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PROBLEMS IN TEXTURE ANALYSIS OF METAMORPHIC ROCKS

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INTRODUCTION

During the last decade the interest in quantitative data on orientation relationships of metamorphic rocks has increased significantly[1-5]. There are several reasons for that. The texture in a given rock specimen contains valuable information on its deformation history. In connection with megascopic data it can be used to conclude about the regime of temperature, pressure and strain which were active in the investigated matter. Therefore, the accurate and complete description of the texture gives important information to perform a petrofabric analysis. Another type of problems is connected with the safety and mining optimization in salt deposits using the anisotropy of macroscopic properties in dependence on texture.

In geology the determination of fabric diagrams (pole figures) of the basic plane of quartz by means of the U-stage technique is well known. A more universal method is the pole figure measurement by R-ray diffraction which allows one to carry out a complete texture analysis. It has been used to investigate quartz, limestone, calcite, salt, etc. Because of the small penetration depth of X-rays into the matter some difficulties arise with increasing grain sizes leading to poor grain statistics. This complication can be completely avoided in the case of very time-consuming single orientation measurements. Another way to avoid these difficulties is the use of neutron diffraction with large beam cross-sections.

At IBR reactors of JINR, Dubna, a number of preferred orientation studies have been done at different quartzitic metamorphic rocks by the neutron time-of-flight (TOF) diffraction[5]. The specimens under investigation (granites, granulites, gneisses) consisted to about 50% of quartz. The remaining part was distributed among albite and plagioclases and some impurities. Therefore, the recorded Bragg pattern is very complex. In the present paper the problems are discussed arising during the pole figure determination of such low symmetric multiphased systems.

POLE FIGURE DETERMINATION

In the TOF diffraction technique the complete Bragg pattern is recorded simultaneously at fixed scattering geometry.

Pole figures are determined rotating the sample with respect to an equal angle, an equal area or any other scan. The pole density is proportional to the investigated intensity of the corresponding Bragg reflection/6/. These investigated intensities are determined by means of a computer fit procedure.

Of course, the recorded Bragg spectrum is a superposition of spectra from all components of the sample. Therefore, analyzing complex substances one faces two main questions concerning the accuracy of determined experimental pole figures:

- What phases and to what degree contribute to the investigated intensity of the investigated reflection?
- What is the experimental background in the spectra?

To answer these questions it is advantageous to have available an approximate phase analysis. On this base the intensity part of TOF diffraction patterns of albite, plagioclases and quartz as well as their superposition have been simulated in Fig.1. The $(20\bar{2}1)$ reflection and the double peak $(11\bar{2}1)/(20\bar{2}1)$, for example, can be seen to be mainly caused by quartz. Assuming weak textures for all the components of the sample the error arising from disturbing intensity contributions to the investigated peak is negligible. The $(11\bar{2}2)$ reflection, on the other hand is a mixture of nearly equal intensity parts of quartz and albite and of to some extent lower contribution from plagioclase as well. Such kinds of peaks cannot be taken into further consideration.

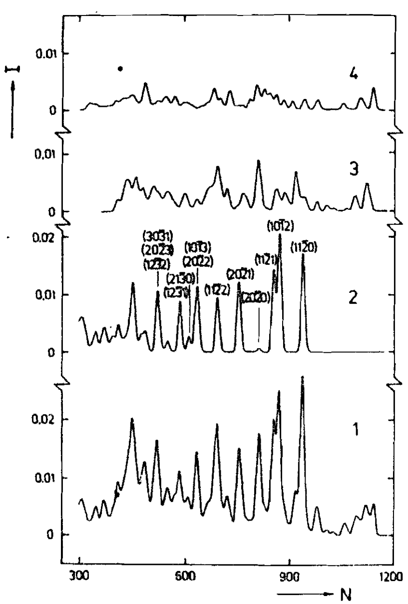

Fig.1. Computer simulated TOF spectra of plagioclase (4), albite (3), quartz (2) and the sum of all three spectra (1).

