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Data Article

Crystallographic orientation and grain size data obtained by Electron Back Scatter Diffraction (EBSD) on quartz analysed in mylonitic quartzite from the Island of Elba (Italy)

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ABSTRACT

Raw Electron Back Scatter Diffraction (EBSD) data on deformed quartz from a mylonitic quartzite sample of the Calamita Schists (Island of Elba, Italy) is available at https://doi.org/10.17632/8c937t6zs4.32. The investigated sample (IESP3SP78) was collected in quartz-rich outcrops exposed at the Praticciolo Cape and was used to realize an oriented thin section (cut parallel to lineation and perpendicular to foliation). Preliminary investigations were carried out by transmitted-light and scanning electron microscopy (SEM), in order to select key areas for EBSD analysis. EBSD mapping was performed on selected areas of deformed quartz, which was the only phase indexed and were processed to derive orientation maps, pole figures, inverse pole figures, misorientation axis distribution in sample and crystal coordinates. While the processed data is available on the original research article ("Fluid-assisted Strain Localization in Quartz at the Brittle/Ductile Transition"; https://doi.org/10.1029/2019GC008270), this contribution is devoted to supply the unprocessed EBSD data, together with a methodological description, aimed to allow the reproduction of the processed dataset. A brief statistical description of the investigated EBSD maps is also available. This data is valuable because it offers grain size and orientation analysis of deformed quartz investigated in a

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natural study case and the present publication makes it accessible to those working on naturally and experimentally deformed quartz.

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Specifications Table

Subject	Geology
Specific subject area	Mineral and rock physics
Type of data	Table Image Chart Graph
How data were acquired	EBSD [(1) JEOL 6610 LV SEM equipped with a NordLys Nano EBSD detector and a (2) JEOL 7001 FEG SEM equipped with a NordLys Max EBSD detector]
Data format	Raw Analyzed
Parameters for data collection	EBSD maps were collected using a 20–25-mm working distance, 70° of sample tilt with respect to the horizontal and accelerating voltage set at 20 keV.
Description of data collection	EBSD patterns were automatically detected and indexed with the software AZTec (Oxford Instruments). Noise reduction was performed using the HKL CHANNEL 5 software (Oxford Instruments).
Data source location	Calamita Schists, Praticciolo Cape, Island of Elba, Italy.
Data accessibility	Mendeley Data https://doi.org/10.17632/8c937t6zs4.32
Related research article	Papeschi, S., Musumeci, G., Fluid assisted strain localization in quartz at the brittle/ductile transition, Geochemistry, Geophysics, Geosystems 20 (2019) 3044–3064. https://doi.org/10.1029/2019GC008270

Value of the Data

- The presented EBSD data, collected on naturally deformed quartz is useful for comparison with other EBSD data on experimentally and naturally deformed quartz.
- This data is useful for structural geologists working on quartz-rich mylonitic rocks and deformed quartz.
- This data includes grain size and crystallographic orientation of quartz grains which may be useful for review studies and global compilations of the distribution and orientation of recrystallized and relic grains.
- The dataset provided includes raw data which can be re-interpreted or analysed through different noise-reduction routines.

1. Data

Raw Electron Back Scatter Diffraction (EBSD) data for three EBSD maps collected on quartz-rich layers on a representative sample of mylonitic quartzite (label: IESP3SP78) from the Calamita Schists (Island of Elba, Italy) are provided. The sample is registered on System for Earth Sample Registration (SESAR) at http://www.geosamples.org/and labelled in agreement with SESAR registration requirements. Further details (location, GPS coordinates, and microphotographs) of the sample IESP3SP78 are directly accessible at https://app.geosamples.org/sample/igsn/IESP3SP78. The dataset containing the EBSD data acquired on IESP3SP78 is provided on Mendeley Data (https://doi.org/10.17632/8c937t6zs4.3) and includes the core files of the EBSD maps (.cpr and.crc files, acquired by

AZTEC) and a folder with full thin section scans of the investigated sample at parallel and crossed polarized light, showing the location of the areas selected for EBSD mapping. In this manuscript we refer to the EBSD maps acquired as Map 1, Map 2 and Map 3, following the nomenclature established in the associated research article [1].

1.1. Map 1: subparallel quartz layers

Map 1 was acquired in a recrystallized quartz layer elongated parallel to the mylonitic foliation. The mapped microstructure is dominated by small (10–100-μm) recrystallized quartz grains with serrated grain boundaries surrounding sparse quartz porphyroclasts (up to 500 μm) with lobate boundaries and amoeboid shape. The mapped area is shown in Fig. 3a in Ref. [1] and the interpreted EBSD map and related pole figures are shown in Fig. 4 in Ref. [1].

1.2. Map 2: conjugate shear bands

Map 2 is located within a coarse-grained quartz layer (grain size > 500 μm) at the intersection of two conjugate shear bands, marked by quartz grains with grain size < 100 μm. Fractures are present in coarse-grained quartz, while small grains display serrated grain boundaries. The mapped area is shown in Fig. 3b in Ref. [1] and the interpreted EBSD map and related pole figures are shown in Figs. 6–7 in Ref. [1].

