# Abstracts

# Shear-migration coupling of grain boundaries in metals: an alternative plastic deformation process

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Nanocrystalline metals ($d \leq 100$ nm) possess a much greater resistance to plastic deformation than those with conventional grain size. One of the specificities of these nanocrystals is that they contain a large proportion of grain boundaries (GBs) but virtually no dislocations. Plastic deformation is then thought to occur using alternative paths. Several experiments have shown that in these small-grain materials, the plastic deformation is carried out predominantly by grain boundaries. The dominant mechanism is the so-called shear-migration coupling. Despite a recent increase in simulations studies, its experimental characterization remains very scarce. Aside from experimental obstacles, the problem is very vast as real grain boundaries possess at least 5 degrees of freedom and contains a potentially infinite number of disconnections, a specific defect that combines a step and dislocation character.
Both in-situ TEM experiments and molecular dynamic simulations using the NEB technique (Nudge Elastic Band) concluded that shear-migration coupling involves the displacement of these disconnections whose origin will be discussed. As dislocations in the crystal, the properties of these disconnections seem to guide the coupling mechanism of migrating grain boundaries. The questions that will finally be addressed here is to whether we should still consider a given GB as a crystalline defect or a network of its own, which mechanical properties (mobility, shear coupling) are governed by its nature or by its defects.

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*Speaker

# High-resolution 3D synchrotron X-rays methods for full field in-situ recrystallization studies

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After 20-years development, the current generation synchrotron techniques, such as 3D X-ray Laue microdiffraction using differential aperture and diffraction contrast tomography, are powerful techniques for measurement of the crystallographic orientations, morphologies and local lattice strains of grains within bulk samples in full 3D. However, it is still challenging to study recrystallization of deformed metals with these techniques. In this presentation, several well-designed experiments performed using these techniques to study the recrystallization, including nucleation at hardness indents, growth of several nuclei into a well-characterized deformation matrix, and strain distribution within recrystallized grains will be presented. It is shown that with high-resolution ($\sim$1 $\mu$m) mapping of both the deformation matrix and the recrystallized grains, the local heterogeneous nucleation and growth of recrystallized grains can be correlated to the local deformation microstructure. Key results are presented and it is discussed how the new results may be incorporated in next generation recrystallization models.

*Speaker

# Dislocation-driven static recrystallization in AZ31B magnesium alloy imaged by quasi-in-situ EBSD experiments

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We performed a series of quasi-in-situ annealing experiments in an SEM-EBSD system to characterize the effect of the deformation microstructure on the first stages of static recrystallization. Six samples of AZ31B magnesium alloy were deformed at different combinations of temperature and strain rates to produce microstructures with variable dislocation densities and arrangements and then heated at 300 °C ($T_h \sim 0.64$) for up to 6 h using similar time steps. All samples recrystallized by the growth of substructure-free grains largely inherited from the deformed state. This process is fast (minutes to hours), stops before full recrystallization, and is driven by local differences in the stored dislocation energy under the tested experimental conditions. We observe a positive correlation between the initial average kernel average misorientation (KAM) and the recrystallization kinetics of each sample and, to a lesser extent, the recrystallization fraction attained at a given time. We also present direct evidence for local control of the dislocation density on the migration kinetics by quantifying the misorientation gradients in the vicinity of the migrating grain boundary. Yet, our data suggest that the reduction in the dislocation energy alone cannot explain the stagnation of the recrystallization front before full recrystallization.

