Grain-Size Piezometry: Subgrains and New Grains in Theory and in Practice

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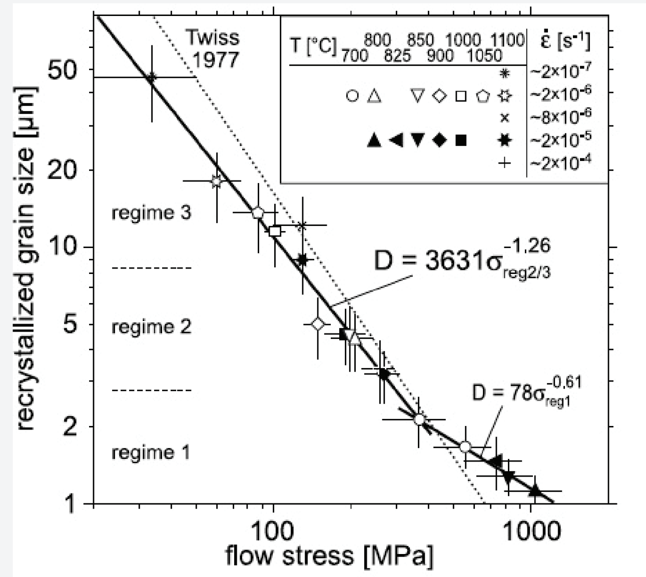
John Platt: University of Southern California. jplatt@usc.edu

1 Introduction

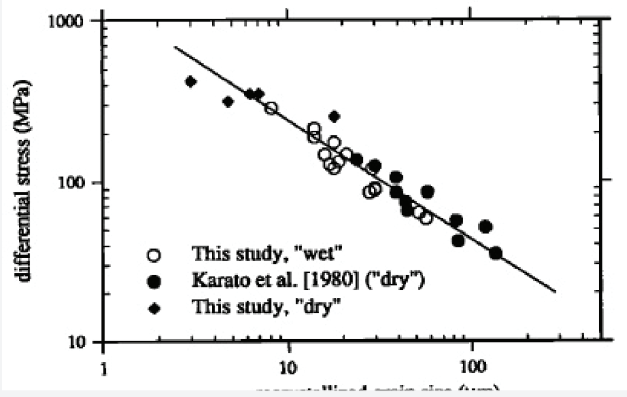
A relationship between differential stress and dynamically recrystallized grain-size has been established experimentally for quartz, olivine, calcite, orthopyroxene, ice, and various metals and salts. At least for quartz, this has been shown to be independent of temperature, strain-rate, or water content.

Current explanations are inconsistent with observational data and basic physical laws.

Here I show that the relationship between subgrain size and stress, which has a physical basis, leads to an understanding of the grain-size piezometer in terms of recrystallization processes.



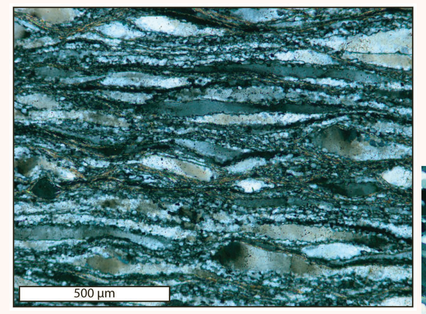
Quartz piezometer: Stipp & Tullis (2003)



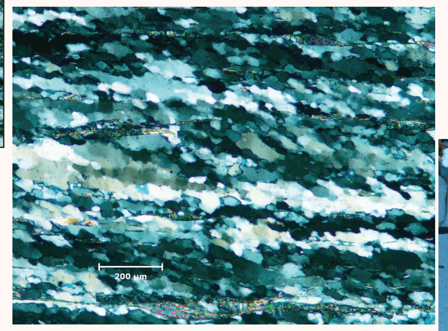
Olivine piezometer: van der Wal et al (1993)

2 Mechanisms of Dynamic Recrystallization

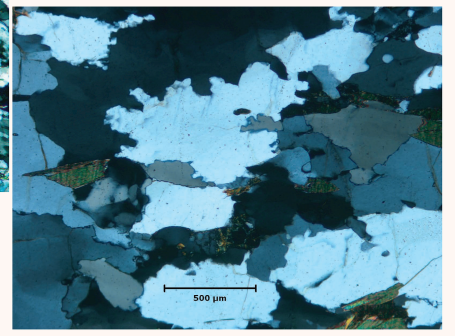
We understand how recrystallization occurs, but there is no overarching theory that explains the stress/grain-size relationship.



