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FABRIC ANALYSIS OF THE QUARTZ COMPONENT IN SAXONIAN GRANULITES USING NEUTRON TIME-OF-FLIGHT DIFFRACTION

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1.Introduction

Orientation distribution of crystallites in a given rock specimen contains valuable information on its deformation history. In connection with megascopic data it can be used to conclude on the regime of temperature, pressure and strain which were active in the investigated matter. Therefore, the accurate and complete description of the relation between crystal and specimen orientation should give important information for petrofabric analysis. In geology fabric diagrams, i.e., representations of the distribution of one crystallographic direction with respect to specimen coordinates are known for many years. In this description the chosen crystallographic axis is fixed, but rotations about it are allowed. A more complete and precise way of determination of the relative orientation of crystal and specimen coordinate systems is given by means of the so-called orientation distribution function (ODF). There are some possibilities to find this function. A very time-consuming method is the direct measurement of orientation data of individual crystals on the universal stage or by electron microscope /1,2/. The calculation of the ODF from pole figure data, determined by neutron or X-ray diffraction using Bunge's series expansion method /3/, seems to be more straightforward. In the last years some investigations of geological samples have been done on this basis /4,5,6/.

In this paper the complete texture analysis of quartz components of three granulite samples is presented. Pole figures have been measured by means of neutron time-of-flight (TOF) diffraction at the Dubna pulsed reactors IBR-30 and IBR-2. The applied experimental method is well suited for the investigation of low symmetric crystal systems because of simultaneous measurement of many pole figures.

2. Series expansion method

All the important points of view of the ODF definition have been discussed by Matthies /7/ in a very detailed manner. In general, the ODF $f(g)$ cannot be measured directly. Therefore, a method has to be found to connect the ODF with experimental results. In the most common technique proposed by Bunge /3/ the ODF is expanded into a series of generalized spherical harmonics

$$f(g) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} C_l^{mn} \; T_l^{mn}(g). \tag{1}$$

The C_l^{mn} are the series expansion coefficients which contain all information concerning the texture (or fabric) of the investigated sample. On the other hand, pole figures (fabric diagrams) are measurable, two-dimensional projections of the three-dimensional ODF. Expanding them into a series of spherical harmonics

$$P_{\vec{h}_i}(\vec{y}) = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} \frac{C_l^{mn}}{2l+1} \, k_l^{m}(\vec{h}_i)\, k_l^{n}(\vec{y}). \tag{2}$$

It can be shown /3,7/ that the series of expansion coefficients C_l^{mn} are the same in equations (1) and (2). The unit vectors $\vec{h}$ and $\vec{y}$ determine crystal and specimen direction, respectively. In this way, a connection is found between pole figures and ODF via series expansion coefficients. Usually, the C_l^{mn} are calculated from eq. (2) with the help of a least square fit. The series expansion cut off l_{max} depends on the number of known pole figures.

According to Friedel's law it is impossible to distinguish in a normal diffraction experiment between crystallographic directions h and $-\vec{h}_i$, i.e., only superpositions

$$\tilde{P}_{\vec{h}_i}(\vec{y}) = P_{\vec{h}_i}(\vec{y}) + P_{-\vec{h}_i}(\vec{y}) \tag{3}$$

can be measured. From these so-called reduced pole figures it is impossible to determine the C_l^{mn} with odd l. In this way, only the "even" part of the ODF $f(g)$ can be reproduced from experimental data, in general cases, leading to "ghost" effects /7/.

3. Symmetry considerations.

Each crystal system is characterized by a set of possible symmetry transformations. This symmetry is strong in the mathematical sense. Less strong symmetry properties can be found for specimen in many cases too, caused by the formation process of the given sample. Rotation symmetry operations should be reflected in ODF, pole figures and inverse pole figures. Inversion and mirror symmetry operations transform right-hand into left-hand coordinate systems and vice-versa. Therefore, they cannot be taken into account in texture analysis.

In the trigonal crystal system the planes (hkil) and (khil) having the same lattice spacings are not equivalent from the symmetric point of view. Reflections of this type coincide in powder diffraction patterns. Therefore, only a superposition of reduced pole figures can be recorded.

$$\tilde{P}_{\vec{h}_i}(\vec{y}) = w_{(hkil)} \tilde{P}_{(hkil)}(\vec{y}) + w_{(khil)} \tilde{P}_{(khil)}(\vec{y}), \tag{4}$$

where $w_{\vec{h}_i}$ is the weight factor which is proportional to the corresponding structure factor. These factors have to meet the condition

$$w_{(hkil)} + w_{(khil)} = 1. \tag{5}$$

Taking into account such kinds of pole figures, the spherical harmonics of eq. (3) have to be substituted by

$$k_l^m(\vec{h}_i) \longrightarrow w_{(hkil)} k_l^m(hkil) + w_{(khil)} k_l^m(khil) \tag{6}$$

if the Miller index l is not equal to zero.

