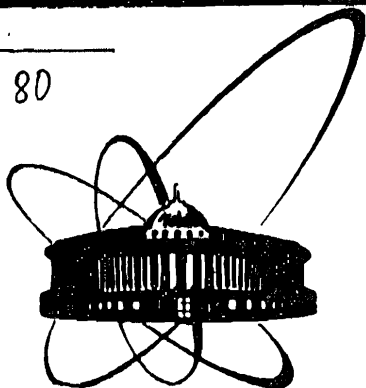


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K.Walther**

**NEUTRONOGRAPHIC FABRIC ANALYSIS  
OF QUARTZ  
IN NATURALLY DEFORMED GNEISS**

Submitted to "Texture and  
Microstructures"

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**1987**

Dedicated to the memory  
of Prof. Dr. Günter Wassermann

## Introduction

The orientation distribution of crystallites in tectonites contains valuable information on deformation processes which have taken place in the Earth's crust. Comparing the preferred orientations in naturally deformed rocks with the results from experimentally deformed material and computer simulations of deformation process, the data can be used to estimate the regime of temperature, pressure, stress and strain as well as the preferred operating mechanisms of deformation which were active in the investigated matter. Therefore, important information for petrofabric analysis can be expected from the accurate and complete description of the relation between crystal and specimen orientations. In this sense, the determination of the orientation distribution function (ODF) is favoured in comparison with fabric diagram measurements like those known in structural geology. The reproduction of the ODF from pole figure data, determined by neutron or X-ray diffraction, is a very straightforward way to calculate this function.

In the last years some preferred orientation studies carried out on this base in different geological materials have been reported<sup>/1-4/</sup>.

In this paper the partial texture of quartz in orthogneisses from the middle Erzgebirge (GDR) is studied. The sample has been taken from the very crest of a recumbent fold structure. All pole figure measurements were carried out using neutron time-of-flight (TOF) diffraction at the pulsed reactor IBR-2 in Dubna<sup>/5,6/</sup>. This method is well suited for the investigation of low symmetric crystal systems like quartz because of simultaneous measuring of several pole figures. Furthermore, this technique allows one to study natural multiphased aggregates with sufficient accuracy<sup>/7/</sup>. The ODF reproduction from experimental pole figures and the determination of recalculated and inverse pole figures have been done by means of spherical harmonics analysis<sup>/8,9/</sup>.

## Geological background and specimen characterization

In the present paper the structural evolution is started to investigate within a folded complex being typical for the upper part of the Earth's crust (5 km depth). From the structural geological point of view this deformation consists in an intensely asymmetric folding of a parallel system of planes (crystalline schistosity,  $sk_1$ ). As a result of this folding a younger crys-

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talline schistosity ( $sk_2$ ) is formed nearly parallel to the orientation of the axial plane of the folds connected with intimate crenulation of the older schistosity ( $sk_1$ ) near the crest of the folds having pencil structures (b-tectonites) in the very crest of the folds (see fig. 1).

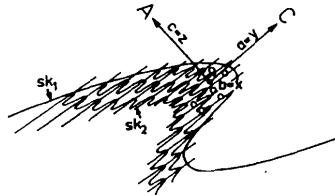


Fig. 1. Structural-geological position of the studied sample.

Together with increasing isoclinal structure of the folds the orientation of the younger crystalline schistosity ( $sk_2$ ) approaches more and more an axial position. So it becomes obvious, that on the limbs of the fold the older and nearly formed crystalline schistositities are approximately parallel. Near to the crest of the fold the intersection angle of both foliations is increasing and reaches  $90^\circ$  in the very crest. The crest is, furthermore, characterized by the morphological dominance of the  $sk_2$ -plane as well as by stretching in  $b=x$  (pencil-structure) combined with rotation around the  $b=x$  - axis.

