Statistical mixture model for separating deviatoric stress tensors from heterogeneous calcite twin data

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Mechanical twinning results in the simple shear of a crystal grain. The twinning in calcite occurs if the resolved shear stress, $\tau$, along the gliding direction of an $e$-plane is greater than a critical value, $\tau_c$, which is known to be around 10 MPa (Lacombe, 2010). The twinning condition, $\tau > \tau_c$, has a geometrical interpretation. That is, a data point on a unit sphere in 5D space corresponds to a twin datum, which consists of the orientation of a twin lamella and its gliding direction; whereas a spherical cap on the sphere represents a deviatoric stress tensor. The twinning condition is equivalent with the condition that a data point exists on the spherical cap that represents the deviatoric stress tensor responsible for the twinning (Yamaji, 2015a). Accordingly, the stress inversion of the orientations of twin lamellae comes down to the search problem to determine the spherical cap that best fits data points on the sphere (Yamaji, 2015b). However, natural data are usually heterogeneous, meaning that twin lamellae that were formed under different stress conditions coexist in a calcite aggregate. In that case, the data points make clusters on the sphere; and the deviatoric stress tensors can be determined by fitting spherical caps to the data points (Yamaji, 2015b).

A computer program was made in the present work to materialize this idea. That is, a probability density function was defined to describe the twinning condition on the sphere. Second, the mixture model of the functions was fitted to data points through genetic algorithm with assuming the number of stresses to be detected was 1, 2, 3, etc. This number was determined using Bayesian information criterion. The program determines the non-dimensional deviatoric stress tensor, which is equal to the deviatoric stress tensor divided by $\tau_c$. The method to determine $\tau_c$ is shown in the poster of the author in this session.

Mechanical twinning results in strain hardening, which can be regarded as the gradual increase of $\tau_c$. A preliminary test using a natural data set did not show this effect.

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