1.3. Map 3: synthetic shear bands

Large areas of the sample are characterized by shear bands that are synthetic with the sense of shear and make a 30–35° angle with respect to the foliation. A representative EBSD map (Map 3) has been acquired on two, paired East-verging shear bands that crosscuts quartz layers with variable grain size and serrated grain boundaries and are characterized by phyllosilicates (white mica and chlorite) and small quartz grains localized on the shear band planes. The location of the mapped area is shown in Fig. 3c in Ref. [1] and the interpreted EBSD map and related pole figures are available in Fig. 8 of [1].

2. Experimental design, materials, and methods

2.1. Field sampling

Sample IESP3SP78 (nomenclature following the SESAR database: http://www.geosamples.org/)was collected at an outcrop of quartz-rich rocks exposed at the Praticciolo Cape in SE Island of Elba (Fig. 1a). The location of the sample is shown on satellite image in Fig. 1b, while Fig. 1c and d shows the outcrop where the sample was collected. The rocks exposed in this area belong to the Calamita Schists, a complex of metapelite and metapsammite defined by Barberi and co-workers [2]. The outcrop is characterized by mylonitic quartzite and quartz-rich mylonitic micaschist containing biotite, andalusite, cordierite, K-feldspar and plagioclase, strongly overprinted by retrograde chlorite and phengite. As shown in Fig. 1c, the exposed rocks present a penetrative mesoscale foliation that dips to SW. The sample was collected based on the presence of conjugate shear bands at outcrop scale (Fig. 1d). In detail, sample IESP3SP78 is a mylonitic quartzite containing quartz (70–80%), sericite, and chlorite, and strongly-retrogressed relics of biotite, andalusite, cordierite, and K-feldspar. The general structure is characterized by lenses/layers of quartz (thickness: 100–500 μm) interlayered with thin, phyllosilicates-rich layers (~10–100 μm in thickness). A detailed description of the sample microstructures is available in Ref. [1].

2.2. Thin section preparation

An oriented polished thin section was realized on a slab of the sample cut parallel to the lineation, marked by mineral aggregates and quartz fibres, and perpendicular to the mesoscopic foliation. Cutting

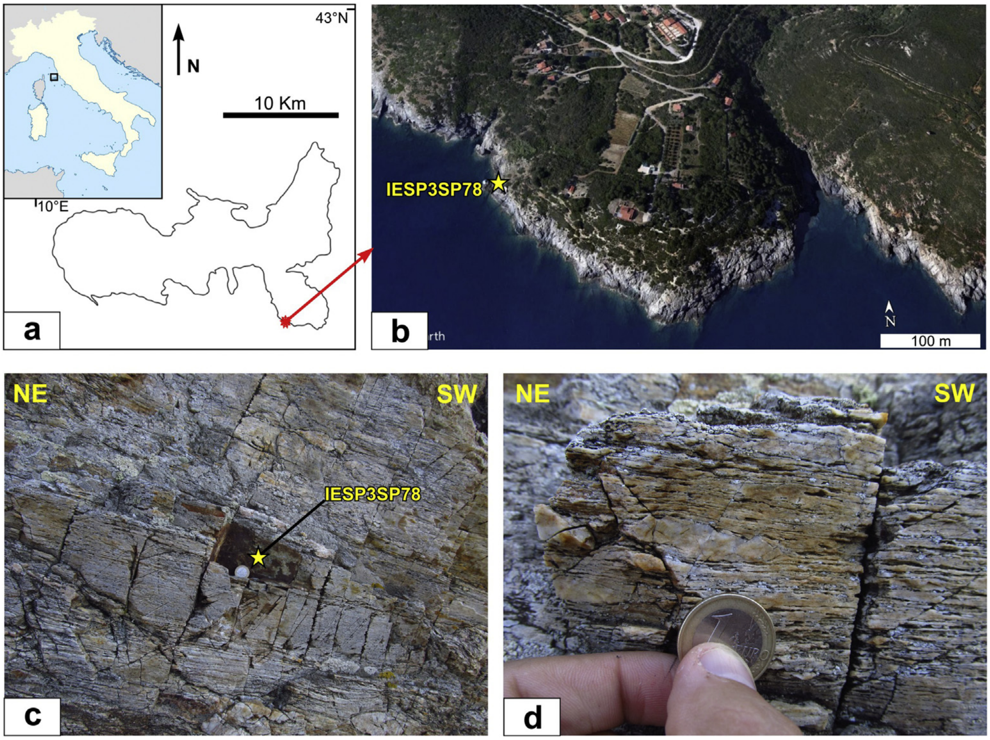

Fig. 1. Field location of the key sample investigated in this study (IESP3SP78) – **(a)** Location of the investigated area (images after wikimedia.commons) and **(b)** Satellite image of the Praticciolo Cape showing the position of the sample (© Google Earth, 2003; retrieved from https://tinyurl.com/y2moluwz). **(c)** Mesoscale view of the outcrop where the sample was collected (yellow star) and **(d)** detail of deformed quartz layers with conjugate shear bands.

and thin section preparation was performed by TS Lab & Geoservices (Navacchio, Italy). Preliminary petrographic investigations and selection of EBSD areas on the thin section were carried out at the microstructural lab of the Department of Earth Sciences in Pisa (resp. G. Musumeci) and at the National Institute for Geophysics and Volcanology (Pisa, Italy)using a ZEISS-EVO Scanning Electron Microscope (SEM) equipped with an Oxford Instruments EDS detector.

