# Dislocation electron tomography
# Applications and association to continuum mechanics and dislocation dynamics

PhD Timmo Weidner, supervised by Alexandre Mussi, Karine Gouriet and Patrick Cordier

UMET Unité Matériaux Et Transformations
Université de Lille

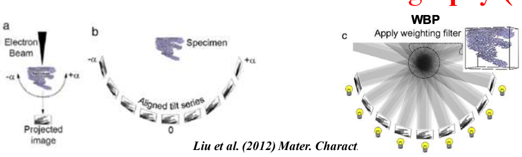
Contact author:
Mail : timmo.weidner@univ-lille.fr

erc
TimeMan

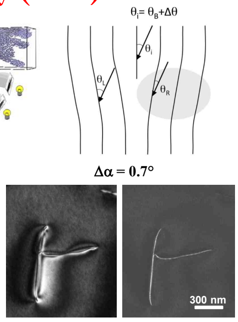
## Motivation

**Understanding Earth's interior dynamics requires linking observable deformation rates to the underlying stress fields through rheology. This relationship is governed by the deformation mechanisms operating at the microscale, which are recorded in the dislocation microstructure.**
**Conventional TEM gives only 2D projections of these structures, but electron tomography [1] provides full 3D reconstructions and quantitative characterization. We use these 3D data to compute internal stress fields within a continuum-mechanics framework and to initialize Dislocation Dynamics simulations using NuMoDis [2]. This approach allows us to investigate how real dislocation networks evolve under stress and to better constrain the rheology of key mantle minerals.**

## Dislocation electron tomography (DET)



*Liu et al. (2012) Mater. Charact.*



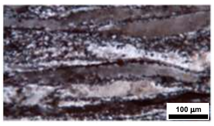
Micrographs of a dislocation under slight tilt variation

In **electron tomography**, we record a tilt series by acquiring TEM images every few degrees over a wide angular range. Using a weighted back-projection (WBP) algorithm, this series is reconstructed into a 3D volume.

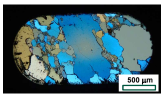
Dislocations are visualized in **diffraction contrast**, which is extremely sensitive to even small orientation changes. As a result, precise alignment of the tilt series is essential for an accurate 3D reconstruction.

### Quartz

We analysed two fine-grained wet quartz specimens, that were naturally deformed at ~350 ± 50 °C and 400–800 MPa [3]: one from the Moine Thrust Zone (MT) in northern Scotland and one from the Main Central Thrust (MCT) in the Himalaya. Since both show identical microstructural behaviour, only the MT specimen is presented here. Quartz is highly beam-sensitive, requiring adapted acquisition conditions—such as reducing the number of projections—to limit radiation damage during tomography.

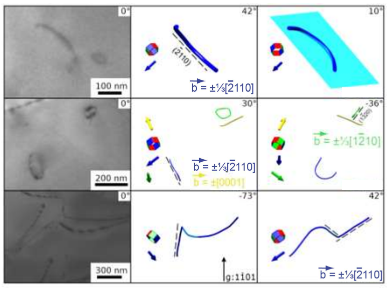


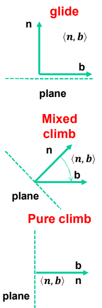
MT thin section



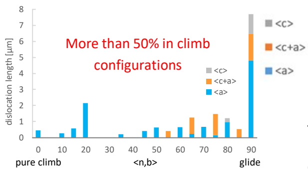
MCT Thin foil

**TEM micrograph**: Selection of dislocation in climb configurations from the MT specimen with identified habit planes and Burgers vectors.



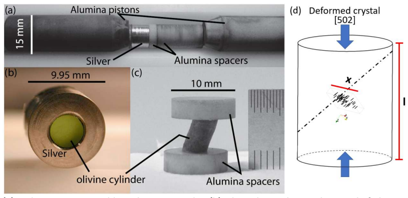

**Slip system statistics:**
Relative angles between the habit plane normal *n* and the corresponding Burgers vectors.
The horizontal axis represents the relative climb–to–glide contribution of the analysed dislocations.




