Shear coupled grain boundary migration as a deformation mechanism in minerals.

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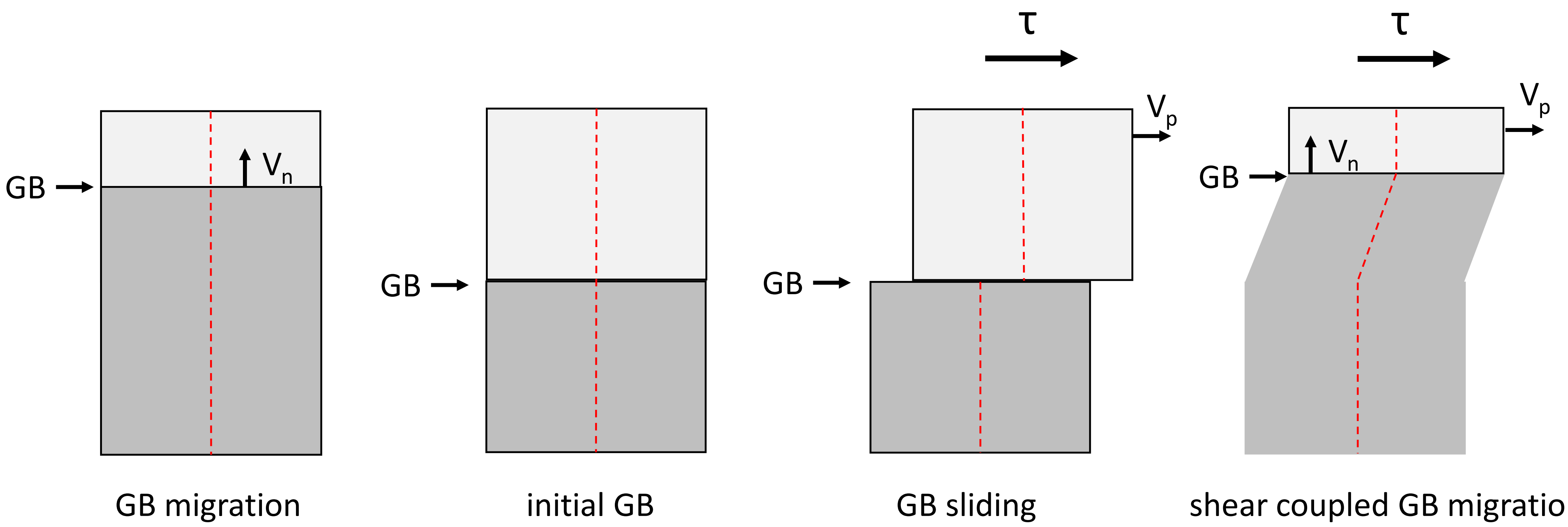
Introduction

The motion of a grain boundary, as in grain boundary (GB) migration, is widely considered to be a process that occurs during recrystallization and recovery, where strain energy differences across the boundary are reduced by movement of the boundary. This movement of the boundary does not deform the lattice, Figure 1.

A GB responds to stress in several ways, Figure 1. Shear coupled GB migration (SC GBM) is now recognized as a common phenomenon for a wide range of boundary misorientation angles [1-6], where there is an atomically ordered structure at the grain boundary. SC GBM involves simultaneous translation and migration of the boundary. Twinning is an example of SC GBM[7].

Figure 1: GB migration, shear coupling and sliding



Diagrams illustrating different types of GB behavior: Vn = velocity of migration, Vp = velocity of translation parallel to boundary. Conventional view of GB migration as recovery processes. Under shear stress, τ , deformation can occur by GB sliding or shear coupled migration.

Examples of shear coupled GBM

Numerous examples of SC GBM are found in bicrystal and polycrystal studies (experimental and modelling) mostly for cubic and hexagonal metals[8], although shear coupling is also found in ionic materials (NaCl[9]) and oxides[10, 11].

Figures 2 and 3 show an example of macroscopic SC GBM and grain boundary sliding (GBS) in deformed polycrystalline magnesium[12].

Figure 4 shows SC GBM and GBS in deformed bicrystals of ice[13, 14].