The polished thin section was then smoothed using an alkaloid colloidal suspension (SYTON) with a Buehler Vibromet 2 for at least 3 hours and then carbon coated to about 3.5-nm thickness at the University of Plymouth (U.K.).

2.3. *Electron Back Scatter Diffraction: acquisition and processing*

Electron Back Scatter Diffraction (EBSD) mapping was carried out at the Electron Microscopy Centre of Plymouth University with a (1) JEOL 6610 LV SEM equipped with a NordLys Nano EBSD detector and a (2) JEOL 7001 FEG SEM equipped with a NordLys Max EBSD detector. The analytical configuration for EBSD mapping was 20–25-mm working distance, 70° of sample tilt with respect to the horizontal and 20 KeV of accelerating voltage. The sample symmetry used was monoclinic, and quartz was the only phase indexed, using trigonal crystal system (Laue group 3/m). EBSD patterns were automatically detected and indexed with AZTec software (Oxford Instruments). Map 1 is a 414 × 310 pixel map acquired with a step of 2.4 μm, Map 2 has a size of 1237 × 927 pixels and was acquired with a step size of 1.1 μm, and Map 3 is 585 × 438 pixels and has a step of 1.3 μm.

Noise reduction, following Bestmann and Prior [3], was performed using HKL CHANNEL 5 software by Oxford Instruments, as following: (1) wild spikes, resulting from misindexing problems (pixels with

Table 1
Grain size statistics of EBSD areas. **EX**: average, expectation; **D^2X**: variance, dispersion; **σ**: standard deviation; **σ/EX**: coefficient of variation; **Xmin**: minimum equivalent diameter value (μm); **Xmax**: maximum equivalent diameter value (μm); **N**: number of detected grains.

Map	EX	D^2X	σ	σ/EX	median	mode	Xmin	Xmax	N
Map 1	20.498	347.95	18.653	0.9100	15.791	7.660	7.165	335.39	890
Map 2	12.965	377.2	19.422	1.498	9.205	3.044	3.0403	612.31	1625
Map 3	13.985	121.76	11.034	0.789	10.779	4.149	4.149	103.98	958

exotic orientation with respect to the surrounding crystal lattice) were corrected by extrapolation (2) zero solution pixels (i.e. pixels that were not indexed); are corrected by extrapolating their orientation from the neighboring pixels and then by iteration (progressively increasing the filtering level from 8 to 5 in Channel 5).

High-angle boundaries were defined at a critical misorientation of 10° and above, allowing grain boundary completion down to 0°, while low-angle boundaries were set for a critical misorientation of 2–10°. The use of a higher symmetry for quartz (3/m instead of 32 Laue group) allows to recognize Dauphiné twin boundaries (twinning between right-handed and left-handed quartz) as grain boundaries with 60° ± 2° of misorientation and <c> as misorientation axis and to disregard them from the grain detection routine. The grain size detection routine of Channel 5 (Tango software) recalculates grain diameters in μm from equivalent-area circles (μm^2). Grains measuring less than 3 times the step size (i.e., containing less than 4–9 pixels) were nullified, as they could represent artifacts generated by the noise reduction routine. Grain size statistics of the processed dataset are available in Table 1.

2.4. Analysis of the processed EBSD dataset

The processed dataset was used to derive (1) orientation maps, colored according to inverse pole figures, (2) pole figures, (3) misorientation axis distribution in sample coordinates and (4) crystal coordinates, all available in [1]. The processed dataset was further divided into subsets according to grain size, orientation and microstructural position.

Orientation maps were colored according to the inverse pole figure of quartz oriented parallel to Y (vertical axis of the Map; corresponding to the Z axis of the finite strain ellipsoid of the sample). Low-angle boundaries are shown in white, high-angle boundaries in black and Dauphiné twin boundaries in red [1]. Inverse pole figures and misorientation axis distributions in crystal coordinates (MOCC) were plotted as equal area, upper hemisphere projections, while pole figures and misorientation axis distributions in sample coordinates as equal area, lower hemisphere projections, using Mambo (Channel 5 software suite). Except for subsets containing relatively small populations of large grains, where plotting all the indexed points in pole figures is useful to visualize the distortion of the crystal lattice, contoured pole figures were realixed on one-point-per grain subsets using 10° half width and 10° cluster size with density shown as multiples of a uniform distribution. The same contouring scheme has been applied to misorientation axis distributions in sample and crystal coordinates.

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Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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