*Speaker

# Deformation of polycrystalline forsterite at 900-1200 °C and grain boundary activity

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To further constrain the plasticity of rocks in the uppermost lithospheric mantle, deformation experiments were carried out on forsterite aggregates using a gas-medium apparatus (Paterson press) at 300 MPa, 900-1200 °C and nearly constant strain rates of $\sim 10^{-5}$ $s^{-1}$. The starting material is a synthetic iron-free forsterite aggregate with an average grain size of $\sim$ 2.8 $\mu$m and ∼2–3 % of iron-free enstatite. Eight deformation experiments were performed as well as an additional static annealing to characterize grain growth. The maximum stresses obtained range from ∼480 to 1870 MPa. Below 1000 °C, where stress significantly exceeds confining pressure, and based on microstructural observations, grain boundary mediated creep is observed, with evidences of sliding and cavitation (gaping) at grain boundaries. At 1050–1200 °C, where pseudo-steady state could be achieved, the microstructures are very different and show evidences of dislocation activity, resulting from the activation of several dislocation slip systems with increasing temperature. When compared to rheology laws previously obtained from similar experiments, the temperature dependence of iron-free olivine creep is similar to the one of its iron-bearing counterpart at high temperature (∼1200 °C); at temperatures ≤1000 °C, however, the strength of iron-free olivine is higher than for iron-bearing olivine. The deformation-induced textures obtained show that grain boundary sliding (GBS) was accommodated by cavitation, which was likely activated in response to large differential stresses, i.e., beyond the Goetze criterion. Given these high-stress conditions, our results cannot be directly applied to deformation of the Earth's mantle at large scale. Nevertheless, they highlight the key role played by the grain-boundary network in accommodating strain at lithospheric temperatures (< 1100 °C), when crystal-plastic mechanisms remain inefficient.

*Speaker

# On-Axis Transmission Kikuchi Diffraction on the SEM. Performances and Applications

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TKD is a very recent technique of orientation mapping in the SEM. In 2012, Keller [1] tried to do EBSD on a thin electron transparent specimen. They got a Kikuchi pattern that could be indexed from a 10 nanometers sized crystal. A new technique was invented: TKD which stands for Transmission Kikuchi Diffraction. The main advantage is a lateral resolution divided by 10 in comparison with the EBSD. In 2016, a new configuration for the TKD, in which the detector is in a horizontal position instead of a vertical position, has been proposed and validated by our team [2]. It is called on-axis TKD because it is symmetrical with respect to the microscope axis. It allows to acquire orientation maps about twenty times faster than the usual TKD. Using a cross correlation software the angular resolution can be as good as 0.01°. The performances of TKD in terms of lateral spatial resolution is about few nanometers. The depth resolution is about few tens of nanometers with a linear dependence with the electron energy and the atomic number Z.
TKD, which has both good lateral and depth resolutions, is the most suitable technique to investigate nanomaterials. It is the first field of application. Many examples will be shown and analyzed, including strongly plastically deformed materials with the calculation of the geometrically necessary dislocation (GND) density. For the other field of application: the electron damage sensitive materials for which it is necessary to use low dose electron beam, the example of bio mineral calcite will be given.

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*Speaker

# Full field modeling of recrystallization in polycrystalline nickel base superalloys

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Full field numerical methods have been developed over the last decades with the aim to simulate explicitly microstructural evolution [1-3] and then to propose enhanced mean-field models [4,5]. The idea behind these "mesoscale" simulations is that the morphology and the topology of the grain boundary (GB) network play an essential role in microstructure evolution. In these approaches, simulations are performed on Representative Volume Elements (RVEs) where the microstructural features are explicitly represented. Boundary conditions applied to the RVE can be representative of what suffered a material point at the macroscopic scale (thermal or thermomechanical cycle). In this context, the state of the art of the used full field simulations dedicated to recrystallization suitable for nickel base superalloys will be detailed and a particular focus on recent results obtained with the level-set (LS) method will be done.

