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NEUTRONOGRAPHIC TEXTURE INVESTIGATION OF METAMORPHIC ROCKS

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Introduction

The interest in precise quantitative petrofabric analysis of metamorphic rocks has increased considerably. Full information on preferred crystalline orientations in a representative rock volume may be obtained using spectroscopic methods of X-ray or neutron diffraction. The low absorption of thermal neutrons by the most of materials combined with extended beam cross sections allows to investigate bulk texture effects even in relatively coarse grained substances like those frequently found in geological specimens. Furthermore, complete pole figures can be measured without special expense for sample preparation.

The most of natural rocks consist of more than one phase. In granulites, and gneisses investigated at the pulsed reactor IBR-2 of the JINR Dubna using neutron time-of-flight (TOF) diffraction there are about 40 percents of quartz among other minerals. Therefore, the TOF diffraction pattern is a superposition of spectra from all components, i.e. there is a lot of overlappings of different reflections. In this case the question arises about the reliability of the experimental pole figures.

Pole Figure Determination

Rock samples are frequently found to consist of a mineral mixture. Then, the diffraction pattern is a superposition of the spectra from all phases of the specimen. Therefore, in texture analysis overlapped reflections must be considered also. This can be done only if an adequate part of the Bragg pattern is known, i.e. using TOF diffraction (1) or angle dispersive method with position sensitive detector (2).

The pole figure values are proportional to the intensity of the corresponding Bragg reflection. The intensities are determined by line profile analysis.

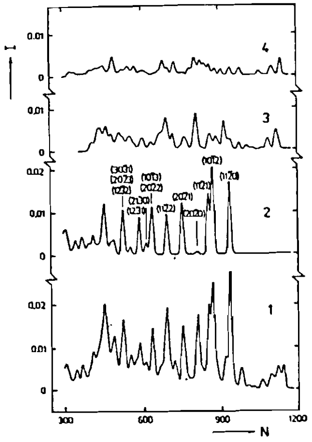

Figure 1. Computer constructed TOF spectra of plagioclase (4), abite (3), quartz (2), and the supperposition of three spectra (1).

Investigating complex substances two main questions arise concerning the accuracy of experimental pole figures:
- What components contribute to the intensity of the considered peak?
- What is the true experimental background in the spectra?

This questions can be considered on the base of phase analysis results. For example, the TOF diffraction pattern of granulite has been superposed in Fig.1 using theoretical spectra of the main components, i.e. quartz, plagioclase and albite. The quartz (20$\bar{2}$1) reflection and the double peak (11$\bar{2}$1) (10$\bar{1}$2) are not too much influenced by other phases. Assuming weak textures, the errors arising from small strange intensity contributions and uncertainties in background subtraction lead mainly to incorrect pole figure normalization. On the other hand, the ($\bar{1}$122) reflection is a mixture of equivalent intensity parts of quartz and albite. Pole figures from such kind of peaks may be much incorrect. In practice, reflections have been selected, where the quartz-caused intensity is more than 60%.

Furthermore, there are some sources for pole figure errors having a more general character:
- Using several detectors at the same time one must expect different characteristics for each one. The error distribution on the pole figure range depends on the applied diffraction technique and the goniometer (3).
- For thick intensely scattering samples multiple Bragg scattering has to be taken into account especially in the range nearly to the overlapping of transmission and reflection geometry.

Therefore, criteria have to be found to check experimental pole figures with respect to their internal and external compatibility before final ODF reproduction.

Pole Figure Check and Correction

According to the series expansion method (4) the $F_l^{\nu}(h_i)$ factors can be found for every pole figure

$$F_l^{\nu}(h_i) = 4\pi \oint \tilde{\tilde{P}}_{h_i}(y)\, k_l^{\nu}(y)\, dy \Big/ \oint \tilde{\tilde{P}}_{h_i}(y)\, dy \; ; \quad dy = \sin\vartheta\, d\vartheta\, d\psi , \qquad (1)$$

where the denominator is the normalization factor of experimental pole figures. Their tilt and azimuth angles are denoted by ϑ and ψ, respectively. The $F_l^{\nu}(h_i)$ and the series expansion coefficients are connected by

$$F_l^{\nu}(h_i)\cdot(2l+1) = \sum_{\mu=1}^{M(l)} C_l^{\mu\nu} k_l^{\mu}(h_i) . \qquad (2)$$

The $C_l^{\mu\nu}$ can be calculated for every pole figure separately, if $M(l)=1$ (5,6) (l=4,6,8,10 for cubic, l=2,4 for hex., l=2 for tetr. and trig. lattices). The $C_l^{1\nu}(h_i)$ (l,ν fixed) must be invariants for different completely accurate pole figures of one specimen. Therefore, variations between the $C_l^{1\nu}(h_i)$ are indicators for external pole figure incompatibility.

