part of the Montagne Noire, is definitively related to the emplacement of an anatectic metamorphic core complex accompanied by granitoid injections. The respective roles of crustal thickening related to the nappe emplacement and the isobaric cooling of mafic/ultramafic bodies at the base of the crust, in relation with magmatic underplating are discussed.

P. H. Thompson & J.P. Bard, *Can. J. Earth Sci.*, **19**, 129-143, (1982).

M Demange, *Acad. Sci. Paris*, 288, (1979).

### PCM4 : MOpm22 : G5 The Numerical Simulation of Microstructures in Geological and Non-Geological Materials

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The ability to accurately interpret microstructures in rocks is important both to field geologists, who need to be able to use these interpretations to unravel the geological history of an area, and also to those working on large-scale geodynamic problems, where the interaction between processes is one of the primary controls on the time-dependant mechanical behaviour of the Earth. This review discusses the attempts that have been made by geologists to numerically simulate the evolution of microstructures in rocks, and compares them with related research in the wider materials science community. Unlike many other branches of materials science, microstructures in geological materials are thought to be the product of a large number of competing processes, and hence are inherently more difficult to characterise.

There are a wide range of techniques that have been used to simulate microstructure evolution, from continuum descriptions such as phase field models at one extreme to molecular dynamics codes at the other. At the same time the term "microstructure" encompasses a wide range of scales, and techniques appropriate to one scale or process will not necessarily be easy to combine.

Until recently attempts to combine deformation and metamorphic processes at the grain scale have been very limited, however in the last 5 years several approaches have been taken, usually resulting in a hybrid code involving a finite element approach plus some other description (such as a Potts model or a front tracking system). While none of these hybrid codes are complete, there is hope that there are now a sufficient number of simulation tools available to us that a geologically useful system can be developed to simulate both the microstructural and mechanical behaviour of rocks.

## Monday PM Session

### PCM4 : MOpm23 : G5 Melting by Numbers: Chemical Versus Textural Melt Fertility

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Petrological experiments can determine what quantity of melt can be produced from an initial source composition at given temperature and pressure conditions. However, samples are generally small (several cm<sup>3</sup>) and cannot cover the full range in chemical and textural variation of source rocks. At a larger scale, field observations indicate that melt is not randomly distributed in partly molten rocks. Obviously, in migmatites formed by dehydration melting of micas or amphiboles, layering and textural anisotropy control the spatial distribution and amount of melt produced. We examined partial melting through numerical modelling, to (i) reproduce numerically the results of experimental melting; (ii) to explore new situations, not yet attainable by experiments, by looking at the intrinsic disposition of the different minerals (random; linear aggregates; stratified). We started with muscovite, followed by biotite, dehydration reactions. They are simulated through a Lagrangian description, which considers a discrete mineral distribution. Melt forms only if the reactant phases are simultaneously in contact. A textural anisotropy of one mineral distribution induces melt layering, which mimics the one observed in migmatites. Optimum melt production is obtained for a mineral assemblage with modal abundances similar to the reaction stoichiometry. In other cases, optimum melt productivity cannot be reached. The thickness of mineral layers also influences melt production. The percentage of melt that can form falls rapidly when the thickness of the layers increases. Whereas fertility is around 25% for a layer one mineral cell thick, it falls to about 5% when the layer is 3 cells thick. Melting occurs at the interface of two layers, but it does not propagate inward. At higher thickness, melt production becomes thickness independent, stabilizing at a low value (about 1%). We applied our model to determine what would be the melt fertility of greywackes in relation to their tectonic environment. The real fertility of some source rocks is lower than the bulk fertility estimated only from the bulk mineral percentage. Consequently, most models of crustal derived magma production involve more material than previously estimated for their source. This is valid for magma forming minerals, but also applies to trace elements and accessory minerals which are incorporated into magmas. This has important consequences for mass balance in orogenic cycles. In particular, we show how the presence of some inert phase (e.g., K-feldspar) is important in damping melt production. Our model can also be applied to metamorphic reactions, modelling reaction progress as a function of mineral distribution.