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†Speaker

# Optimized manufacture of nuclear fuel cladding tubes by numerical modeling of processes and microstructure evolution analysis

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Within the manufacturing route of Zirconium alloy cladding tubes, each process can have an influence on the chemistry, microstructure and properties of the intermediate and final products. An overall vision of the manufacturing processes is then necessary for a global optimization of the manufacturing route. The strong relationship between processes is illustrated by the evolution of chemical composition during VAR melting, its influence on the microstructure evolution during quenching and hot extrusion, and the potential effect of microstructure on ductile damage during cold pilgering. Together with the characterization of intermediate products, the numerical modeling of each manufacturing step is used for the optimization of the products quality through the mastering of the main process parameters.
Numerical modeling of VAR process on SOLAR software is able to assess the chemical composition of the ingot, including the impurities such as chlorine, as a function of the melting parameters. The quenched microstructure, which consists of alpha needles arranged in parallel plate or basket weave microstructures, is highly dependent on the chlorine content and is thus linked to the melting parameters. The evolution of this microstructure during hot extrusion will depend on the initial microstructure (parallel plate or basket weave) and the extrusion parameters, which can be assessed by the numerical modeling of extrusion on FORGE software coupled with a dynamic continuous recrystallization model. In the case of a low recrystallization ratio, the ductility of the alloy can be reduced and it is therefore necessary to optimize the cold-pilgering parameters in order to avoid ductile damage of the tubes. Finite element analysis of the cold pilgering process, including ductile damage models, was developed for this purpose on FORGE software and is used to optimize the rolling parameters.

*Speaker

# Texture formation during hot rolling of ferritic stainless steel

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Formability of ferritic stainless steel thin sheets is strongly affected by the crystallographic texture resulting for the production process (hot rolling, annealing, cold rolling, annealing). The final product texture can be optimized intensifying the (1 1 1) fiber which improves deep drawing performance but also limits ridging (heterogeneous plastic deformation leading to ridges along the rolling direction). Due to the absence of phase transformation during the overall process, final texture is strongly inherited from the hot rolling texture. The present study aims at better understanding how crystallographic texture is progressively built during hot rolling, especially trying to identify the origin of the strong $(h\,k\,l)\langle 1\,1\,0\rangle$ fiber observed in industrial hot rolled coils (and known to promote ridging) instead of the (1 1 1) fiber supposed stable in plane strain compression. Single pass hot rolling trials followed by quenching have been performed in laboratory at different temperature and strain level. Deformed microstructures and textures have been quantitatively characterized by EBSD. Hot rolled samples have been annealed to study static recrystallization mechanisms and the resulting texture. A model of abnormal subgrain growth has been used to explain the orientation selection occurring during new grain nucleation, the critical step defining the final texture. A reasonable scenario describing texture evolution during the succession of deformation passes and inter-pass times of the roughing mill schedule is proposed coupling deformation texture calculations with a crystalline plasticity model (GF-VPSC) and recrystallization texture calculations based on abnormal subgrain growth.

*Speaker

# A new lagrangian strategy for the simulation of boundary migration applied to microstructure evolutions

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The Level-set (LS) method [1] is used to model dynamic interfaces in the context of large deformations and topology changes. This approach is classicaly used in simulations of microstructure evolutions [2] using a Finite Element (FE) framework where the interfaces are implicitly defined and captured by refined meshes. This process can be very costly in terms of CPU-time and the presence of vacuum regions is unavoidable. A new model to simulate these microstructure evolutions using a completly Lagrangian mouvement of the interfaces will be presented.
The new model consist of two steps : the pre-procesing and the evolution computation. In the first step, Interfaces given by an initial LS field are discretized by means of local remeshing operations [3] producing a body-fitted mesh free of vacuum regions, then, an identication and reconstruction algorithm tags and classifies every node of the mesh in relation to the topologic entity that it represents (3D volume, 2D boundary, 1D boundary or multiple point).
In the second step, for each increment, local variables such as the curvature $\mathbf{k}$ and normal $\mathbf{n}$ to the interface are computed only for the nodes belonging to the boundaries, the velocity $\mathbf{v}$ is then defined in function of these local variables and other field data depending on the evolution mechanisms considered [2]. This velocity is locally applied to the nodes of the interfaces after a flipping check on every element belonging to the local mesh patch, discarding every movement that produces a flip. Finally special local remeshing operations are made. These operations are oriented to maintain the quality and to solve the previous discarded movements of the mesh without compromising the boundary topology already defined allowing to solve the next time increment.
Results for this new Lagrangian model will be presented and compared to more classical approaches based on the solution of a convective-diffusive partial differential equations (PDEs) of the LS fields. It will be illustrated that this new method is very accurate and enables to simulate efficiently massive multiphase problems. To the authors knowledge, no other FE model in the literature reports similar capabilities.