Such deformation process is in a wide range independent of different types of parent rocks, their chemical composition and regional geological position. According to critical minerals in the present case the deformed system of planes ( $sk_1$ ) corresponds to a crystalline schistosity formed by regional metamorphism under the conditions of the amphibolite-facies ( $p > 4,5$  kbar,  $T > 400-500^\circ C$ ). Nearly the same or even, somewhat lower metamorphic conditions are to be taken into consideration due to the development of the younger crystalline schistosity ( $sk_2$ ). These data are derived from the occurrence of younger biotite following the  $sk_2$ -planes.

The studied sample is a pencil gneiss from the very crest of an asymmetric recumbent fold with a half wave length of about 1 km (fig. 1). It has been taken in a quarry 1.5 km southern from Jpehstadt at the boundary to Czechoslovakia. The geological unit is an orthogneiss complex ("redgneiss") of the Erzgebirge-anticlinorium named "Reitzenhainer Rotgneisstrunktur"<sup>10/</sup>. The sample is cut as a plate with about 1 cm thickness parallel to the  $c=z$  axis and an area of about  $15 \times 20 \text{ cm}^2$  in the  $ab=xy$  plane. By means of X-ray phase analysis proved by microscope modal analysis the main minerals are determined contributing to the pencil-gneiss specimen under investigation : quartz 35%, plagioclase 35 %, K-feldspar 15 %, muscovite 10 %, biotite 5 %.

## Experiments

The presented fabric analysis of quartz in pencil-gneiss has been done at the pulsed reactor IBR-2 in Dubna using neutron time-of-flight (TOF) diffraction. The method is similar to the energy-dispersive X-ray technique<sup>11/</sup>. It is characterized by a simultaneous recording of all nonforbidden Bragg reflections in one diffraction pattern at constant scattering geometry. This means, all pole figures under investigation are measured at the same time by only one scan of the texture goniometer.

The experiments were carried out at the spectrometer NSWR<sup>12/</sup>. Some important parameters of the equipment are :

total flight path :	$L_1 + L_2 = 34.2 \text{ m}$	
detector positions :	$2\theta_1 = 80^\circ$	transmission
	$2\theta_2 = 100^\circ$	geometry
	$2\theta_1 = 140^\circ$	reflection
	$2\theta_2 = 100^\circ$	geometry
beam diameter :	$D = 5 \text{ cm}$	

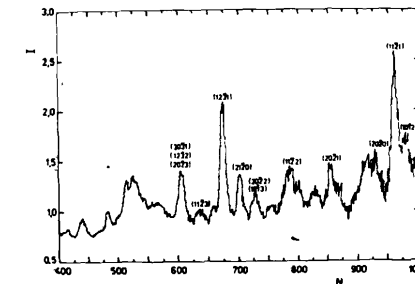


Fig. 2. TOF diffraction pattern of pencil-gneiss ( $2\theta = 80^\circ$ ).

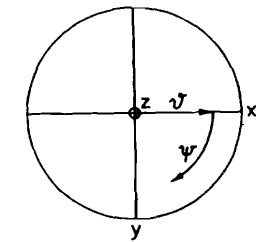


Fig. 3. Pole figure angles.

In fig. 2 the TOF diffraction pattern at  $2\theta = 80^\circ$  is shown, which is normalized to constant neutron flux. The channel numbers are proportional to the neutron wavelength. Using two detectors in transmission and reflection geometry as well, complete pole figures could be determined by rotating the goniometer around its normal situated in the horizontal scattering plane (azimuth angle  $\psi$ ), and around the vertical axis (tilt angle  $\mathcal{J}$ ). The pole figures were measured in constant  $-\mathcal{J}$  - circles (see fig.3). The steps are equidistant  $\Delta\mathcal{J} = 10^\circ$ . The  $\Delta\psi$  -steps vary in dependence on  $\mathcal{J}$  (see the table). The pole figure ranges for transmission and reflection geometry and the results from different detectors have been compared by means of special calibration circles.

