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How tightly does calcite *e*-twin constrain stress?

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ABSTRACT

Mechanical twinning along calcite *e*-planes has been used for paleostress analyses. Since the twinning has a critical resolved shear stress at ~10 MPa, not only principal stress axes but also differential stress can be determined from the twins. In this article, five-dimensional stress space used in plasticity theory was introduced to describe the yield loci of calcite *e*-twinning. The constraints to paleostress from twin and untwin data and from calcite grains twinned on 0, 1, 2 and 3 *e*-planes were quantified by using their information contents, which were defined in the stress space. The orientations of twinned and untwinned *e*-planes are known to constrain not only stress axes but also differential stress, *D*, but they loose the resolution of *D* if the twin lamellae were formed at *D* greater than 50–100 MPa. On the other hand, it is difficult to observe twin lamellae subparallel to a thin section. The stochastic modeling of this effect showed that 20–25% of twin lamellae can be overlooked. The degradation of the constraints by this sampling bias can be serious especially for the determination of *D*.

1. Introduction

Calcite *e*-twinning is useful for understanding tectonics in the upper crust, because calcite is a common mineral and records deformations at low temperatures and low differential stresses (e.g., Turner, 1953; Groshong, 1972; Jamison and Spang, 1976; Laurent et al., 1981; Pfiffner and Burkhard, 1987; Burkhard, 1993; Nemcok et al., 1999; Constantin et al., 2007). Calcite *e*-twin has been used to infer not only the orientations but also the magnitudes of paleostresses. Researchers have often applied stress tensor inversion to natural data (Lacombe, 2010, and references therein), though they utilize Etchacopar's (1984) method, which is based on the assumption that *e*-planes are twinned if the resolved shear stress along their gliding directions exceed a critical value. It has been scarcely pursued theoretically since the study by Jamison and Spang (1976) how tightly calcite *e*-twins constrain stress based on the assumption.

This paper aims at the theoretical investigation of the constraints from calcite *e*-twins to establish the basis for improving the stress inversion scheme. In this paper, the theoretical analyses of Takeshita et al. (1987), Fry (2001) and Sato and Yamaji (2006) are reformulated to relate stress and the orientations of twinned and untwinned *e*-planes to define the yield locus of calcite e-twinning and to quantify the constraints from *e*-twin lamellae. The present study is based on the fact that the twinning occurs if resolved shear stress along the gliding direction of a twin plane exceeds a critical value, τ_c, which is assumed to be 10 MPa (Lacombe, 2010, and references therein) throughout of this paper, meaning that the twins are useful to investigate tectonics at the depths of about 0.5–5 km (Lacombe, 2007; Lacombe et al., 2009).

Here, we introduce, first, the five-dimensional stress space in which the yield loci of *e*-twinning is defined. Second, by using information theory, the constraints from twin and untwin data are quantitatively estimated, because several researchers utilized not only the attitudes of twinned *e*-planes but also those of untwinned ones in their stress inversion (Laurent et al., 1981, 1990; Etchecopar, 1984). Fry (2001, Fig. 3) explained why untwin data are necessary to constrain differential stress. The constraints from grains twinned on 0, 1, 2 and 3 *e*-planes are evaluated as well. In case the number density of twin lamellae is low, attention must be payed to sampling bias, because the bias degrades the constraints. It is shown that 20–25% of twin lamellae are overlooked due to the low angles made by the lamellae and the observation plane, e.g., a thin section. Thus, the bias can have distortive effects on paleostress analysis.

2. Notations and basic equations

In this section we introduce mathematical symbols and important terms for the following analyses. Let $\boldsymbol{c}$ be the unit vector indicating the host *c*-axis of a twin lamella, the unit normal of

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which is denoted by $\boldsymbol{e}$ (Table 1). The vectors are represented by (3×1)-matrices. The angle made by $\boldsymbol{c}$ and $\boldsymbol{e}$ is denoted by α, which is about 26.25° (Twiss and Moores, 2006, p. 499). We pay attention to the 'footwall' of a twin lamella to consider the gliding direction and shear stress on the lamella. Corresponding to the choice that compression is positive in sign, the unit normal, $\boldsymbol{e}$, is defined to point inward of the footwall block (e.g., Yamaji, 2007, p. 62). The unit vector, $\boldsymbol{g}$, indicates the gliding direction of the footwall.