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*Speaker

# A new level set-finite element formulation for anisotropic grain boundary migration

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Grain growth in metallic materials causes coarsening of the microstructure which greatly impacts the mechanical properties of components. Therefore, predicting the evolution of microstructures undergoing grain growth is crucial to controlling the microstructure and, by association, the properties of formed metal parts. However, the "microstructure" is potentially a rich data set comprised of hundreds of thousands of grains with their own crystallographic orientations and potentially different phases. Thus, the intricacy of the description of this mesoscale in a given model will ultimately define the complexity one will have to deal with. For example, looking to predict the grain growth of a monophase microstructure submitted to a heat treatment it becomes necessary to give an explicit description of the grain boundary. The grain boundary at the mesoscopic scale can be characterized by 5 intrinsic parameters [1], three related to its misorientation M and two related to its inclination n. This parameterization of the grain boundary space must be taken into account if one wishes to reliably predict the behavior of individual grain boundaries during heat treatments (twin boundaries for example). The internal structure of the grain boundary renders the energy densities of these boundaries "anisotropic", in the sense that the energy density varies differently in different directions. The presence of these variations in the energetic density of the boundaries generates supplemental terms in the equations for grain boundary movement [2]. This work aims to formulate, develop and implement a grain growth simulation framework that can take into account the full anisotropy of grain boundary energy density using a level-set (LS) description of the microstructure and a finite element (FE) resolution of the physical problem. An analytical benchmark for verifying the inclination anisotropy is developed so as to test the formulation. The model is also tested using classical "Grim Reaper" test cases for triple junctions. The response of the numerical model on generated polycrystals is then evaluated. To the authors' knowledge, no other model in the literature has demonstrated its capability of taking into account fully anisotropic energy densities in a polycrystal setting.

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*Speaker

# Modeling and simulation of recrystallization and grain growth

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A range of alternative numerical approaches is available for simulation of recrystallization and grain growth. The talk will provide some examples of different modeling strategies and their applicability to different microstructure phenomena. In particular, issues related to the assumptions and simplifications that are inevitable in numerical modeling of physical processes, such as recrystallization and grain growth, will be emphasized. The intent is to inspire a critical mindset in the adoption and implementation of numerical models and in the judgement of the results obtained using such models.

*Speaker

# Material parameters identification in the context of full field modelling of grain growth and recrystallization

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Industrial processes improvement for the obtention of metallic materials with high-end mechanical properties and/or satisfying finishing surfaces mainly relies nowadays on an accurate understanding of microstructure evolutions throughout complex thermomechanical paths. As systematic experimental observations at each step of the process can rarely be performed due to time constraints, the modelling of the different mechanisms occurring at the mesoscopic scale is of interest since several decades now.
At first, mainly based on experimentally-driven analytical expressions (Burke & Turnbull law for grain growth [1]; JMAK relation for recrystallization kinetics [2-4]), models describing microstructure evolutions have evolved toward a more precise description of the microscale. With respectively implicit and explicit representation of the microstructures, mean field and full field modelling are getting of prime importance to have a better insight of microstructure evolutions under varying thermomechanical conditions.
These models are based on phenomenological and physics-based equations used to describe the microscale mechanisms. Inside these equations, several material-dependent parameters need to be identified in order to be able to accurately predict the microstructural evolutions of a given material. Similarly to what is done with material parameters identification for rheological laws, an experimental dataset is used to refine models' parameters on a considered range of application in terms of temperature and strain rate.
An identification procedure for an existing grain growth and dynamic recrystallization full field modelling framework [5] will be presented and discussed regarding some key aspects: sensitivity of the identified material parameters to both experimental dispersion and/or analysis parameters, statistical repeatability of the procedure and also the range of validity of the identified parameters. The optimisation and automatisation of the procedure will also be detailed.
The overall modelling framework, from experimental data through identification to simulation, that will be presented is expected to provide a precise following of the microstructural evolutions and to complement experimental observations toward a better understanding of the underlying mechanisms occurring at the mesoscopic scale during forming processes of metallic materials.