The mathematical background used in this paper has been outlined in detail in /8/.

4. Experiments and data handling

The TOF texture investigations on the granulite samples 1 and 2 of the Granulite massif (southern GDR) have been done at the pulsed reactor IBR-30 of the JINR Dubna. Some important experimental parameters are:

- flight path 32 m
- $2\Theta =$ 90°
- beam diameter 50 mm
- specimen dimensions about 10 x 100 x 150 mm^3
- record time per spectrum 2 h

The investigation of the third sample has been done by means of the spectrometer NSWR /9/ at the IBR-2 reactor. The measurements have been carried out using two detectors simultaneously. The Bragg angles were $2\Theta = 80^\circ$ and $2\Theta = 100^\circ$ in the transmission case and $2\Theta = 100^\circ$ and $2\Theta = 140^\circ$ in the reflection case, respectively. Other parameters were approximately the same. The samples were situated in an automatic three-circle texture goniometer to ensure all necessary specimen rotations about three perpendicular axes. The symmetries of samples 1 and 2 were found to be approximately monoclinic, i.e., only one half of the complete pole figure was to be covered by experimental points, where one TOF diffraction spectrum yields one point in every considered pole figure. For the third rock full pole figures have been measured. To decrease experimental expanse scans similar to equal area ones were recorded on the pole figures, i.e., the tilt angle steps were $\Delta\Phi = 10^\circ$ in each case, but the azimuth angle steps $\Delta\Psi$ varied in dependence on Φ.

The TOF diffraction patterns for the three perpendicular directions of the sample coordinate system ND (normal of the sheet), DD (lineation) and TV (transverse) of granulite 1 are shown in Fig.1. From all the measured spectra the integrated intensities of Bragg reflections have been determined using a modified variant of the computer fit program ORION /10/. The investigated granulite samples consisted of about 50% quartz. The reflections from other components contributed to the background, which is assumed to be orien-

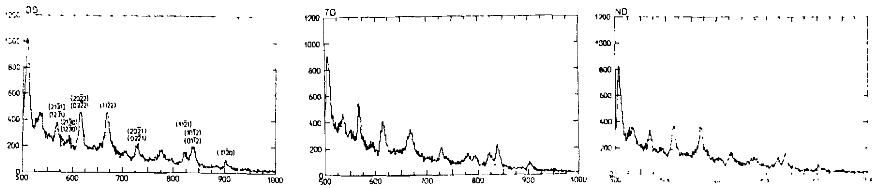

Fig. 1. TOF-diffraction patterns of granulite for the sample positions DD, TD and ND.