Grain-boundary bulging recrystallization (BLG). Quartz mylonite, Moine Thrust Zone, NW Scotland



Subgrain rotation recrystallization (SGR). Quartz mylonite, Snake Range, Nevada



Migration recrystallization (GBM) in quartz. Ruby Mtns, Nevada

high stress
low T

Different recrystallization mechanisms may require different stress / grain-size relationships

low stress
high T

References

Cross, A.J., Prior, D.J., Stipp, M., Kidder, S., 2017. The recrystallized grain size piezometer for quartz: An EBSD-based calibration. Geophysical Research Letters 44, 6667–6674.

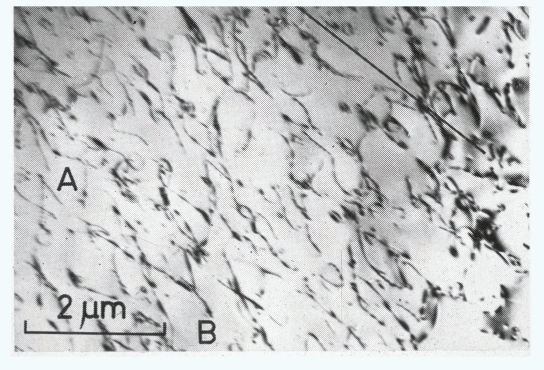
Platt, J.P., Behr, W.M., 2011. Grainsize evolution in ductile shear zones: implications for strain localization and the strength of the lithosphere. Journal of Structural Geology 33, 537-550.

Stipp, M., Tullis, J., 2003. The recrystallized grain size piezometer for quartz. Geophysical Research Letters 30, 2088, 3-1 - 3-5.

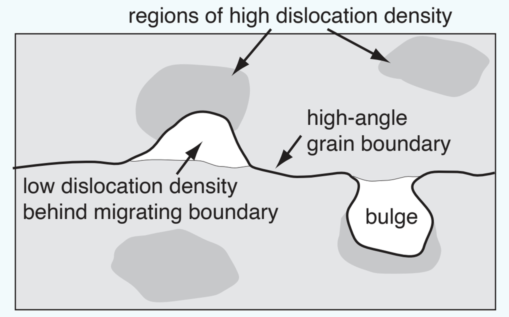
van der Wal, D., Chopra, P., Drury, M., Fitz Gerald, J.D., 1993. Relationship between dynamically recrystallized grain size and deformation conditions in experimentally deformed olivine rocks. Geophysical Research Letters 20, 1479-1482.

3 Stress during Dislocation Creep

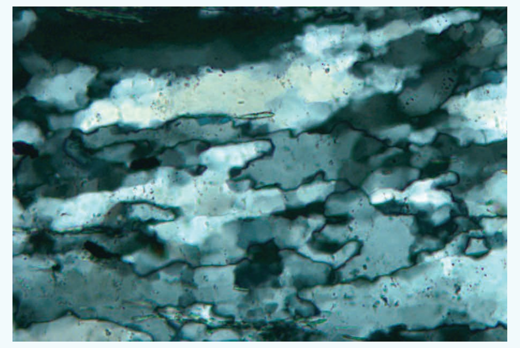
Dislocation creep leads to an increase in dislocation density, which increases the stress required for creep, because of the elastic strains associated with the dislocations. This may be counteracted by recovery processes, which can lead to a steady state dislocation density. Dislocations are lines within a volume, hence dislocation density ρ is related to stress σ by:
$\rho = Gb\sigma^2$, where G is the shear modulus, and b is the Burgers vector (lattice spacing).



