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Large strain shearing of halite: Experimental and theoretical evidence for dynamic texture changes

Hans-Rudolf Wenk [a,*], Marina Armann [b], Luigi Burlini [b], Karsten Kunze [c], Mauro Bortolotti [a]

[a] Department of Earth and Planetary Science, University of California, Berkeley, California 84720, USA
[b] Geological Institute, ETH Zürich, 8092 Zürich, Switzerland
[c] Electron Microscopy (EMEZ), ETH Zürich, 8093 Zürich, Switzerland

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ABSTRACT

We report results from torsion experiments on polycrystalline halite (NaCl) to shear strains $\gamma = 8$ and observe a very complex texture evolution. The same behavior was reproduced with polycrystal plasticity simulations, suggesting that we capture the underlying mechanisms. While crystal shapes gradually rotate into the shear plane, crystal orientations change continuously and dynamic texture patterns evolve with increasing shear. This is highly significant for ultra-large deformation, as for example implied from geodynamic modeling for the deep earth, where seismic anisotropy patterns may develop and locally disappear again as material is deformed during convection. The study also suggests that caution is required when interpreting deformation mechanisms from simple shear preferred orientation patterns.

1. Introduction

Simple shear is important in material science as well as earth sciences. In metallurgy, shear is relevant in high-speed cutting (Dudzinski et al., 2002), in geology it occurs in ductile faults and in geophysics shear is involved in convection in the deep earth. Many aspects remain enigmatic and a combination of large-strain shear experiments combined with numerical modeling provides new insights.

Simple shear deformation is fascinating because, on the crystal lattice scale, all deformation by dislocation glide occurs in simple shear and an arbitrary deformation of a crystal is accommodated by slip on a combination of different slip systems. On a macroscopic scale, incremental simple shear (Fig. 1b) is related to pure shear (Fig. 1a) by a 45° rotation against the sense of shear. At low strains preferred orientation patterns from coaxial pure shear and non-coaxial simple shear show such a relationship. This has been shown not only for fcc metals (Canova et al., 1984; Bolmaro and Kocks, 1992) but also for non-cubic minerals such as olivine (Zhang and Karato, 1995), calcite (Barber et al., 2007) and quartz (Dell Angelo and Tullis, 1989). While the overall deformation and strain on individual crystals may be similar, the strain path is entirely different, with a monoclinic deformation symmetry for simple shear versus orthorhombic symmetry for pure shear. This symmetry is expressed in the preferred orientation patterns.

There are two interpretations for textures produced during simple shear. On the one hand polycrystal plasticity theory predicts crystal lattice rotations, mainly in the sense of shear, due to activity of slip systems and confinements by the surrounding grains. These rotations occur at different speed, depending on the activities and orientation of slip systems. Fig. 2a illustrates lattice rotation increments for a grain of halite during shear deformation to $\gamma = 17.3$ in 2% strain steps. Texture maxima occur where rotations are slowest. There are no stable orientations, in contrast to pure shear or compression (e.g. Wenk et al., 1989a).

On the other hand, an intuitive interpretation suggests that one slip plane aligns with the macroscopic shear plane and a slip direction with the macroscopic shear direction (Schmid et al., 1981). In halite, at low temperature, {110} are the easiest slip planes and $<\bar{1}10>$ the easiest slip directions. Indeed, if all crystals were aligned this way – essentially a single crystal – homogeneous deformation could occur without any rotations and one could use preferred orientations to infer the active slip systems. This "easy slip" interpretation has two main pitfalls: it does not explain how grains reach this orientation; and in most crystals more than one slip system exist, which constantly change their activity due to rotation. With a single slip system one could not deform a polycrystal by dislocation glide without having it break apart. In a cubic crystal such as halite, there are six symmetrically equivalent {110} planes. Torsion deformation experiments on halite to large strains shed new light on whether textures continue to evolve during shear or reach a stable position.

Deformation of halite aggregates has been of longstanding interest, in part sparked by projects to use salt rocks as repositories for nuclear waste (Hwang et al., 1992), CO_2 or gas storage due to its limited permeability. In addition, salt domes represent cap rocks for oil and

* Corresponding author.
E-mail address: wenk@berkeley.edu (H.-R. Wenk).

