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Fabric transitions in quartz via viscoplastic self-consistent modeling part I: Axial compression and simple shear under constant strain

Luiz F.G. Morales [a,*], Geoffrey E. Lloyd [b], David Mainprice [c]

[a] Deutsches GeoForschungsZentrum (GFZ), Section 3.2 Telegrafenberg, 14473 Potsdam, Germany
[b] Institute of Geophysics and Tectonics, School of Earth and Environment, University of Leeds, Leeds LS2 9JT, UK
[c] Géosciences Montpellier, Université Montpellier 2, Place Eugène Bataillon, Batîment 22, 34095 Montpellier, France

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ABSTRACT

Quartz is a common crustal mineral that deforms plastically in a wide range of temperatures and pressures, leading to the development of different types of crystallographic preferred orientation (CPO) patterns. In this contribution we present the results of an extensive modeling of quartz fabric transitions via a viscoplastic self-consistent (VPSC) approach. For that, we have performed systematic simulations using different sets of relative critical resolved shear stress of the main quartz slip systems. We have performed these simulations in axial compression and simple shear regimes under constant Von Mises equivalent strain of 100% ($\gamma = 1.73$), assuming that the aggregates deformed exclusively by dislocation glide. Some of the predicted CPOs patterns are similar to those observed in naturally and experimentally deformed quartz. Nevertheless, some classical CPO patterns usually interpreted as result from dislocation glide (e.g. Y-maxima due to prism <a> slip) are clearly not developed in the simulated conditions. In addition we reported new potential preferred orientation patterns that might happen in high temperature conditions, both in axial compression and simple shear. We have demonstrated that CPOs generated under axial compression are usually stronger that those predicted under simple shear, due to the continuous rotation observed in the later simulations. The fabric strength depends essentially on the dominant active slip system, and normally the stronger CPOs result from dominant basal slip in <a>, followed by rhomb <a> and prism [c] slip, whereas prism <a> slip does not produce strong fabrics. The opening angle of quartz [0001] fabric used as a proxy of temperature seems to be reliable for deformation temperatures of ~400 °C, when the main slip systems have similar behaviors.

1. Introduction

Quartz is a common crustal mineral that deforms plastically in a wide range of temperatures and pressures, from very low metamorphic grades just above diagenesis, to sub-solidus temperatures. Such a broad range of metamorphic conditions, together with different imposed deformation geometries that aggregates may experience naturally and experimentally, leads to the development of different microstructures and crystallographic preferred orientation (CPO) distributions (e.g. Hirth and Tullis, 1992, 1994; Law and Johnson, 2010; Schmid and Casey, 1986; Tullis et al., 1973). The development of CPO in quartz might have multiple origins, from mechanical rotation of crystals in very low-grade metamorphic rocks (e.g. Stallar and Shelley, 1995) to dissolution–precipitation (e.g. Hippertt, 1994; Hippertt and Egydio-Silva, 1996). In most cases however, the CPO of quartz is interpreted in terms of dislocation activity and the activation of different crystal slip systems.

Numerical modeling of CPO development has been conducted in the last four decades by different approaches. These studies were initially conducted via kinematic (Etchecopar, 1977) or relaxed-constrain Taylor (Lister and Paterson, 1979; Lister et al., 1978) approaches. However, the 1990s saw an evolution in the development of different modeling methods that simulated the development of preferred orientations in different types of materials. Such evolution was due mainly to improved understanding of the physical processes underpinning the development of CPO in crystalline materials, combined with a significant improvement in computational processes that allowed the development of complex codes capable of incorporating a number of different parameters that influence CPO development. These approaches include equilibrium-based models (e.g. Chastel et al., 1993), isotropic models (Takeshita et al., 1990), n-site models (Wenk et al., 1991), and viscoplastic self-consistent models (Lebensohn and Tomé, 1993). All of these methods have in common the assumption that deformation is accommodated by dislocation glide on a limited number of crystallographic planes in specific crystallographic directions. Furthermore, they all consider also that polycrystalline behavior can be averaged by considering the response of individual microscopic (grain) responses. Thus, the lower bound state assumes that the stress in the

* Corresponding author.
E-mail address: luiz.morales@gfz-potsdam.de (L.F.G. Morales).

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aggregate is homogeneous, whereas in the upper bound state it is the strain in an aggregate that is homogeneous (Sachs, 1928; Taylor, 1938).

An important aspect considered in only a few of the numerical models of CPO development is dynamic recrystallization (e.g. Etchecopar, 1977; Lebensohn et al., 1998; Wenk et al., 1997). Although the occurrence of dynamic recrystallization in parallel with crystal-plastic mechanisms is well-know from experiments and nature, the mechanisms by which the recovery occurs (i.e. subgrain rotation recrystallization, grain boundary migration, etc.) and their impact on the CPO development remain poorly constrained. More recently, integration of viscoplastic self-consistent methods with bi-dimensional microstructural network configurations defined by computer codes such as ELLE has provided new opportunities to better study the effects of dynamic recovery mechanisms concurrent with crystal plasticity (e.g. Griera et al., 2011).

Other processes that are normally not considered in these approaches but are of great importance for the development of CPOs is the effect of dislocation climb and twinning (in quartz, more specifically, Dauphiné twinning). Dislocation climb modeling has to consider the effect of diffusion of atoms in the lattice, as well as the shear components of applied stress in addition to the resolved shear stress described by the diagonal components of the applied stress matrix (e.g. Lebensohn et al., 2012), leading to complex computations. Dauphiné twinning is an important mechanism because it is potentially a grain weakening mechanism due to its effect on stiffness/compliance of quartz single crystals, as it switches −ve & +ve orientations, such as the <a>-axes and the rhombs (e.g. Lloyd, 2004; Menegon et al., 2010; Pehl and Wenk, 2005; Wenk et al., 2006, 2007, 2009a).

