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Peek inside the black box of calcite twinning paleostress analysis

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Abstract: Calcite e-twinning has been used for stress inversion purposes since the fifties. The commonly used technique is the Etchecopar method (e.g. Laurent *et al.*, 1981), based on testing of 500-1000 randomly generated reduced stress tensors using a penalization function f_L. A systematic search of all possible reduced stress tensors with a new penalization function f_R double checked with a spatial distribution plot is suggested.

Keywords: stress inversion, paleostress analysis, calcite, mechanical twinning.

Extensive research of the deformation mechanisms of calcite monocrystals and polycrystalline aggregates during the last century provided evidence of several glide and twinning systems present in calcite. Twelve different glide systems on five different crystallographic planes and three different twinning systems have been defined (Bestmann and Prior, 2003). Only twinning systems are suitable for stress inversion purposes because they are easy to observe under an optical microscope, their orientation can be measured using either a universal stage or EBSD and only one glide vector *g* with only one shear sense is possible for each twin plane. The dominant twin lamellae are the *e*-twins (they cut the edges of the rhombohedron, figure 1a), the other two are very rare, mainly present only in laboratory experiments performed under special conditions. Mechanical *e*-twinning is the dominant deformation mechanism for calcite at low temperatures (below 400 °C, e.g. De Bresser and Spiers, 1997; figure 1b), low confining pressures and low finite strains (8%, e.g. Turner, 1953; De Bresser and Spiers, 1997).

An *e*-plane twins only if the shear stress τ_i acting along the plane exceeds the critical resolved shear stress (τ_c) value. The commonly used value of τ_c in stress inversion is 10 MPa, which was experimentally determined by Turner *et al.* (1954). The magnitude of τ_c is independent of normal stress σ, magnitude and temperature (e.g. Turner *et al.*, 1954; De Bresser and Spiers, 1997; figure 1b). In order to cause twinning, the stress tensor acting upon an *e*-plane must have appropriate principal direction orientation and sufficient differential component. The magnitude of the shear stress is controlled by the Schmid criterion μ, which is a function of the orientation of the σ_1 vector (Handin and Griggs, 1951; figure 1c). The σ_1 must lie in the right dihedron not containing the optical axis *c* (Fig. 1d). The most favorably oriented σ_1 and σ_3 stresses are coplanar with the *c*-axis and the *e*-twin normal vector and form a 45° angle with the *e*-twin normal vector (Fig. 1e). This was the basic idea of TDA (Turner dynamic analysis), a simple graphical stress analysis method proposed by Turner (1953).

The Lacombe and Laurent (e.g. Laurent *et al.*, 1981) modification of the Etchecopar stress inversion method (Etchecopar *et al.*, 1981) has until the present time been the most sophisticated calcite twinning stress inversion method. This contribution is focused on an explanation of basic features of this stress inversion, discusses its limitations and tests possible improvements of the method.