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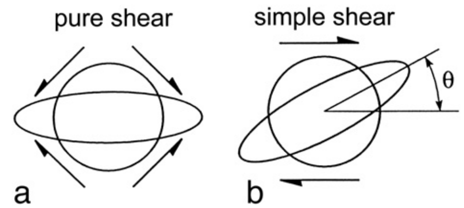

Fig. 1. Relationship of pure shear (a) and simple shear (b). The finite strain ellipse of simple shear is inclined against the ellipse of pure shear against the sense of shear.

gas reservoirs (Jackson and Talbot, 1986; Carter et al., 1993). Our main interest is linked to deep earth rheology since halite has the same structure and similar slip systems as magnesiowüstite, which is a major phase in the lower mantle.

2. Experiments

Experiments on halite single crystals established deformation mechanisms (Carter and Heard, 1970) and deformation experiments on polycrystals documented texture development, mainly in compression geometry (Kern and Braun, 1973; Franssen, 1994), with a few experiments in extension (Skrotzki and Welch, 1983; Lebensohn et al., 2003), pure shear (Skrotzki et al., 1995) and simple shear (Franssen and Spiers, 1990). Interpretation of preferred orientation patterns has relied on comparison of measurements on experimentally deformed samples with polycrystal plasticity simulations. Halite was the first mineral to which the Taylor theory was applied (Taylor, 1938; Siemes, 1974). Application of the viscoplastic self-consistent model to halite deformed in extension revealed differences between the Taylor model that relies on strain compatibility and the self-consistent approach that is closer to stress equilibrium (Wenk et al., 1989b). These differences were further explored by comparison with finite element simulations (Lebensohn et al., 2003). All these experiments and simulations were done to moderate amounts of strain (<100% von Mises equivalent strain ε_{VM}, for definition see Hosford, 2005). However, in the torsion experiments presented here much larger strains were achieved (>600%, i.e. shear $\gamma = \sqrt{3}\ \varepsilon_{VM} = >8$).

Fine grained (150–200 µm) wet (water content ~35 ppm as measured by FTIR at the University of Utrecht) synthetic halite aggregates were prepared by cold pressing and annealing of analytical grade NaCl powder. The water content enhances climb and thus reduces hardening that often leads to early recrystallization (Ter Heege et al., 2005; Pennock et al., 2006). In these experiments we wanted to avoid recrystallization by nucleation as well as grain boundary migration (Humphreys and Hatherly, 1996), in order to concentrate on deformation by dislocation glide. Torsion experiments were carried out in a high pressure/high temperature Paterson deformation apparatus (Paterson and Olgaard, 2000) to large shear strain at a constant temperature of 200 °C, confining pressure of 250 MPa and at two constant twist rates, corresponding to nominal shear strain rates of $\dot{\gamma} = 3\times10^{-3}\ \mathrm{s}^{-1}$ (sample P0742) and $\dot{\gamma} = 3\times10^{-4}\ \mathrm{s}^{-1}$ (all others). In torsion every small volume element of the sample undergoes deformation by simple shear at a constant strain rate. From the deformed samples polished sections were prepared perpendicular to the cylinder radius at the outer sample margin. Textures were measured by electron backscatter diffraction (EBSD) using an EDAX-TSL OIM system with DigiviewFW detector installed on a SEM CamScan CS44LB.

