Grain boundary microstructures and their control on deformation mechanisms in high-grade quartz-rich rocks

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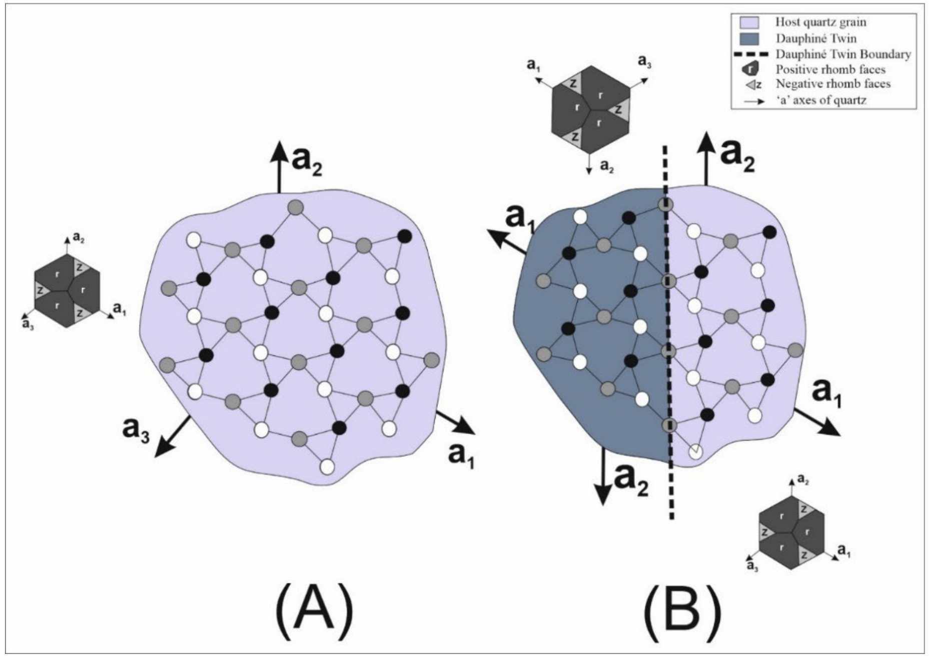
Grain boundaries in quartz

- High angle boundaries (> 10°)
- Low-angle boundaries (< 10°)
- Twin boundaries or special boundaries?

Dauphiné twins…

Requires a rotation of 60° about the 'c' axis. These DTBs are generally formed during β-quartz to α-quartz transition at 573ºc at 1 atm.



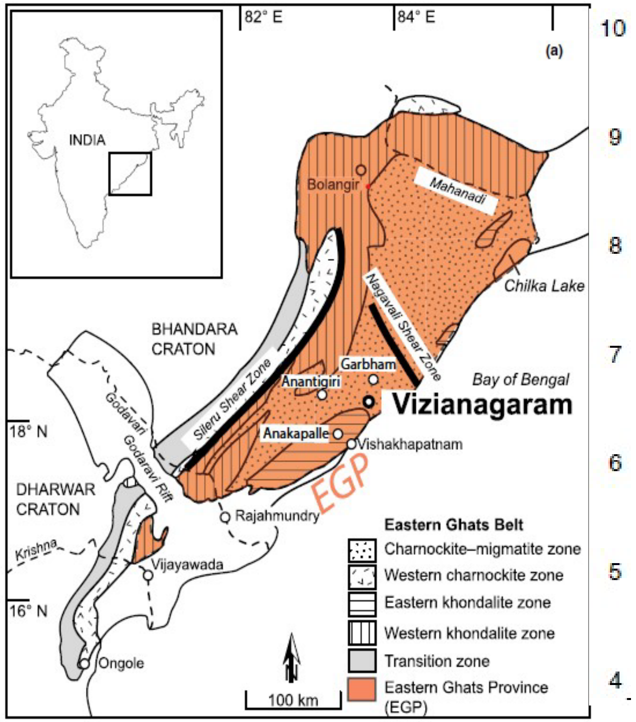
Formation of DTBs during β-quartz to α-quartz transition at 573ºc at 1 atm; after Dey et al., (2024)

Twin Law	Angle between 'c' axis
Japan twins	84.55°
Esterel twins	76.32°
Sardinian twins	64.83°
Breithaupt twins	48.90°
Cornish twins	42.97°

Study Area and Samples

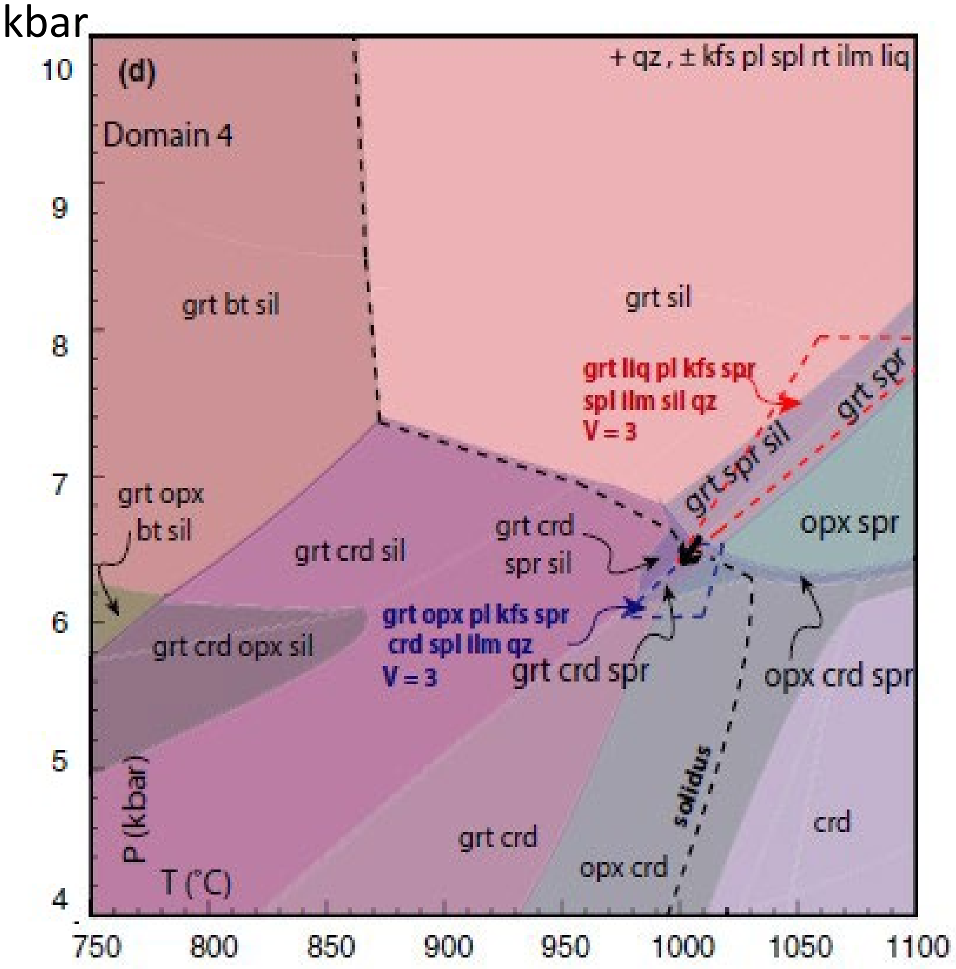
Vizianagaram, Southern Eastern Ghats Province (sEGP), India

A well-documented ultra-high temperature (UHT) domain (c. 1000 ◦C at 7-8 kbar;) of the Indian Shield.

