The Black Box of the Stress Analysis Based on Calcite Twinning

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Since the deformation origin of calcite twin lamellae (e-twins) and their crystallographic laws have been determined in the end of the 19th century, it was recognized as the main deformation mechanism of calcite polycrystalline aggregates at low temperatures, low confining pressures and low finite strains (8 %; e.g. Turner 1963, DeBresser, Spiers 1996).

The e-plane will twin if, and only if the shear stress \( \tau \) exceeds the critical value \( \tau_c \approx 10 \text{ MPa} \), which is believed to be independent of normal stress, temperature and strain rate (e.g. Laurent et al. 1981). This is one of basic assumptions of the Etchecopar inverse method modified by French authors Laurent, Lacombe et al. (e.g. Lacombe, Laurent 1996). It is based on applying numerous (500 to 1000) randomly generated reduced stress tensors and then selecting the best-fit tensor using a penalisation function. When a stress tensor \( [T] \) is applied on a set of twin planes, there are four possibilities for any twin plane: 1) the plane is twinned and \( [T] \) should twin it (compatible twinned plane); 2) the plane is untwinned and \( [T] \) should not twin it (compatible untwinned plane); 3) the plane is twinned and \( [T] \) should not twin it (incompatible twinned plane); 4) the plane is untwinned and \( [T] \) should twin it. In an ideal case only compatible untwinned and twinned planes occur. In most cases all four cases are present. Whereas incompatible untwinned 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 \( [T] \).

A penalization function with solutions for all stress tensors and a systematic search of all possible stress tensors within engaged range should be preferred. Such procedure commonly provides more maxima (minima) of the penalization function but eliminates all wrong solutions. 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. 1b). It provides less scattered maxima clusters and no solution–less stress tensors.

Even thought calcite stress inversion method by Laurent et al. (e.g. 1981) provides credible solutions and has been proven by experiments, a detailed revision of the penalization function used revealed some uncertainties due to its discreteness. The presented penalization function is less discrete then \( [T] \) by Laurent and Lacmbe (e.g. 1981), but in some cases it requires additional parameters to provide a unique solution (e.g. the lowest sum of stresses along incompatible untwinned lamellae).

Laurent et al. (1981) proposed a criterion (so called penalization function \( f \)) for selecting the best-fit tensor (fig. 1a). It is a sum of differences of shear stresses for incompatible untwinned lamellae and the least shear stress for compatible twinned lamellae, considered as the critical value for twinning \( \tau_c \). It is clear, that the value of this function is strongly dependent on the amount of incompatible untwinned lamellae and compatible twinned lamellae. As shown in Fig. 1, there exist stress tensors with \( f = 0 \), which represent stress tensors with no solution, the spatial distribution of which depends on the shape ratio \( \Phi \). The number of such "solution–less tensors" decreases with decreasing number of stress tensors examined and with increasing number of grains. Using this penalization provides results that may not always be reliable.

\[
a = \sum_{i=1}^{n} (\tau_i - \tau_c) \\
b = \frac{n_{CT}}{w_{CT}} + \frac{n_{CU}}{w_{CU}} - \frac{n_{TU}}{w_{TU}}
\]

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References