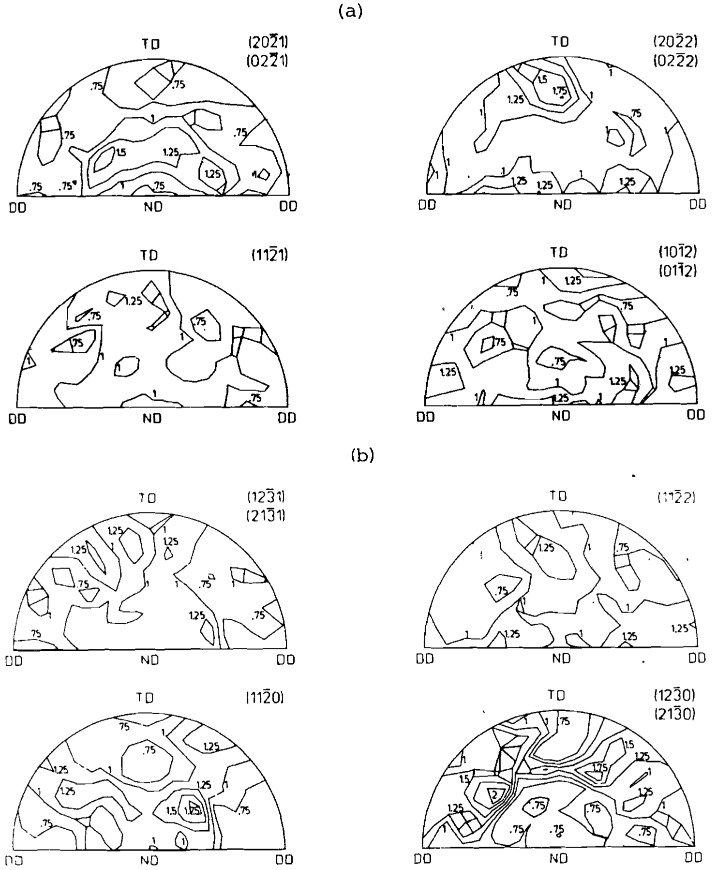

Fig. 2. Experimental pole figures of granulite 1.

tation dependent, and can influence the intensities of quartz reflections also. Therefore, the model TOF spectra have been calculated taking into account the main components of granulite : quartz, albite, sanidine and muscovite. For texture analysis the Bragg reflections have been taken into account, where the quartz part was higher than 70%. Furthermore, the determined pole figures proved their mutual consistence as compared with the C_2^{mn} coefficients, which can be calculated for every pole figure separately. In this way a different number of pole figures (see figs.2-4) has been selected for further texture analysis by means of computer programs QUARZ /8/ and QUARZ 2 . For mathematical treatment the point network on pole figures has been decreased to $\Delta\phi = \Delta\psi = 5$ degrees in all cases using quadratic interpolation. The series expansion cut-off was $l = 14$ for all the samples.

5. Geological remarks

Granulites are metamorphic rocks which developed under conditions of high temperature and pressure. Their texture and composition is characterized by the fact that during their development conditions of dry facies were existing. Therefore, the primary minerals are generally free of water. By secondary processes water-bearing materials enter into the system. Granulites are typical for the lower half of the Earth's crust, but locally they are outcropping in geological units with intense erosion or intense tectonic development which brought them on the recent surface (more than 10 km above the depth of origin). One of these occurences of granulites on the Earth's surface is the Granulite massif in the southern part of the GDR.

The age of rocks is not exactly known. Pyroxene-enriched inliers within the granulites (pyroxenite, granulite,pyriclasite and others) have according to /11/ a Rb-Sr-isochrone of 2970±250 mio years b.p. It cannot be excluded that these ultramafics came into their positions from the upper mantle by later movements. In general, it should be supposed that the Saxonian granulites originated in the time of Lower Proterozoic (between 2500 and 1700 mio.years b.p.).

Two types of granulites are known: acid ones (mesoperthite, plagioclase quartz) and mafic ones (pyroxenes, plagioclase). Probably, the members of the first group are sedimentary rocks, those of the second group mafic volcanic rocks /12/. The acid granulites hold the largest parts of the massif.

The tectonic structure is explained in /12/ as a system of nappes which developed as plastic rock flow. The nappes became deformed in later times by crossfolding and were metamorphosed by inflow of water leading to metagranulitic biotite gneisses from granulites, especially in the bording zones of the massif. The nappes were primarily folded with fold axes in E-W direction.

The granulites are metamorphic rocks with planar fabric which is less intense than in ordinary gneisses. The lineation is weak. Two types of quartz distributions are to differentiate: Schistose-platy granulites have a well-paper quartz, the grained granulites have a disk-quartz distribution. The type of the quartz texture differs highly and depends on the tectonic level and on the mineralogical composition. Granulites with larger parts of biolite are without texture caused by the secondary metamorphism whereas cross girdle fabrics seem to be related to areas with cross folding.

Quartz fabrics studies can influence geological ideas, if they are in accordance with the detailed knowledge about the structural history of the studied areas. A lot of results about the quartz fabrics investigations were published on the Granulite massif of the southern GDR /13-18/.

Deformed rocks are characterized in different degree by an orientation of minerals. A close relationship exists between the symmetry of minerals and of the rock bodies as a whole. The deformation takes place under pressure, temperature and OH reactions. Additionally metamorphism imposes thermodynamic conditions on deforming rock units defined by temperature and activities of H_2O, CO_2 and O_2. The elements of the deformation history can be reconstructed to some degree by texture measurements. Furthermore, the path of deformation can be studied by model calculations, using the Taylor theory of plastic deformations. But these results seem to be overdetermined when compared with natural textures. Therefore, it is necessary to measure the texture