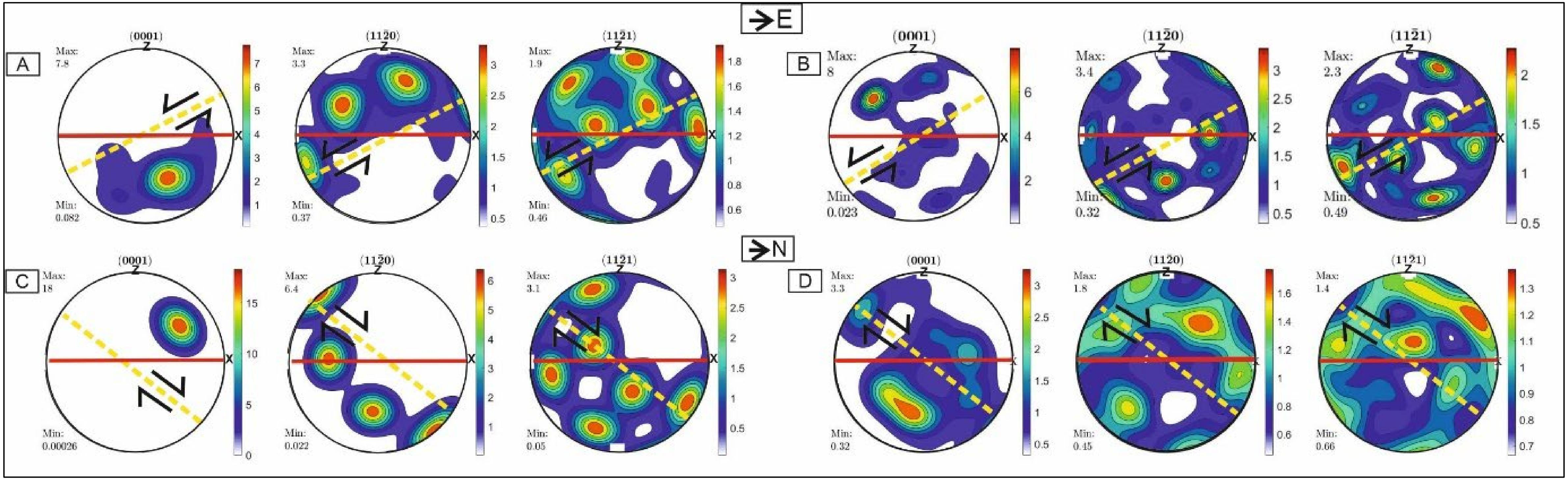


Map of the Eastern Ghats Belt to show the study area (after Mitchell et al., 2019)

UHT followed by isothermal decompression (Mitchell et al., 2019)

