Dauphiné twinning as evidence for an impact origin of preferred orientation in quartzite: An example from Vredefort, South Africa

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ABSTRACT

Large meteorite impacts cause great changes to geologic features on Earth, ranging from cratering and ejecta blankets to phase transformations in minerals. In this report we describe the effect of a shock wave on the crystallographic orientation of quartz crystals in quartzite from the Vredefort impact site in South Africa. Preferred orientation of bulk quartzite samples was measured by time-of-flight neutron diffraction. With a random distribution of *c*-axes, a weak but distinct difference between the orientation distribution of positive and negative rhombs was observed, as illustrated with pole figures and inverse pole figures. Results for the natural Vredefort sample are compared with deformation experiments in which the reorientation occurs as a result of mechanical Dauphiné twinning under stress. We conclude that stresses during the impact produced twinning and that the direction of the compressive shock wave can be inferred from the preferred orientation pattern. Specifically, positive rhombs become aligned perpendicular to the direction of compressive stress.

Keywords: Vredefort impact site, Dauphiné twinning, quartz crystals, preferred orientation.

INTRODUCTION

The Vredefort crater in South Africa has long been suggested to be an impact structure (Daly, 1947), but only with the recognition and detailed analysis of features such as pseudotachylites (Shand, 1916; Reimold, 1995; Gibson et al., 1997b), high-pressure phases like coesite and stishovite (Martini, 1978; White, 1993), and shatter-cone features (Dietz, 1961) has the shock-origin interpretation become generally accepted and Vredefort emerged as a classical example of a meteorite impact site (Gibson and Reimold, 2001). The impact has been dated as 2.0 Ga (Gibson et al., 1997a; Moser, 1997; Trieloff et al., 1994), and it occurred in Precambrian igneous and metamorphic rocks, including quartzites. Maximum shock pressures are estimated as 20–50 GPa (Melosh, 1989; Leroux et al., 1994). In this study we use methods of quantitative texture analysis to investigate the effect of shock deformation on the orientation distribution of quartz grains.

It is well known that quartz crystals subjected to high stress undergo mechanical Dauphiné twinning (Zinserling and Schubnikov, 1933; Wooster et al., 1947; Thomas and Wooster, 1951). During twinning, only a slight displacive rearrangement of atoms occurs (Frondel, 1945), without any breakage of bonds or permanent macroscopic strain (Fig. 1). However, the change in crystallographic orientation is profound. It corresponds to a twofold rotation about the *c*-axis that reverses positive and negative rhombs and is recognizable in diffraction patterns (e.g., intensity of 70% for neutron diffraction of the positive rhomb $\{10\bar{1}1\}$ and 30% for the negative rhomb $\{01\bar{1}1\}$). In terms of elastic properties, the pole to the positive rhomb is close to the stiffest direction of quartz, and that of the negative rhomb close to the softest direction. The original elastic loading experiments were done on single crystals. Similar loading experiments were performed on polycrystalline quartz, and distinct changes in orientation patterns were observed without changes in the overall sample shape (Tullis, 1970; Tullis and Tullis, 1972). At differential compressive stresses of 1–2 GPa, crystals with negative rhombs perpendicular to the compression direction were reoriented by Dauphiné twinning in a way that the positive unit rhomb $\{10\bar{1}1\}$ became preferentially aligned perpendicular to compression. We thus surmised that a 20 GPa shock wave that passed through a quartzite might also produce Dauphiné twinning such that crystals become energetically more favorably oriented.

SAMPLE CHARACTERIZATION AND TEXTURE ANALYSIS

We investigated a sample of quartzite collected at Weltevrede farm between Parys and Sasolburg in Kromellenboogspruit, ~30 km from the Vredefort impact center (Fig. 2). This quartzite, part of the West

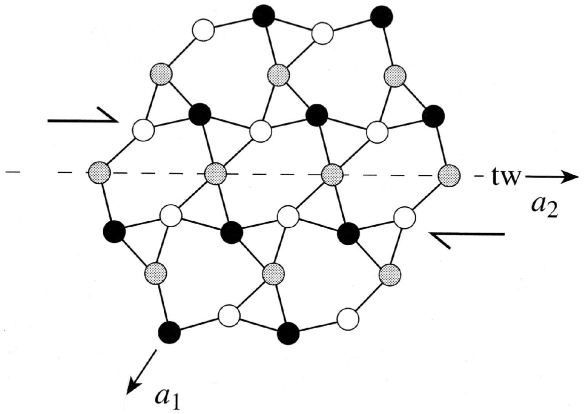

Figure 1. Model for structure of Dauphiné twin (tw) in quartz produced by shear. Only silicon atoms are shown (circles); gray shades indicate different levels along *c*-axis; a_1 and a_2 are crystallographic axes.

