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

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Abstract

We report results from torsion experiments on polycrystalline halite (NaCl) to shear strains γ = 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.

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1. Introduction

Simple shear is important in material science as well as earth sciences. In metallurgy, it is relevant in high-speed cutting (Dudzinski et al., 2002), in geology shear 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; Bolzamo and Kocks, 1992) but also for non-cubic minerals such as olivine (Zhang and Karato, 1995), calcite (Barber et al., 2007) and quartz (Del Ángelo 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 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 γ = 17° 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 <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 slip systems. 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), CO₂ or gas storage due to its limited permeability. In addition, salt domes represent cap rocks for oil and …
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; Lebedsohn 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 (Lebedsohn et al., 2003). All these experiments and simulations were done to moderate amounts of strain (<100% von Mises equivalent strain εVM, for definition see Hosford, 2005). However, in the torsion experiments presented here much larger strains were achieved (>600%, i.e. shear ε = 3εVM ≈ 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 clump and thus reduces the hardness 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 8×10⁻³ s⁻¹ (sample P0742) and 8×10⁻² 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 ε = 1 to ε = 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 (ε = 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 (ε = 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 (ε = 5 in Fig. 3c and ε = 8 in Fig. 3d) subgrain rotation is most pronounced, resulting in an apparent grain-size reduction. However, even at ε = 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 140 × 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 (γ = 1). This distribution attenuates and becomes more asymmetric, with a strong asymmetric 100 maximum (γ = 2). With increasing strain, the 100 maximum rotates towards the shear plane normal and the 110 maximum in the shear direction increases in strength (ε = 3 and ε = 5). At the highest strain (ε = 8), the preferred orientation can be described as a "rotated cube" with a 100 maximum normal to the shear plane and two 100 maximums 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][110]- slip and the high strain texture to [100][111]- 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; Lebedsohn 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 α is between 2 and 3, then the power law can be approximated by a power law with a stress exponent α = 2 (Ashby, 1989). The stress exponent α is between 2 and 3, and the stress exponent β is between 2 and 3 (Ashby, 1989). For a stress exponent α = 2 and a stress exponent β = 3, the linear part of the power law is a straight line with a slope of 1/α. For a stress exponent α = 3 and a stress exponent β = 3, the linear part of the power law is a straight line with a slope of 1/β. For a stress exponent α = 2 and a stress exponent β = 2, the linear part of the power law is a straight line with a slope of 1/α. For a stress exponent α = 3 and a stress exponent β = 2, the linear part of the power law is a straight line with a slope of 1/β. For a stress exponent α = 2 and a stress exponent β = 1, the linear part of the power law is a straight line with a slope of 1/α. For a stress exponent α = 3 and a stress exponent β = 1, the linear part of the power law is a straight line with a slope of 1/β. For a stress exponent α = 2 and a stress exponent β = 0, the linear part of the power law is a straight line with a slope of 1/α. For a stress exponent α = 3 and a stress exponent β = 0, the linear part of the power law is a straight line with a slope of 1/β. For a stress exponent α = 2 and a stress exponent β = -2, the linear part of the power law is a straight line with a slope of 1/α. For a stress exponent α = 3 and a stress exponent β = -2, the linear part of the power law is a straight line with a slope of 1/β. For a stress exponent α = 2 and a stress exponent β = -3, the linear part of the power law is a straight line with a slope of 1/α. For a stress exponent α = 3 and a stress exponent β = -3, the linear part of the power law is a straight line with a slope of 1/β. For a stress exponent α = 2 and a stress exponent β = -4, the linear part of the power law is a straight line with a slope of 1/α. For a stress exponent α = 3 and a stress exponent β = -4, the linear part of the power law is a straight line with a slope of 1/β. For a stress exponent α = 2 and a stress exponent β = -5, the linear part of the power law is a straight line with a slope of 1/α. For a stress exponent α = 3 and a stress exponent β = -5, the linear part of the power law is a straight line with a slope of 1/β. For a stress exponent α = 2 and a stress exponent β = -6, the linear part of the power law is a straight line with a slope of 1/α. For a stress exponent α = 3 and a stress exponent β = -6, the linear part of the power law is a straight line with a slope of 1/β. For a stress exponent α = 2 and a stress exponent β = -7, the linear part of the power law is a straight line with a slope of 1/α. For a stress exponent α = 3 and a stress exponent β = -7, the linear part of the power law is a straight line with a slope of 1/β. For a stress exponent α = 2 and a stress exponent β = -8, the linear part of the power law is a straight line with a slope of 1/α. For a stress exponent α = 3 and a stress exponent β = -8, the linear part of the power law is a straight line with a slope of 1/β. For a stress exponent α = 2 and a stress exponent β = -9, the linear part of the power law is a straight line with a slope of 1/α. For a stress exponent α = 3 and a stress exponent β = -9, the linear part of the power law is a straight line with a slope of 1/β. For a stress exponent α = 2 and a stress exponent β = -10, the linear part of the power law is a straight line with a slope of 1/α. For a stress exponent α = 3 and a stress exponent β = -10, the linear part of the power law is a straight line with a slope of 1/β.
random orientations were simulated to deform in 1000 steps with a mimicks subgrain formation with increasing misorientations. 2000 updated until they reach an aspect ratio (long to short axis) of 4. This assume that no work hardening occurs and that grain shapes are only (strain rate sensitivity 1/8=). For input of the plasticity model we need to know slip systems, their differences in orientation and grain deformation. The individual orientations at various strain steps were transformed into an OD and from this, pole figures were calculated, similar to the procedure with EBSD measurements. These pole figures on the right side of Fig. 4 illustrate simulated texture changes with increasing strain. The simulated pole figures show a similar transition from a texture with 111 normal to the shear plane and 110 in the shear direction to a texture with 110 normal to the shear plane and 110 in the shear direction, just as in the experiments. In addition to texture patterns, the simulations also provide information about mechanisms and they can be extended to much larger strains than attained in the experiments.