### PCM4 : MOpm24 : G5 Numerical Modelling of the Evolution of Single Phase or two Phase Microstructures during Dynamic Recrystallization: Implications for Strain Localization and Flow Behaviour

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Marked differences in developing microstructures were observed in numerical simulations of deformation and dynamic recrystallization in one phase or two phase materials. These differences are expressed in different rates of recrystallization, development of crystallographic preferred orientation, strain localization and flow behaviour.

Simulations were performed with the 2-D numerical modelling system Elle. With Elle, it is possible to simulate a variety of concurrent microstructural processes that are active at the grain scale during progressive deformation. Individual grains are defined by polygons. Each grain can

# PCM4

## Quantitative Modelling of Microstructures

be made up by a number of second-order polygons (subgrains). A data file stores a complete description of the microstructure at a specific time interval and contains information about geometry, viscosity, strain, stress, dislocation density and age of each individual grain. A shell program iteratively combines an ordered set of individual processes which are each described by separate stand-alone codes to simulate the effect of a single grain-scale process over a small time increment. The data file is changed according to the operation of one micro-process. In our model we simulate viscous plane simple shear strain flow, crystal lattice rotation, formation of subgrains, rotational recrystallization, recrystallization by nucleation, grain boundary migration and recovery.

Experiments were run with initially coarse and fine grained quartz aggregates and initially coarse and fine grained two phase aggregates, where the two phases represent quartz (soft) and feldspar (hard). Settings were chosen to model deformation at greenschist to lower amphibolite facies conditions. Experiments were run to a finite strain of 2 in strain and time increments of 0.05 and 1 Ma, respectively.

Strain localization is seen in both microstructures, but is more profound in polyminerally microstructures. In a coarse grained polyminerally microstructure, the rate of recrystallization in the "soft" phase is markedly higher than in monomineralic fabrics. Combined with the higher rate of recrystallization is the increased tendency of a strong crystallographic orientation with the basal planes parallel to the flow plane. Calculations of the change in the overall viscosity of the microstructure show strain softening with increasing finite strain and degree of recrystallization. A power-law relation between softening and strain was observed, with an exponent that is highest in the 2 phase samples.

### PCM4 : MOp25 : G5 The Effect of Interface Slip on the Rotation and Stabilization of Monoclinic Particles in Simple Shear

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Analytical theory and experimental observation predicts that elliptical particles embedded in an isotropic, linear-viscous matrix undergoing simple shear flow should not develop a stable orientation. However, many natural porphyroclasts are not strictly elliptical but are more prismatic, with straight faces and a generally monoclinic symmetry. Some natural examples develop a very strong shape preferred orientation, more characteristic of a stable end orientation than the transient or oscillating fabric expected for continually rotating particles. One possibility is that the imposed flow is not simple shear: a component of pure shear results in a stable end orientation for particles above a critical aspect ratio. However, it is also possible that the monoclinic prismatic shape could promote slip on the long straight faces and thereby slow down the rotation or even stabilize particles in an orientation close to the shear direction. The current analogue scale-model study considers the rotational behaviour of prismatic, monoclinic rigid particles in a linear viscous matrix (PDMS) to large values of shear (using a ring-shear rig), to make direct comparison with natural measurements of several thousand individual porphyroclasts from different mylonitic shear zones. The rotational behaviour of a monoclinic particle with no slip on the interface is very similar to that of an ellipse with its long axis parallel to the longest particle dimension. There is no stabilization and only a very minor difference is observed for opposite senses of shear, reflecting the particle's monoclinic symmetry ('sigmoidal' vs 'inverse sigmoidal' shape relative to the shear direction). With slip at the boundary (a lubricating liquid soap layer), the particle reaches a stable orientation that is different depending on the sense of rotation. When the longest side is the first to rotate close to the shear direction, the particle stabilizes in this orientation to form a 'sigma clast', similar to typical mica fish or feldspar augen. For the opposite sense of rotation, there is initially oscillation between positions with the short or long side near parallel to the shear direction, before a final stable position with the short side parallel to the shear direction is established. Both these

stable fabrics, with sigma or inverse sigma geometry depending on the developing porphyroclasts' shape (in turn strongly dependent on the presence or absence of extensional crenulation cleavage or shear bands), are observed in natural mylonites.