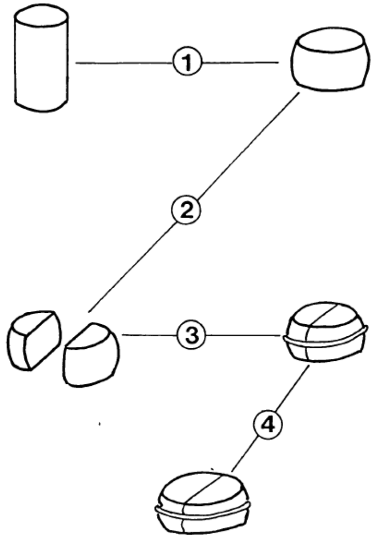
Twinning is also widely observed in materials with both low and high symmetry materials[15].

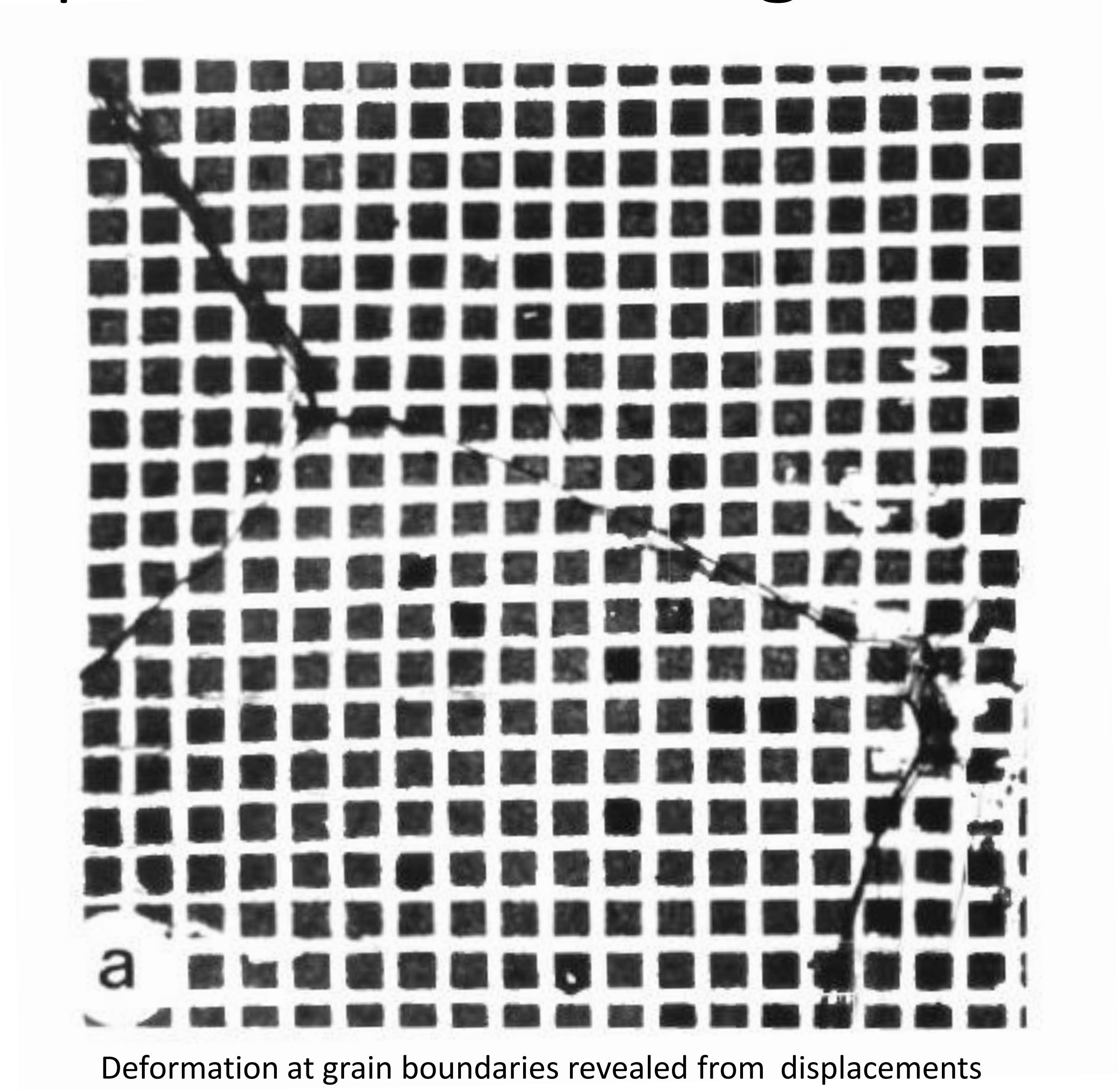
Figure 2: GBS and shear coupled GBM in magnesium

Magnesium deformed in uniaxial compression at 0.5 to 0.95 of the melting temperature, Tm, Drury 1984 [12].