Table: Dependence of angle steps  $\Delta\psi$  on tilt angle  $\psi$

$\psi$	0°	10°	20°	30°	40°	50°	60°	70°	80°	90°
$\Delta\psi$	36°	30°	36°	30°	24°	20°	18°	15°	10°	10°

Pole figure determination and data handling

The values of pole figures are proportional to the intensity of their Bragg reflection at the corresponding specimen position. These intensities were determined from TOF spectra by means of a computer fit. The quartz phase of the gneiss has only been considered. Because of several other components in the material having low lattice symmetries, the diffraction patterns contain a large amount of peaks. Therefore, problems in the fit procedure arise due to overlappings and coincidences of reflections:

- In regions consisting in dense sequences of reflections it may be impossible to find reliable points for background correction. Consequently, outcoming errors have to be expected. They are reflected in the pole figure normalization and simulate incorrect sharpness of texture.
- Narrowly overlapped or coincided reflections cannot be separated by means of the fit. As a result, the determined intensities are expected to include influences from other phases. An approximate phase analysis (components of more than 5 percents) can be used to simulate the TOF spectra of single phases and to select weakly "contaminated" peaks for further consideration.

In the present fabric analysis the quartz reflections have been picked up where the influence of other phases was lower than 30%. For the understanding of weak textures of all components the arising errors are supposed to be small. Accurate and mutually consistent pole figures are the base for the mathematical texture analysis. Efforts have been made to check the quality of pole figures and to correct them for the errors discussed above. The applied criteria and methods are outlined in more detail in /7/.

The mathematical texture analysis up to the ODF calculation has been carried out using the well-known series expansion method<sup>/8/</sup> up to  $l = 14$  for even  $l$  only. In the applied formalism real and imaginary terms were considered separately. In the trigonal system the lattice planes (hkil) and (khil) are not symmetrically equivalent although they have the same lattice spacing and are, therefore, overlapped in powder diffraction patterns. Consequently, pole figures of this type cannot be measured separately. They are taken into account with respect to the method outlined in /2/.

Results

From time-of-flight diffraction patterns of the pencil gneiss specimen 6 pole figures have been determined and selected for further consideration according to the check described in the previous paragraph. The specimen coordinate system has been chosen in a way, that the quartz pencils in the gneiss representing the direction of the tectonic b-axis are parallel to the sample x-axis. An approximately orthorhombic symmetry of pole figures could be attained after the rotation of the sample coordinate system around the z-axis for about 20 degrees and around the y-axis for about 8 degrees. The system is turned around the z-axis in fig.4. The deviation between the tectonic and primary specimen

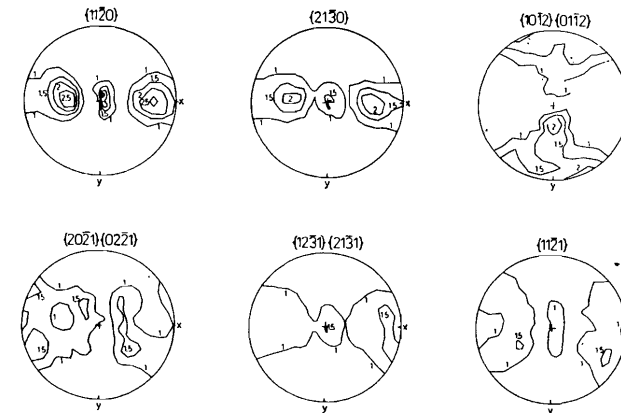


Fig. 4. Experimental pole figures.

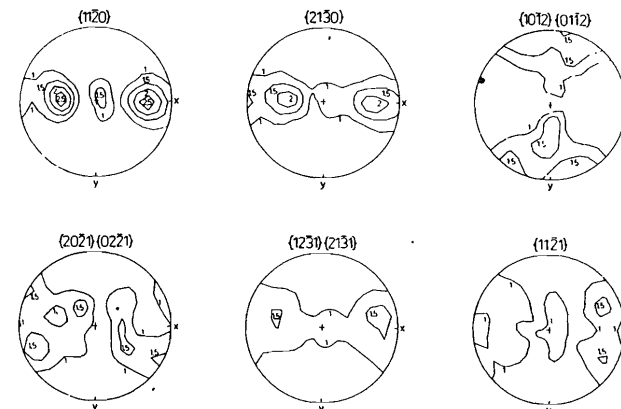


Fig. 5. Recalculated pole figures (initial set).

coordinate system can be explained by the uncertainties at sample preparation and at sample calibration in goniometer. The initial set of pole figures has been recalculated from  $C_{ij}^v$ -coefficients (fig.5). The differences in texture components are less than 10% of the pole density.