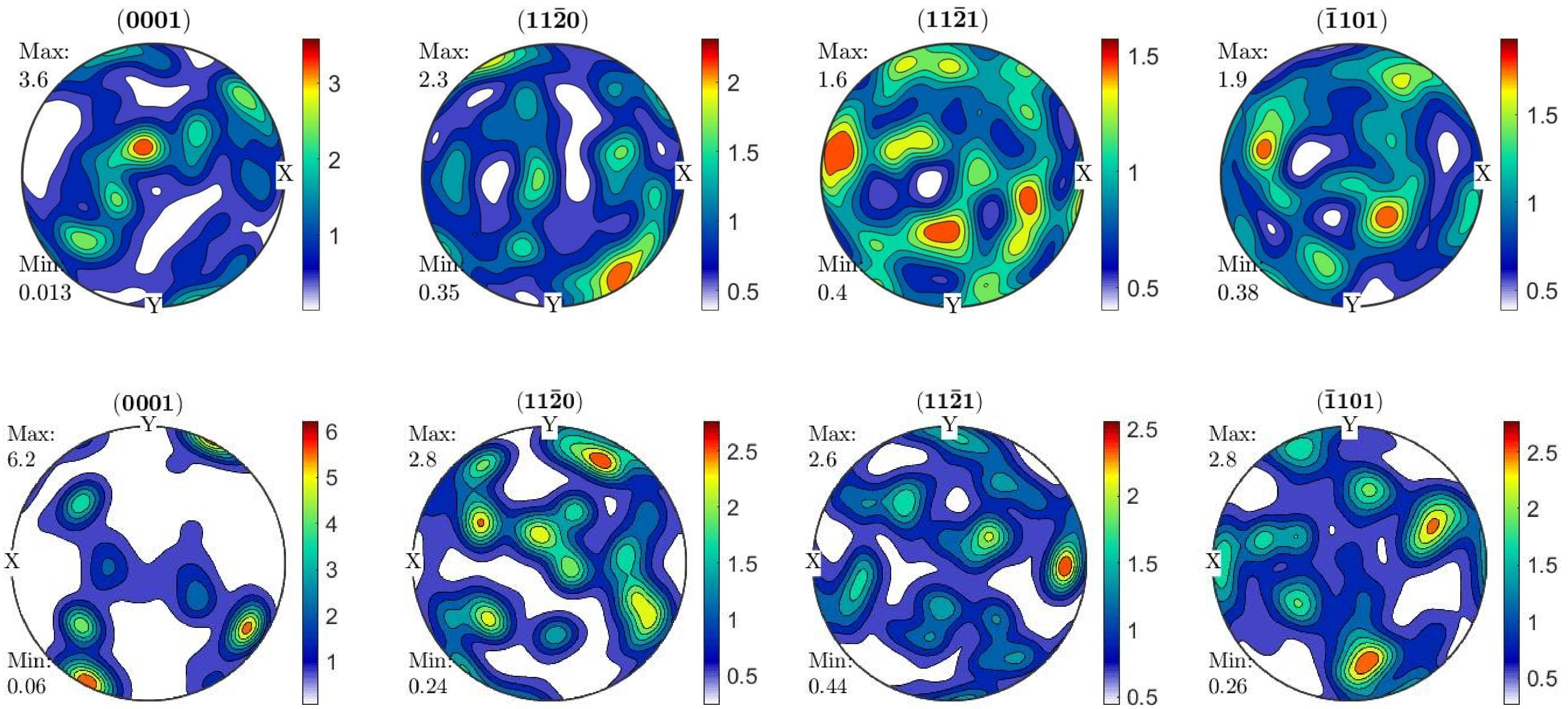


Pole Figures from EBSD Data



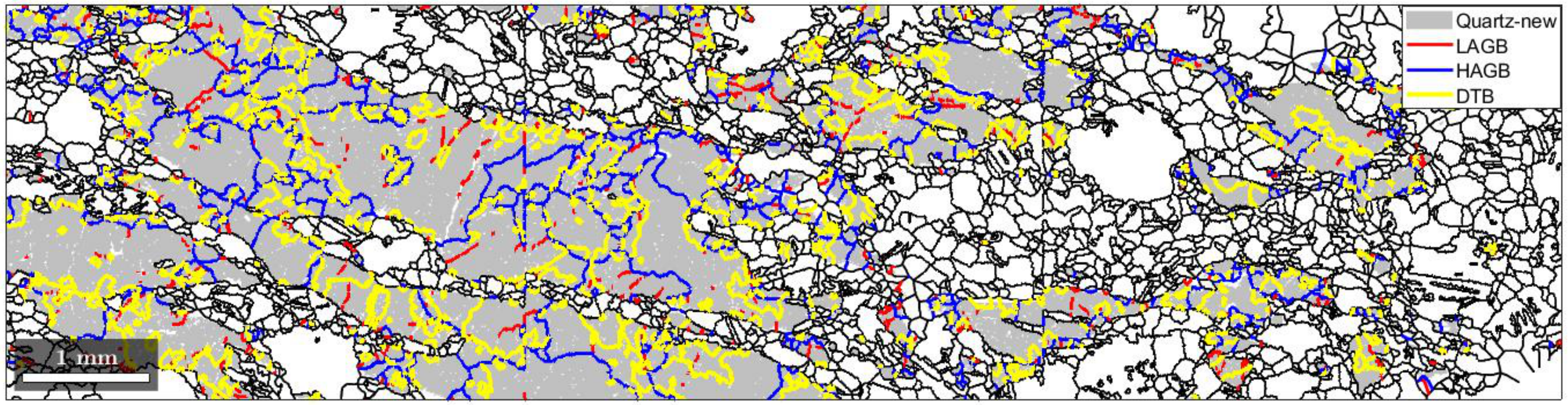
CPOs of quartz grains show a strong preferred orientation, with the asymmetry consistent with thrust sense and activation of rhomb<a> slip system in S_1/S_2 fabrics (A, B) and down-dip extension with rhomb<a> slip in S_3 fabric (C, D).

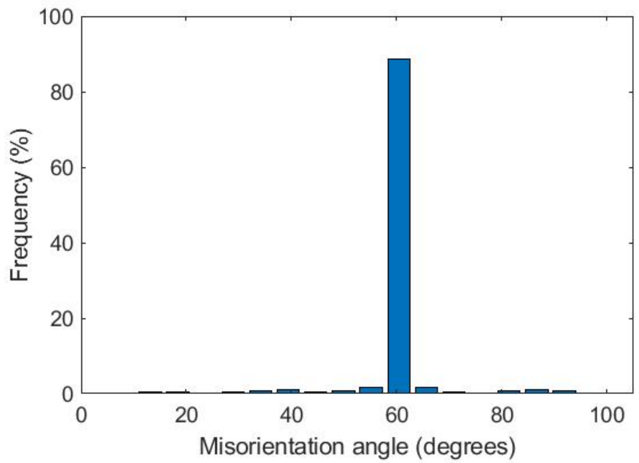
Disrupted CPO data

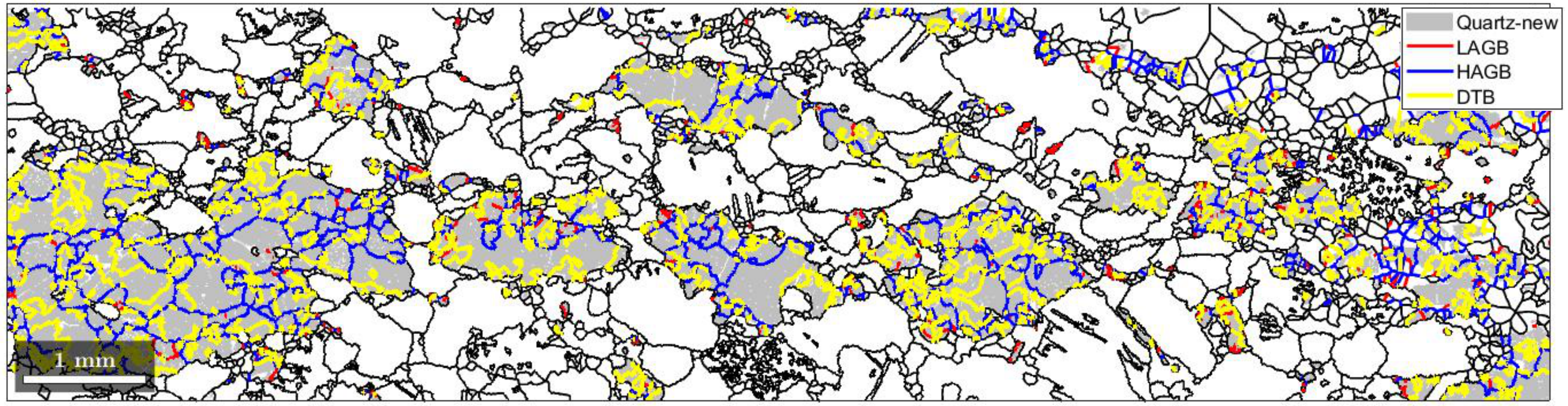


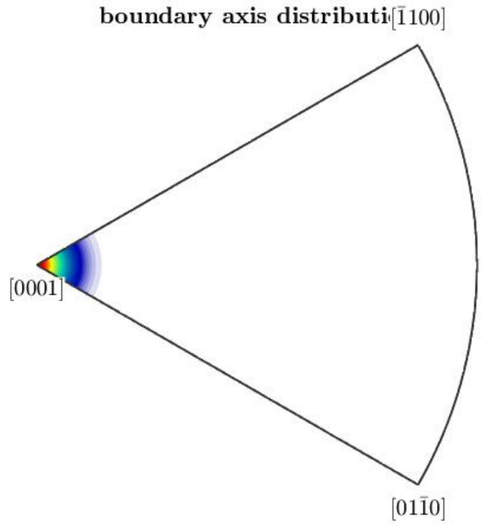
Possible Reasons?