In practice, from texture analysis of the quartz component of the studied metamorphic rocks those reflections have been selected for which the quartz-caused intensity is more than 60%.

The time required for computer fit increases rapidly with increasing number of reflections taken into account. Therefore, it seems to be optimal to divide the diffraction pattern in groups of no more than five peaks for

integral intensity determination. From Fig.1 uncertainties have to be expected in background subtraction. In general, the zero level will be chosen too high. Consequently, the normalization factor of the experimental pole figures will become too small and the measured texture will seem to be sharper than it is in reality. On the other hand, this error can be partly compensated by intensity contributions of other phases to the considered peak.

Therefore, it is necessary to find some criteria for checking the experimental pole figures with respect to their accuracy and mutual compatibility before mathematical texture analysis.

METHODS FOR CHECKING AND CORRECTION OF POLE FIGURES

In the series expansion method, the pole figure $\vec{h}_i = (hk\ell)$ can be written as/7,8/:

$$\tilde{P}_{\vec{h}_i}(\vec{y}) = 4\pi \sum_{\ell=0(2)}^{\infty} \sum_{\mu=1}^{M(\ell)} \sum_{\nu=1}^{N(\ell)} \frac{C_\ell^{\mu\nu}}{2\ell+1} k_\ell^{\mu}(\vec{h}_i)\, k_\ell^{\nu}(\vec{y}), \qquad (1)$$

Using the orthogonality of spherical harmonics the $F_\ell^\nu(\vec{h}_i)$ factors can be found

$$F_\ell^\nu(\vec{h}_i) = 4\pi \frac{\oint \tilde{P}_{\vec{h}_i}(\vec{y})\, k_\ell^\nu(\vec{y})\, d\vec{y}}{\oint \tilde{P}_{\vec{h}_i}(\vec{y})\, d\vec{y}}. \qquad (2)$$

These $F_\ell^\nu(\vec{h}_i)$ factors and the series expansion coefficients $C_\ell^{\mu\nu}$ are connected by the equation

$$F_\ell^\nu(\vec{h}_i) = \sum_{\mu=1}^{M(\ell)} \frac{C_\ell^{\mu\nu}}{2\ell+1} k_\ell^{\nu}(\vec{h}_i). \qquad (3)$$

In the case of $\ell = 2$ there holds $M(\ell) = 1$ for hexagonal, tetragonal and trigonal crystal symmetries, i.e., the $C_\ell^{1\nu}$ can be calculated for each pole figure separately. Of course, if there are no errors in pole figure determination, $C_\ell^{1\nu}$ should not depend on pole figures. Therefore, the differences between $C_\ell^{1\nu}(\vec{h}_i)$ are the indicator for the mutual consistency. If there is any reference pole figure, the other $C_\ell^{1\nu}(\vec{h}_i)$ can be corrected to some degree by adding a constant background value to the pole figure values in eq.(2). The numerator of eq.(2) does not change because of the orthogonality of spherical harmonics, but the denominator varies the pole figure normalization. Another error source is the overestimation of some pole ranges. If there is a reference pole figure having the same tilt in the crystal coordinate system the factors $F_\ell^1(\vec{h}_1)$ and $F_\ell^1(\vec{h}_2)$ have to be identical. The overestimated tilt angle range in a pole figure can be found by simultaneous consideration of $F_{\ell}^{\nu}(\vec{h}_i)$ discrepancies and the tilt angle dependence of spherical harmonics. Of course, this method is limited to a few pole figures only.

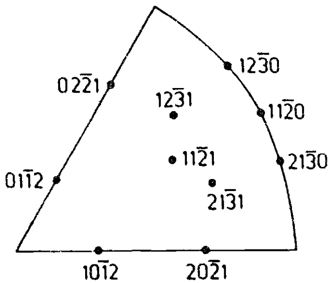

Fig.2. Positions of experimental points in the inverse pole figure.