### PCM4 : MOp26 : G5 Numerical Modelling of Simple Shear Flow around Rigid Objects in different Matrix Materials

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The preferred orientation of certain objects such as mica fish in mylonites suggests that they reach a stable orientation during progressive deformation. However, theoretical and most experimental studies suggest continuous rotation of rigid objects in simple shear flow. We applied the 2D finite difference code FLAC to study the effect of matrix rheology, the existence of inhomogeneities in the matrix, boundary conditions and a slipping object-matrix interface on strain distribution and on rotation rate of rigid objects. The results of these numerical simulations are compared to microstructures in thin sections to get a better understanding of deformation around relatively rigid objects, the rheology of the matrix material, and the stable orientation of these objects. A model consisting of a central object embedded in a less competent matrix is used for the simulations. Results of the experiments show that strain is localised around the elongated object in experiments with (1) a Mohr-Coulomb type matrix, when (2) soft layers are present in the matrix, or (3) in the case of a soft object-matrix boundary in a power-law or Newtonian viscous matrix. In each of these cases rotation rate of the object is reduced and strain is localised, compared to the rotation rate and the relatively homogeneous deformation in homogeneous power-law or Newtonian viscous matrix materials. In mylonites with mica fish, the mica trails that link mica fish may indicate strain localisation along discrete bands (C-planes). Processes like dynamic recrystallisation at the rim of the mica crystal could reduce the coherence between object and matrix. The results of the numerical simulations indicate that an object can reach a stable orientation when strain is localised around the object, which suggests that minor parts of the matrix rheology can have a significant effect on the geometry of the final microstructure. The stable orientation of mica fish in mylonitic rocks is probably the result of strain localisation around the object, anisotropy of the matrix and a reduced coherence on the object-matrix boundary. This implies that the preferred orientation of objects such as mica fish can not be explained with a homogeneous power-law viscous rheology of the matrix, as has been attempted by many workers. This result may also apply to structures that involve other relatively rigid objects in mylonite zones.

### PCM4 : MOp30 : G5 Quantitative Models of Metamorphic Microstructures

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The development of metamorphic textures at the thin-section scale can be simulated by an approach that models nucleation and reaction mechanisms using kinetic and thermodynamic techniques. Nucleation of new phases in a rock is treated using the method of Carlson et al. (1995), modified to account for variations in the local metastable mineral assemblage due to the heterogeneous distribution of minerals. The overall reaction for each domain of local equilibrium is monitored using a differential thermodynamic approach (Spear, 1988) and the local reactions responsible for the growth and dissolution of individual minerals are modeled using a local equilibrium, irreversible thermodynamic approach (Foster, 1999). The end result of the procedure is a simulated thin-section picture showing the calculated rock texture. The method is illustrated using a pelitic bulk composition that crosses garnet, staurolite and aluminum silicate-forming reactions. This type of rock has eight end-member textural permutations among garnet, staurolite and aluminum silicate that are commonly observed in metamorphic terranes. The results of the calculation show that textures of this type are related to the specific P-T-t path the rock experienced.

The simulations also show that variation in the size of domains of local equilibrium can have a profound effect on the processes of nucleation and growth during metamorphism. If the domains of equilibrium are large, nucleation and growth is dominated by a single mineral assemblage composed of all the phases in the rock, a scenario that is typically assumed in many metamorphic studies. Alternatively, if the domains of equilibrium are small, nucleation and growth is dominated by a number of different mineral assemblages, leading to several different nucleation and growth possibilities in the same rock. For example, consider a biotite-chlorite-muscovite pelite crossing the garnet and staurolite isograds. If the size of local equilibrium domains is small, garnet nucleation and growth begins after the garnet isograd is crossed and continues even after the staurolite-forming (garnet-consuming) reaction has begun in the rock, provided that some domains have not equilibrated with previously nucleated staurolite and garnet due to limited transport. Similarly, staurolite nucleation and growth takes place in two domains: one with a metastable garnet assemblage, and one with a metastable garnet-free assemblage where garnet has not yet nucleated. Because domains of local equilibrium typically enlarge near the thermal maximum as T increases and dT/dt decreases, a rock may equilibrate with the expected whole-rock equilibrium assemblage at the maximum temperature, yet much of the mineral growth took place under metastable conditions in domains of local equilibrium.