Grain Boundary Misorientation Characterization









Distribution of DTBs (in yellow), LAGBs (Low-angle grain boundary; red) and HAGBs (High-angle grain boundary; blue) in the studied samples (after Dey et al., 2024)

These twin boundaries are high in abundance and are not restricted to the grain interiors. In many places, these DTBs intersect the RHAGBs.

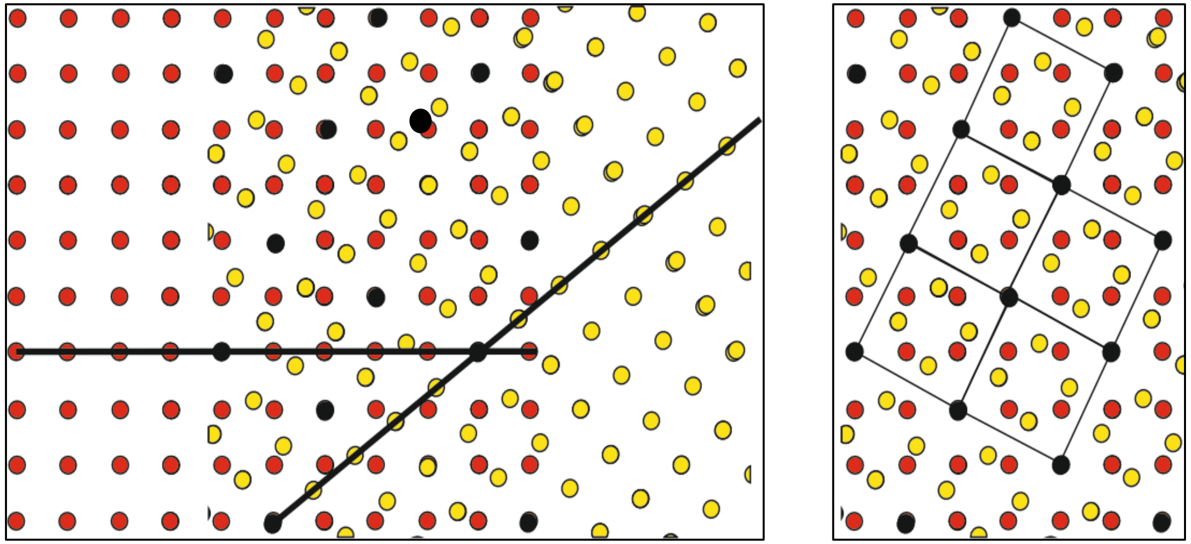
CSL boundaries

Why are these DTBs so special?

The Dauphiné twin boundaries are the most common example of the 'Coincident Site Lattice (CSL)' boundaries in quartz (Mclaren, 1986)

'Coincident Site Lattice' (CSL) boundaries

- **CSL boundaries have low-energies compared to the RHAGBs.**
- **Metals are thermo-mechanically processed to increase the frequency of low $\sum(\leq 29)$ CSL boundaries.**



Σ5 Coincidence Site Lattice

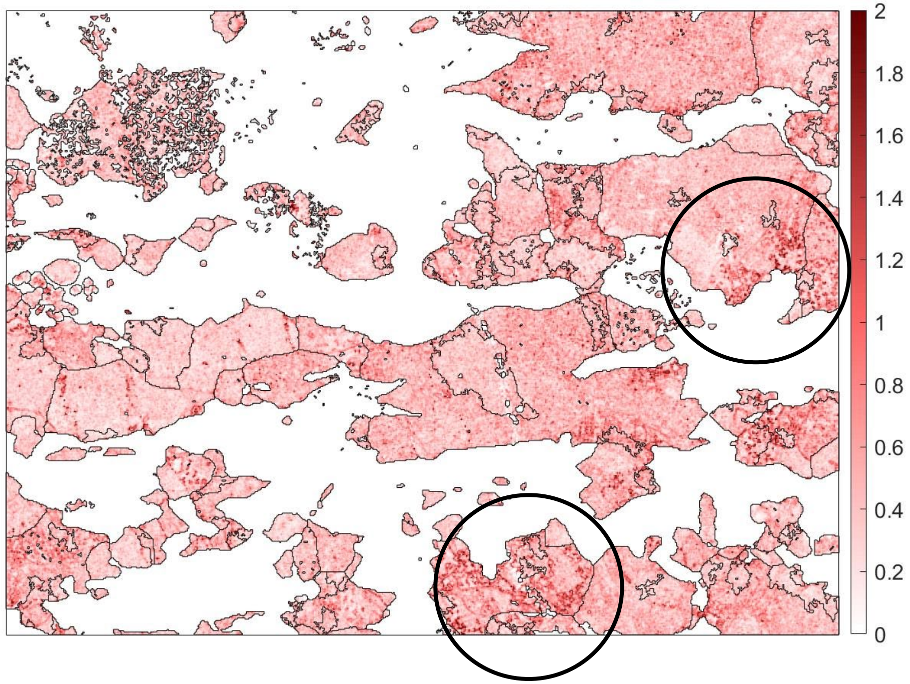
Similar to metals, rocks in nature undergo thermo-mechanical processing by deformation and metamorphism, but the existence and importance of CSL relationships in rocks has yet to be convincingly demonstrated

Problems!