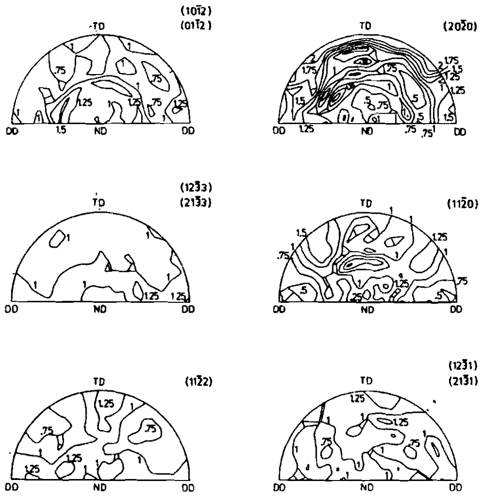

Fig. 3. Experimental pole figures of granulite 2.

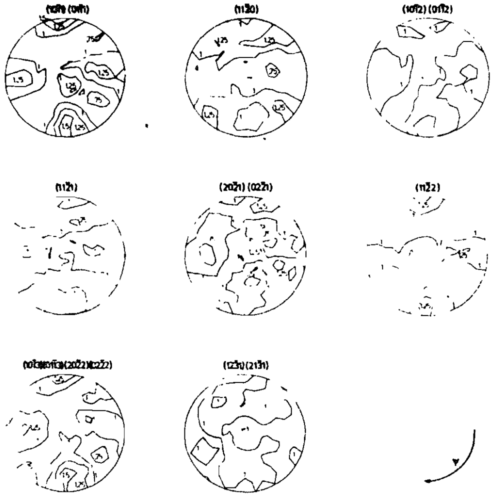

Fig. 4. Experimental pole figures of granulite 3.

as detailed as possible. This can be done especially by neutron texture analysis.

Theoretical models show the influence and importance of the symmetry of the kinematic field, possible glide systems and the strain history. Preferred orientations of lattice include information about the kinematics of rock deformation. Since the physical properties of rocks depend on the fabrics and the crystal structure of the constituents, and since the texture depends on the deformation history it is of practical and scientific importance to use the possibilities of neutron diffraction to know the lattice orientation and the differences in orientation type and density for different lattice planes - as markers for the transport mechanism of rock masses.

6. Results

From experimental pole figures in figs. 2 to 4 the series expansion coefficients have been determined. Using the known C_l^{mn} the input sets of pole figures are recalculated. They reproduce the main characteristics of experimental pole figures, like those shown in fig.5 for granulite 3, referring to sufficient reliability of experiments and data handling. Traditionally, the knowledge of the basic plane pole figure(0003) is important for the interpretation of quartz fabrics. Because of the small structure factor of (0003) reflection and the neighbourhood of the strong (11$\bar{2}$2) peak, it is nearly impossible to measure this pole figure by neutron diffraction. Therefore, it has been calculated from the known C_l^{mn} . Fig. 6 shows the (0003) pole figure together with the hexagonal edge pole figure (1010) for granulite 1. Fig. 8 demonstrates the corresponding results for granulite 3. In both samples the texture types are very similar. In the basic plane pole figures typical two girdle structures can be seen taking into account the full pole figure area in Fig.6. Comparing with samples 1 and 3 the (0003) pole figure of granulite 2 in fig. 7 shows axisymmetric features in its centre.

The inverse pole figures of ND, DD and TD for all the samples are represented in figs. 9 to 11, respectively. In compliance with the known pole fi-

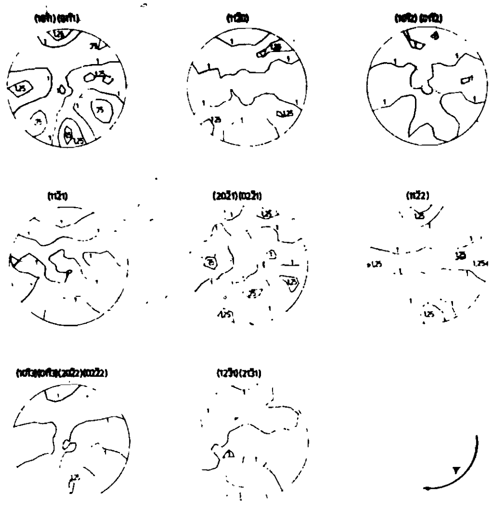

Fig. 5. Recalculated pole figures of granulite 3.