If the value of $k_l^{1}(h_i)$ is low, the $C_l^{1\nu}(h_i)$ responds sensitively even to small changes in $F_l^{\nu}(h_i)$. In this case the accuracy of numerical integration (equ.1) plays an important role.

As long as all $C_l^{1\nu}(h_i)$ have the same sign, their magnitude may be fitted adding a constant background to the pole figures in equ. 1. According to the orthogonality of the spherical harmonics only the denumeration will be varied by changing the pole figure normalization, i.e. the texture sharpness. A reference pole figure should be choosen with respect to a stable $C_l^{1\nu}(h_i)$ (i.e. $k_l^{1}(h_i)$ high) and a sufficient experimental certainty.

Even if the external compatibility of pole figures is satisfactory, the pole figures reproduced from $C_l^{\mu\nu}$ must not agree with the experimental ones.

Some error sources are remarked in the previous section. The situation may be improved by mutual variation of const. ϑ circles. The sums over a const. circle in experimental and reproduced pole figures may be compared to do that. Taking into account the behaviour of Legendre polynomials the signs of $F_l^1(h_i)$ as well as $C_l^{11}(h_i)$ may be changed also.

Analogously, overestimations of azimuth ranges may be corrected comparing $C_l^{1\nu}(h_i)$, $F_l^{\nu}(h_i)$ $(\nu > 1)$ and the behaviour of $\cos n\psi$ or $\sin n\psi$ terms of the spherical harmonics, respectively.

Furthermore, all pole figures may be misnormalized in the same way. A too sharp texture of pole figures under consideration is then compensated by negative pole density ranges in other pole figures or inverse pole figures (5). The non-negative pole density condition has to be satisfied by further background variation.

Experimental Results

At the JINR Dubna preferred orientations of the quartz component in granulites and gneisses have been studied. As examples the experimental and reproduced pole figures are shown to demonstrate the usefulness of the described check and correction methods. For the study of granulite (Fig. 2) (7) pole figures have been selected with respect to the C_2^{11} criterion only. No background variations have been carried out. The main characteristics of the experimental pole figures are reflected in the reproduced ones.

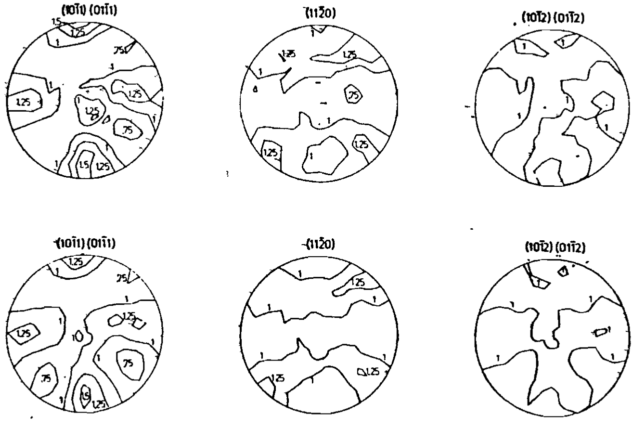

Figure 2. Two experimental pole figures (on the top) and the corresponding reproduced ones for granulite.

A better coincidence of both pole figure sets has been obtained for pencil gneiss (8) (Fig. 3). The C_2^{11} were fitted by background variations. Only some relatively sharp maxima in the incident data are smoothed out in the reproduced ones, being explained by the low expansion degree (l=14).

