ESF -EUROCORES

Mineral SubStructure Dynamics

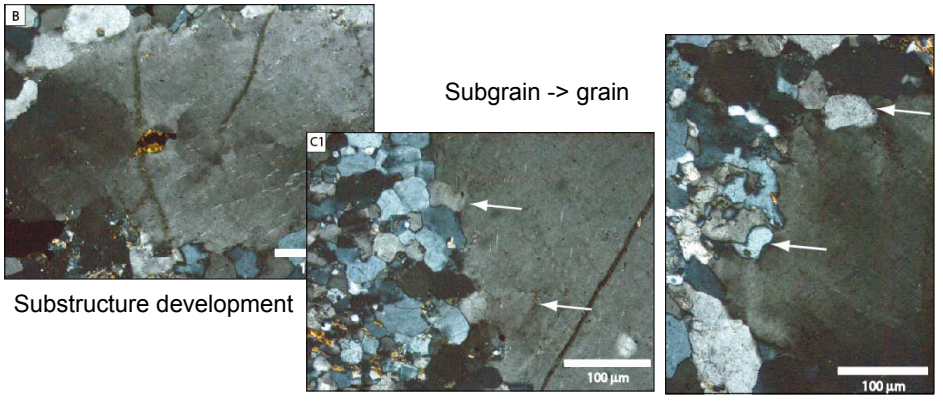
Subgrain structure development in rocks and metals

Subdynamics.geo.su.se

6 PIs (Piazolo, Prior, Urai, Jessell, Cordier, Bons)
Borthwick, Tatham, Schmatz, Griera, ,Becker
4 AP (Drury, Spiers, Juul Jensen, Köhn)
Valcke, Pennock,

Main technique: Coupling/Comparison of
In-situ & classical Experiments – Multi–scale Numerical Simulations

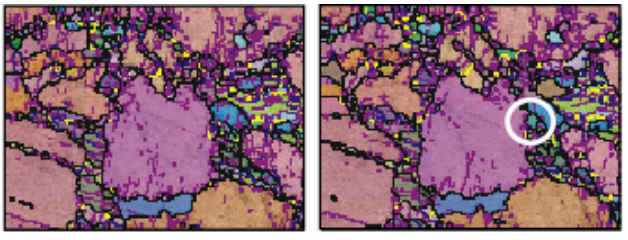
Education:
Bringing modellers and experimentalist closer
(exchanges, workshops etc.)



Substructure development

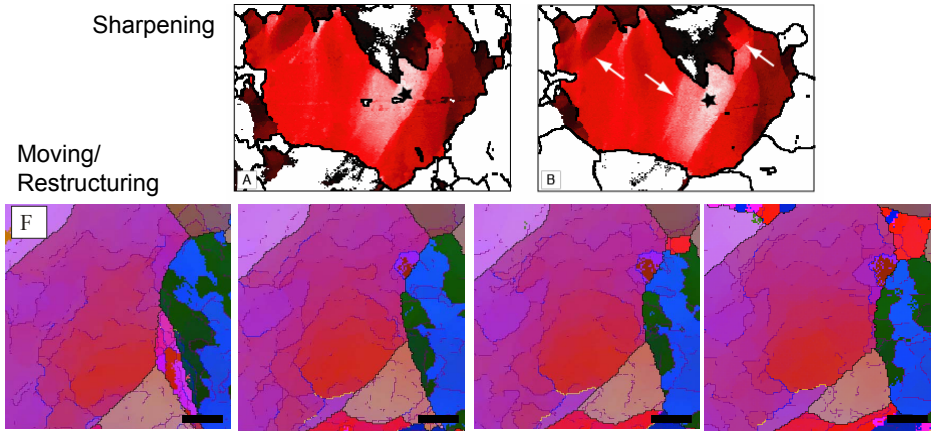
Subgrain -> grain

New grain
Nucleation

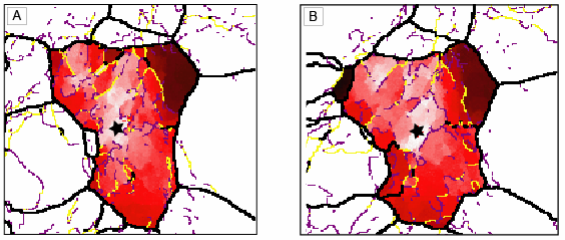


Sharpening

Moving/
Restructuring



Moving/
Restructuring
coupled with
GBM



SubStructure Dynamics

- How do new (sub-) grains nucleate and evolve?
- What are the properties and behaviour of subgrain boundaries?
- How do processes at different scales interact, from dislocations to whole grains?