- **What are the effects of these grain boundaries on the deformation mechanisms of quartz aggregates?**

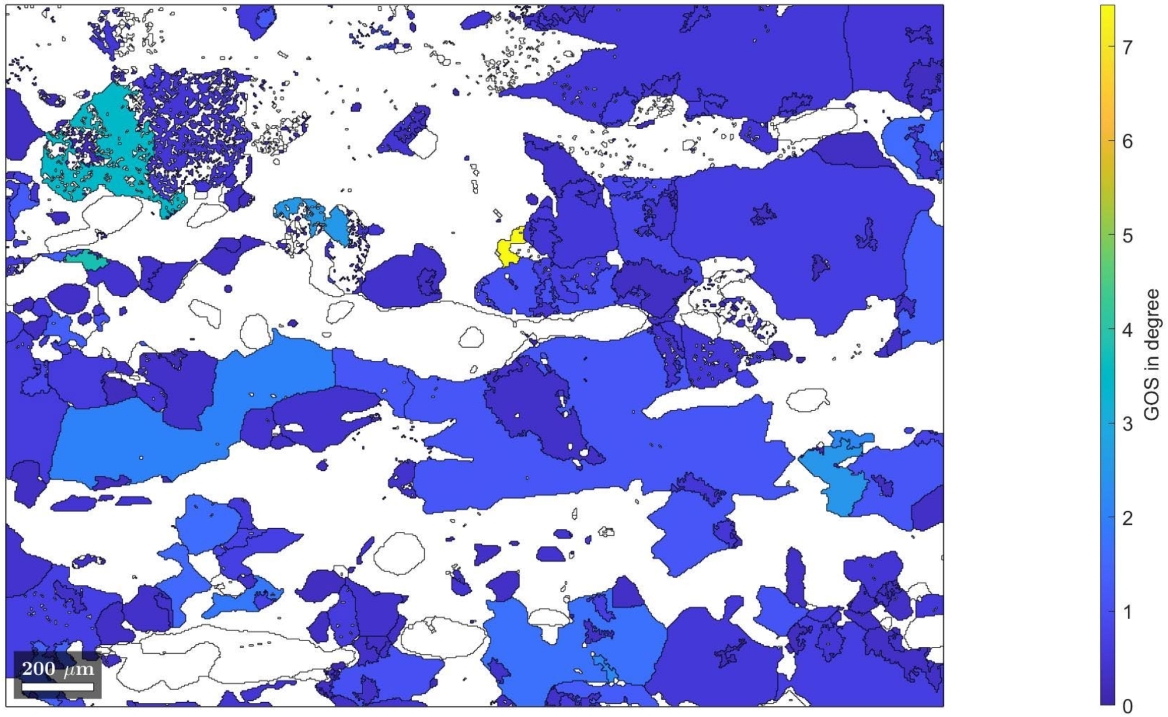
- **What role do these CSL relationships of DTBs play in the microstructural evolution of quartz-rich rocks?**