TEM image of high density of tangled dislocations in work-hardened quartz.



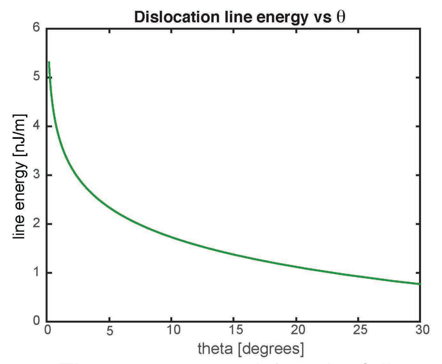
Grain-boundary bulging (BLG) is driven by dislocation density ρ: the boundary migrates into areas of high ρ, leaving new lattice behind with a lower elastic strain energy.
Bulge size may be controlled by the scale of variations in ρ. A lower limit is placed by the Dmin line (see panel 6); an upper limit by the spacing of subgrain walls (see panel 5).



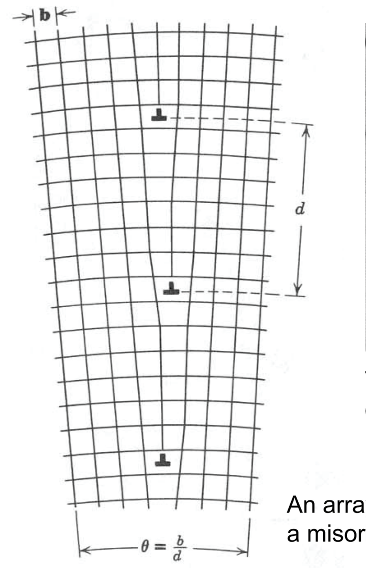
Optical image of grain-boundary bulging in deformed quartz, Santa Catalina Island, California

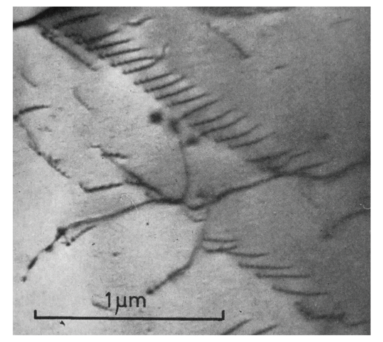
4 Subgrains are Key

Thermally activated recovery processes allow dislocations to organize into arrays that lower the elastic strain energy. These arrays create a misorientation θ of the crystal lattice across them, such that $\theta = b/h$, where h is the dislocation spacing in the array. The arrays bound lattice volumes known as subgrains, with distinct but small (<10°) differences in orientation.



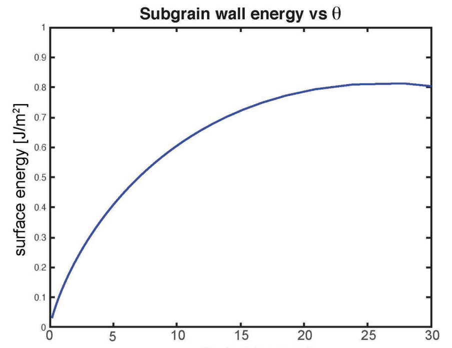
The energy per unit length of dislocation line *decreases* with θ



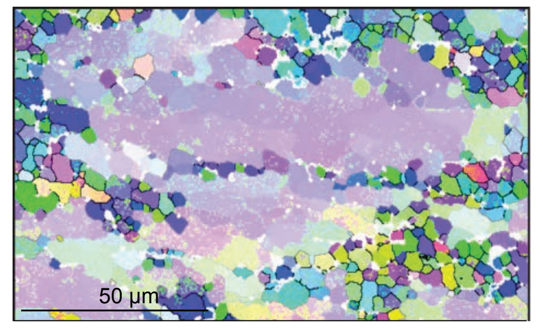


TEM image of an array of edge dislocations

An array of edge dislocations creates a misorientation of the lattice θ.



