Comparative quantitative analysis of quartz textures in monomineral and multiphase rocks using neutron diffraction at IBR-2, Joint Institute for Nuclear Research Dubna (Russia)

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Introduction

Many manmade and natural materials are composed of crystals with generally non-random crystallographic orientation (texture). Rocks show a great variety of textures and compositions, generally containing several phases with very different physical and chemical properties. The texture is a fingerprint of the earth's history and, simultaneously, informs on anisotropies of elastic, magnetic and thermal properties of rocks constituting the crust and upper mantle. Nowadays, knowledge has reached a level that provides a quantitative framework of texture information. Progress of quantitative texture analysis in geosciences is based on the improvements of the experimental techniques with special emphasis on diffraction methods and use of neutron. Many fundamental investigations in modern geology and geophysics are developed due to the application of neutron diffraction analysis to study of structure, texture and properties of geological materials as well as to model the behavior of rocks at high temperatures and pressures.

Of all minerals quartz has received the most attention with respect to texture studies. This is due to its importance in controlling the rheology of many rocks, but also to the large variety of texture types found under different deformational conditions. Mean while a point in the understanding of the development of quartz texture has been reached to deduce at least some aspects of deformation history of a rock empirically.

The project lets the neutron diffraction texture analysis application in description of type and symmetry of quartz texture in monomineral and multiphase rocks and to reveal the possible deformational condition (strain symmetry) and process of texture formation. The project is aimed at: the introduction into the modern mathematical texture analysis, the determination of the orientation distribution of crystallites in the polycrystalline aggregate, the interpretation of this distribution in terms of the processes which lead to its formation. The project could provide practical exposure and experience in neutron diffraction application in condensed matter (e.g., rocks) study.

Project description

Experimental setup

The pulsed reactor IBR-2 represents a worldwide well known powerful machine, last but not least for experiments with geomaterials, because the used neutron time-of-flight method is able to meet several requirements for studies on geological specimens. Thermal neutrons offer the advantage of high transmission through matter. That means, large sample volumes are accessible, allowing good grain statistics even for coarse grained and inhomogeneous specimens. Simultaneous detection of all allowed Bragg-reflections is permitted with high precision and it is possible to study minerals with lower crystal symmetry (large unit cell), of which consist most of the rocks of the upper and middle earth's crust.

Fig.1: View of the SKAT texture diffractometer

The time-of-flight texture diffractometer SKAT (spectrometer for quantitative analysis of textures) is located at the end of a more than 100 m long flight path on beam 7a of the IBR-2 pulsed reactor (Fig. 1).

The main characteristics of the diffractometer SKAT may be summarized as follows:

- 19 detector modules are arranged on a ring carrier around the incident neutron beam at a unique scattering angle of 2Q = 90° (Fig. 2a); (Ullemeyer et al., 1998). Neutrons, scattered at lattice planes with the same spacing, i.e. belonging to the same pole figure, are recorded by the detectors at the same time-of-flight.
- The sample is positioned in the centre of the ring and rotated around a horizontal axis Z at an angle of 45° with respect to the incident neutron beam Supposing that the detector modules include an angular range of 180° on the ring, complete pole figures may be measured by a single sample revolution (Fig. 2b).