Crystallographic preferred orientation development



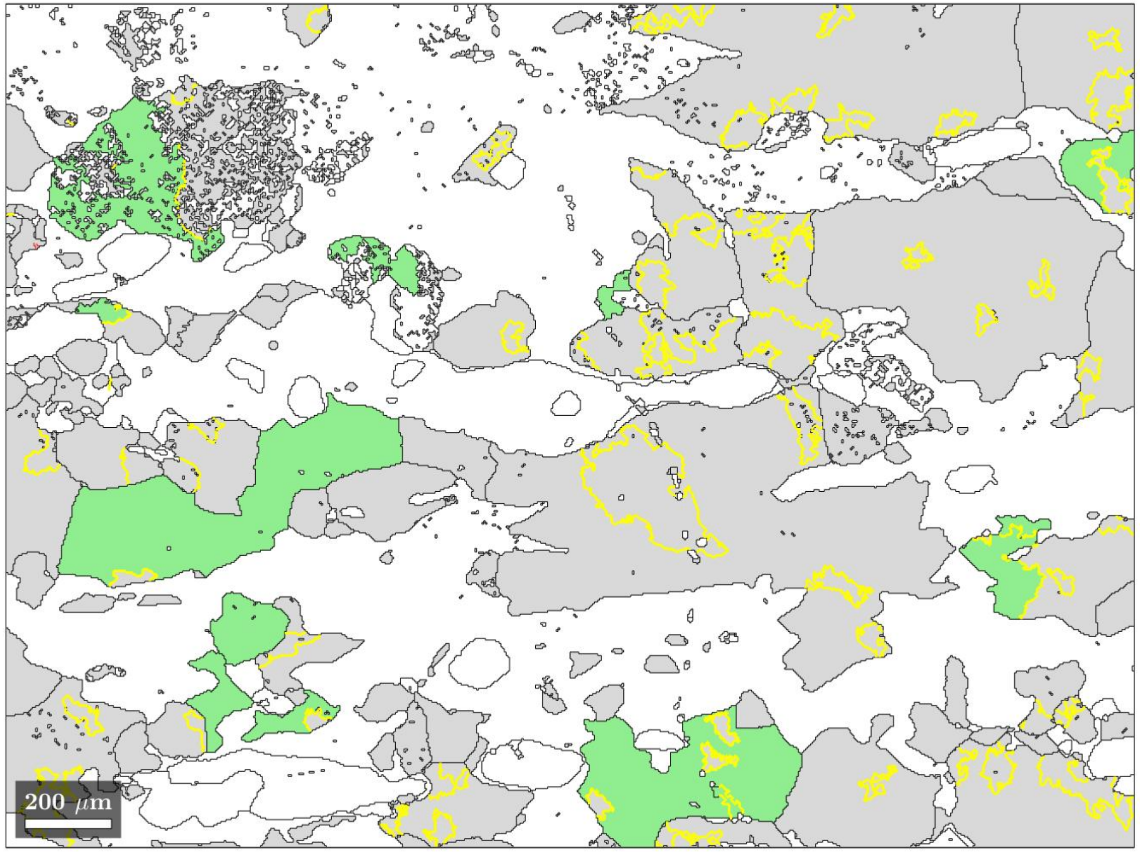
Kernel Average Misorientation (KAM) map

Grain Orientation Spread (GOS) map



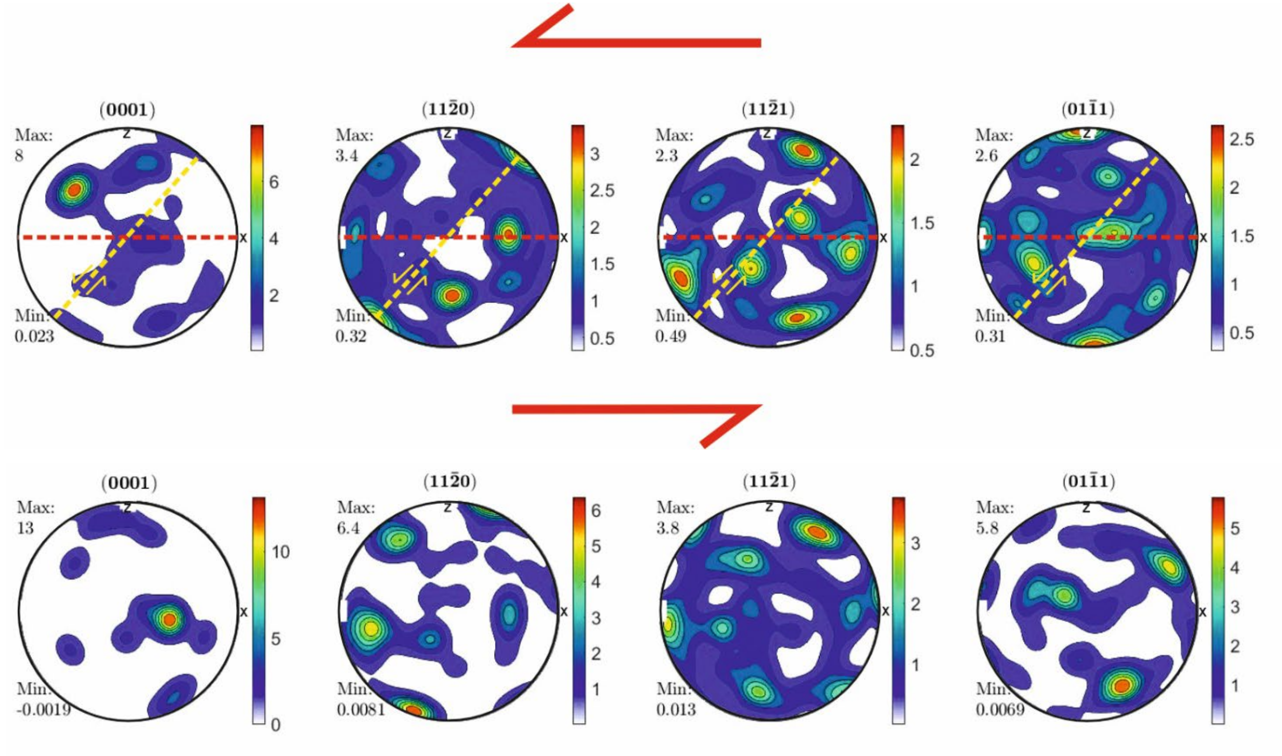
Crystallographic preferred orientation development

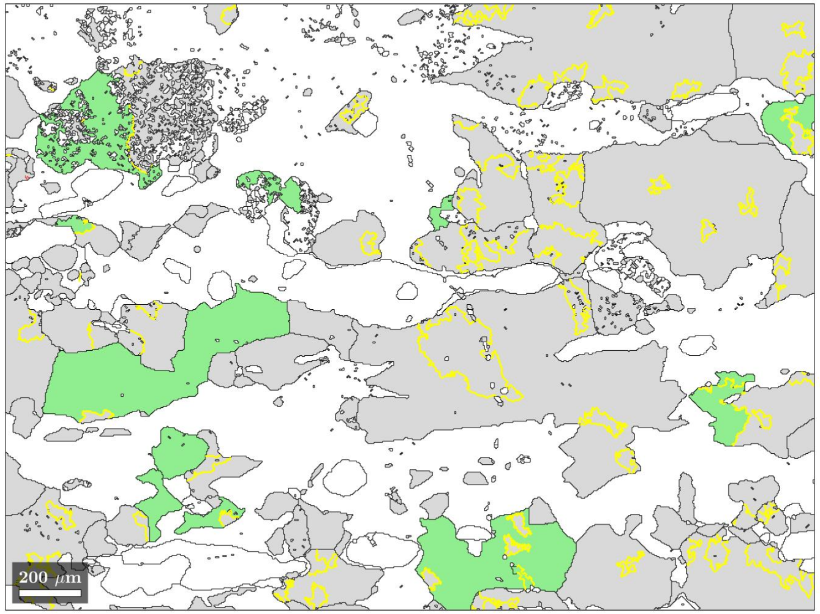
Strain variation grains map based on GOS threshold value