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*Speaker

# A semi-topological approach for mean-field models of dynamic and metadynamic recrystallization

David Piot *

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La présente communication présente une partie de la thèse de Smagghe (2017). Elle se concentre sur le développement d'une approche originale semi-topologique pour la modélisation en champs moyens des recristallisations dynamique et métadynamique. Cette démarche générique, qui permet d'utiliser des modèles en champs moyens, chaînés entre eux dans les cas multipasses, pour une prévision précise des distributions de la taille des grains, est illustrée dans le cas particulier du forgeage libre de l'acier inoxydable austénitique AISI 304L pour de grosses pièces de chaudronnerie nucléaire.

*Speaker

# Grain growth based on Orientated Tessellation Updating Method

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This work is part of a more general idea consisting in developing a macroscopic model of grain growth whose state variables contain for each material point the statistical descriptors of the microstructure (e.g., disorientation, grain size and shape distributions). The strategy is to determine macroscopic free energy and dissipation potentials on the basis of a large number of computations at the scale of the polycrystal. The aim is to determine enriched macroscopic evolution laws. In order to test this upscaling strategy it is necessary to establish a simulation tool at the scale of the polycrystal. It should be sufficiently simple and fast to enable a large number of simulations of various microstructures, even if it leads to neglect some phenomena occurring at this scale. A fast approach based on Orientated Tessellation Updating Method (i.e., grain growth is obtained through an evolution law directly written on the weights of a Laguerre-Voronoi tessellation) has been proposed recently. The energy per unit surface associated to crystal disorientation at each grain boundary enables to calculate the driving force. In addition, the dissipated power associated to any virtual motion of the grain boundaries enables to obtain the evolution law. However, this approach did not consider proper boundary conditions with crystal desorientation at the boundary of the tessellation, which is limiting if the tessellation is a representive volume element. In this contribution, this difficulty is overcome and proper RVE can be simulated with boundary conditions and mass conservation.

*Speaker

# Dynamic recovery and recrystallization at large strains in aluminium and titanium alloys: experiments and models

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Titanium alloys are materials used in many industrial applications due to their high specific strength and corrosion resistance. The alloys are usually formed by means of forging and rolling. In this lecture I will show some basics on titanium alloys: allotropy, behaviour under thermal and thermomechanical loads, microstructural evolution and mechanical properties. I will present some experimetal results obtained out of compression, torsion and dilatometric tests, as well as the relevant microstructural features obtained from microscopy. We will discuss the dynamic and static recovery, recrystallization and phase transformation ocurring during hot deformation and heat treatments, respectively. Finally, I will show some developed mesoscale models used to describe these phenomena using dislocation densities, crystal misorientation distributions, grain and subgrain sizes as internal variables.

*Speaker

# Microstructure evolution during multiaxial processing of Ti-6Al-4V

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Subtransus multiaxial hot forging of $\alpha + \beta$ Ti-6Al-4V titanium alloy with a $\beta$-transformed microstructure aims at obtaining an equiaxed microstructure through $\alpha$ phase globularization. Microstructure evolution related to this process depends on parameters such as temperature, strain and strain rate, which vary with time and space in industry, and holding times1. Strain localization can occur in the form of shear bands, as a function of alpha lamellae initial orientation2. Other phenomena such as continuous dynamic recrystallization are observed3. As a result, multiaxial processing of titanium alloys leads to significant microstructural gradients. In this study we focused on the effect of time-space variations of the parameters on globularization kinetics and development of such gradients.
Thanks to the MaxStrain Gleeble device we were able to reproduce complex thermomechanical treatments to $\beta$-transformed Ti-6Al-4V samples. Stress and strain fields obtained with finite element modelling of the MaxStrain test were compared to experimental microstructure. This experimental method offers the opportunity to get closer to industrial open die forging conditions, and to study microstructural evolution of Ti-6Al-4V in such conditions.