If there is a sufficient number of corrected pole figures to carry out the mathematical texture analysis, a good consistency of experimental and recalculated pole figures is required. But even in the case of excellent consistency further correction may be necessary. In the quartz texture analysis which has been carried out at JINR, Bragg reflections have been considered corresponding to the points in the inverse pole figure most of which are far from the centre of it as is shown in Fig.2. If all the pole figures are misnormalized in the same way, any inverse pole figure gets to high values in its outer range. The only possible compensation to fulfill the normalization condition for the inverse pole figure are the physically senseless negative ranges in its centre. This situation can be corrected by pole figure background manipulations in Eq.(2) also. Up to now the only objective criterion for the degree of correction is the non-negative pole density condition. The latter procedure influences the sharpness of texture, but not its type.

EXPERIMENTAL RESULTS

At the JINR, Dubna, the preferred orientations of the quartz component in granulites /4/, gneisses and granites have been studied. As examples the experimental and reproduced pole figures are shown to demonstrate the usefulness of the described checking and correction methods. For the investigation of granulite (Figs. 3 and 4) as well as granite (Figs.5 and 6) pole figures have been selected with respect to the $C_2^{1\nu}$ criterion only. No background variation has been carried out. The recalculated pole figures of granite reproduce only some general characteristic of incident ones. There is no evident specimen symmetry. The agreement of experimental and reproduced pole figures is quite satisfactory in the case of granulite. In the pole figures an approximative orthorhombic sample symmetry can be also observed referring to plane deformations in the formation process of the rocks.

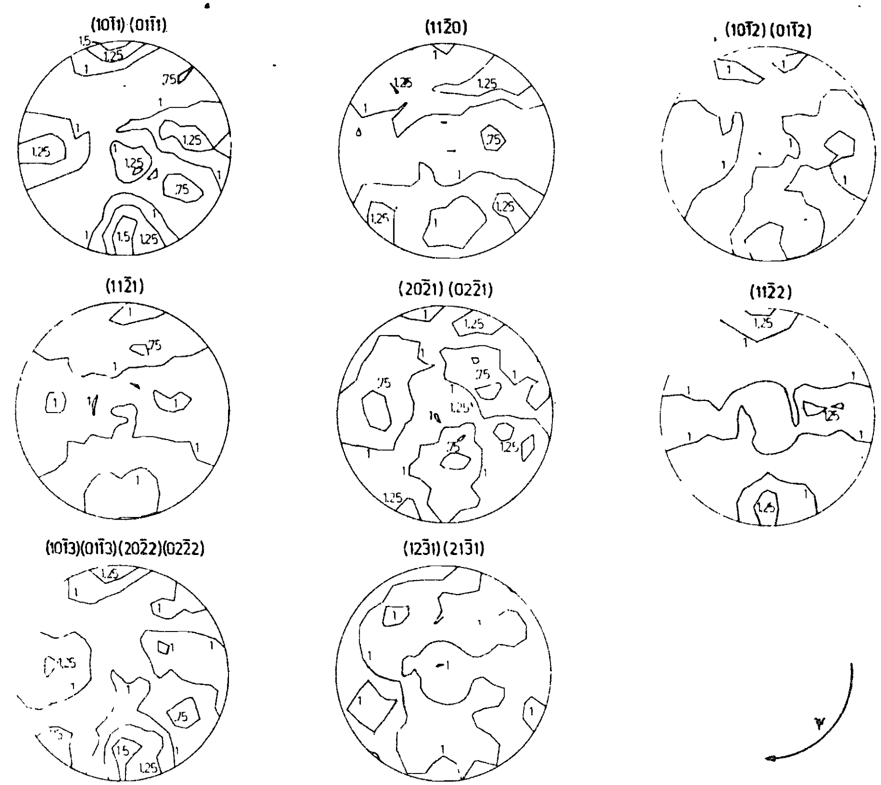

Fig.3. Experimental pole figures of granulite.