Split cylinder tests at 475-600 °C, Strain rate = 2×10^{-4} s^{-1}

1) Deformation to a strain of 0.42.
2) Sectioning, polishing and deposition of 25 micron gold squares.
3) Sample re-assembly and heating for 3-5 minutes
4) Deformed a second time by strains 0.05 to 0.1.



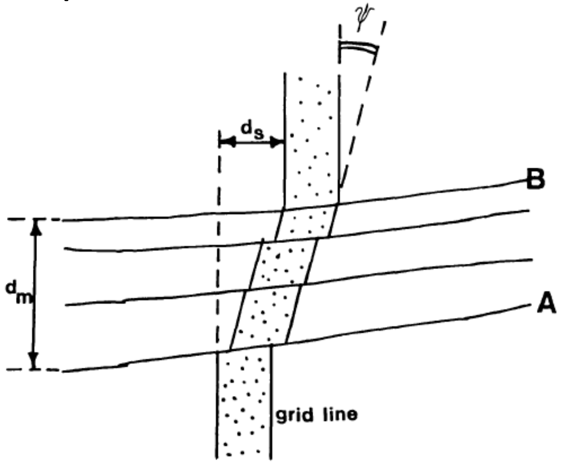


Deformation at grain boundaries revealed from displacements and distortion of marker grid [12].

Figure 3: GBS and shear coupled GBM in magnesium

Magnesium deformed in uniaxial compression at 0.5 to 0.95 Tm

Deformation involves lateral (**ds**) sliding displacements and shear Ψ in the region (**dm**) swept by grain boundary migration.



a) **Grain boundary sliding.**

b) **Grain boundary migration and shear.**

c) **Grain boundary sliding, migration & shear**. Lateral displacements at the initial and final position of the boundary. The region swept by grain boundary migration is sheared.

d) **Grain boundary migration and shear**. The region swept by grain boundary migration is sheared.

In this example deformation at GBs occurs by a combination of grain boundary sliding and shear coupled grain boundary migration. Individual boundaries, can slide, shear couple, or show mixed behavior[12].