Furthermore, the pole figures of some important morphologic forms have been recalculated (fig. 6). The pole figure of the basal plane  $\{0001\}$  shows an intense maximum at  $y=a$  and a tendency to a weak girdle from  $y=a$  to  $z=a$ . Moreover, it is compared with a fabric diagram of quartz axes determined by U-stage technique (200 axes in an a-c-section). The principal coincidence of both results is

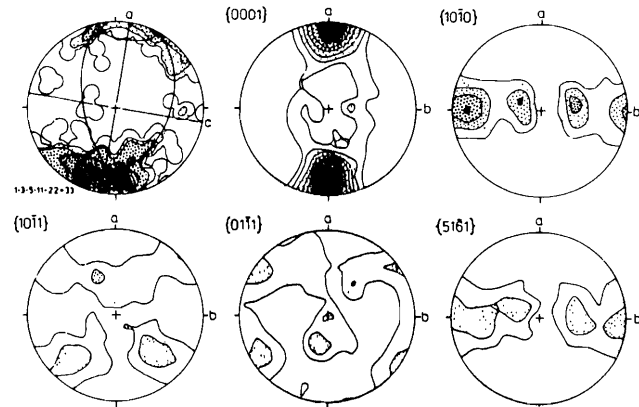


Fig. 6. Quartz axes diagram (200 axes) (left on the top) and recalculated pole figures of morphologic forms.

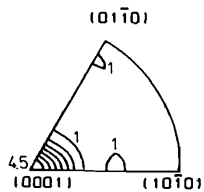
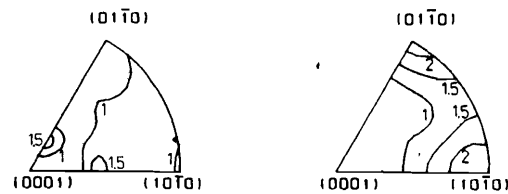


Fig. 7. Inverse pole figures of the specimen coordinate axes (z,x,y - axes from the left hand side).

quite satisfactory. In the optically determined fabric diagram no tendency to the girdle formation can be found. This lack may be explained by the consideration of quartz grains from the pencils only. In the diffraction experiment the quartz grains of the matrix having very small grain sizes are contributing to the pole figures also. On the other hand the separation of the maximum at  $b=y$  into two in the fabric diagram having an angle distance of about 20 degrees is not observed in the  $\{0001\}$  pole figure. It is supposed to be smoothed out in consequence of the relatively low series expansion degree and the chosen point density on the experimental pole figures.

Fig. 7 shows the inverse pole figures for the specimen coordinate axes. Beside the strong maximum at (0001) in the y-direction no other significant texture component is observed. The existence of only one marked component is confirmed by the ODF in fig. 8. The two maxima at  $\pm y$  in the  $\{0001\}$  pole figure are reflected by high intensities in the ODF at  $\beta \approx 90^\circ$ ,  $\alpha_1 = 90^\circ$  and  $\alpha_2 = 270^\circ$ , respectively. Fig.9 represents the skeleton lines of both components in dependence on Euler angle  $\gamma$ . Each line shows two maxima having a distance of

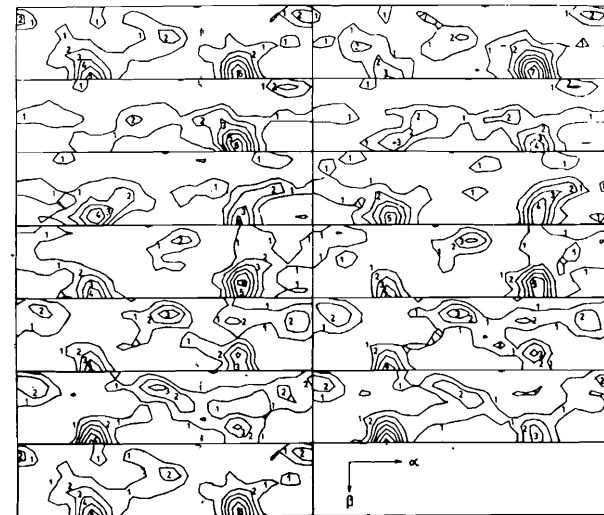


Fig. 8. Quartz ODF of pencil-gneiss.