Geology; April 2005; v. 33; no. 4; p. 273–276; doi: 10.1130/G21163.1; 5 figures.

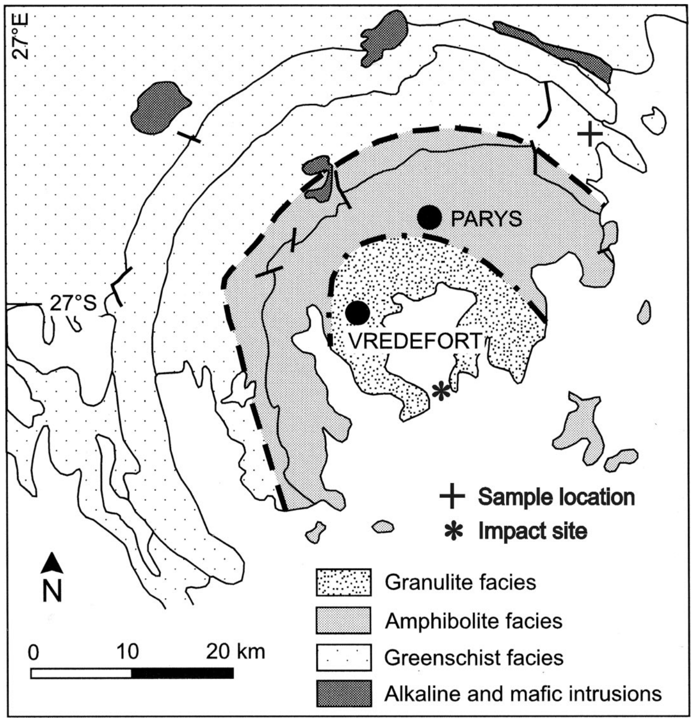

Figure 2. Geological sketch map of Vredefort Dome area in South Africa, indicating impact site and sample locality. Also shown is pre-impact metamorphic grade in ring structure (from Gibson and Reimold, 2001).