A good coincidence between experimental and recalculated pole figures has been found in the case of gneiss (Fig.7 and 8) using all correction possibilities which have been described in the previous paragraph. Only some relatively sharp maxima in the incident data have been smoothed to some extent in the reproduced ones in the same way as in granulite and granite. An orthorhombic specimen symmetry can be also seen in the pole figures of gneiss.

CONCLUSIONS

In this paper some methods are proposed to check and to improve the accuracy and consistency of experimental pole figures from very complex materials like natural rocks. The considerations should have importance in the study of other multiphased and lowsymmetric systems also.

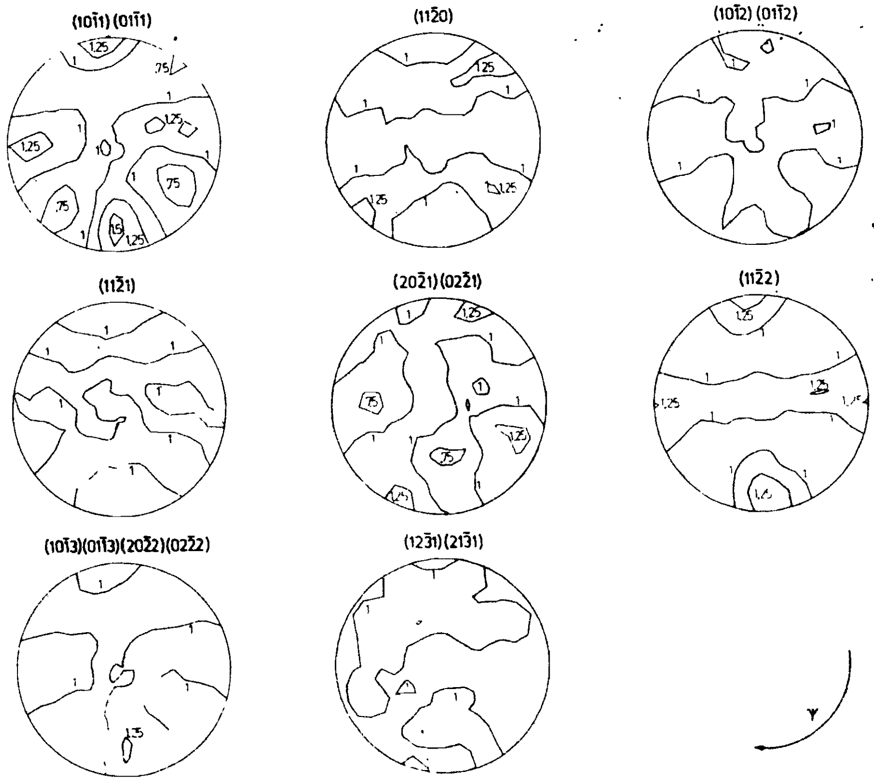

Fig.4. Recalculated pole figures of granulite.

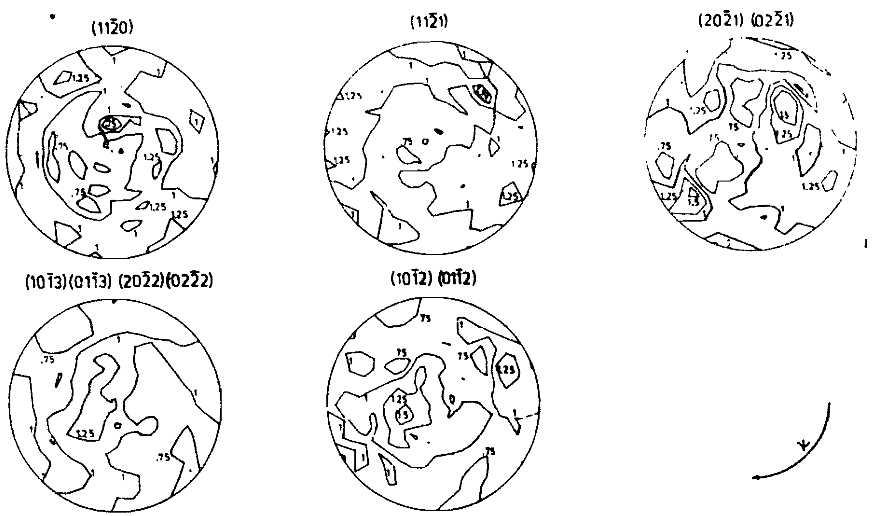

Fig.5. Experimental pole figures of granite.