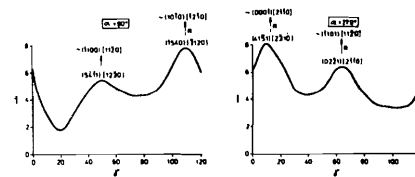


Fig. 9. Skeleton lines of ODF maxima in dependence on  $\gamma$ .

$60^\circ$ . The skeleton lines are drawn for the maximum values of the corresponding ODF component even if  $\beta$  tends to lower angles, especially in the neighbourhood of  $60^\circ$ . The fluctuations of  $\beta$  are explained by the incomplete orthorhombic symmetry of pole figures.

#### Interpretation

The pole figures of the principal morphologic forms of quartz (basis, prisms I and II, rhomboeders, trigonal dipyramide, trapezoeder) have been determined for coordinate system relations  $a=y, b=x, c=z$ . Rotating the specimen coordinate system to the orientation  $a=z, b=x, c=y$ , one can compare the maxima of pole figures with the crystallographic stereogram of right-hand-quartz (right-hand and left-hand quartz cannot be distinguished in the diffraction experiment). The coincidence is quite good (see fig.10) confirming satisfactory experimental accuracy. The differences between experimental and stereographic points (of about  $10^\circ$ ) are explained by the incomplete pole figure symmetry. Some orientations differing from the stereogram are assumed to correspond to the weak  $ac=yz$  - girdle in the  $\{0001\}$  pole figure.

The fabric type of the quartz phase in the pencil gneiss under investigation corresponds to the maximum I - preferred orientation of Sander /13/ combined with the tendency to an  $ac$ -girdle formation. Hofmann describes this kind of preferred orientations in his hierarchy of the evolution of the partial fabric of quartz in the Erzgebirge anticlinorium /16/ to be characteristic for the upper crust regions. According to /14/ the basal slip with the accompanying external rotations of  $c$  toward  $G_4$  leads to the  $c$ -axes maximum parallel to  $G_4$  for temperatures below  $800^\circ\text{C}$  and strain rates  $\dot{\epsilon} = 10^{-5} \text{ sec}^{-1}$  or other equivalent ( $T, \dot{\epsilon}$ ) values from fig. 11. In this region of the diagram plastic flow is operating without any recrystallization. The formation of girdle fabrics is explained by combined operation of basal and prismatic slip, where increasing influence of prismatic slip increases the opening angle of the girdle.

The comparison of the determined fabric type with experimentally deformed quartzites refers to deformation conditions at relatively low temperatures ( $< 500^\circ\text{C}$ ), but higher strain rates ( $\dot{\epsilon} \leq 10^{-4} \text{ sec}^{-1}$ ) /1/.

According to Taylor-Bishop-Hill computer simulations /15/ the investigated texture corresponds to the "model quartzite A" in the range between axial extension and flattening, where the dominating slip system is  $(0001)[a]$  (see fig. 12).

Finally, the important influence of the water content in quartz on its deformation behaviour has to be mentioned. It has been reported in /14/ that a synthetic quartz crystal containing water molecules ( $8.8 \times 10^{-3} \text{ H/Si}$ ) could be deformed above a critical temperature of  $380^\circ\text{C}$  under stresses by 10 to 20 times lower than a natural "dry" crystal. This hydrolytic weakening

is attributed to the enhanced mobility of dislocations by hydrolysis of the strong covalent  $\text{Si} - \text{O}$  bonds.