Orientation maps of selected areas near and parallel to the external surface of the deformed samples (where shear deformation is a maximum) illustrate a microstructure with increasingly elongated grains (Fig. 3) with progressive shear from $\gamma = 1$ to $\gamma = 8$. The foliation correlates well with the macroscopic deformation illustrated by strain ellipses. The grain elongation is inclined towards the shear plane with the sense of shear, and the angle is reduced with increasing strain. Deformation is fairly homogeneous but some grains deform more than others, depending on their orientation. This is most pronounced at low strain ($\gamma = 1$, Fig. 3a). The sheared elongated grains contain slip bands and polygonally shaped subgrains. The misorientations between subgrains remain minor (<15°) as indicated by the modest color changes inside the grains in the orientation map (Fig. 3a). With increasing shear strain ($\gamma = 3$), misorientation between subgrains increases with values sometimes exceeding 15°, indicating that subgrains rotate to form new grains, but most original grains are still recognizable (Fig. 3b). With further straining, grains become more elongated, consistent with the finite strain ellipse. In the high shear strain samples ($\gamma = 5$ in Fig. 3c and $\gamma = 8$ in Fig. 3d) subgrain rotation is most pronounced, resulting in an apparent grain-size reduction. However, even at $\gamma = 8$ some original grains are recognizable with distinct color patterns. There is no evidence for nucleation and growth along grain boundaries and little grain boundary migration.

500,000 single orientation measurements over a maximum area of 7×9 mm were then used to calculate an orientation distribution (OD) with 5°×5°×5°cells and smoothing with a 7.5° Gauss filter. From the OD, pole figures were constructed which we apply to display texture development. While the evolution of strain is regular, changes in orientation patterns with shear strain are striking and unexpected (Fig. 4, left side). At low strains, 111 and 110 pole figures have a "hexagonal" appearance with a 111 maximum normal to the shear plane and a 110 maximum in the shear direction ($\gamma = 1$). This distribution attenuates and becomes more asymmetric, with a strong asymmetric 100 maximum ($\gamma = 2$). With increasing strain the 100 maximum rotates towards the shear plane normal, and the 110 maximum in the shear direction increases in strength ($\gamma = 3$ and $\gamma = 6$). At the highest strain ($\gamma = 8$) the preferred orientation can be described as a "rotated cube" with a 100 maximum normal to the shear plane and two {100} maxima at 45° to the shear direction. At all stages of the deformation history, there is a wide spread of orientations, as is obvious from the color differences in the orientation maps (Fig. 3) as well as from the pole figures with many orientations not associated with the maxima (pole figure minima are larger than 0.2 multiples of a random distribution or m.r.d.).

Could the systematic texture changes be due to changes in slip mechanisms? Using the easy slip interpretation we could ascribe the low strain texture to {111}<$\bar{1}$10> slip and the high strain texture to {100}<011> slip. Here polycrystal plasticity simulations to large strains may help us understand.

3. Model

For polycrystal plasticity we used the viscoplastic self-consistent computer code VPSC (Molinari et al., 1987; Lebensohn and Tomé, 1994), modified for large strains. The viscoplastic approach assumes that the strain rate is linked to the stress by a power law. If the stress exponent

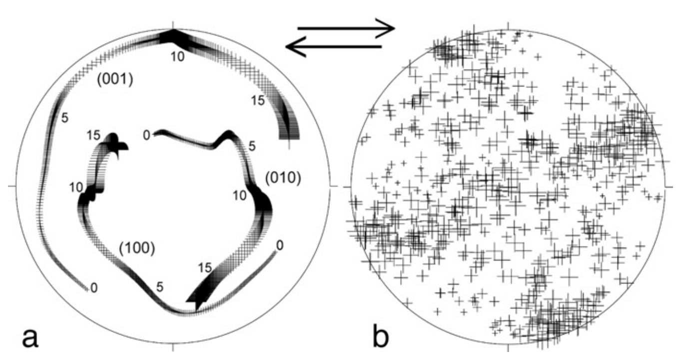

Fig. 2. Viscoplastic simulation of simple shear deformation of halite. (a) Rotation trajectories of {100} poles for a single grain (initial orientation Bunge Euler angles $\phi_1 = 320°$, $\Phi = 75°$ and $\phi_2 = 24°$) to $\varepsilon_{vm} = 10$ ($\gamma = 17.3$) in 0.02 increments. Some shear strain values γ are indicated along the trajectories. Note that the rotations are generally in the sense of shear. (b) {100} pole figure with 200 orientations after $\varepsilon_{vm} = 3$ ($\gamma = 5.1$). Equal area projection, the symbol size is proportional to the grain deformation, the trace of the shear plane is horizontal and shear sense is dextral.