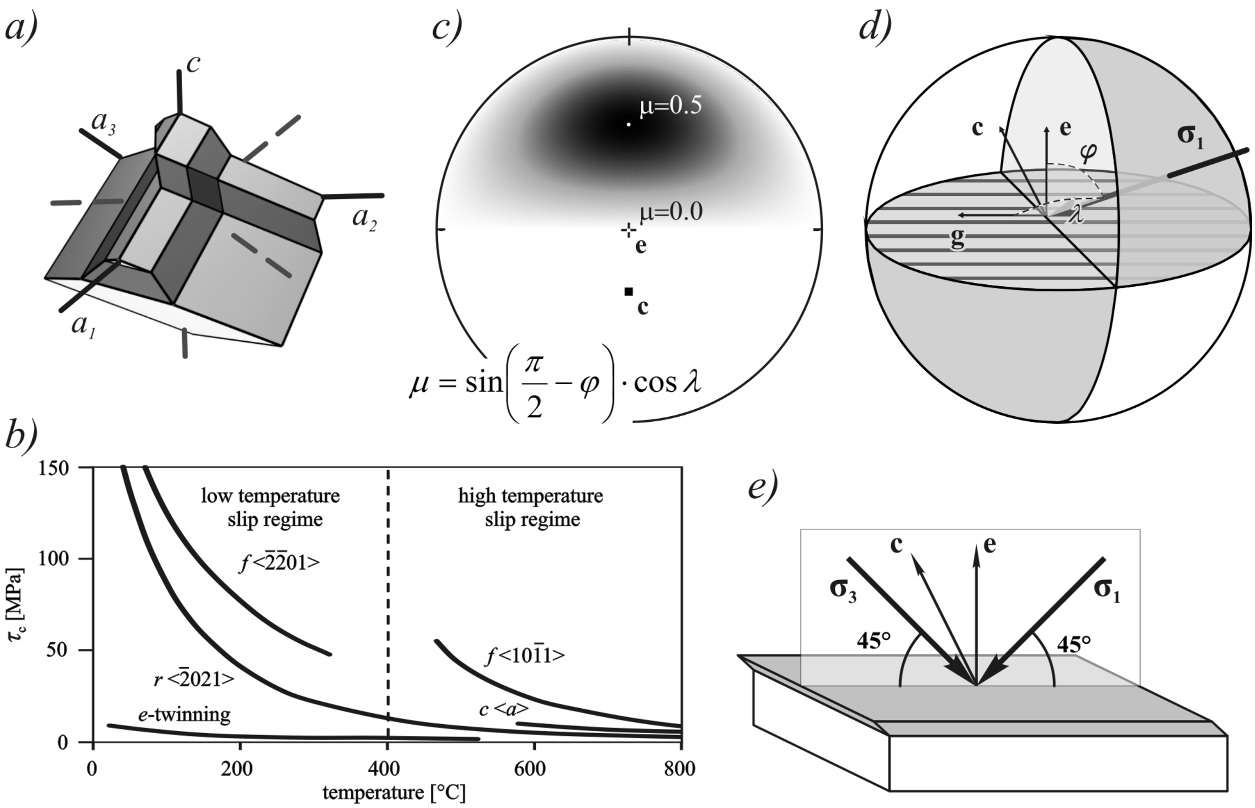


Figure 1. Basic characteristics of calcite *e*-twinning. (a) The orientation of *e*-twins in calcite, the *e*-twins cut the edge of the rhombohedron, (b) the relationship between critical resolved shear stress (τ_c) and temperature for the main glide and twin systems in calcite, *e*-twinning is the main deformation mechanism at temperatures below 400 °C (De Bresser and Spiers, 1997), (c) the magnitude of the Schmid criterion μ for one twin lamella (modified after Jamison and Spang, 1976), (d) orientation of the glide vector *g* in a twin plane (*g* is coplanar with *c* and *e* vectors), σ_1 must lie in the grey right dihedron in order to cause twinning along the *e*-plane, (e) the most favorably oriented normal shear stresses are coplanar with *c* and *e* vectors and form a 45° angle with the *e*-twin normal vector.

Results

As noted above, an *e*-plane will twin if, and only if the shear stress τ_i exceeds the critical value $\tau_c \approx 10$ MPa. The Etchecopar inverse method modified by Laurent, Lacombe and others is based on applying numerous (500-1000) randomly generated reduced stress tensors (the τ_c for twinning is independent of normal stress) and then selecting the best-fitting tensor using a penalization function *f*. When a stress tensor [T] is applied to a set of twin planes, four possibilities exist for any particular twin plane (Fig. 2a):

(1) compatible twinned plane (the plane is twinned and [T] should twin it);

(2) compatible untwinned plane (the plane is untwinned and [T] should not twin it);

(3) incompatible twinned plane (the plane is twinned and [T] should not twin it);

(4) incompatible untwinned plane (the plane is untwinned and [T] should twin it).