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*Speaker

# Texture evolution during dynamic recrystallization in olivine-rich rocks

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Understanding how dynamic recrystallization (DRX) modifies the texture and microstructure of polycrystalline aggregates during plastic deformation is key for predicting the effect of DRX on the polycrystal strength. We characterize the evolution of the texture and microstructure during DRX in three natural olivine-rich rocks deformed in axial extension at a temperature of 1473 K and confining pressure of 300 MPa by electron backscatter diffraction (EBSD). The similarity in morphology between subgrain cells in the porphyroclasts and recrystallized grains and the orientation relations between porphyroclasts and recrystallized grains imply that the new grain boundaries developed by progressive subgrain rotation or continuous DRX (CDRX). This process produces a dispersion of the texture. However, the change in orientation between parent, sub-structured relic, and recrystallized grains is more complex than a gradual increase in misorientation with increasing distance to the centre of the parent grain (consecutive necklace model). Some sub-structured relic and recrystallized grains display high misorientation (up to 90°) relative to the parent grain independent of their distance to it. Recrystallized grains have dominantly olivine [1 0 1] axes aligned with the extension direction and on average higher Schmid factors for the "easy" [1 0 0](0 1 0) slip system than the parent grains. We use the EBSD data to assess the slip systems contributing to the development of both low and high- angle grain boundaries and the associated changes in texture and to explore how high-angle misorientations between adjacent parent and DRX grains may be produced during by CDRX, in absence of major grain boundary sliding or migration.

*Speaker

# Xenolith Constraints on Rheology of Heterogeneous Deep Crust Beneath the Eastern Mojave Desert, California

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Lower crustal xenoliths from a Tertiary dike in the Eastern Mojave Desert, California are lithologically heterogeneous. They broadly reflect igneous and sedimentary protoliths, but two features stand out: 1) high proportion of metapelites compared to typical lower crustal xenolith suites; 2) abundant modal garnet. Previous work by Hanchar et al. (1994) interpreted garnet-rich metasedimentary xenoliths as residues of deep crustal melting. Here, we use electron backscatter diffraction (EBSD) large area mapping to investigate rheology of three major compositional categories represented in the metasedimentary suite: quartzose, quartzofeldspathic, and aluminous. We focus on the modally abundant rheology-controlling minerals quartz and plagioclase. Quartz microstructures in quartzose xenoliths are consistent with dynamic recrystallization (DRX) via grain boundary migration and subgrain rotation (SGR). In quartzofeldspathic and aluminous compositions, quartz grains display sparse interconnected bands, but isolated grains are common. Using quartz pole figure data, we find crystallographic preferred orientations (CPOs) consistent with operation of $\{m\}\langle c\rangle$ and $\{m\}\langle a\rangle$ slip systems and less commonly, $\{c\}\langle a\rangle$ and $\{r\}\langle a\rangle$ slip systems. Plagioclase microstructures are characterized by grains with deformation twinning, as well as by dynamic recrystallization via SGR. Plagioclase pole figures exhibit CPO consistent with the $[0\,0\,1](0\,1\,0)$ and $[1\,1\,2](1\,1\,\bar{1})$ slip systems. Our data lead to several findings with respect to strain accommodation between rock compositions, and thus have implications for bulk rheology of heterogeneous crust. First, quartz in quartzose xenoliths accommodates more deformation than quartz in other xenolith types, suggesting phase topology as a first-order control on deformation amongst diverse lower crustal compositions. Second, some samples have quartz and plagioclase CPOs consistent with dislocation creep; however limited interconnectedness and interstitial nature of the phases appear incompatible with crystal-plastic deformation. Instead, we propose CPO could develop from shape-preferred orientation induced through partial melting. Our results provide insight into contributions of various rock compositions in lower crustal strain localization and melt.