A calcite grain has three sets of planes for *e*-twinning, which have three-fold symmetry about the *c*-axis. A set of *e*-planes is characterized by the paired vectors, $\boldsymbol{e}$ and $\boldsymbol{g}$. Each of the three sets has two states, twinned or untwinned. Following Venkitasubramanyan (1971), we refer to calcite grains with 1, 2 and 3 twinned planes as singlets, doublets and triplets, respectively. In addition, we use the term, 'zeroplets,' to refer to untwinned grains.

Twinning is assumed to occur on a twin set if the resolved shear stress parallel to the gliding direction, τ, satisfies

$$\tau \geq \tau_c. \tag{1}$$

Otherwise, the potential set is left untwinned. A stress tensor is said to be compatible with a twin datum, if this condition is met on the *e*-plane from which the datum is obtained. Likewise, a stress tensor is said to be compatible with an untwin datum, if this condition does not hold on an untwinned *e*-plane. A stress tensor is said to explain a twin datum, if Eq. (1) is satisfied on the *e*-plane.

Table 1
List of symbols. Vectors in the physical space and five-dimensional space are denoted by boldface letters and arrows, respective, such that $\boldsymbol{g}$ and $\vec{\sigma}$.

$\boldsymbol{c}$	Unit vector representing the orientation of *c*-axis
$\vec{c}^{(1)}, \ldots, \vec{c}^{(M)}$	Uniformly distributed points on S
D	Differential stress
diag (a,b,c)	3×3 diagonal matrix with the diagonal components, *a*, *b* and *c*
$\boldsymbol{e}$	Unit vector normal to twin lamella
$\boldsymbol{g}$	Unit vector indicating griding direction
$H(\,)$	Heaviside step function
I	Information content
$\boldsymbol{I}$	3×3 identity matrix
I_t	Information content of a twin datum
I_u	Information content of an untwin datum
M	Number of points, $\vec{c}^{(1)}, \ldots, \vec{c}^{(M)}$, distributed with uniform intervals on S
P	Probability
$\boldsymbol{P}$	Elementary orthogonal projector
$\boldsymbol{Q}$	Orthogonal matrix representing the orientations of stress axes
S, S	Unit sphere in five-dimensional space and its area
$\boldsymbol{s}$	Shear stress (vector)
$(\,)^{\mathrm{T}}$	Matrix transpose
$\boldsymbol{T}$	Deviatoric stress tensor
T_{II}	Second basic invariant of $\boldsymbol{T}$
$\vec{x}$	Position vector in the five-dimensional stress space
α	Angle between $\boldsymbol{c}$ and $\boldsymbol{e}$
$\boldsymbol{\varepsilon}$	Reduced strain tensor
$\varepsilon_{\mathrm{II}}$	Second basic invariant of $\boldsymbol{\varepsilon}$
$\vec{\varepsilon}$	Epsilon-vector, five-dimensional unit vector corresponding to a twin or untwin datum
θ	Angle made by $\boldsymbol{g}$ and $\boldsymbol{s}$
λ	Normalizing factor for ς
Φ	Stress ratio
$\boldsymbol{\sigma}$	Stress tensor
$\boldsymbol{\sigma}^0$	Reduced stress tensor with the eigenvalues, 0, Φ and 1
$\vec{\sigma}$	Sigma-vector, five-dimensional unit vector corresponding to ς
ς	Reduced stress tensor with the eigenvalues, $(2-\Phi)/3\lambda$, $2(\Phi-1)/3\lambda$ and $-(\Phi+1)/3\lambda$
ς_{II}	Second basic invariant of ς
σ_1, σ_2, σ_3	Principal stresses
τ	Resolved shear stress along $\boldsymbol{g}$
$\underline{\tau}$	Non-dimensionalized resolved shear stress
τ_c	Critical resolved shear stress
Ψ	Radius of a spherical cap on S