The energy per unit area of subgrain wall *increases* with θ

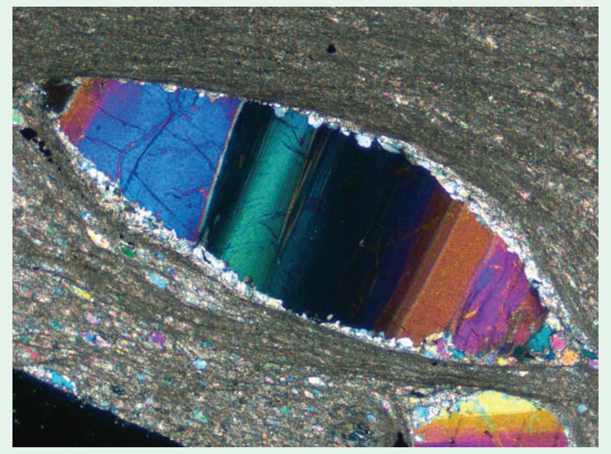


EBSD image showing subgrains in quartz porphyroclasts and recrystallization by BLG and SGR.

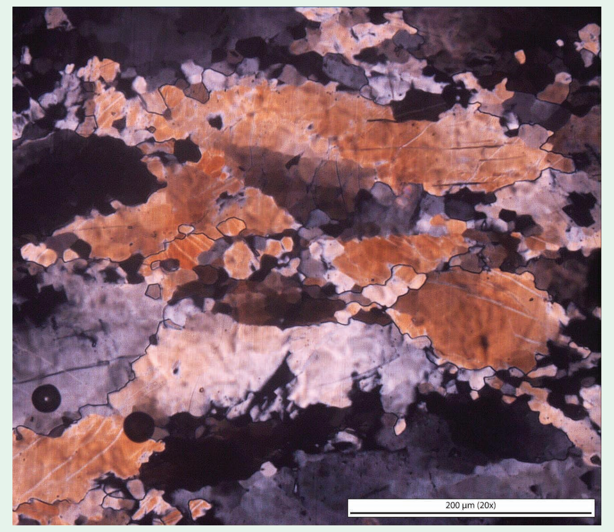
5 Controls on Subgrain Size

Subgrain walls stabilize when dislocation strain energy/unit area in the wall = strain energy/unit area outside the wall. At this point, dislocations can't break out of the wall, and the wall can only move slowly. This provides a criterion for stabilization, such that the critical spacing h_c of dislocations in the subgrain wall is:
$h_c = [1 - \ln(h_c / 2\pi R_0)]/\{\sqrt{\rho}[\ln (R_0\sqrt{\rho})]\}$.
R_0 is function of dislocation structure – value ~ b/3
This equation requires a numerical solution, but is close to $h_c = q/\sigma$, where q is ~0.9.

Once the subgrain structure has stabilized, dislocations can continue to accumulate in the walls, increasing the misorientation, without changing the size of the subgrains.
Only *geometrically necessary dislocations* (GND) accumulate in walls – these produce lattice distortion. The subgrain size d is a function of the total dislocation density and the proportion ϕ of GND.
$d = 3/(\phi h_c \rho)$.
Since h_c depends on $1/\sigma$, and ρ depends on σ^2, d depends on $1/\sigma$. d therefore defines a subgrain piezometer.
The slope of the piezometer is independent of material properties, but the intercept depends on ϕ, which is difficult to predict or calculate, and hence has to be determined from observational data.



Optical image of lattice distortion in an olivine porphyroclast, Finero massif, Italian Alps. The distortion is accommodated by geometrically necessary dislocations (GND) that have accumulated in subgrain walls.