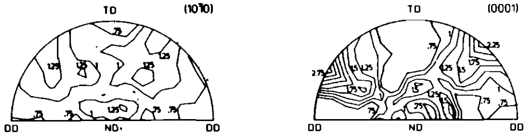

Fig. 6.Recalculated pole figures of granulite 1 for the basal plane and the hexagonal edge.

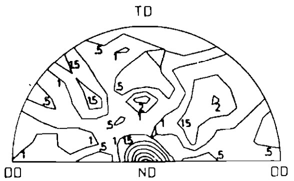

Fig. 7. Recalculated (0003) pole figures of granulite 2. The pole density in the centre is 4.3.

Fig. 8. Recalculated pole figures of granulite 3 for the basal plane and hexagonal edge.

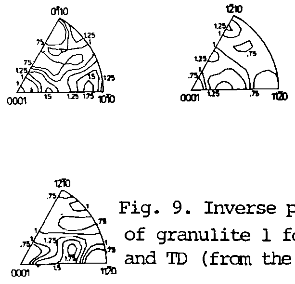

Fig. 9. Inverse pole figures of granulite 1 for ND, DD and TD (from the left).

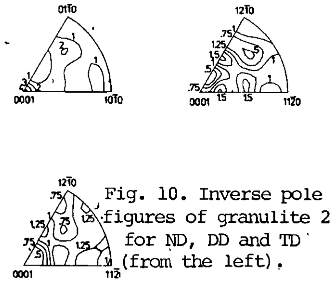

Fig. 10. Inverse pole figures of granulite 2 for ND, DD and TD (from the left).

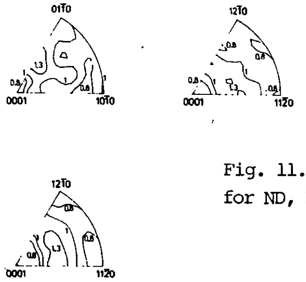

Fig. 11. Inverse pole figures of granulite 3 for ND, DD and TD (from the left).

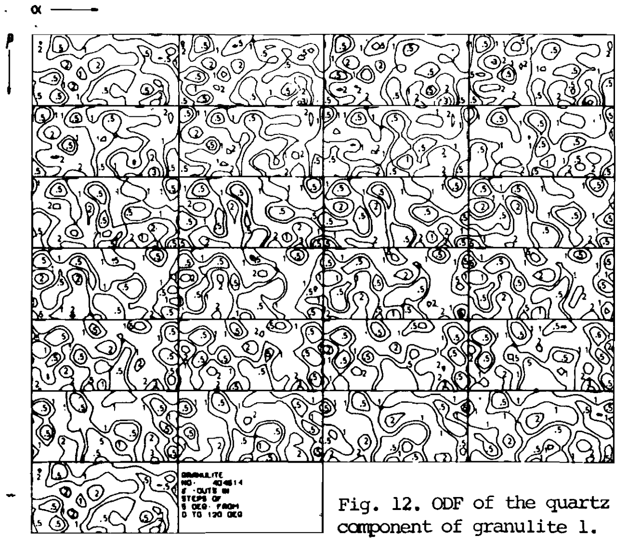

Fig. 12. ODF of the quartz component of granulite 1.

gures the inverse pole figures of granulite 1 and 3 do not show any significant texture components. The pole density is lower than 2 in all the inverse pole figure range. In the ND inverse pole figure of granulite 2 relatively high intensity is concentrated in the direction of the trigonal axis.

Fig. 12 represents the ODF of granulite 1. The main maximum with an intensity of 4.3 is found at $\alpha = 150^{\circ}$ and $\beta \approx 87^{\circ}$. Besides of this range of high orientation density the ODF of granulite 1 does not show any more essential texture components.

In the ODF of granulite 2 in fig. 13 a zone of high intensity is concentrated in the neighbourhood of $\beta = 0$. The orientation density of this range is nearly independent of α and γ. In coincidence with pole figures and inverse pole figures, such behaviour describes a concentration of trigonal quartz axes in the normal direction of the investigated rock plate.

Fig. 14 shows the ODF of granulite 3. Four components with a distance of about 90° in α refer to the approximately orthorhombic symmetry of the investigated specimen.

The discussed ODFs contain the even l information only. The influence of ghost effects is expected to be small because of the relatively weak texture of the samples.

In the orientation of investigated granulites dominate (0001), (11$\bar{2}$0) and (12$\bar{1}$0) components, respectively. The intense orientation of the prism can be explained by the influence of temperature of approximately 600° C. Higher values are to be excluded (thermobarometric investigation is going on). Prism and basal activity are dominating. The basal-switch mechanism corresponds to the transition of plane strain to flattening. The third active system is (1101).