4. Discussion

A detailed analysis reveals that during the whole strain history, an average of 4-6 individual slip systems are active in each grain (with an strain increment of 0.02, resulting in a final von Mises equivalent strain of $\gamma_{VM}=20$ (in plane strain), corresponding to a shear $\gamma=3$ $\gamma_{VM}=28$. To our knowledge these are some of the largest strain texture simulations that have been performed. The results are fairly robust to minor changes in the assumed parameters and here we are interested in the overall pattern. For the same conditions, we performed both self-consistent simulations and Taylor simulations and results are similar. It appears, based on details of the texture patterns, that initially the self-consistent deformation is more applicable, i.e. grains deform differently, depending on orientation, to maintain stress equilibrium. With increasing strain the Taylor model describes details better and homogeneous deformation is approached, with all grains of similar shape.

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Fig. 4. Pole figures of halite deformed in simple shear. (left) EBSD measurements on samples from torsion experiments at 200 °C. (right) Polycrystal plasticity simulations, starting with self-consistent assumption (50% and 100%) and continuing with homogeneous strain at higher deformation. Equal area projection, linear contour intervals. The trace of the shear plane is horizontal and shear sense is dextral.

Fig. 5. Viscoplastic polycrystal plasticity simulation of large strain simple shear deformation of halite to γ=35. Bottom shows activity of slip systems (in %), and above some {100} pole figures and plots of main grain elongation axes. The trace of the shear plane is horizontal and shear sense is dextral.

activity of > 5%), two or more of which contribute more than 20% to the
strain in most grains. Initially (in the random aggregate) 54% of the
strain is accommodated by the easiest (110) systems, 36% by (111)-slip
and 10% by the hardest (100) systems (Fig. 5). From the texture pattern
(Fig. 4, γ = 0.9) we could have guessed that (111)-T10- slip is mainly
active because (111) planes are preferentially oriented in the shear
plane, which is clearly not the case. As texture evolves (110) slip
becomes less favored and already at γ = 3.5 activity drops below 20%,
while activity on the harder (111) and (100) systems steadily increases
(to > 50% for (111) and 35% for (100)). At γ = 5, the “rotated cube
texture”, the dominant slip system (> 50%) is (111)-T10- and thus the
rotated cube texture is not due to prevailing (100)-011- slip as one
may have intuitively suspected. A surprising conclusion is that large
strain simple shear experiments can be misleading when it comes to
the interpretation of slip systems from texture patterns. If the goal of
an experiment is to infer slip systems from preferred orientation, low
strain compression experiments are more relevant than high strain
torsion experiments.