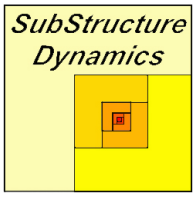
Nucleation and interal structure of (sub-)grains (during and after deformation & phase transformation):

Questions:

- How are they defined?
- Are there different types (with different properties)?
- What is their internal structure and what significance does this have?
- Where exactly do they originate?
- Spatial and temporal distribution?
- What properties do they have?
- How do these properties influence material properties?
- Prediction of nucleation and coupled properties

Answers:

- Through experiments – observations
- Multi-scale numerical simulations (disloc-> grain)

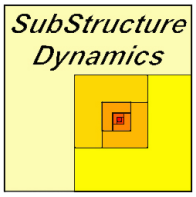


Behaviour of subgrain boundaries during / after deformation & phase transformation

Questions:

- How are subgrain boundaries to be defined?
- Which type of dislocations form which subgrain boundaries?
- Physical properties of subgrain boundaries (surface energy/activation energy)
- How do they evolve with time – within grain?
- Evolution subgrain boundaries with relation to GBM/grain boundaries?
- Prediction of subgrain boundary behaviour

Answers:
Through experiments – observations
Multi-scale numerical simulations (disloc-> grain)

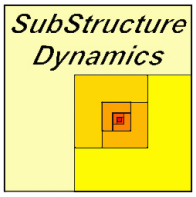


Numerical Prediction of substructure dynamics

Questions:

- How can substructures be predicted?
- What are relevant parameters to test numerical results against experimental results? How can we assess the validity of numerical results
- How do we solve the multi-scale problem – discrete, continuum, statistical
- How do we make sure that competing processes are accounted for?

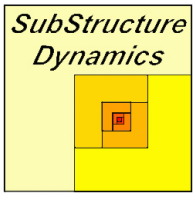
Answers:
Set up of rigorous testing schemes
Multi-scale numerical simulations using hybrid models, statistical methods etc.



Need to:
- Integrate different numerical codes
- Conduct in-situ and classical experiments
- Numerical modelling of physical experiments
- Compare results
- Refine theory used for numerical simulations

Experimental techniques:
In situ experiments 2D
a) in SEM: static & dynamic (Liv, St)
b) See-through: dynamic with fluid films (Aach)
In situ experiments 3D
3DXRD: static (Risö, St,Tüb)
Classic experiments
- Single crystal deformation (Ut)
- Polycrystal deformation (Ut)

Main numerical technique Numerical Platform:
ELLE modified (disloc. Dynamics, Elle (subgrain-grain),
FFT (elastic/viscoelastic), spring model Lattice)



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Specific "Projects" in ELLE

1) Elle 3D – both for grain scale and subgrain scale
2) Elle_FFT – viscoelastic/elastic deformation, work term, dislocation density, dislocation type, crystallographic orientations
   Use FFT to infer dislocation density, dislocation type from crystall. Orientations (EBSD data)
3) disloc_dynamics: prediction of dislocation dynamics (once they are in there!) – statistical prediction for larger scale (substructure)
4) Elle_substructure: a) taking disloc dynamics up one scale
   b) internal substructure development and interaction with/of subgrain boundaries and their interaction with grain boundaries
5) Elle_grain boundary fluid: effect of fluid on grain boundary properties & substructure development
6) Elle_dynamic recrystallization: taking all the above to predict dynamic recrystallization -> influence on microstructure development -> rheology
7) Elle_Lattice – talking to each other

Common Data structure / Interface

to allow full integration and competing process analysis