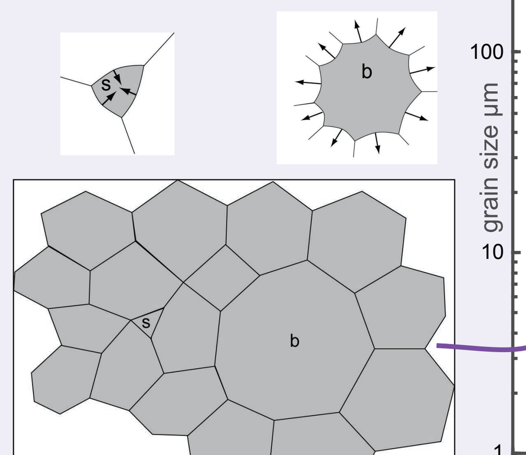


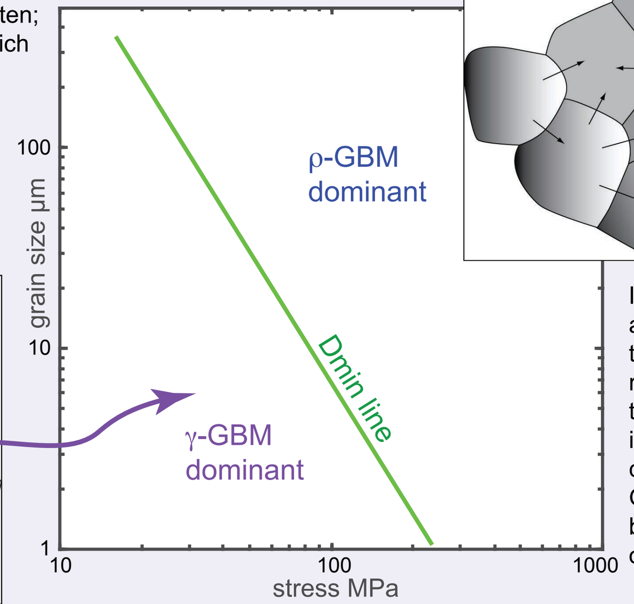
Optical image of experimentally deformed calcite, showing subgrain rotation recrystallization (SGR). The size of the subgrains is similar to that of the new grains, and the stress is known, which provides a way of determining the value of ϕ for the subgrain piezometer.

6 Controls on Grain-boundary Migration

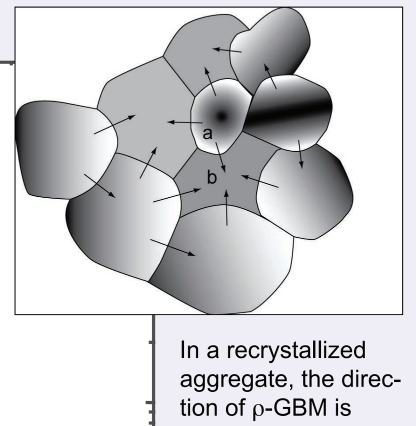
Grain-boundary migration is an essential part of dynamic recrystallization. It is a thermally activated process involving diffusion across the boundary. It may be driven by lattice strain energy (ρ-GBM) or by surface energy (γ-GBM). These processes produce very different microstructures.

γ-GBM causes grain-boundaries to straighten; and small grains shrink and disappear, which results in an increase in mean grain size.





After Platt & Behr (2011)



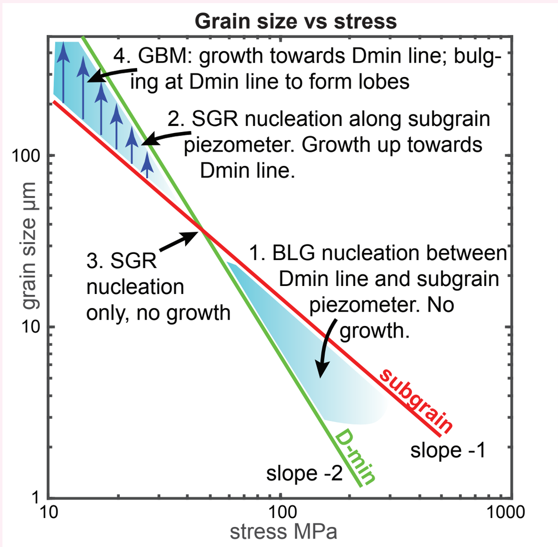
In a recrystallized aggregate, the direction of ρ-GBM is random with respect to grain centers, and it does not result in a change of grain size. Grain boundaries bulge in the direction of motion.