If an ideal stress tensor is chosen, only compatible untwinned and twinned planes occur. However, in most cases, all four possibilities are present. The whole procedure is focused on selecting the best fitting stress tensor with the least possible number of incompatible planes. Whereas the presence of incompatible twinned planes can be caused by polyphase deformation or stress perturbations during deformation, the incompatible untwinned planes are caused by wrong orientation or shape ratio of [T]. This means that incompatible untwinned lamellae can be most effectively used as a criterion for estimating the best-fitting tensor.

Laurent *et al.* (1981) proposed a penalization function f_L which is a sum of differences of shear stresses for incompatible untwinned lamellae τ_j and the least shear stress for compatible twinned lamellae

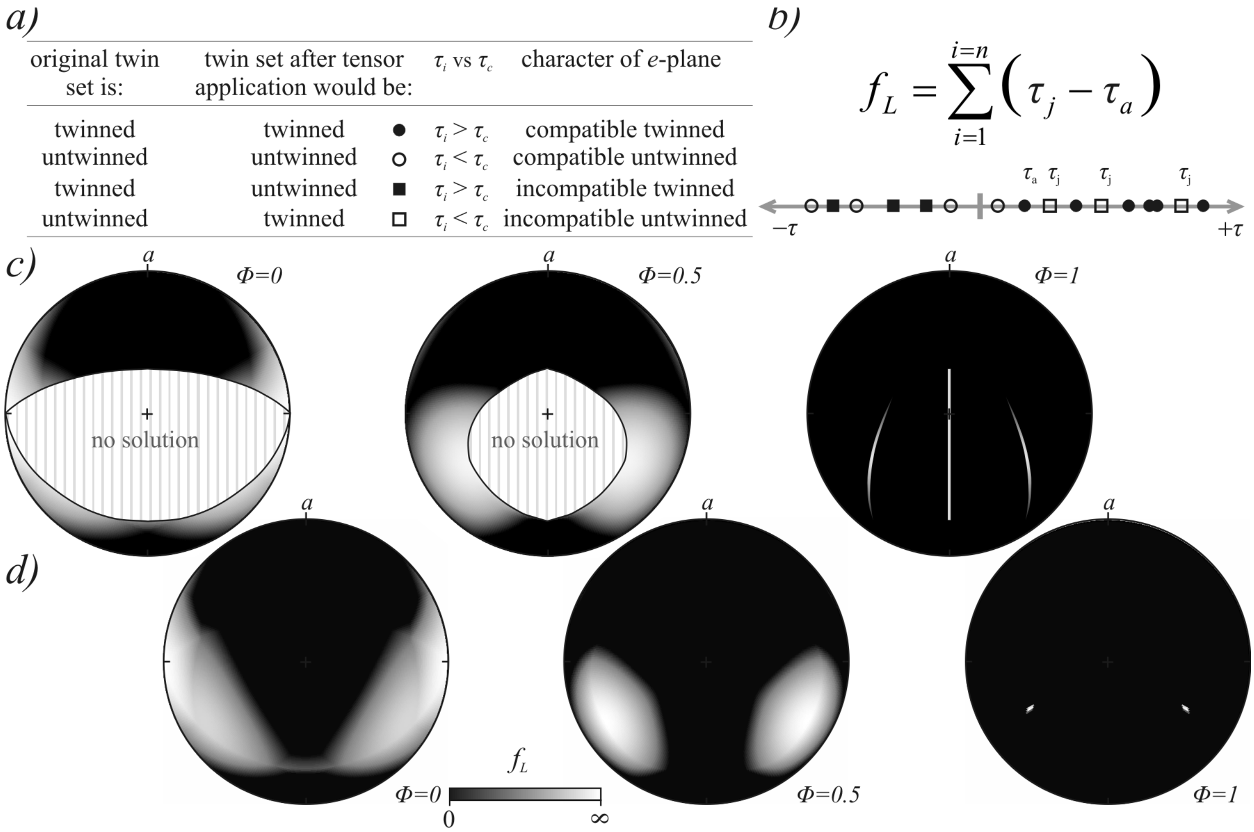


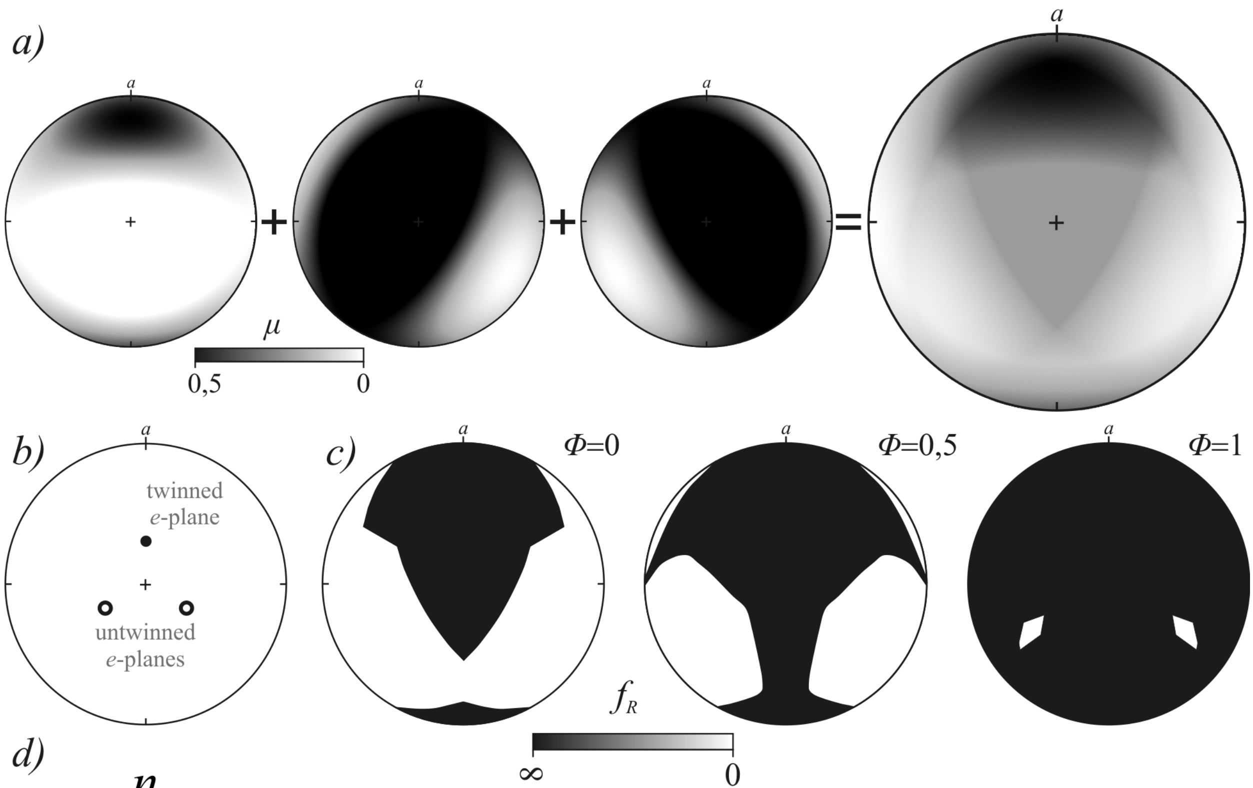
Figure 2. Formula and spatial distribution of the penalization function f_L. (a) Classification table of *e*-planes after stress tensor application, (b) f_L formula and graphical expression of the classification table (after Tourneret and Laurent, 1990), (c) spatial distribution of f_L for three different stress tensor shape ratios, the solution-less tensors being filtered, (d) spatial distribution of f_L for three different stress tensor shape ratios, the solution-less tensors being unfiltered. Note: each point on the diagrams represents the lowest value of f_L for 180 stress tensors with the same σ_1 direction; see figure 3b for the input data.

τ_a, considered in the following calculations as the critical value for twinning τ_c (Fig. 2b). The stress tensor with the lowest f_L is chosen as the best-fitting tensor. It is clear that the value of this function is strongly dependent on the amount of incompatible untwinned lamellae and compatible twinned lamellae.