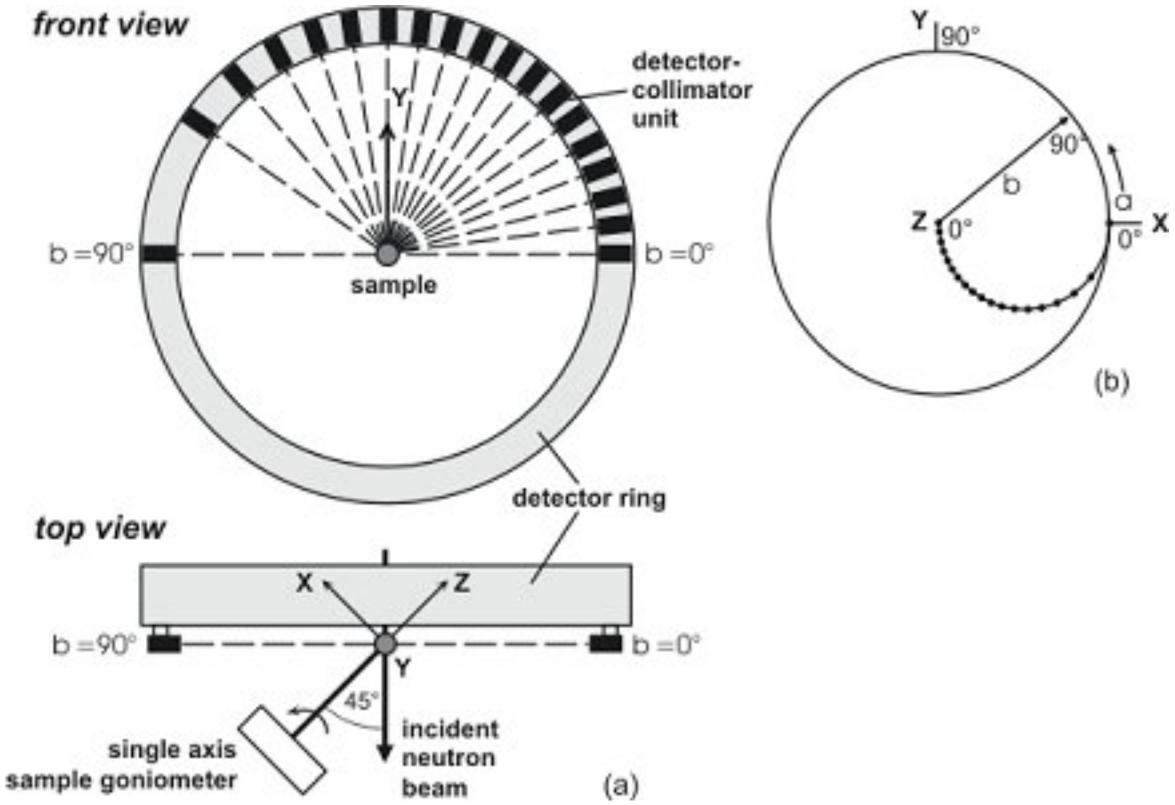

Fig.2: a) Scheme of the SKAT texture diffractometer. The given arrangement of detector-collimator units corresponds to a constant pole angle step size of Db = 5°. b = 0° indicates the centre, b = 90° the boarder of the pole figure.
b) Geometrical relationships at the SKAT, projected onto the pole figure plane XY. a, b: pole figure angles azimuth, inclination (pole angle). Sample directions indicated on the half circle correspond to azimuth angle a = 0°.

From the above mentioned constancy of 2Q follows that all Q dependent intensity corrections may be neglected. Accordingly, a rather low error level of the results of texture analysis is expected. The measurements are comparatively fast, since 19 sample directions are measured at the same time.

Measuring procedure (practical work)

1. Familiarize with the principle of operation of the SKAT texture diffractometer.
2. Estimate the necessary exposition time and measure diffraction pattern of quartz-bearing rock samples by the SKAT diffractometer.
3. Familiarize with AutoIndex and GeoTOF programs. Use the AutoIndex program for indexation of spectra of both monophase and multiphase materials in interactive mode. Use the GeoTOF program

for calculation of pole density distribution (pole figures) from the measured diffraction spectra.
4. Using Beartex program for the comparative quantitative texture analysis of quartz texture component. Interpretation of the data in terms of the possible orientation mechanism and deformation path.

Result presentation

The report should include preamble with the main purpose of the project, description of the rock samples and method, experimental results containing typical time-of-flight diffraction patterns of quartz sample, pole figures classification of investigated samples and conclusions.

Standard of knowledge
The students should have got knowledge of physics of the solid body, crystallography and neutron diffraction experimental technique. A numerical data on mineralogy and physics of the Earth is desirable.

Literature

1. Bunge, H.J. (1982) Texture analysis in materials science // Butterworths. London.
2. Kocks, U.F., Tome, C.N., Wenk, H.-R. (1998) Texture and anisotropy // Cambridge university press. 676 p.
3. Nikitin, A.N. and Ivankina, T.I. (2004) Neutron Scattering in Geosciences. Paricles&Nuclei. Scientific review journal, 4, vol.5, 35, 2, 348-407.
4. Schmid, S.M. and Casey, M. (1986) Complete fabric analysis of some commonly observed quartz c-axis patterns. Am.Geophys.Un.Geophys.Monogr. vol. 36, 263-286.
5. Ullemeyer K., et al. (1998) The SKAT texture diffractometer at the pulsed reactor IBR-2 at Dubna: experimental layout and first measurements // Nucl. Ins.and Meth. In Phys. Res. A 412, 80 - 88.
6. Wenk H.-R. (1985) Preferred orientation in deformed metals and rocks: An introduction to modern texture analysis // FL: Academic Press. Orlando. 610 p.

Students
Concurrently, 2-3 students may work in the team.

Head of the project
Tatyana I. Ivankina

OCCUPATION: geophysicist, educator

POSITION HELD:
Ph.D. in Geophysics
Associate Professor

Senior Researcher, Condensed Matter Department Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Moscow region (1998-2007).

SCIENTIFIC CONTRIBUTIONS:
Achievements include application of neutron diffraction to study of methamorphic, geodynamic and evolution processes in the lithosphere of the Earth on the basis of crystallographic textures of deep and surface rocks. Interpretation of seismic anisotropy of lithosphere on the basis of texture analysis of deep rocks.

SELECTED PUBLICATIONS:

Ivankina T.I., A.N.Nikitin, W.Voitus and K.Walher (1991). Texture analysis and investigation of piezoelectric properties of natural quartz, Textures and Microstructures, vol.14-18, 421-429.
Nikitin A.N. and Ivankina T.I. (1995). On the possible mechanisms of the formation of piezoelectric active rocks with crystallographic textures. Textures and Microstructures, vol.25, 33-43.
Ivankina T.I., Nikitin A.N.,.Ullemeyer K., et al. (1998).Investigation of structure and texture transformation processes in rocks, Schriftenr. Geowiss., 6, 49.
Ivankina T.I., A.N.Nikitin, et al.(2000). Textures and physical properties of marbles deformed at 20-250 ÿЄ C, High Pressure Research, vol.17,335-346.
Nikitin A.N., T.I.Ivankina, D.E.Burilichev, K.Klima, T.Locajicek and Z.Pros (2001). Anisotropy and texture of olivine-bearing mantle rocks at high pressures, Physics of the Solid Earth, AGU, vol.37, 1, 59-72.
Ivankina T.I., Kern H.M. and Nikitin A.N. (2005) Directional dependence of P- and S-wave propagation and polarization in foliated rocks from the Kola superdeep well: Evidence from laboratory measurements and calculations based on TOF neutron diffraction. Tectonophysics, 407, 25-42.