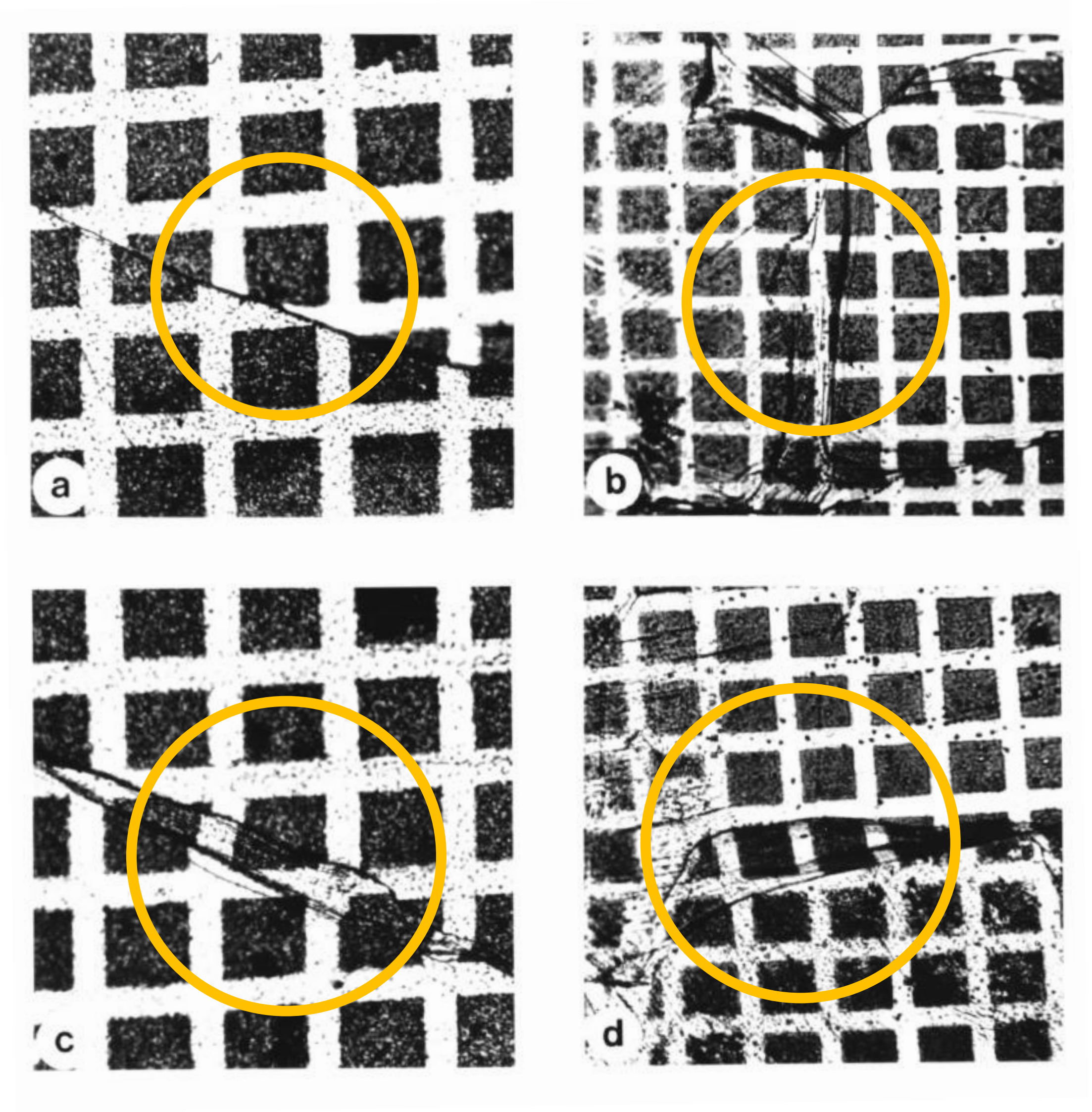
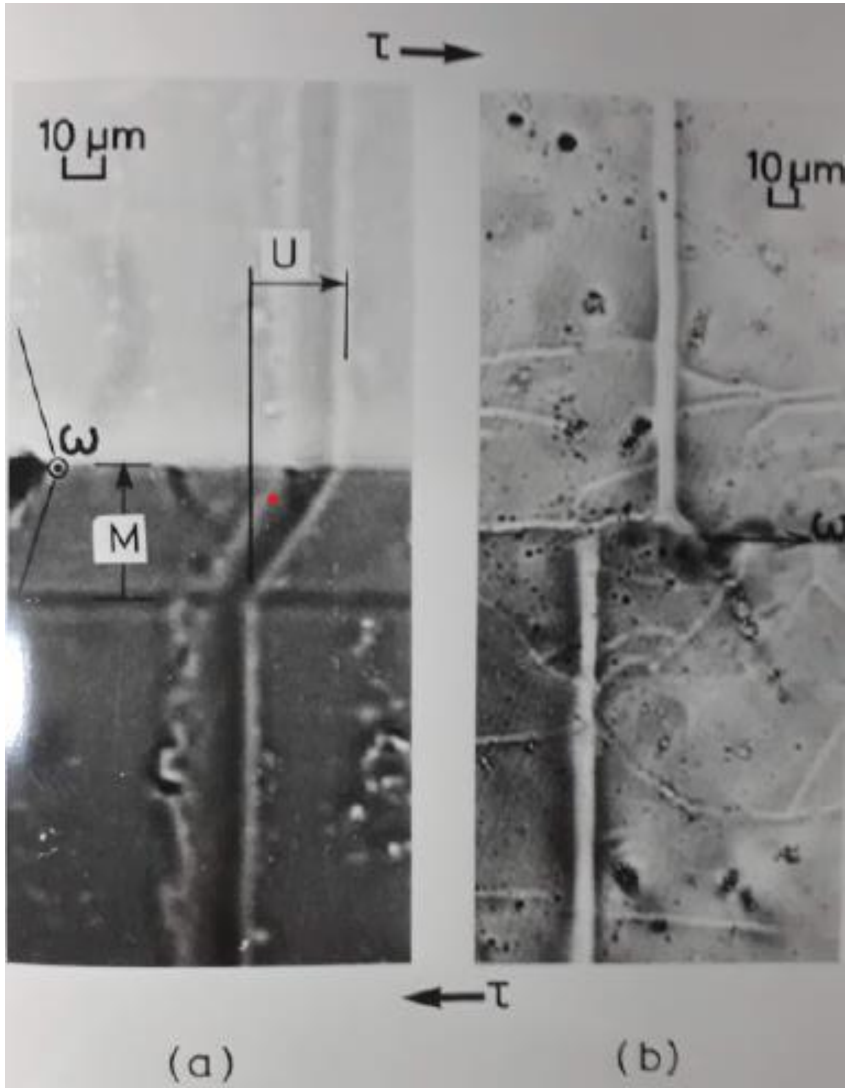