The study also highlights differences between shape changes and
orientation changes during simple shear deformation. As deformation
proceeds, grains become increasingly stretched and the long axes rotate
towards the shear direction, both observed in experiments (Fig. 3) and in
simulations (grain major axis “pole figures” are illustrated in Fig. 5,
bottom). With increasing deformation, grain shape axes cease rotating,
while crystallographic orientations continue to change. From γ < 0 to
γ = 5 the lattice of most grains rotates by over 90° (Fig. 2a), and this
spinning continues with increasing strain. Slip planes do not rotate into
the shear plane and stay there, yet their rotation rates decelerate. This is
most striking when viewed in a movie of texture evolution displaying
the continuous rotations and changes in patterns during deformation to
a shear γ = 35 (supplementary material). Some snapshots of the movie
are shown in Fig. 5 (top), illustrating that texture strength increases and
then attenuates in repeating cycles. Because of the lattice rotations,
simple shear textures never become exceedingly strong. The “tumbling”
of orientations is more rapid for higher strain rate sensitivity (lower
stress exponent) (Toth et al., 1988). It is also more pronounced if many
slip systems are available, as in cubic crystals but applies to all materials
that deform by dislocation glide, including quartz (Wenk et al., 1989a).

High shear/high temperature deformation experiments on per-
close (MgO), which is isostructural with halite and has similar slip
systems, produced similar textures to those for halite, though in some
cases the material recrystallized (Yamazaki and Karato, 2002;
Heidelbach et al., 2003). Magnesiowüstite (MgFeO, one of the
important minerals of the lower mantle, is much weaker than the
primary lower mantle minerals perovskite and postperovskite (Long
et al., 2006) and may control the rheology in the deep Earth.
Geodynamic convection simulations suggest that during slab subduc-
tion into the lower mantle, very large strains accrue and much of it in
simple shear (McNamara et al., 2002; Wenk et al., 2006). Furthermore,
at deep earth conditions, materials are highly rate sensitive and thus
orientation patterns may continuously evolve, without reaching a
steady state or producing strong texture patterns. We have calculated
MgO P-wave velocity surfaces corresponding to the simple shear
textures in Fig. 5, by averaging single crystal elastic properties of MgO
(at lower mantle conditions over the OD, and this illustrates cycles of
anisotropy development followed by attenuation (Fig. 6). This may be
a reason for the overall weak seismic anisotropy in the lower mantle
(Garnero et al., 2004) and for local heterogeneity (e.g. in the D” zone
(Lay et al., 1998; Panning and Romanowicz, 2004; Sidorin et al., 1999)).

5. Conclusions

Fabric development in simple shear is not monotonic and thus
cannot be extrapolated. Simple shear deformation experiments on
halite to large strains and polycrystal plasticity modeling illustrate
that emerging orientation distributions are complex, with dynamic
changes as deformation proceeds and no convergence into strong
texture patterns. Individual grains do not rotate into “easy slip”
orientations and thus shear experiments are inadequate to infer slip
systems. The results illustrated for halite are directly applicable to
cubic metals as well as the lower mantle mineral magnesiowüstite. In
the deep earth, simple shear deformation, compounded by recrys-
tallization (Wenk et al., 1997), may produce heterogeneous and not
to very strong texture patterns and thus only local and weak anisotropy.

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Fig. 6. P-wave velocity surfaces for MgO assuming texture patterns shown in the pole figures of Fig. 5 (top). Note the cyclical development and attenuation of anisotropy. Equal area projection. The trace of the shear plane horizontal. Velocity contours in 10 km/s.
Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.epsl.2009.01.036.

References


Schmidt, H.C., Casey, M., Starkey, J., 1981. An illustration of the advantage of complete texture analysis described by the orientation distribution function (ODF) using quartz pole figure data. Tectonophysics 78, 101–117.