The application of electron tomography of dislocations has revealed complex dislocation microstructures that challenge the standard concept of glide confined to well-defined planes. Approximately half of the analysed dislocations were found in **mixed climb** configurations, showing that the plastic strain produced by climb is comparable to, or even greater than, that produced by glide. We interpret this as a consequence of the very slow natural strain rates, which give diffusion processes sufficient time to operate. Such configurations have never been reported in laboratory experiments for **quartz**, nor previously in natural specimens.
Expanding on the work in quartz, I made preliminary observations of similar mixed-climb configurations in **olivine** from the Oman ophiolite [4]. These results indicate that under geological conditions—**high temperatures** and **low strain rates**—glide (stress-driven) is slowed down, while climb (diffusion-controlled) has time to operate.

**Quantitative analysis at grain scale**
**mixed climb in minerals**

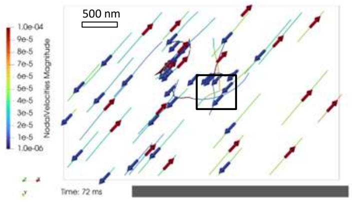
## Discrete Dislocation Dynamics (DDD)



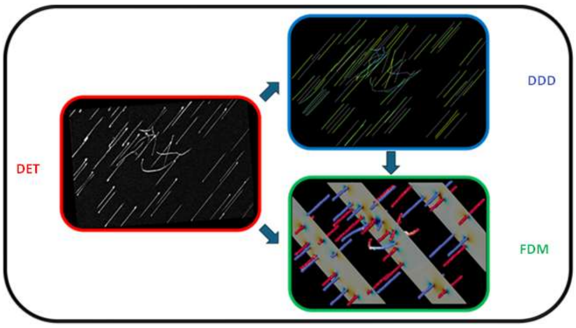
**(a) High pressure assembly without iron jacket (b) Silver plug with a single crystal of olivine inside**
**(c) Post-deformation olivine crystal (d) Sketch of the compressed cylinder with the compression direction and the orientation of the thin foil within the specimen (enlarge to make it visible). Axis grid indicates the orientation in the simulation box. (a)-(c) from [5]**

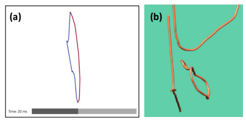
A further step is to implement the real dislocation microstructure into a Dislocation Dynamics (DD) code, NuMoDis [2], in order to investigate the temporal evolution of the microstructure under stress. Here we report the analysis of a single crystal of olivine [5], deformed under uppermost-mantle conditions (300 MPa, 806 °C) with a maximum compressive stress of 754 MPa applied along [502]. The strain rate was $\dot{\varepsilon}$ = 5.1 × $10^{-5}$ $s^{-1}$, and the sample dimensions were 6.32 mm × 4.19 mm (length × diameter).

The simplicity of the microstructure limits the number of observable interactions, but it was nevertheless possible to observe a collinear annihilation, consistent with observations in other regions of the same sample.



**Time evolution of the real microstructure implemented in the DDD code NuMoDis: dislocation configuration after 72 ms. The rectangle marks the location of a dislocation crossing.**



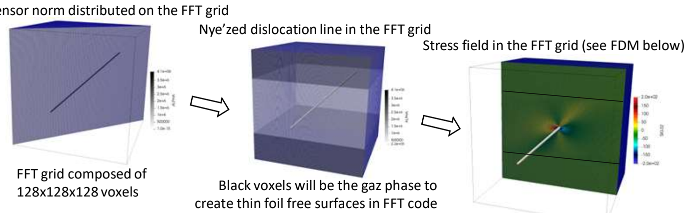



(a) **Residual loop** from collinear interaction laying in **two different planes (b)** similar loop found **experimentally** in other sample from the same study

**Perspectives:**

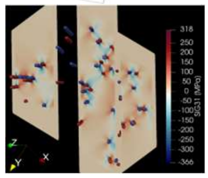
- Implement an improved velocity law based on the ***kink-pair** mechanism*
- Refine the treatment **of image forces** for more accurate dislocation–boundary interactions
- Include **cross-slip** as an additional deformation mechanism in future simulations

## Field dislocation mechanics (FDM)




To study the local mechanical fields associated with our microstructure, we use a **Field Dislocation Mechanics** (FDM) approach [6]. The idea is to generate a continuous dislocation density field from the discrete dislocation segments obtained by tomography [7]. The elasto-static equation of FDM for periodic heterogeneous materials are then solved numerically using Fast Fourier Transform algorithms. Free surfaces are introduced by adding a gas phase.