Given a stress tensor, $\boldsymbol{\sigma}$, the resolved shear stress along the $\boldsymbol{g}$ direction upon the plane normal to $\boldsymbol{e}$ is

$$\tau = -\boldsymbol{g}^{\mathrm{T}}\sigma\boldsymbol{e} \tag{2}$$

The minus signs in Eq. (2) correspond to the fact that deformation occurs in the direction to relieve stress. The lateral translation of Mohr circles on a Mohr diagram does not affect shear stresses. Accordingly, we assume that the minimum principal stress equals zero, and consider the stress tensor of the form,

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^0 D, \tag{3}$$

where $D = \sigma_1 - \sigma_3$ is differential stress, and

$$\boldsymbol{\sigma}^0 = \boldsymbol{Q}\ \mathrm{diag}(1, \Phi, 0)\ \boldsymbol{Q}^{\mathrm{T}}, \tag{4}$$

$\boldsymbol{Q}$ the orthogonal matrix representing the principal orientations, and $\Phi = (\sigma_2 - \sigma_3)/(\sigma_1 - \sigma_3)$. Φ is called stress ratio, and has a value between 0 and 1. It follows from Eqs. (2) and (3) that

$$\tau = -\boldsymbol{g}^{\mathrm{T}}\boldsymbol{\sigma}^0\boldsymbol{e}D. \tag{5}$$

The tensor, $\boldsymbol{\sigma}^0$, carries the information of the attitude ($\boldsymbol{Q}$) and shape (Φ) of stress ellipsoid, the size of which is denoted by D.

3. Yield locus

In this section, we introduce the yield locus of calcite *e*-twinning. The locus is represented by a solid figure in five-dimensional stress space. Although the space and the locus are the concepts of abstract plasticity theory, it is worth introducing them, because (1) not only a multi-axial state of stress but also twin and untwin data are represented by position vectors in the space, and (2) the constraints from twin and untwin data on differential stress have geometric interpretations. In addition, the constraints from twin and untwin data are quantitatively estimated in the space.

3.1. Sigma- and epsilon-vectors

It is convenient for theoretical considerations to introduce the deviatoric stress tensor,

$$\boldsymbol{T} = \boldsymbol{\sigma} - \left(\frac{\sigma_1 + \sigma_2 + \sigma_3}{3}\right)\boldsymbol{I}.$$

Combining Eqs. (3) and (4), we have $\sigma_3 = 0$, $\sigma_2 = \Phi D$, $\sigma_1 = D$ and

$$\boldsymbol{T} = \left(\boldsymbol{\sigma}^0 - \frac{\Phi + 1}{3}\boldsymbol{I}\right)D, \tag{6}$$

Now, suppose the tensor,

$$\varsigma = \frac{1}{\lambda}\left(\boldsymbol{\sigma}^0 - \frac{\Phi + 1}{3}\boldsymbol{I}\right), \tag{7}$$

where the denominator in the right-hand side of this equation,

$$\lambda = \sqrt{(\Phi^2 - \Phi + 1)/3}, \tag{8}$$

is always positive in sign, and has the minimum, 1/2, at $\Phi = 1/2$ and the maxima, $1/\sqrt{3} \approx 0.58$, at $\Phi = 0$ and 1. Then, Eq. (6) is rewritten as $\boldsymbol{T} = \varsigma\lambda D$. The tensor, ς, has the second basic invariant,

$$\varsigma_{\mathrm{II}} \equiv \frac{1}{2}(\varsigma : \varsigma) = \frac{1}{2}\left(\varsigma_{11}^2 + \varsigma_{22}^2 + \varsigma_{33}^2\right) + \varsigma_{23}^2 + \varsigma_{31}^2 + \varsigma_{12}^2 = 1, \tag{9}$$