*Speaker

# Deformation of oceanic crust at slow-spreading ridges: microstructures in gabbros from the SouthWest Indian ridge (IODP Hole U1473A)

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We identify and quantify ductile deformation processes in oceanic gabbros from the slow-spreading SouthWest Indian Ridge (SWIR). The crustal architecture of slow-spread ocean crust results from complex interactions between magmatism, hydrothermalism and tectonics. The 800m deep IODP Hole U1473A was drilled at the summit of the Atlantis Bank, a submarine massif of gabbros at the SWIR, during IODP expedition 360. We describe deformed zones using petrographic observations made on 127 samples along the core. Ductile deformation is common, and is generally strongly localized. The deformation initiated during accretion under magmatic conditions, and continued until late brittle conditions. Gabbros show variably foliated magmatic microstructures (sub-ophitic and granular). Porphyroclastic microstructures demonstrate that post-magmatic, solid-state, high-temperature deformation occurred. Pyroxene clasts are generally partially recrystallized at their edge, while olivine clasts show evidences of recovery. Plagioclase represents ∼50% of the mineralogical assemblage, and plays a major role in the accommodation of high-temperature deformation in gabbros. It shows a strong recrystallization, often complete and forming a fine-grained matrix. Deformation is often localized, expressed by mylonitic and ultramylonitic zones, some being overprinted by deformation at decreasing temperatures. Electron Backscatted diffraction (EBSD) data in the plastically deformed gabbros points to weak to moderate textures or crystallographic preferred orientations (CPO), dominated by the early magmatic flow. The latter has developed a classic magmatic fabric with the foliation defined by (010) and the lineation by [100]. This type of CPO is persistent during plastic deformation, and observed in all samples. The misorientation related to plastic deformation in plagioclase grains is consistent with a (010)[001] principal slip system, which is inconsistent with the CPO described above (it should produce a lineation defined by [001] if starting from a random orientation). The strength of CPO tends to decrease from moderately deformed samples to highly deformed ones (mylonites and ultramylonites), which could be explained by the overprint of plastic deformation and recrystallization.

*Speaker

# Grain growth in polycrystals - 3D experimental observation and phase field modeling

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We report on a combined experimental observation and concomitant phase field simulation of 3D grain growth in pure iron. An ensemble of initially 1500 grains has been followed over 15 time steps of annealing at 800 C by means of X-ray diffraction contrast tomography. A statistical analysis of the evolution of the grain microstructure [1] showed that the growth of the average grain size is somewhat consistent with classical isotropic grain growth models, while the growth rates of individual grains are not consistent with these models.
Using a classical phase field model [2], the reduced mobilities for a large number of grain boundaries have been fitted [3]. Apart from a small fraction of low angle boundaries, the data do not indicate a clear correlation between the reduced grain boundary mobility and the five macroscopic degrees of freedom. The reduced mobilities are observed to vary with time and there is experimental evidence that topological transitions in the grain boundary network can lead to sudden jumps in the mobility. The observations indicate that the grain growth behavior for the large majority of boundaries seems to be governed by mechanisms other than those underlying the classical models of grain growth [4].

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*Speaker

# Misorientation dependence of the grain boundary migration rate: role of elastic anisotropy

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In addition to temperature, pressure and impurity concentration, it is known that the velocity of a grain boundary also strongly depends on its macroscopic degrees of freedom, i.e. the inclination of the boundary plane and the crystallographic misorientation. The understanding of this crystallographic dependency is of crucial importance as it affects the development of recrystallization textures. In FCC metals and particularly in Al, overwhelming data of GB migration rates are available from growth selection and bicrystals experiments. Both kind of experiments show that the misorientation of the fastest moving boundaries correspond to a rotation around a $\langle 1\,1\,1\rangle$ axis with an angle close to 40°.