In this contribution, the viscoplastic self-consistent approach (Lebensohn and Tomé, 1993) is used to investigate crystallographic preferred orientation transitions in quartz via a systematic modeling of the influence of multiple slip systems in quartz preferred orientations. For that, we assumed systematic changes in the relative critical resolved shear stress (CRSS) for the main slip systems in quartz during axial compression and simple shear. We assume that the main control on the activation of different slip systems in quartz is temperature, and the quartz slip systems are activated in the following order with increasing temperature: <a>(c) → <a>{r/z} → <a>{m} → [c]{m}. This assumption is justified by the classical works of Hobbs (1968), Baeta and Ashbee (1970) and Tullis et al. (1973) that indicate that prismatic slip in quartz is dominant over basal slip in higher temperatures (and vice-versa) and that the increasing temperature leads to a switch between basal <a> to rhomb <a> slip. According to Lister and Dornsiepen (1982) and Mainprice et al. (1986), at 'normal' geological strain rates, the change from basal to prismatic glide occurs at 600–700 °C. The increase in temperature nevertheless does not imply that "low" temperature slip systems become inactive, but that "low" and "high" temperature slip systems may occur together (e.g. Egydio-Silva et al., 2002; Kruhl, 1996; Menegon et al., 2011; Tommasi et al., 1994). It is important to note that this classical view has been questioned in the last few years (see review by Toy et al. (2008)) and some authors clearly demonstrate that CPO in quartz may also be strain-dependent (e.g. Heilbronner and Tullis, 2006), and this will be discussed in the second part of this paper where we will present the detailed fabric transitions in quartz using the same systematic approach of slip system combinations under high strain simple shear. Finally, in the third part of the paper we will discuss the characterization of orientation distribution functions, orientation matrices and different parameters of CPO quantification resulting from the simulations presented in parts 1 and 2.

2. Methodology

2.1. Viscoplastic self-consistent modeling (VPSC)

In this paper, we explore the possibilities of the viscoplastic self-consistent approach (Lebensohn and Tomé, 1993) using the software VPSC7 compiled for Mac OS X. Through this approach, the overall response of the aggregate is averaged from known properties of the constituent grains, and the effective medium assumption is considered to calculate the interactions between each grain with the surrounding ones. In the VPSC approach, strain compatibility and stress equilibrium are averaged at the aggregate scale, and the microscopic stress and strain rate may differ significantly from the macroscopic values. The plastic anisotropy is also considered in this approach. Although this factor has a minor influence in quartz because of the relatively large number of slip systems, it is significant in materials with few slip systems.

The VPSC approach considers that deformation takes place when one or more slip systems become active. The shear rate induced in a slip system (s) by a given local deviatoric stress (s_{ij}) is described by a viscoplastic law of form (Eq. (1))

$$\dot{\gamma}^{s} = \dot{\gamma}_0 \left(\frac{\tau_r^s}{\tau_0^s}\right) = \dot{\gamma}_0 \left(\frac{r_{ij}^s s_{ij}}{\tau_0^s}\right)^{n^s} \tag{1}$$

where $\dot{\gamma}_0$ is the reference strain rate, n^s is the stress exponent (i.e. for diffusion creep, n = 1, for dislocation creep in silicates, $3 \le n \le 5$), τ_r^s and τ_0^s are the CRSS and the activation stress respectively for a given crystal slip system and r^s is the Schmid tensor, which defines the orientation of the slip system in relation to the stress axes.

The sum of the shear rates over all slip systems gives the microscopic strain rate ($\dot{\varepsilon}$) per grain. To determine the microscopic state ($s, \underline{\dot{\varepsilon}}$) of each

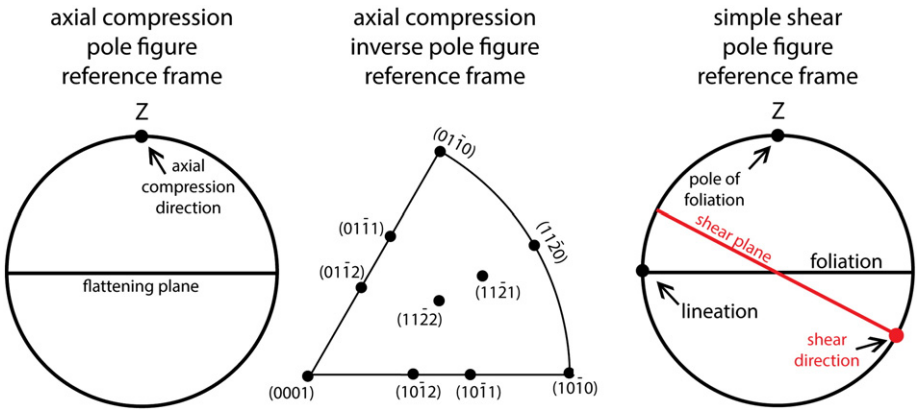

Fig. 1. Reference frames used in this paper, for axial compression and simple shear simulations. In the axial compression pole figures, the crystallographic orientation data is plotted in relation to the axial compression direction (Z) and the flattening plane (E–W vertical plane). In simple shear, the data is plotted in relation to the strain ellipsoid main features (foliation/lineation–E–W vertical plane/E–W horizontal pole) and in relation to the imposed shear plane/shear direction (NE–SW vertical plane/NE–SW horizontal pole). In the inverse pole figures the axial compressional direction is plotted in relation to the main crystallographic forms of quartz.