Figure 4. GBS and shear coupled GBM in ice



Two examples of grain boundary displacement in experimentally deformed ice bicrystals, at conditions similar to that found in natural ice.

(a) Simultaneous translation and migration of a boundary under a shear stress, τ, normal to the rotation axis, ω. This corresponds to shear coupled GBM.

(b) Pure sliding under a shear stress, τ, parallel to the rotation axis, ω. This corresponds to GBS.

ω is perpendicular to the plane of viewing in (a) and parallel in (b) so τ is the same direction for image view.

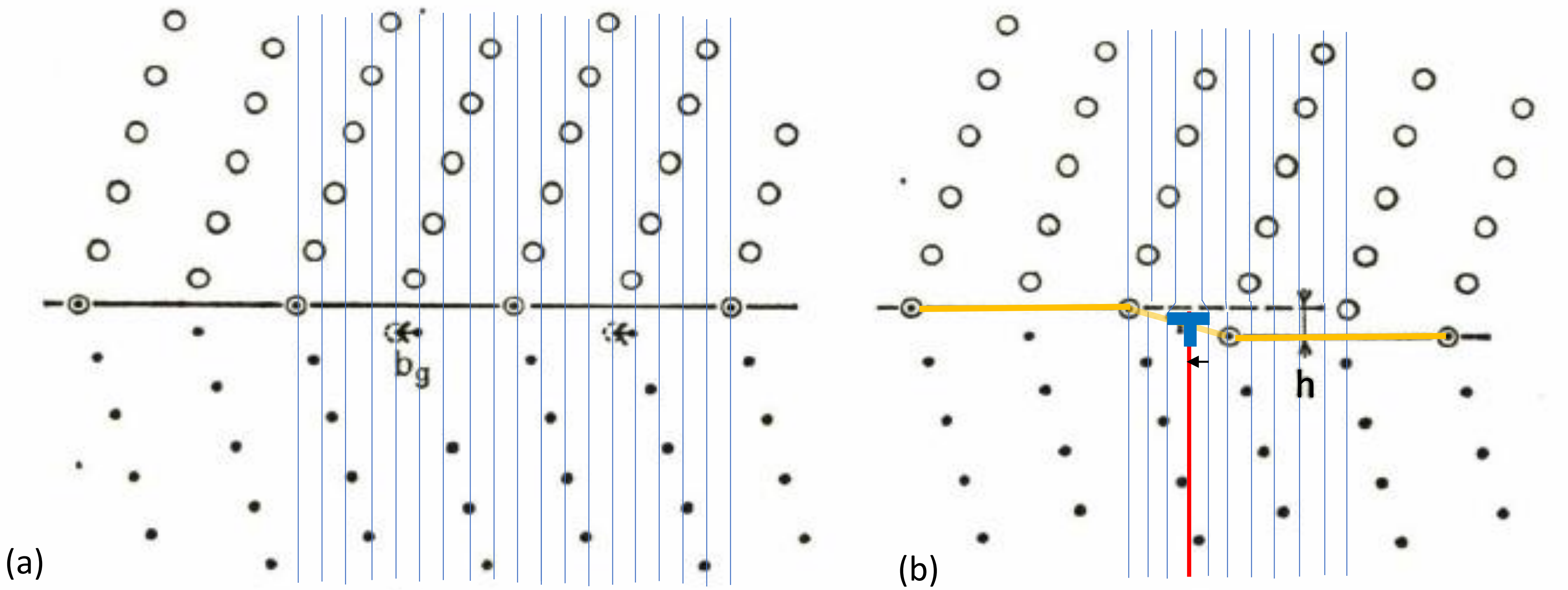
bicrystal rotation, ω, is 34^{o} about <10-10>; applied load 0.1 – 0.2 MPa; temperature -20 ^{o}C [13, 14]