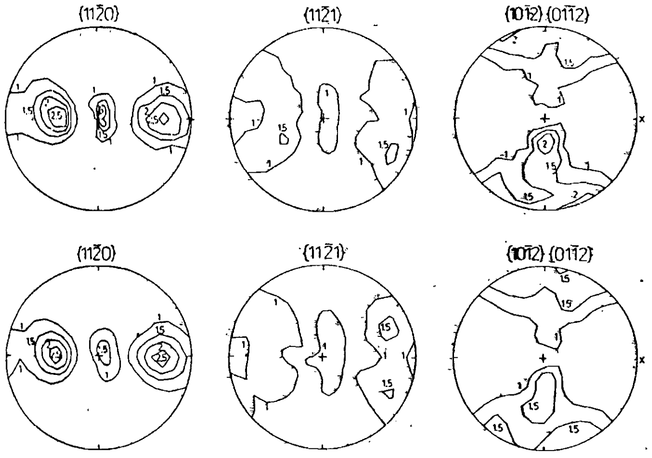

Figure 3. Three experimental pole figures (on the top) and the corresponding reproduced ones for pencil gneiss (8).

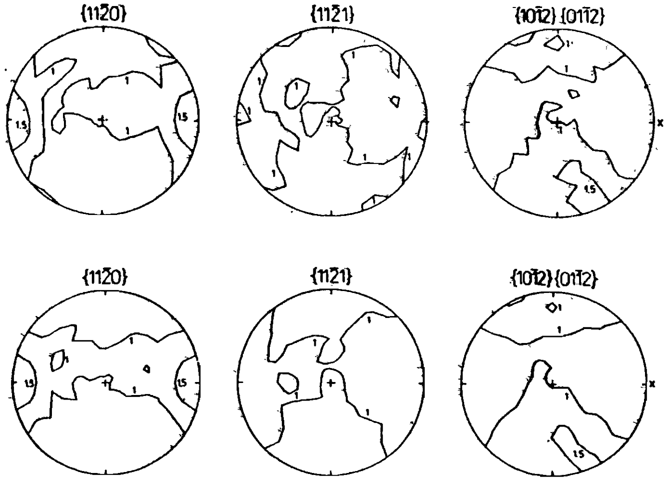

Figure 4. Three experimental pole figures (on the top) and the corresponding reproduced ones for gneiss B379 (9).

For the second gneiss specimen (B379 (9)) (Fig. 4) a ϑ circle fit was carried out besides the background variation. The RP-values in the table show that the pole figure compatibility is somewhat better than for pencil gneiss.

Table . RP values for two different gneiss samples. For overlapped reflections only one Miller index is given

	1121	1121	1012	1231	2021
PENCIL GNEISS	11.8	8.5	12.4	6.1	10.4
B379	6.6	7.8	6.6	8.9	7.4

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Фельдманн К., Фуэнтес Л., Вальтер К. E14-87-677
Нейтронографические текстурные исследования
метаморфных горных пород

Нейтронная дифракция по времени пролета является подходящим методом для исследования преимущественных ориентаций в низкосимметричных образцах, как например, в кварцевых горных породах потому, что полный брэгговский спектр измеряется одновременно. Ненормированные значения полюсной плотности определяются программой подгонки в качестве интегральных интенсивностей соответственных дифракционных отражений. Большинство естественных горных пород состоит из некоторых минералов. Поэтому времяпролетный спектр является суперпозицией спектров ото всех компонент, т.е. ожидаются многократные взаимные перекрытия различных пиков. В таких случаях возникает вопрос о верности экспериментальных полюсных фигур. На основе полных полюсных фигур обсуждаются методы и критерии для проверки и коррекции их собственной и взаимной согласованностей. Описанные подходы могут иметь значение и для изучения других низкосимметричных или многофазных образцов. Демонстрируется эффективность этих методов для избранных экспериментальных результатов.

Работа выполнена в Лаборатории нейтронной физики ОИЯИ.

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Feldmann K., Fuentes L., Walther K. E14-87-677
Neutronographic Texture Investigations
of Metamorphic Rocks

The neutron time-of-flight (TOF) diffraction is well suited for preferred orientation studies in low symmetric materials, for example, in quartzitic rocks, because of the simultaneous recording of the whole Bragg pattern. The unnormalized pole figure values are determined as integrated intensities of the corresponding diffraction peaks by a computer fit of the TOF spectrum. Unfortunately, many of natural rocks consist of more than one mineral. Therefore, the TOF diffraction pattern is a superposition of spectra from all components, i.e. there is a lot of overlappings of different reflections. In this case the question arises about the reliability of the experimental pole figures. On the basis of complete experimental pole figures methods and criteria are discussed to check and to improve their internal and external compatibility. These procedures may have importance in the study of other low symmetric or multiphased systems also. The efficiency of the presented methods is demonstrated for selected experimental results.

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

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