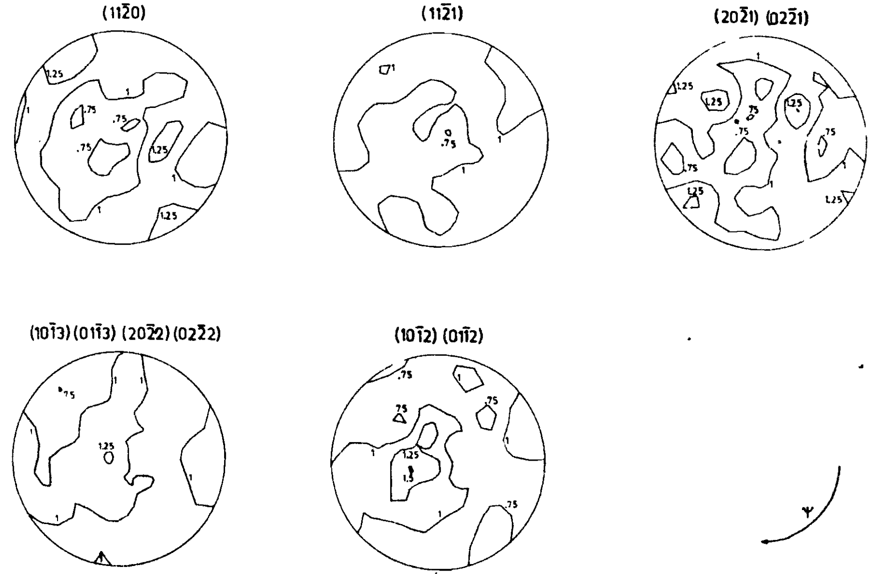

Fig.6. Recalculated pole figures of granite.

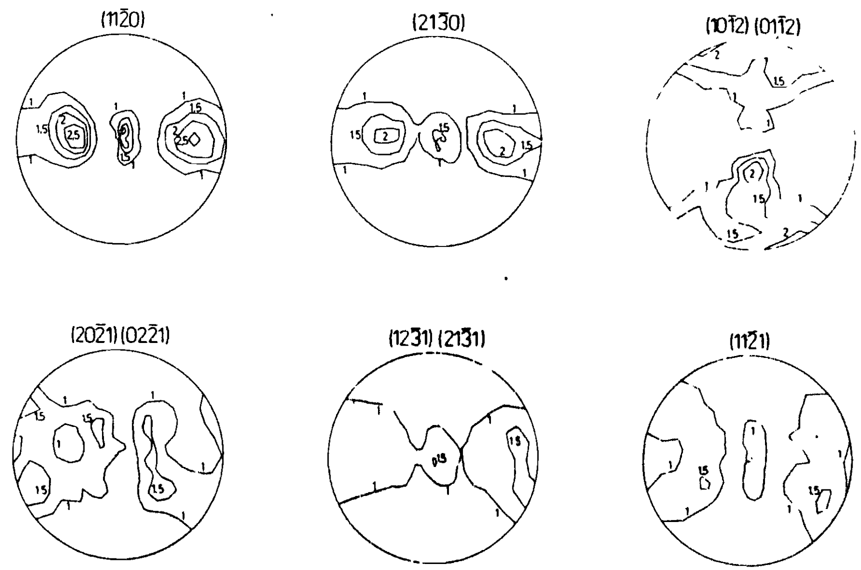

Fig.7. Experimental pole figures of gneiss.