This method allows quantitative analysis at the grain scale, providing access to the full strain and stress tensors, relative CRSS, and the 3D mechanical fields at nanometre scale [8].


Reconstructed internal stress field in $\sigma_{31}$ [MPa] in the (001) plane, with the [001] dislocation facing toward the viewer

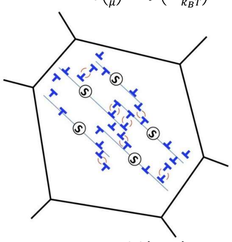
**To balance the incompatible distortion of the dislocations you need a nonzero elastic displacement field**

## Influence of climb in rheology

### Climb as recovery: climb controls strain rate

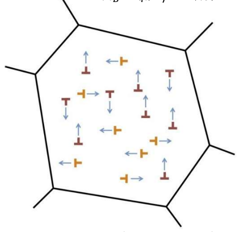
Use of 2.5D Dislocation Dynamics (DD) showed **dislocation creep** in **MgO** [9]:

$$\dot{\varepsilon} = \dot{\varepsilon}_0 \left(\frac{\sigma}{\mu}\right)^n exp\left(-\frac{H}{k_B T}\right)$$

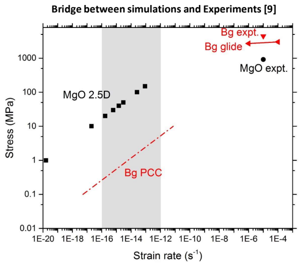

Weertman model (1955)

2.5D Dislocation Dynamics (DD) showed **Pure climb** in **$MgSiO_3$** ( Reali et al. 2019):

$$\dot{\varepsilon} = \frac{D_{Mg}^{sd} \mu b}{\pi k_B T} \left(\frac{\sigma}{\mu}\right)^3 \Big/ \ln\left(\frac{4\mu}{\pi\sigma}\right)$$


Pure climb model (Nabarro 1967)

### Climb as strain mechanism



**Values at 30 GPa and 2000K, experiments by (Girard et al. 2016)**

Combined study demonstrates a transition in deformation. **Bridgmanite weaker than periclase** at lower mantle strain rates, with **pure climb** as the dominant mechanism [9].

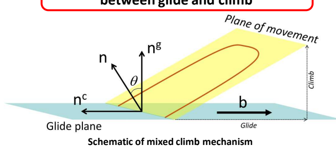
**Significance of climb at natural strain rates**

- → further investigations of climb on a microscopic level needed
- → 3D microstructure visible with **tomography**

### Mixed climb: climb as strain mechanism

$\sim v^c = v^g$

**Approximately the same velocities between glide and climb**



Schematic of mixed climb mechanism

**Experimental studies show evidence of mixed climb in both quartz and olivine [3,4].**

**Need for careful consideration of natural conditions in both empirical and theoretical studies**

**References:**
[1] Mussi et al., *Tectonophysics* 803 (2021): 228754.
[2] Drouet et al., *Journal of Nuclear Materials* 449.1-3 (2014): 252-262.
[3] Weidner et al., *Journal of Geophysical Research: Solid Earth* 129.7 (2024): e2024JB029083.
[4] Demouchy et al., *PEPI* 346 (2024): 107125.
[5] Demouchy et al., *PEPI* 220 (2013): 37-49.
[6] Djaka et al., CMAME 315 (2017): 921-942.
[7] Bertin, *International Journal of Plasticity* 122 (2019): 268-284.
[8] Weidner et al., Modell. Simul. Mater. Sci. Eng. 32.1 (2023): 015004.
[8] Cordier et al., *Nature* 613.7943 (2023): 303-307.

**Visit our website:**
**www.timeman.univ-lille.fr**

**This work was supported by funding from the European Research Council under European Union's Horizon 2020 Research and Innovation Program under grant agreement N°787198**