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Deformation behaviour and elastic properties of gypsum polycrystals: implications for lithosphere-scale geological processes

Gypsum plays an important role in many lithosphere-scale geological processes. We used neutron diffraction to perform quantitative texture analysis on a set of gypsum samples deformed over a range of well-characterised conditions. The resulting pole figures provide a better understanding of the deformation behaviour of gypsum and enable it to be defined in terms of active deformation mechanisms. Moreover they allow the calculation of elastic properties to be made, which helps with the geophysical interpretation of seismological investigations on a lithosphere-scale.

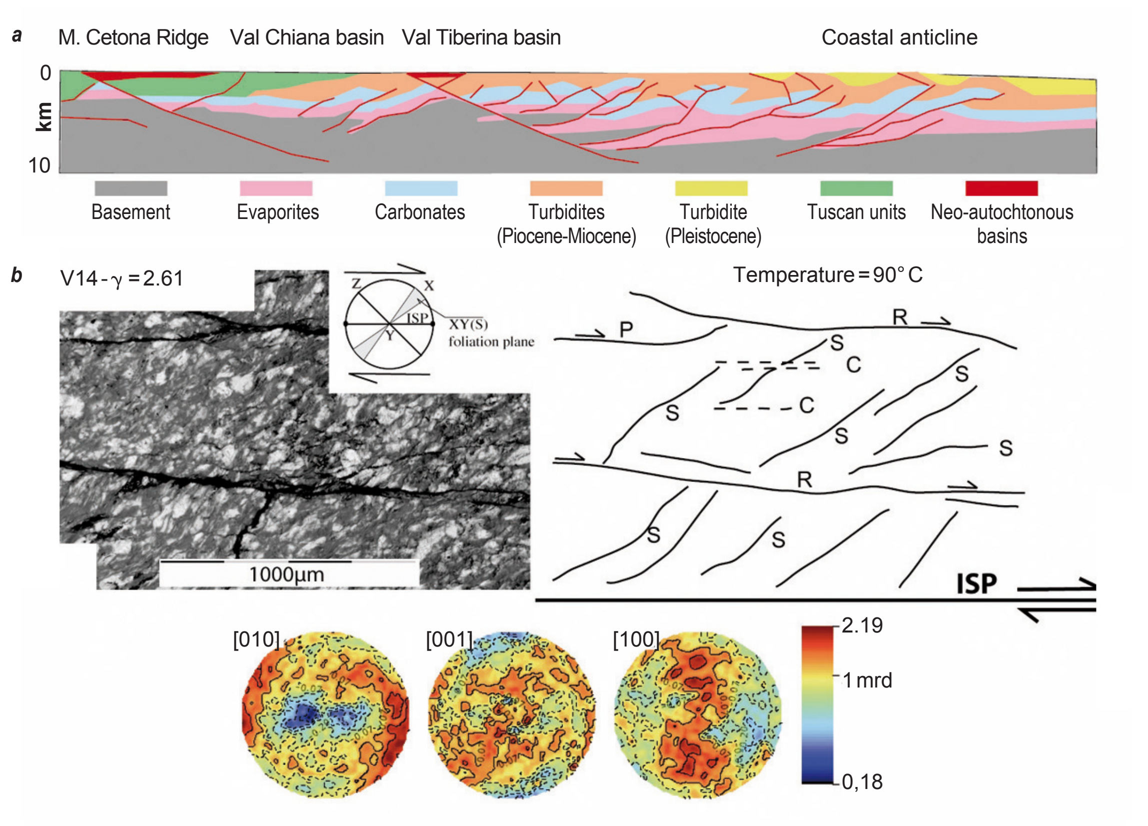

Figure 1: ***(a)*** *An example of the occurrence of evaporites within sedimentary sequences involved in tectonic processes. Geological interpretation of the seismic reflection line CROP-03, from Mount Cetona to the Adriatic Sea [2]. Evaporites are in pink.* ***(b)*** *Microphotograph image of the sample V14, experimentally deformed at strain rate (γ) = 2.61; X, Y, Z represent principal orientations of the rock samples, defined by the maximum (X), intermediate and minimum (Z) direction of alignment of gypsum grains, where the S (foliation) plane corresponds to the plane containing the X and Y directions. Schematic representation of microstructures developed during torsion deformation with the Imposed Shear Plane (ISP), where P-R-S-C planes are shear planes marked by micro-fractures or by shape preferred orientation of gypsum grains. Main axes pole figures obtained from the analysis of D20 neutron data performed with MAUD are shown at the bottom.*

Gypsum, together with halite and anhydrite, is the main rock-forming mineral of evaporitic rocks. Evaporites, interlayered within sedimentary sequences (**figure 1**), play an important role in localising deformation: evaporitic levels have often been found in horizontal layers where the deformation of rocks localises and permit lower strata to be thrust over those above [1].

A good knowledge of the mechanical behaviour and elastic properties of evaporites is of great importance in several fields: in the oil industry, because evaporites often form the cap of oil and gas reservoirs; in environmental management, where rock salt formations are being considered for nuclear waste disposal and depleted hydrocarbon reservoirs for gas storage (e.g. CO_2, H_2S). Once the mechanical properties have been rationalised, numerical modelling may be used to explore geological systems in which they play a role – for example the Northern Apennines extensional system (**figure 1a**) where deformation within evaporitic layers is accompanied by seismic activity [2].

One way to study deformation behaviour and elastic properties of rocks within the Earth's lithosphere is to perform laboratory experiments in which known conditions of, for example, confining pressure, temperature, differential stress, pore pressure are imposed on a rock sample and measurements are made of its deformation and the velocity of seismic waves, both P ('primary' or compressional) and S ('secondary' or shear). Such experiments, carried out over the last few decades, have widely demonstrated that texture is one of the most important intrinsic rock properties (together with mineralogical composition) controlling deformation behaviour and elastic properties; it is also important in understanding many other properties of rocks, including magnetic and electrical. Here we report quantitative texture analysis of experimentally deformed gypsum rock by neutron scattering and show that the elastic properties differ between single-crystal and polycrystalline aggregate samples.