Carlson WD, Denison C, Ketchum RA, *Geological Journal*, **30**, 207-225, (1995).

Foster, CT, *Canadian Mineralogist*, **37**, 415-429, (1999).

Spear, FS, *Contrib. Mineral. Petrol.*, **99**, 249-256, (1988).

### PCM4 : MOp31 : G5 The Correct use of Shear Bands as Kinematic Indicators

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Shear bands are defined as local shear zones developed in deforming rocks at an angle to the principal foliation (White, 1979). Although their use as shear sense criteria has been questioned and conjugate sets have been described, shear bands are frequently used to derive the direction of non-coaxial flow.

Here, we show that three different, but roughly similar looking structures may form that all may be (mis-)interpreted as shear bands and which may lead to a misinterpretation of shear sense (Passchier in press). They are: (i) Co-rotating counter-shearing zones with a deflection of the host rock inconsistent with the local shear sense (i.e. co-rotating a-type flanking folds). This structure is favored by secondary shear zone with a high angle to the foliation and by flow types with a high non-coaxial component. (ii) Counter-rotating co-shearing zones with a deflection of the host rock inconsistent with the local shear sense (i.e. counter-rotating a-type flanking folds). This structure forms if the secondary shear zone has a low angle to the foliation and if the flow has a high coaxial component. (iii) Counter-rotating co-shearing zones with a deflection of the host rock consistent with the local shear sense (i.e. shear bands). This structure develops if the secondary shear zone has a low angle to the foliation and if the flow has a high non-coaxial component.

We note that the significance of the difference between co-rotating (structure (i)) and counter-rotating structures (structures (ii) and (iii)) for the interpretation of shear sense has been recognized in the past (Grasemann and Stüwe in press), but that the distinction between counter-rotating a-type flanking folds (structure (ii)) and shear bands (structure (iii)) is completely new. While this difference is not critical for the interpretation of the shear sense, it is nevertheless of profound importance: it can be used to quantify the flow type in deformed rocks!

We describe natural examples for all three structures and show that they are kinematically and mechanically consistent with the results of a plane-strain finite element model for the non-coaxial deformation of a non-linear viscous medium.

Grasemann, B & Stüwe, K, *J. Struct. Geol.*, (in press).

Passchier, C W, *J. Struct. Geol.*, (in press).

White, S, *J. Struct. Geol.*, **1**, 333-339, (1979).

## PCM4 Quantitative Modelling of Microstructures

### PCM4 : MOPm32 : G5 Modeling Formation of Mafic Segregations with Felsic Halos as a Solid-State Diffusion Process

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Mafic segregations surrounded by felsic halos, sometimes called "flecks", are common in high-grade metamorphic terrains, and their formation is often attributed to partial melting. Fisher (1970), however, attributed the formation of such flecks in Sweden to solid-state diffusion process triggered by overstepping of a metamorphic reaction. A seven-meter zone of the 1.1 b.y. Baltimore Gneiss near Baltimore, U.S.A., cut by a ~1.5-meter pegmatite, locally contains flecks with striking appearance. These flecks are ellipsoids, <1 cm thick, flattened parallel to the foliation. On foliation planes, each comprises a ~5 cm mafic core surrounded by irregular leucocratic mantle, up to 15 cm in diameter. The matrix, or host rock, is a homogeneous biotite-muscovite-quartz-feldspar gneiss.

Texture and compositions of the minerals vary within these flecks. The core biotite is greenish brown and more Fe-rich than those in the matrix, which are dark brown. Garnets are present only in the core and in the neighboring pegmatite, but they differ in composition and zoning pattern. Feldspars vary in habit, but are nearly uniform in composition. The core minerals are less perfectly oriented than those in matrix, suggesting that the flecks are younger than the foliation.

Assuming that the segregation occurred by diffusion in a closed system, except for volatiles, starting from an initially homogeneous rock with the composition of the present matrix, the Al-conserved reactions were written for each zone of the fleck from textural, modal, and chemical data. The net, fleck-forming reaction derived by using the reactions and observed zone proportions is a breakdown of biotite and muscovite to form garnet and microcline.