Mechanisms of shear coupled GBM

In low misorientation angle boundaries, the mechanism of SC migration involves cooperative glide of lattice dislocations. At higher misorientations disconnections are involved, which consist of a grain boundary dislocation and step [4, 8b, 8c, 9, 13, 14, 16, 29]. Shear coupled GBM by motion of disconnections has been observed in in-situ studies [30].

Providing there is some form of bicrystal symmetry across a boundary that provides the basis for a disconnection configuration, SC is possible. The displacement shift complete (DSC) lattice is the basis for describing the possible disconnections[8c]. Several disconnections may be possible in any boundary and the one which is activated will depend on several factors, including stress and temperature[4, 5, 8b, 10]. Several coincident site lattice (CSL) structures, with an associated DSC lattice, have been modelled for ice (hexagonal)[13, 14, 17, 18]. Figure 5 shows the boundary structure shown in Figure 4 and the mechanism for shear coupling.

Figure 5: Shear coupled GBM in ice



The shear displacement observed in ice (Figure 4) fits with the disconnection model [13, 14]. (a) CSL model for a 34° tilt boundary in ice. The blue lines are part of the DSC which defines the Burgers vectors of grain boundary dislocations [8c]. (b) A shift of the lower left part of the black lattice by **bg**, produces a disconnection. The extra half plane of the dislocation is shown in red. Motion of the disconnection produces shear and GBM.

Discussion: implications for ice deformation

In polar ice sheets and glaciers grain boundary migration and dynamic recrystallization are important processes[19, 20]. On the grain scale, deformation in ice occurs by basal slip accommodated by non-basal slip and/or by strain accommodation at GBs. Pimenta and Duval [21] proposed that strain accommodation was by GBM, while Goldsby and Kohlstedt [22] proposed strain accommodation was by GBS. Extrapolation of grain size sensitive flow laws imply that GBS is important in polar ice sheets [23, 24], however dominant GBS is not consistent with the strong crystallographic preferred orientations in polar ice [25]. The recognition of SC GBM in ice may resolve this controversy, as migration and sliding can both accommodate strain at grain boundaries and produce a range of grain size sensitive creep regimes in ice.

Studies on SC-GBM [4] show a transition at high homologous temperatures from SC-GBM to GBS. This may be related to a change in boundary defect structure or the onset of pre-melting. The experimental example of SC-GBM in ice bicrystals was at 0.93 Tm. Ice in polar ice sheets is at 0.8-1.0 Tm, with pre-melting occurring around 0.95 Tm, depending on impurity content. This suggests that in ice sheets there may be a transition from SC-GBM in the upper, cold ice to dominant GBS in the hot, deeper ice.

Discussion: shear coupled GBM in minerals

GBS and SC GBM are both plastic modes of deformation that can occur when GBs have an ordered structure. Identifying the atomic structure of the interface is essential to understanding the possible deformation mechanisms. There is now a huge number of molecular dynamics and experimental studies in the materials literature investigating SC-GBM and it's role in creep, recrystallization, grain growth and grain boundary engineering. The role of SC-GBM in minerals is harder to predict and may well be limited by lower crystal symmetry and by the effects of grain boundary fluids. Nevertheless, the role of GBM as a strain accommodation mechanism has been observed in rock analogues[27]. SC-GBM occurs in synthetic rock-salt [9] and has been proposed in olivine [28]. We have shown here that SC GBM also occurs in ice [13, 14] (Figure 4) and we suggest that the mechanism is likely to occur in other cubic, hexagonal and trigonal minerals. Twin boundaries are a well known example of SC in geological materials: other more general boundaries may also shear couple but more research is needed to investigate the deformation conditions where SC-GBM occurs in the Earth.

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