According to /14/ the asymmetry in the inverse pole figures can be produced by the glide systems with trigonal symmetry. In general the low intensity of texture components in granulite is to be explained by the secondary heating of the rocks which has weakened the texture intensity.

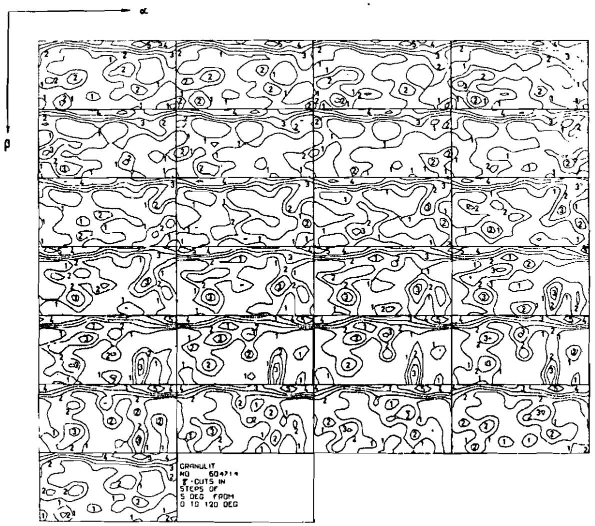

Fig. 13. ODF of the quartz component of granulite 2.

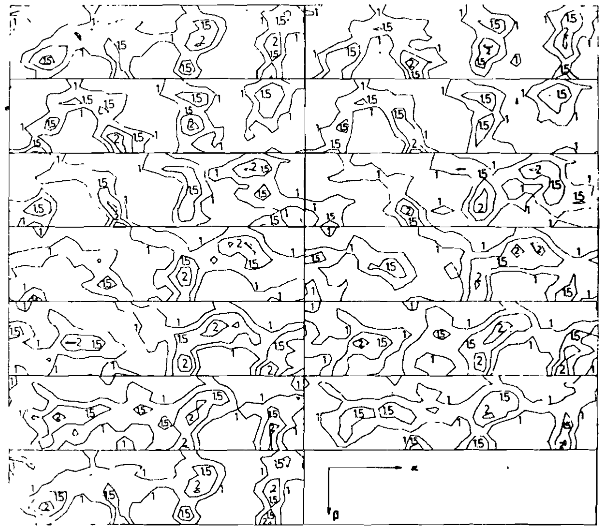

Fig. 14. ODF of the quartz component of granulite 3.

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Вниманию организаций и лиц, заинтересованных в получении публикаций Объединенного института ядерных исследований

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Банквитц П. и др. E14-86-23

Текстурный анализ кварцевой части саксонского гранулита с помощью нейтронной дифракции по времени пролета

Гранулированный массив в южной части ГДР залегает в верхней части Саксонско-Тюрингской зоны европейских варисцидов. Возраст его пород, по всей вероятности, моложе протерозойского. В данной работе представляются полные количественные текстурные анализы в трех образцах гранулита с большим содержанием кварца. Исследования были проведены с помощью нейтронной дифракции по времени пролета на импульсных реакторах ИБР-30 и ИБР-2. Несмотря на низкую симметрию, структура кварцевой составляющей обнаруживает влияние базисной и призменной активации для текстурообразования гранулита. Текстура всех исследуемых образцов была относительно слабая. Это можно понять как следствие последующего восстановления после первоначального образования.

Работа выполнена в Лаборатории нейтронной физики ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна 1986

Bankwitz P. et al E14-86-23

Fabric Analysis of the Quartz Component in Saxonian Granulites Using Neutron Time-of-Flight Diffraction

The Granulite massif in the southern GDR is an inlier within the Saxothuringian zone of the European Variscides. The rocks are probably of Lower Proterozoic age. The full quantitative fabric analysis (texture analysis) of the three specimen of different quartz granulites has been done using neutron time-of-flight diffraction at pulsed reactors IBR-30 and IBR-2 of the JINR,Dubna. In spite of the low symmetry of orientation the quartz fabric shows the influence of basal and prism plane movements for the origin of the texture of the granulites. The textures of all investigated samples were found to be relatively weak. This fact is explained by the later recovery of the rocks after their formation.

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

Communication of the Joint Institute for Nuclear Research. Dubna 1986