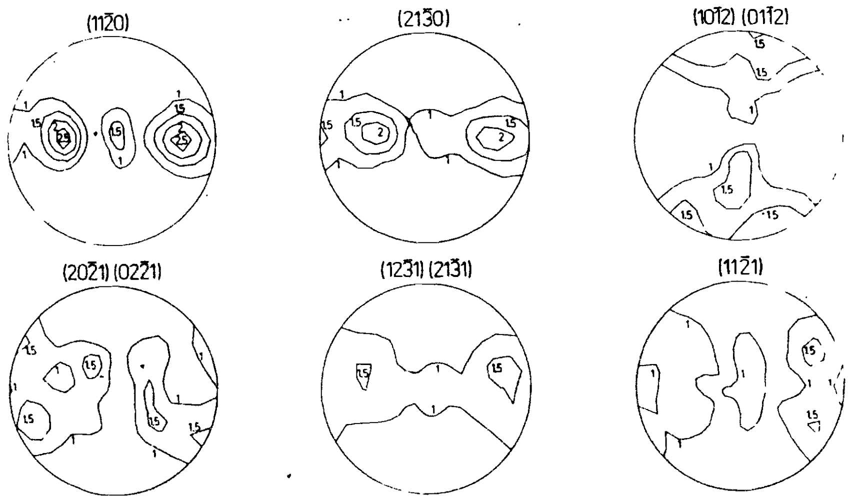

Fig.8. Recalculated pole figures of gneiss.

The carefull background handling is shown to have great influence on the quality of pole figure determination. Therefore, for texture analysis of materials having a large number of reflections and overlappings in their Bragg pattern experimental techniques should be preferred to obtain not only information on the integrated intensity of the studied peak, but also on the behaviour of its neighbourhood. Such methods are the energy dispersive diffraction of X-rays or neutrons (TOF), or the use of position sensitive detectors in the conventional angle dispersive techniques.

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Фельдманн К., Фуэнтес Л., Вальтер К. E14-86-360
Проблемы текстурного анализа метаморфных горных пород

В нейтронной дифракции по времени пролета полный дифракционный спектр снимается одновременно. Такая экспериментальная техника является эффективным способом для исследования текстур низкосимметричных соединений, в том числе кварцевых горных пород. Ненормированные полюсные плотности определяются в виде интегральных интенсивностей соответствующих брэгговских отражений с помощью программы подгонки. Большинство горных пород состоят из нескольких фаз. Те гранулиты, граниты и гнейсы, которые исследовались в ОИЯИ, Дубна, содержали 50 процентов кварца, помимо других компонент. Поэтому время-пролетная брэгговская картина является суперпозицией спектров от всех фаз, т.е. имеется большое число перекрывающихся рефлексов. В этом случае возникает вопрос о надежности экспериментальных полюсных фигур. В данной работе представлены критерии для проверки и возможности повышения качества полюсных фигур. Приведенные соображения могут иметь значение при исследовании текстур и других низкосимметричных или многофазных образцов. В качестве примера показываются результаты текстурного анализа в некоторых исследованных кварцевых горных породах.

Работа выполнена в Лаборатории нейтронной физики ОИЯИ.

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Feldmann K., Fuentes L., Walther K., E14-86-360
Problems in Texture Analysis of Metamorphic Rocks

The neutron time-of-flight diffraction is well-suited for the investigation of preferred orientations in low symmetric materials, like for example in quartzitic rocks, because of the simultaneous recording of the complete bragg pattern. The unnormalized pole figure values are found by a computer fit of the integrated intensities of the corresponding Bragg reflections. Most of the natural rocks consist of more than one phase. In granulites, granites and gneisses, which have been investigated at the JINR Dubna, there are about 50 per cents of quartz among other components. Therefore, the TOF diffraction pattern is a superposition of spectra from all phases, i.e. there is a lot of overlappings of different Bragg peaks. In this case the question arises about the reliability of the experimental pole figures. Some possibilities and criteria are discussed to check up and to improve the quality of pole figures. These methods may have importance in the study of other low symmetric or multiphases systems too. Furthermore, texture analysis results are presented for several investigated quartzitic rocks.

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

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