The gypsum samples studied are cores about 9 mm thick and 7-15 mm long obtained from natural gypsum (gypsum > 99%) deformed in torsion experiments up to high shear strain values (up to $\gamma = 5$), at confining pressure of 300 MPa and at various temperatures (from 70°C to 90°C) and strain rates (between 10^{-3} and $10^{-5}s^{-1}$).
A complete texture characterisation could be completed in 4 hours for a 1 cm^3 volume of rock. Although this is relatively small, it is still much larger than the volume that could be analysed with any other analytical technique. The measurements were made with the D20 instrument whose detector spans a 2θ range of 153.6° with a resolution of 0.1°, and the neutron wavelength was 2.41 Å. An Eulerian cradle allows rotation about the χ and φ angles. Scans were operated from $\chi = 0$ to 90° (with a 5° step) using a fixed incidence angle ω of 10° (corresponding to the (020) Bragg position of gypsum) and from $\varphi = 0$ to 355° (also with a 5° step). Each diffraction pattern was collected for 4 seconds and quantitative texture analysis was performed using the Rietveld based programme MAUD [3].

Figure 1b shows an example of a pole figure obtained in this manner for gypsum. Pole figures are very useful in their own right, as they help to relate the deformation mechanisms that are active or dominant under specific conditions (e.g. pressure, temperature, deviatoric stress) to the evolution of the preferred orientations of grains or crystallites in the sample. But that is not all. The full set of information obtained from quantitative texture analysis i.e. the Orientation Distribution Function (ODF), derived from the pole figure, can be used as input data to calculate many properties, such as elastic macroscopic tensors (from which derive the P and S wave velocity and anisotropy), provided we know the single crystal tensor of the property we want to investigate and the abundance of different minerals (if we are dealing with polymineralic rocks). We investigated the relations between our quantitative texture analysis and seismic velocities.
Figure 2 shows the wave velocity distribution for the P (compressional) mode (Vp) and the two S (shear) modes S1 and D2 (velocities S1 and S2 respectively) within one of the samples studied, calculated with the software BEARTEX [4] using the ODF, refined from the pole figures of **figure 1** using MAUD [3].

In a single crystal of gypsum (**Table 1**), the largest diagonal components of the elastic stiffness tensor are c_{11} and c_{33}. Consequently, the velocities of the P waves are higher in the 100 and 001 crystallographic directions, and lower in the 010 direction (**figure 2**); however, the Vp anisotropy is small since the 3 diagonal components of the tensor are similar.

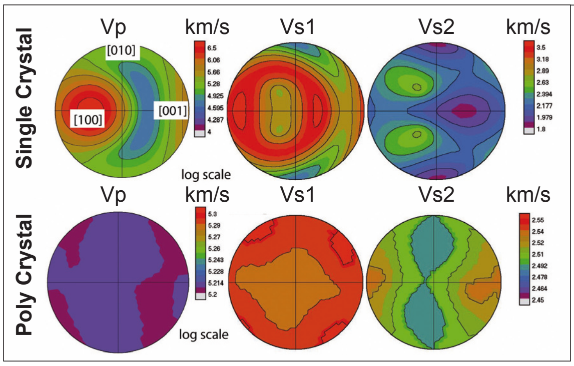

Figure 2: *Distribution of P and S wave velocities obtained from the calculation with BEARTEX. Respectively, Vp, Vs1 and Vs2. Input data for this calculation are the elastic stiffness tensor for gypsum single crystal and the ODF obtained from **figure 1**.*

In our polycrystals, since the crystallographic preferred orientation (i.e. texture) is not very strong (**figure 1b**), a further smoothing of the seismic anisotropy is produced. This is what is shown in the values for calculated velocities of P waves in the region of 5.2-5.3 km/s, whatever the direction of the pole figure. For S waves a slightly larger anisotropy is shown, because the off diagonal values and the diagonal components c_{44}-c_{66} are more different from each other, compared to c_{11}, c_{22} and c_{33} (**Table 1**).

Textured polycrystalline gypsum aggregates show seismic anisotropy that is different from that predicted from the properties of the single-crystal model, and which is widely used for the interpretation of deep seismic data. The elastic tensor produced by quantitative texture analysis may correct this error and improve our knowledge of lithosphere-scale geological processes.

Single Crystal					
78.60	41.00	26.80	0.00	-7.00	0.00
41.00	62.70	24.20	0.00	3.10	0.00
26.80	24.20	72.60	0.00	-17.40	0.00
0.00	0.00	0.00	9.10	0.00	-1.60
-7.00	3.10	-17.40	0.00	26.40	0.00
0.00	0.00	0.00	-1.60	0.00	10.40

Poly Crystal					
62.91	32.79	33.16	-0.03	0.00	-0.02
32.79	62.93	34.11	0.00	-0.22	0.01
33.16	34.11	62.97	0.01	-0.02	0.11
-0.03	0.00	0.01	14.50	0.00	0.10
0.00	-0.22	-0.02	0.00	14.85	0.01
-0.02	0.01	0.11	0.10	0.01	15.01

Table 1: *Elastic stiffness tensor for a single crystal of gypsum and the corresponding geometric homogenised tensor for polycrystalline gypsum; polycrystalline gypsum tensor components were calculated using the ODF obtained from quantitative texture analysis. The values correspond to the elements of the tensors C_{ij}, where i and j are from 1 to 6, and are in GPa.*

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