When a grain boundary starts moving, the stress field seen by a specific dislocation changes immediately because the distance from the interface is modified. Indeed, a grain boundary possesses an intrinsic stress field, whereas the dislocation stress field depends also on the boundary position. Because of elastic anisotropy, polycrystals have actually heterogeneous elastic moduli and image stresses are appended to the dislocation self-stress field in order to satisfy the boundary conditions at interfaces. Such image forces can repel or attract dislocations towards the grain boundary and may have significant influence on dislocations self-organization near interfaces in the absence of externally applied stress. More importantly is the fact that the elastic energy of dislocations depends on the distance to the grain boundary since migration is driven by a reduction of the stored energy. In classical theories, migration leads to an elastic energy reduction due to the decrease of the total dislocation density as the grain with the highest dislocation density is consumed. However, is seems sound to assume that the elastic energy reduction should be effective throughout the whole migration process, even on small distances where the dislocation density on both sides remains unchanged.

In this work, numerical computations of image forces and stored energy during the growth of a strain free grain within a recovered matrix containing a dislocation array are performed based on a the Leknitskii-Eshelby-Stroh (LES) analytical formalism (or sextic equation formalism). Considering the migration of a planar grain boundary towards an initially equilibrated dislocation array, a decrease of the stored energy is observed when image forces are attractive and an increase when image forces are repulsive. For a finite array of 20 edge dislocations in Al at 600 K and a grain boundary motion over ∼100 atomic spacing, the magnitude of the energy variation is of the order of one dislocation line energy, which is significant although the Zener anisotropy ratio of Al is quite low with $A = 1.24$. The elastic energy variation will indeed increase with the elastic anisotropy of the material, the number of dislocations and the migration distance. Finally, by sweeping the whole orientation space for FCC crystals, it is also shown that grain boundaries close to a $\langle 1\,1\,1\rangle$ 40° misorientation are among those that display the highest attractive forces on edge dislocations, which makes a direct link with the reported experimental observations.

*Speaker

# Using second-order bounds to parametrize the anisotropic elastic tensor of snow, firn and ice microstructures

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The continuous "recrystallization" of highly anisotropic crystals in the snowpack under metamorphism influences the mechanical properties of snow. Experimental estimation of the elastic properties of snow is difficult, and hence parameterizations are required for various applications. To this end, we employ second-order bounds and FE-simulations to derive a parametrization of the effective, anisotropic elastic tensor of snow. The characterization of the microstructural anisotropy requires a geometrical fabric tensor, which is computed from the two-point correlation function. We evaluated a wide variety of snow samples from seasonal to polar snow for relative densities from 0.07 to 1, which showed a good correlation between numerical computations and effective medium theories. The comparison of the results with previous work on the elastic tensor of snow based on fabric tensors also shows a good agreement. In particular, for temperature gradient metamorphism samples, a definite improvement in the coefficient of determination is obtained when anisotropy is included in the parameterization in addition to density.

*Speaker

# Accounting for elastic anisotropy in crystal plasticity within the context of olivine dynamic recrystallization using a level-set framework

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Because olivine is the major constituent of upper mantle rocks, its mechanical properties and microstructural evolutions play an important role in the lithosphere rheology. In this study, we investigate the deformation of olivine polycrystals and the underlying dynamic recrystallization through full field modeling. Our numerical finite element framework is based on the level-set approach for the polycrystal description and the modeling of grain boundary migration, including capillarity and stored energy driven pressures and new grain nucleation. The rheology of the olivine aggregate is described through a crystal plasticity model that we have developed and that takes into account the elastic anisotropy of the olivine crystal, based on published experimental data. In addition to predicting grain size evolutions, this methodology also allows to track the development of lattice preferred orientation (LPO) during deformation. These important features are predicted using the proposed approach during the deformation of olivine aggregate (see figure) with and without accounting for elastic anisotropy. Ultimately, this kind of models could be used to infer mean field rheological laws for large-scale geodynamic models.

*Speaker