Analyses of the phase relations show that once garnet nucleates in the matrix assemblage, activity gradients would develop between the stable core assemblage with garnet and the metastable matrix assemblage. This favors migration of Fe toward the garnet leading to growth of still more garnet, and migration of K from the core to the mantle to form microcline. The observed migration of Mg is up its chemical potential gradient, and may have been driven by the cross coefficient coupled to that of Fe. The segregation is explained as a diffusional process driven by the gradients between two mineral assemblages which were not in equilibrium with each other. The garnet nucleation could have been related to the emplacement of the neighboring, garnet-bearing, discordant pegmatite. The coexistence of Fe-rich biotite with garnet in the core suggests that the fleck formation may have involved addition of Fe and/or loss of Mg. A possible cause of the garnet nucleation, therefore, is an influx of fluid from the pegmatite which was not in equilibrium with the matrix.

Fisher GW, *Contrib. Mineral. Petrol.*, **29**, 91-103, (1970).

### PCM4 : MOPm33 : G5 Microstructural Analysis of Mass-Flow Textures in High Grade Igneimbrites: The Example of Nuraxi Tuff

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Nuraxi tuff is a Miocene densely welded rhyolitic ignimbrite from Sulcis volcanic area (SW Sardinia, Italy) characterized by a prominent parataxitic fabric and flow-banding foliation throughout most of its thickness. The vitrophyric, 1-2 m thick, basal zone of the tuff is characterized by the presence of several flow structures such as imbricated lithics and fiamme, rotated crystals, parallel stria imprinted on parting planes, variably elongated vesicles with internal curved structures. The flow structures are arranged in a regular vertical pattern visible at various localities. A detailed study of preferred orientation of crystals, type and geometry of rotating structures, vesicle shapes and microfolds was undertaken through image analysis of a sequence of oriented thin sections of the basal

vitrophyric zone taken at different stratigraphic levels and in areas where a secondary, gravity-driven laminar flow (rheomorphism) couldn't affect the deposit.

Results allowed the reconstruction of the strain fabric, calculation of the minimum lateral displacement and the vertical shear strain profile. The ratio of pure vs. simple shear strain components in the deformation fabric was calculated in order to define deformation mechanisms of hot particles and the relative amount of load compaction, generally assumed as the main process which determines welding of pyroclastic deposits. Field data and microscopic observations were used to discuss the relationships between primary flow and welding in Nuraxi ignimbrite and its implications on transport and depositional mechanisms in high temperature pyroclastic flows.

### PCM4 : MOPm34 : G5 The Rounding Kinetics of Olivine in Fe, Fe-S

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Pallasite meteorites are mainly composed of olivine and metal. Olivine crystals in pallasites may be macroscopically rounded (type "R") or macroscopically angular (type "A"). Studying the rounding kinetics of olivine provides constraints on the genesis and thermal history of pallasites: was it possible to get "R" type from "A" type in a time compatible with the cooling history of the pallasites parent bodies?

Two different processes may account for the rounding of olivine in pallasites: bulk diffusion in olivine or diffusion at the olivine surface. Both processes result in a reduction of the whole interfacial energy. In the case of surface diffusion, we performed a numerical model for which the matter flux along the interface is proportional to the gradient of curvature (assuming an isotropic interfacial energy), following a model by Saiki (1997). This model gives the evolution of the crystal shape with time: the appearance of "rolls" on the surface near highly curved zones may be a discriminative feature compared to bulk diffusion process. The kinetics of rounding depends on the initial shape; for the borderline case of an initial corner, the inward advance of the crystal surface is proportional to the time to a power approaching 1/4. For the bulk diffusion process, a greater exponent is expected.

In parallel, experimental rounding of a single olivine crystal (cut in cubic shape in order to start from a well-known initial geometry), surrounded by solid or liquid Fe or Fe-S, is performed in piston-cylinder apparatus. The rounding kinetics is highly dependent on temperature. The experimental results serve to calibrate the numerical model, which in turn can be used as a quantitative predictive model.

Saiki K, *Geophysical Research Letters*, **24**, 1519-1522, (1997).