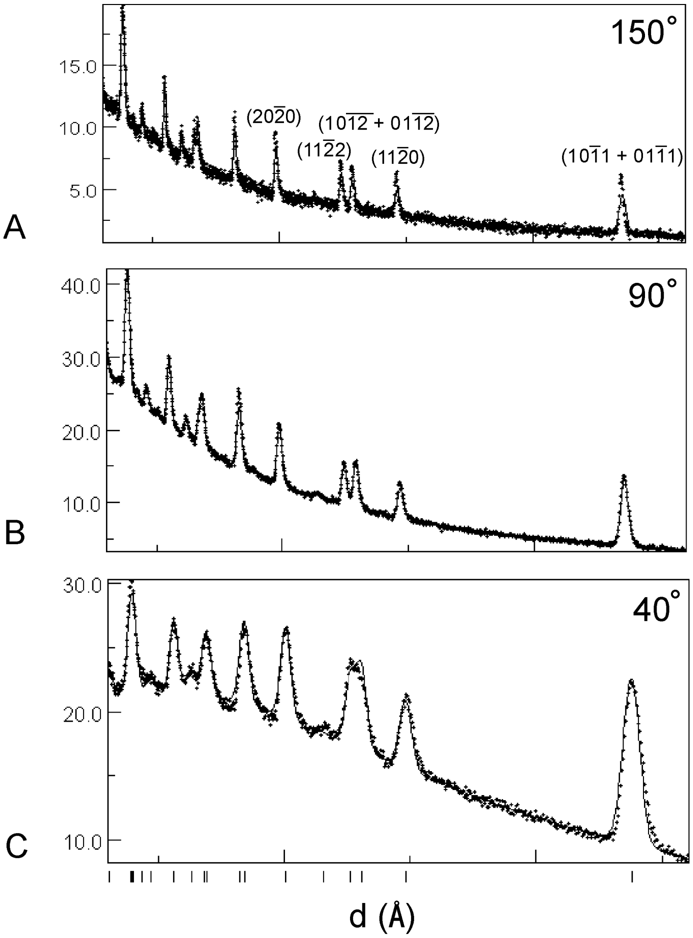

Figure 3. Time-of-flight neutron diffraction spectra for Vredefort quartzite that were used for Rietveld texture refinement. Examples of 150° (A), 90° (B), and 40° (C) detectors. Dot pattern is measured spectrum, and line indicates Rietveld fit. Some quartz diffraction peaks are indexed, with calculated peak positions indicated below. Abscissa is d-spacing.

Rand Group of the Witwatersrand Supergroup, has a sedimentary age of 2.7–2.9 Ga (Armstrong et al., 1991), and underwent greenschist facies metamorphism prior to the meteorite impact (Phillips and Law, 1994). Martini (1978, 1991) discovered small amounts of coesite and stishovite in this rock, as well as planar deformation features in quartz that are typical of shock deformation (Carter, 1965; Leroux et al., 1994). The average grain size of quartz is 0.3–0.5 mm. Some fine-grained muscovite occurs along the quartz-grain boundaries. A preliminary survey of thin sections with the petrographic microscope and gypsum plate revealed no significant preferred orientation of *c*-axes.

We used neutron diffraction to determine the complete orientation distribution. The main reason for applying this technique is that with optical microscopy and a universal stage only the orientation of *c*-axes can be determined, but not the difference between positive and negative rhombs, which is critical to assess Dauphiné twinning. Dauphiné twins are invisible in transmitted light because host and twin share the same *c*-axis. A second reason is that, to ensure statistical significance, a large sample volume needs to be investigated and averaged, particularly in the case of coarse-grained samples with very weak textures (Matthies and Wagner, 1996). This is difficult to achieve with X-ray diffraction or electron microscopy, techniques that rely on surface analyses. With neutron diffraction, attenuation is minimal and large bulk samples can be investigated.

The sample analyzed was a cylinder, 6 mm in diameter and 10 mm long, containing >2000 crystallites. We employed the texture capabilities of the time-of-flight neutron diffractometer high-pressure preferred orientation at Los Alamos (Wenk et al., 2003). The sample was irradiated with a beam of polychromatic pulsed neutrons, 12 mm in diameter, and a flux of 2×10^7 neutrons cm^{-2} s^{-1}. Diffraction from the sample was recorded with 720 ^{3}He tubes, mounted on 30 detector panels and arranged on 3 rings around the incident beam at diffraction angles $2\theta = 40°$, 90°, and 150°. Each detector recorded a diffraction spectrum from differently oriented crystals. The sample was rotated around the cylinder axis to improve orientation coverage. From a combination of 180 spectra from 30 detectors in 6 sample orientations, the orientation distribution function (ODF) was calculated with the Rietveld method and the tomographic EWIMV texture algorithm as implemented in the software package MAUD (Lutterotti et al., 1997). The Rietveld method obtained a best fit between measured spectra and calculated intensities by refining instrument parameters, background, crystallographic parameters, microstructural characteristics, and texture, which influence peak positions, peak intensities, and peak shapes. Figure 3 displays typical spectra for 150°, 90°, and 40° detectors, comparing measurements (dot patterns) and the Rietveld fit (line). Note that the resolution (in d-spacing) decreases with diffraction angle. This was not critical for quartz with widely spaced diffraction peaks. Although the diffraction peaks for positive and negative rhombs occur at identical d-spacings, the relative-intensity contributions are different, and this is the basis for the resolution of trigonal symmetry and separation of pole figures for positive and negative rhombs (Baker et al., 1969).

