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TOF Neutron Diffraction to Characterize Polycrystalline Rocks: Quartz Textures as Examples

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Neutron diffraction is increasingly used to characterize properties of polycrystalline materials. Such properties include microstructure (grain size, grain shape, defect densities), texture (crystallographic preferred orientation) and stress. Time-of-flight facilities as IPNS, ISIS, JINR and LANSCE have been particularly important because they record continuous spectra that can be analyzed for peak positions, peak intensities and peak shapes with the Rietveld method as implemented in computer codes like GSAS and MAUD. At these facilities analyses can not only be performed at ambient conditions but at temperature, pressure and stress as well. Earth scientists have made increasing use of these new opportunities to study the complexities of polycrystalline aggregates, particularly in fields of rock deformation and rock mechanics, structural geology and seismic anisotropy. The goal of such studies is to better understand the stress and strain evolution rocks and relate it to the orientation distribution.

This report highlights some issues for quartz. Samples were analyzed on the HIPPO TOF diffractometer at LANSCE. In a sample suite of granitic mylonites from Southern California, consistent texture patterns were observed for quartz and biotite, including trigonal pole figures expressed in positive and negative rhombs. These trigonal textures can be explained as due to mechanical Dauphiné twinning, opening the prospect to use them as paleopiezometers. Such complex polymineralic rocks with many overlapping diffraction peaks eluded a quantitative texture characterization until the Rietveld method became available. Another example is a quartzite from the Vredefort meteorite impact site. High pressure phases such as coesite and stishovite are indicative of high shock pressures. The c-axis orientations of quartz are random, but there is a slight yet systematic difference between positive and negative rhombs that can only be ascertained with neutron diffraction and excellent grain statistics. Again the orien-

tation pattern is explained as due to Dauphiné twinning during passage of the shock wave. A third example is the effect of the trigonal-hexagonal-trigonal phase transformation on texture. Highly textured quartzites were heated to 650ºC and texture measurements were done in situ in a furnace. Interestingly upon cooling the sample returned exactly to the original trigonal texture, indicating a texture memory. Similar variant selections have been documented in metals (e.g. hcp→bcc and bcc→fcc, as well as shape-memory alloys) and the causes are still poorly understood. Neutron diffraction at high temperature now provides quantitative experimental data that can serve as basis for mechanical models. Most likely, stresses from neighboring grains in these elastically very anisotropic materials imposes the texture memory and such stresses can also be quantified by neutron scattering. Contributions from Jenny Pehl, Sven Vogel and Darrick Williams are gratefully acknowledged.