Strain variation grains map with DTBs

Crystallographic preferred orientation development

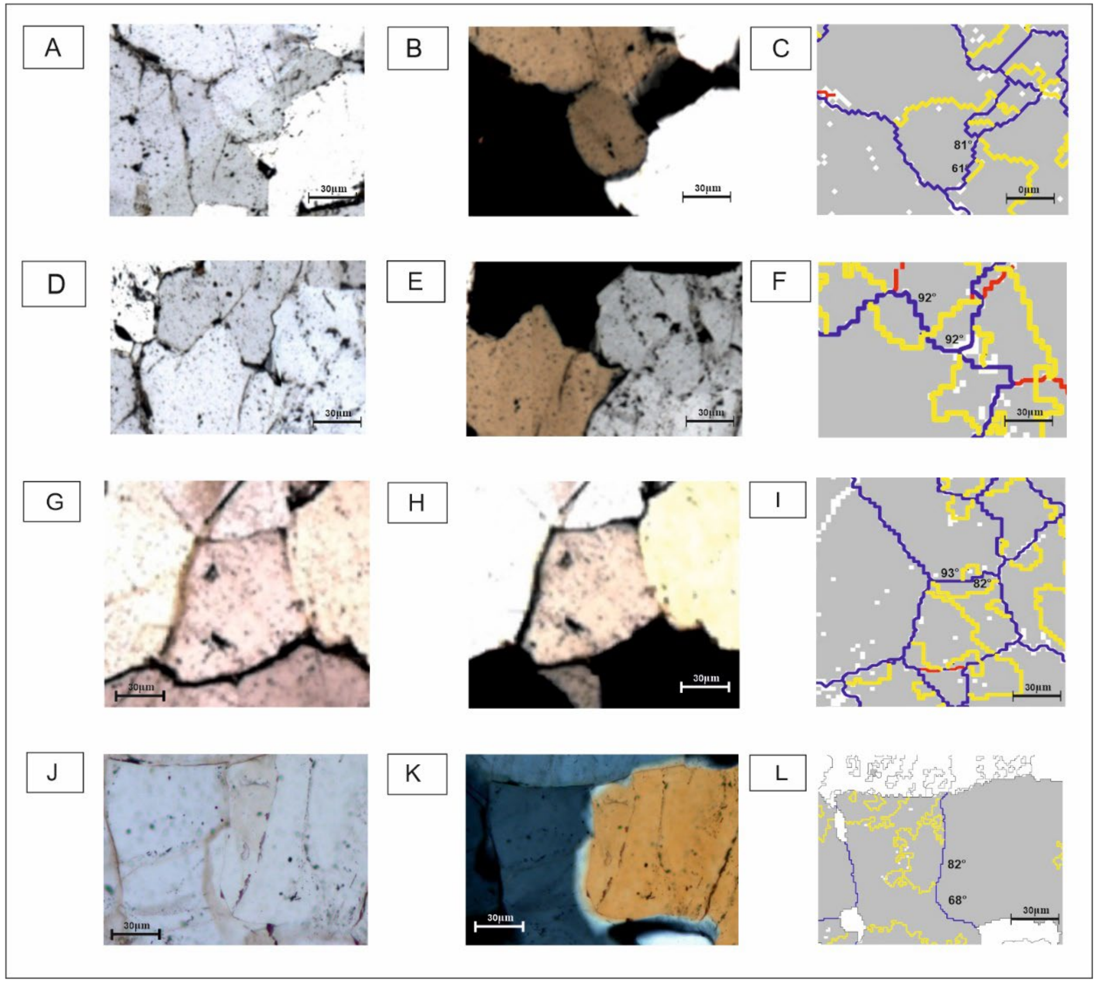


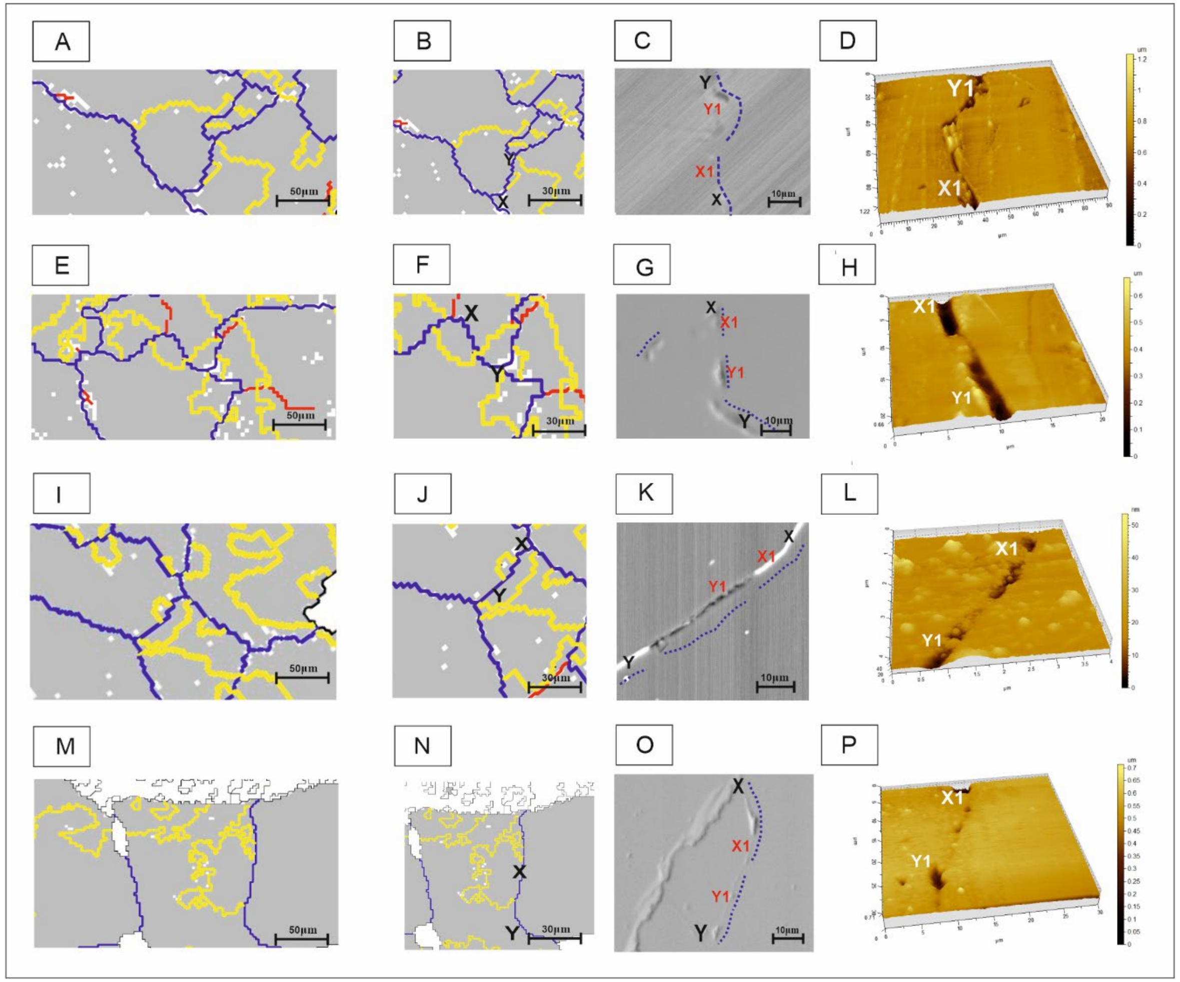


CPO of strained grains shows a rhomb <a> slip system and CPO of unstrained grains from the same sample do not show any clear distribution.

The presence of DTBs can cause strain partitioning due to stiffness differences between positive and negative rhombs of quartz.