The discrete ODF obtained with the Rietveld refinement in $5° \times 5° \times 5°$ cells in orientation space was smoothed with a 7.5° gauss filter. As a result, pole figures for several lattice planes were recalculated. For *c*- and *a*-axes, highly irregular patterns were observed; these are due to poor grain statistics and confirm the qualitative assessment with the petrographic microscope that the *c*-axis distribution is basically random. However, pole figures of rhombohedral lattice planes produce weak but well-defined patterns, with positive rhombs $\{10\bar{1}1\}$ and

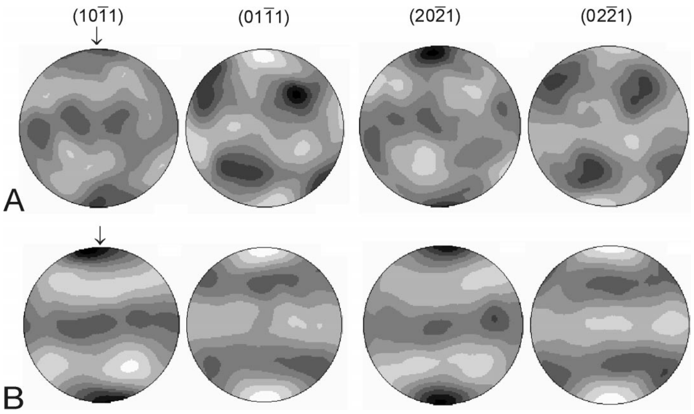

Figure 4. Pole figures for rhombohedral lattice planes of quartz, recalculated from orientation distribution. A: Vredefort quartzite (maximum is 1.30 multiples of random distribution [m.r.d.]; minimum is 0.75 m.r.d.). B: Experimentally deformed novaculite (sample W-1170) (maximum, 2.0 m.r.d.; minimum, 0.40 m.r.d.). Equal-area projection; linear gray-shade scale. Dark shades indicate high pole densities; light shades indicate low densities. Arrow indicates symmetry axis (compression direction).

$\{20\bar{2}1\}$ displaying a single maximum (and small circle girdles from symmetrically equivalent poles), and negative rhombs displaying minima in the orientations where positive rhombs show maxima (Fig. 4A). These normalized pole figures express pole densities in multiples of a random distribution (m.r.d.). The maximum pole density is 1.3 m.r.d., and the minimum is 0.75 m.r.d. This is quite weak, yet statistically significant and reproducible. The pole figures have been rotated such that the primary maximum for positive rhombs is on the periphery at the top and marked with an arrow. Based on the conclusions of Tullis (1970), it thus appears that this is the direction of compression, i.e., the direction from which the shock wave arrived.

EXPERIMENTAL ANALOG

To test this conclusion, we compared the Vredefort quartzite with an experimentally deformed sample of novaculite (a sedimentary quartz rock from the Ouachita Mountains in Arkansas, with a grain size of 5 μm and no initial preferred orientation). At a temperature of 200 °C and a confining pressure of 0.1 GPa, we subjected it to a compressive stress of 1 GPa for 2.5 h. The cylindrical sample was analyzed in an identical way by neutron diffraction, and pole figures are shown in Figure 4B. Pole figures are more symmetrical and homogeneous owing to the smaller grain size, and textures are slightly stronger owing to the static nature of the experiment. The maximum is 2.0 m.r.d., and the minimum is 0.4 m.r.d. However, the pole figures display a pattern similar to that of the Vredefort sample, with a maximum for $\{10\bar{1}1\}$ and $\{20\bar{2}1\}$ in the compression direction, and a minimum for $\{01\bar{1}1\}$ and $\{02\bar{2}1\}$, respectively.