The authors' software TwinCalc was used for testing the behaviour of the penalization function f_L using numerically generated input data. A complete search of all possible stress tensor orientations (1° step) for different shape ratios $\Phi = (\sigma_2\text{-}\sigma_3)/(\sigma_1\text{-}\sigma_3)$ (selected or all possible with 0.1 step) was used rather than the standard procedure with randomly generated stress tensors.

During the testing of the f_L on one calcite grain it turned out that some stress tensors have $f_L = 0$, but they are not favorably oriented for twinning (Fig. 2c), which means that $\tau_a = 0$. The spatial distribution of these *solution-less tensors* depends on the shape ratio Φ. Such solutions have to be filtered. The f_L spatial distribution diagrams plotted without the solution-less tensors filter shows a huge minimum of the function for obviously incorrectly oriented stresses (Fig. 2d). The number of such solution-less tensors decreases with an increasing number of grains. Moreover, testing only a small amount of stress tensors without filtering the solution-less ones can lead to spurious solutions.

The spatial distribution diagram of the f_L reveals its clear resemblance to the right dihedra method (compare figure 2c with figure 1) and it led the authors to test this option. The twinned *e*-planes define right dihedra for suitably oriented stresses and untwinned *e*-planes define right dihedra for unsuitably oriented stresses. If we add the Schmid criterion distribution contours and count up the right dihedra for twinned



d)

$$f_R = \frac{n_{CT}}{w_{TU}} + n_{CU} w_{TU} - n_{IU} w_{TU} \qquad w_{TU} = \frac{\textit{number of twinned planes}}{\textit{number of untwinned planes}}$$

Figure 3. Comparison of right dihedra method and penalization function f_R. (a) Equal area plots of the Schmid criterion for one twinned and two untwinned *e*-planes, the result after summation is the function of possibility of suitable orientation of σ_1, which is most likely located in the darkest area, (b) one calcite grain with vertical *c*-axis, one twinned and two untwinned *e*-planes used for testing of the penalization functions, (c) spatial distribution of f_R for three different stress tensor shape ratios, (d) equations used for calculation of the f_R function, where n_{CT} is the number of compatible twinned planes, n_{CU} is the number of compatible untwinned planes and n_{IU} is the number of incompatible untwinned planes.

and untwinned *e*-planes, we obtain a function of possibly suitable oriented stresses. Surprisingly, it is similar to the spatial distribution of the f_L, but does not favor the wrongly oriented stresses. Testing on numerically generated data showed that a relatively good result can be obtained using this direct calculus instead of a total search procedure, but obviously the maxima are smoother, so it should be used just for a quick overview.

The disadvantage of the Etchecopar inverse method used for calcite twins is that the maxima of the penalization function f_L are smooth. At this time it seems that the most useful penalization function is a weighted sum of compatible twinned and untwinned planes minus incompatible untwinned planes (Fig. 3). The stress tensor with the highest values of the function is chosen as the best-fitting one. This f_R penalization function is more discrete than f_L, but when tested on numerically generated polycrystalline data provided sharper maxima and no solution-less stress tensors (Fig. 4).

Conclusions

Testing of the Etchecopar stress inversion method using numerically generated as well as natural data showed that some zero values of the f_L penalization function do not represent the most favorably oriented stress tensors, but are spurious. Systematic testing of a large number (millions) of stress tensors is suggested to avoid spurious solutions.