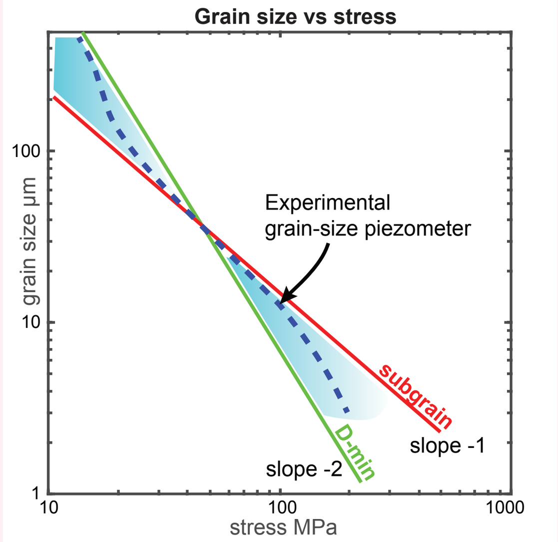
In stress – grain-size space, there is a minimum grain size that can survive elimination by γ-GBM. This defines the Dmin line: Dmin = $-4\gamma/E_d$, where γ is the surface energy/unit area, and E_d is the dislocation energy/unit volume. $E_d \sim \sigma^2/G$, so:
Dmin ~ $-4\gamma G/\sigma^2$.
The Dmin line separates regions where γGBM is dominant from regions where ρGBM is dominant.

7 Tying It All Together

The intersection of the subgrain piezometer with the Dmin line defines several different recrystallization regimes:

1. A high stress zone where grains nucleate by BLG between the two lines;
2. A low stress zone where grains nucleate by SGR along the subgrain piezometer, and then grow up towards the Dmin line.
3. Near the intersection, grains nucleate by SGR and don't change size.
4. At very low stresses, grain growth followed by bulging along the Dmin line leads to GBM microstructures



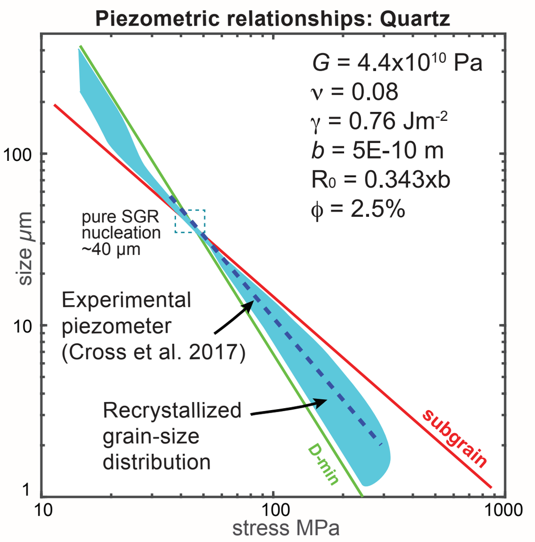


The experimentally determined grain-size piezometer is a fit to these different processes, and lies between the Dmin line and the subgrain piezometer, with a slope ~1.5.

Its position is determined by the intersection of the two lines, where nucleation is by SGR and no growth occurs.

There's no Grand Unified Theory for dynamic recrystallization!

8 Applications



Quartz. The Dmin line is constrained by the elastic constants and the surface energy γ. γ depends on the elastic modulus and has an uncertainty of ±30%.

The subgrain piezometer has a slope very close to 1 for all materials. Its position is determined by its intersection with the Dmin line, where nucleation is by SGR and no growth occurs. For quartz this occurs at a grain size of ~40 µm.

The recrystallized grain size distribution reflects nucleation processes, as described in Panel 7.

Olivine. The piezometric relations were calculated in the same way as for quartz, using the elastic constants for olivine.

The position of the subgrain piezometer is determined by its intersection with the Dmin line, where nucleation is by SGR and no growth occurs. For olivine this is at ~100 µm, but has a large uncertainty.

This method can be applied to any material for which we have the relevant data.