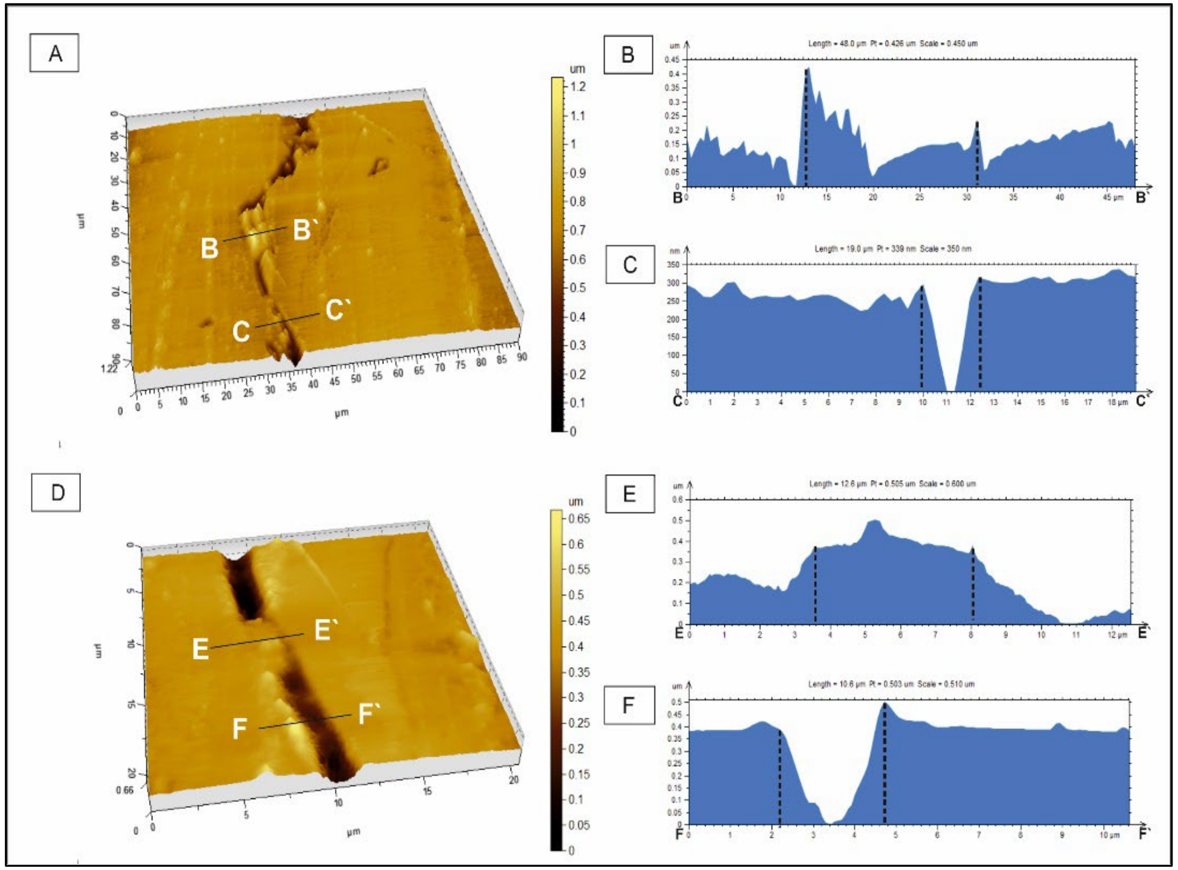
Site-specific nanoscale profiling





Dey et al., 2024

Grain boundaries under AFM

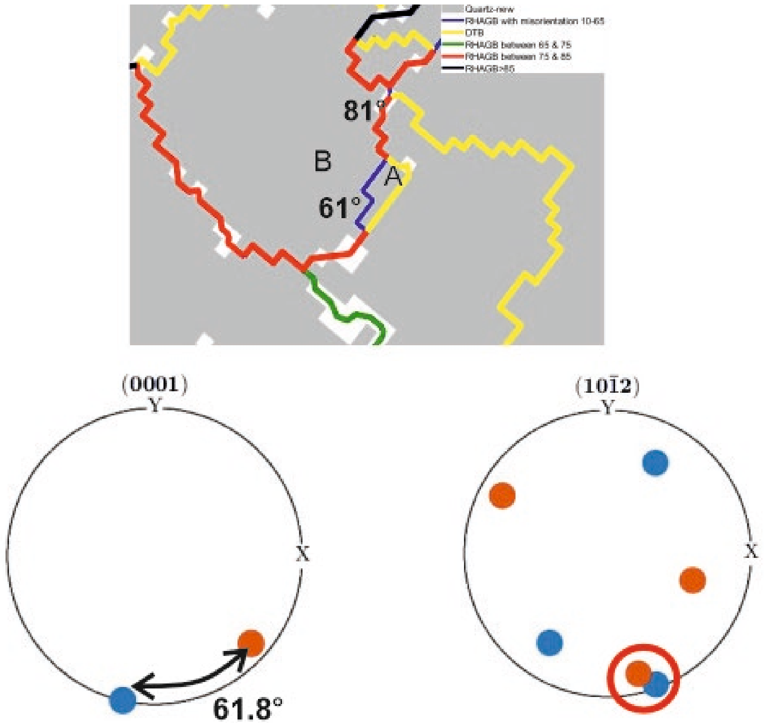


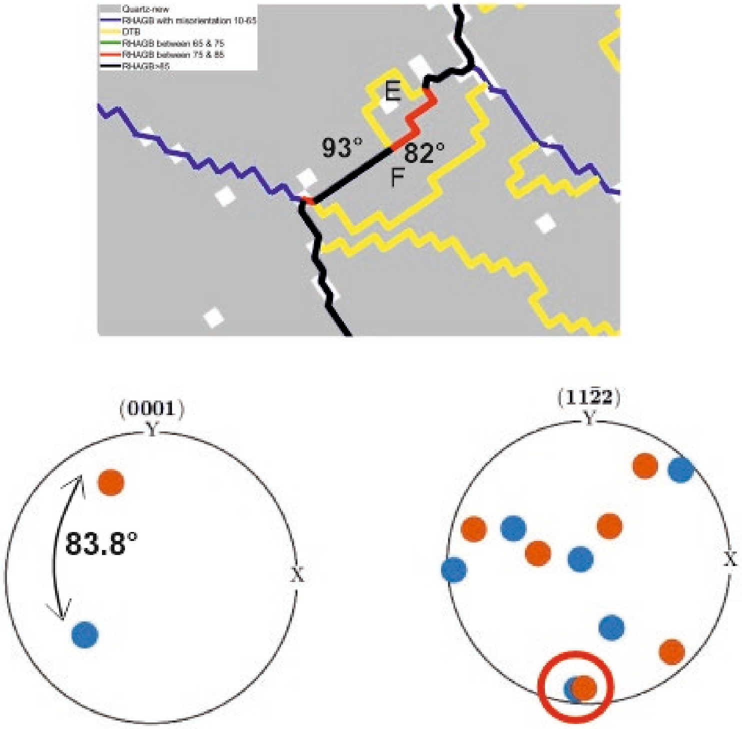
- Random grain boundary domains generally have a high concentration of defects and less cohesion.
- They are seen to have deeply indented channels, rather than the smooth surfaces of the grain interior, **owing to material removal during the process of chemical mechanical polishing** (CMP).
- `They also appear open due to the widening of grain boundary domains during decompression (Kruhl et al., 2013).

The correlation of the domains suggests that the DTBs do not show any discernible channel traces, even on the nano-scale.

DTBs are more stable and compact domains with respect to the RHAGBs.

RHAGB Misorientation Distribution





Change in misorientation distribution across the RHAGB near the RHAGB-DTB intersection. The neighbouring grains across the RHAGB segments follow different twin laws of quartz (A, B: Sardinian twins; C, D: Japan twins; Zhao et al., 2013; Dey et al., 2024).

DTBs are modifying the RHAGB segments at the DTB-RHAGB intersection points into low energy boundaries with symmetry relationships that are similar to other twin laws of quartz

Key points…

- **The formation of DTBs can prompt a general reduction of grain boundary surface energy.**

- **The evolution of these special high-angle misorientations in quartz-rich systems can control the CPO development during deformation.**

- **It becomes important to understand the timing of the twin formation relative to an evolving kinematic deformation geometry to correctly decode the deformation history.**

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