INTERPRETATION OF THE ORIENTATION PATTERNS

In the case of axially symmetric deformation, inverse pole figures are efficient representations of preferred orientation. These pole figures are also calculated from the ODF. The inverse pole figures in Figure 5 display the probability of finding a compression direction (symmetry axis of the pole figure) relative to crystal coordinates. Inverse pole figures for the Vredefort quartzite (Fig. 5A) and the experimentally deformed novaculite (Fig. 5B) show a striking similarity, with maxima between $\{10\bar{1}1\}$ and $\{20\bar{2}1\}$, and minima between $\{01\bar{1}1\}$ and $\{02\bar{2}1\}$. Pole densities at (0001) are 1 m.r.d. in both samples, confirming that the *c*-axis distribution is random. Note that the maximum for positive rhombs is correlated with a minimum for negative rhombs, and if the two sides are averaged across a mirror plane at 30° in the 60° sector, the texture becomes more or less random. This feature indicates that the preferred orientation can be explained solely by Dauphiné twinning, depleting orientations with negative rhomb lattice planes perpendicular to the compression direction. As the aggregate attains a preferred orientation of the positive and negative forms, the *c*-axis distribution does not change. The inverse pole figures document that the Vredefort quartzite has a weaker texture than the novaculite; twinning has not been as efficient, presumably because of strain heterogeneities. As noted by Tullis (1970), the preferred orientation pattern is similar to that for the inverse of Young's Modulus of α-quartz (Hearmon, 1946) (Fig. 5C), and thermodynamic arguments have been used to relate twinning to the elastic energy in a stressed polycrystalline solid (Tullis and Tullis, 1972; McLellan, 1978). For axial compression the elastic energy is minimized if positive rhombs, corresponding to soft directions, are perpendicular to the applied stress.

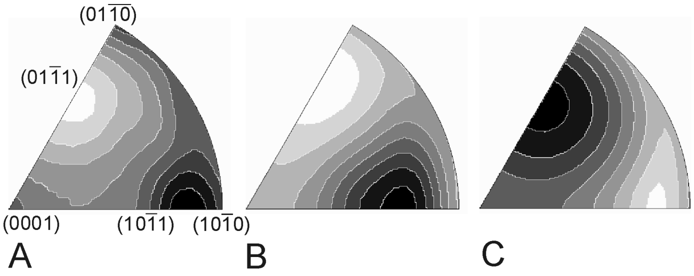

Figure 5. Inverse pole figures of compression direction (symmetry axis in Fig. 4). A: Vredefort quartzite (maximum, 1.3 multiples of random distribution [m.r.d.]; minimum, 0.7 m.r.d.). B: Experimentally deformed novaculite (maximum, 2.0 m.r.d.; minimum, 0.4 m.r.d.). C: Stiffness surface for quartz, illustrating elastic anisotropy (maximum, 130 GPa; minimum, 69 GPa). Equal-area projection; linear gray-shade scale. Dark shades indicate high pole densities and high stiffness; light shades indicate low densities.

OUTLOOK

The investigation suggests that for Vredefort quartzite with no initial preferred orientation, a shock wave produced during meteorite impact changed the orientation pattern of quartz grains by Dauphiné (elastic) twinning. From pole figures we can infer the stress direction (in this case, the tops of the pole figures in Fig. 4). This reorientation occurred without plastic deformation by slip. It may be surprising that the twinning pattern in quartz has not changed for >2 b.y. However, this region has been tectonically very stable, and in the same sample highly metastable stishovite (Martini, 1978) and glass (Dressler and Reimold, 2001) are also preserved. Naturally, this unexpected observation of Dauphiné twinning in quartzites subjected to meteorite impact calls for systematic studies of series of oriented samples, not only at Vredefort, but at other impact sites, such as Meteor Crater in Arizona. A prerequisite is no episode of tectonic deformation since the impact event. Also, in the future quartzites should be investigated that have been experimentally deformed under shock conditions, rather than at slow strain rates as was the case for the experimental sample available for this study.

Mechanical twinning has been documented in many materials. Geologically most important is twinning in calcite, which is widely observed in deformed carbonate rocks. Contrary to Dauphiné twinning in quartz, e-twinning in calcite produces a large strain with profound changes in preferred orientation patterns (e.g., Takeshita et al., 1987). Calcite twinning has been used to estimate stress magnitudes during tectonic deformation (Jamison and Spang, 1976; Rowe and Rutter, 1990). Because stresses required to induce elastic Dauphiné twinning are small, it has been assumed that twins in quartz are not reliable paleopiezometers and so reflect some late-stage local stress events (Tullis, 1980). However, it should be noted that tectonically and experimentally plastically deformed quartzites display distinct orientation distributions of positive and negative rhombs, though in more complicated patterns (Baker and Wenk, 1972; Schmid et al., 1981; Helming et al., 1994, Heidelbach et al., 2000, Lloyd, 2000). It is likely that in those cases the systematic trigonal pattern is also produced by Dauphiné twinning during deformation and thus is a direct expression of differential stresses. So far the patterns in tectonic quartzites have not been interpreted.

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