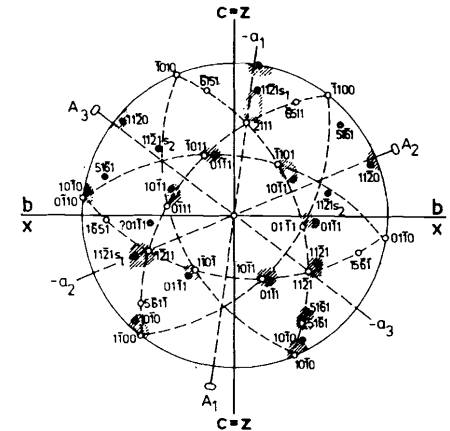


Fig. 10. Comparison of texture components from the experiment (heavy circles) with points in the right-handed quartz stereogram (open circles). The shaded areas indicate deviations.

Fig. 11. Variation of the preferred orientation of quartz  $c$ -axes with temperature and strain rate in quartzites. The numbers in parentheses indicate the average opening half-angle of the girdle.

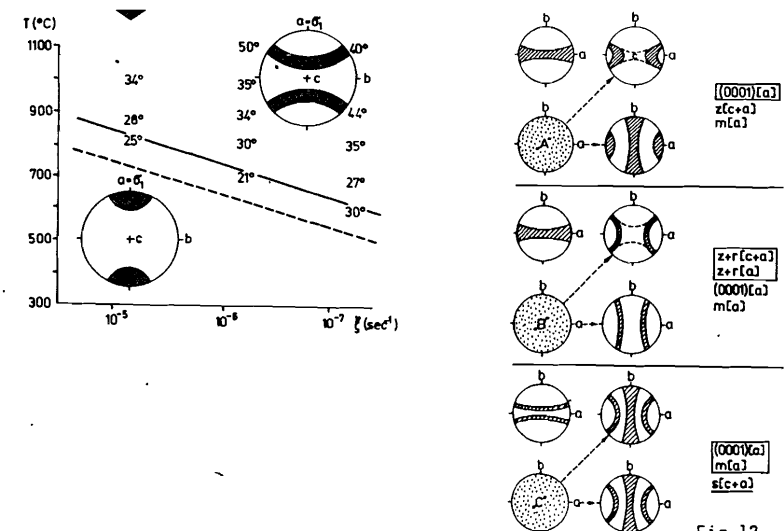


Fig. 12.

Results of Taylor-simulations for three different models characterized by the noted slip systems which were assumed to be active in the deformation process /15/. The vertical direction denotes axial extension, the horizontal one characterizes axial shortening and in the diagonal the flattening takes place.

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Дрекслер Л.П. и др. E14-87-345

Нейтроннографический текстурный анализ кварца  
в естественно деформированном гнейсе

С помощью дифракции нейтронов по методу времени пролета были исследованы кристаллические преимущественные ориентации зерен кварца в стебельчатом гнейсе из Рудных гор /юг ГДР/. Обнаружены отдельные компоненты текстуры, где тригональная ось параллельна тектоническому "а"-направлению. В кварце полюсная фигура "с"-оси, имеющая максимум при  $\pm\alpha$ , связана с поясом слабой интенсивности, не обнаруженном в оптических измерениях. Из сравнения экспериментально деформированного кварцита с модельными расчетами сделан вывод о приблизительных условиях формирования стебельчатого гнейса.

Работа выполнена в Лаборатории нейтронной физики ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1987

Drechsler L.P. et al. E14-87-345

Neutronographic Fabric Analysis of Quartz  
in Naturally Deformed Gneiss

The crystalline preferred orientations of quartz grains in pencil gneiss from the Erzgebirge (southern GDR) are studied by means of neutron time-of-flight diffraction. A single component texture has been found where the trigonal axes are parallel to the tectonic a-direction. In the quartz c-axis pole figure strong maxima at  $\pm\alpha$  are connected by a girdle of weaker intensity being not found in U-stage measurements. From the comparison with experimentally deformed quartzites and model calculations the approximate formation conditions of the given pencil gneiss could be deduced.

The investigation has been performed at the Laboratory of Neutron Physics, JINR.

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