The penalization function f_L provides smooth maxima. The newly suggested penalization function f_R provides sharper maxima and, therefore, more accurate solutions to the stress inversion. The best way to

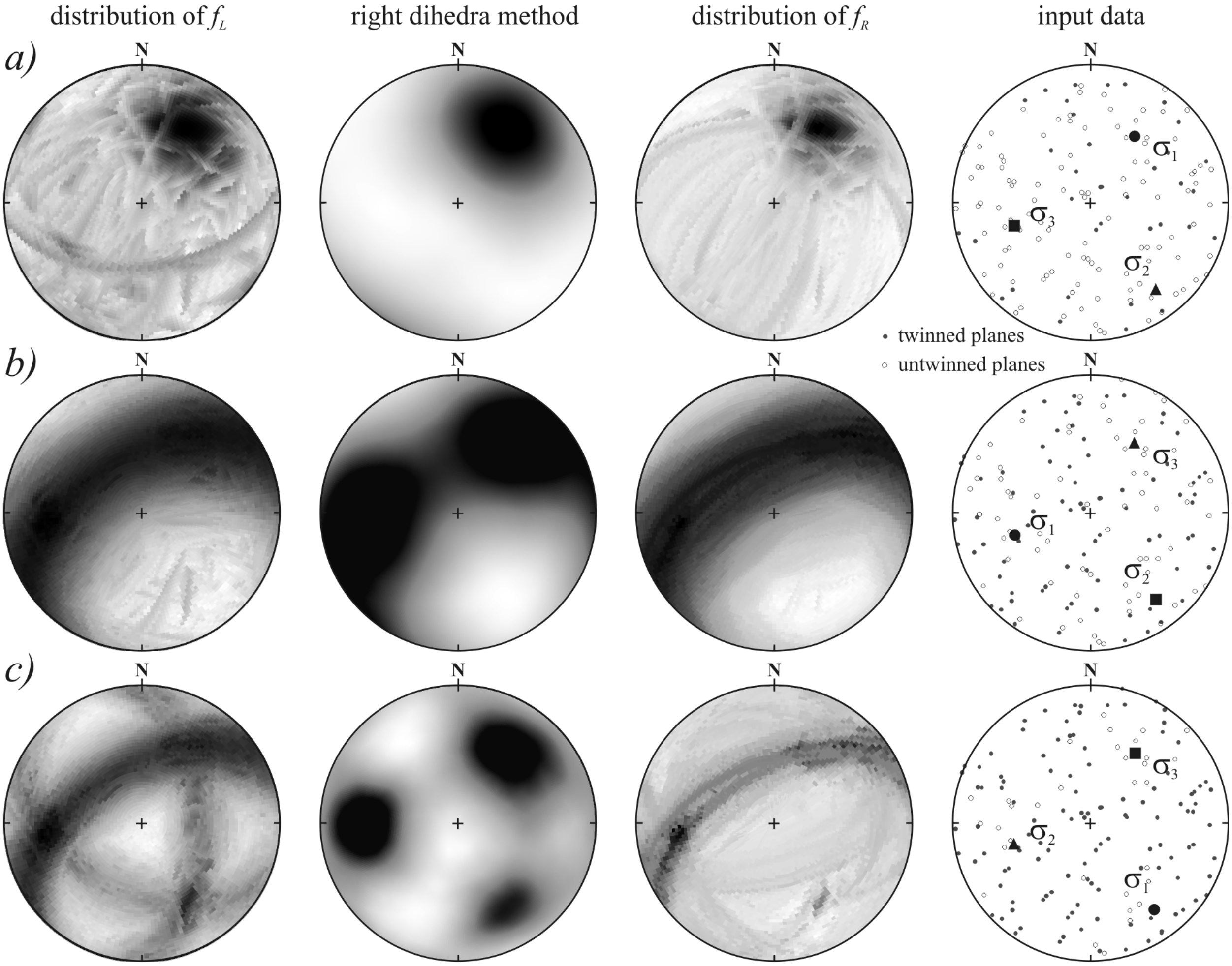


Figure 4. Comparison of penalization functions f_L, f_R and the right dihedra method. Modeled on 50 numerically generated, homogenously oriented calcite grains, strained by (a) one, (b) two and (c) three differently oriented stress tensors with 50 MPa differential stress and Φ = 0.5. All three functions form maxima around theoretical σ_1 directions, but the f_R function seems to form the sharpest maxima, especially in polyphase deformation.

obtain unambiguous solutions is a combination of both methods, double checked by using the spatial distribution diagrams.

Acknowledgements

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