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Editorial

Calcite Deformation Twins: From Crystal Plasticity to Applications in Geosciences

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E-twinning is the dominant mechanism of plastic deformation of calcite at low temperature (<300 °C), and in most limestones, e-twins are, at the crystal scale, the dominant microstructures. Intracrystalline twin lamellae are caused by lattice rotation between rows of atoms along the {01–12} (or {018}) e-plane in response to shear stress. Once a twin is formed, progressive deformation can either create new twins elsewhere or deform the twinned rock portion by other mechanisms. Mechanical twinning accommodates only a very limited amount of the bulk strain accommodated by the rock, so twinning deformation generally co-exists with other deformation mechanisms, such as brittle failure and cataclasis, porosity reduction, pressure solution, or dislocation creep.

Recent experimental work has enabled significant progress in the understanding of the initiation and growth of calcite twins and of their controlling factors, as well as of the contribution of twinning to the deformation of calcite grains at various conditions [1–5]. Coevally, inversion techniques that allow for the determination of principal stress or strain orientations and differential stress magnitudes from naturally deformed calcite-bearing rocks have been developed [6–8]. These techniques were widely applied in paleo-tectonic studies, e.g., as in [9–13].

Despite significant advances, one pending question about twinning in calcite is related to the existence of a critical resolved shear stress and (if it does exist) to its actual significance. Many paleopiezometric approaches have been built around the concept of a constant critical resolved shear stress for twinning, with a value of ~10 MPa being commonly adopted (e.g., [14–16]). In this view, the so-called critical resolved shear stress would correspond to the stress associated with plastic twin propagation across the grain (controlled by external stress and governed by a Schmid-type criterion) rather than to the stress associated with twin nucleation (likely controlled by the local lattice structure and stress concentrations). The idea that the critical resolved shear stress is the empirical stress at which a statistically significant number of twin nucleation sites become suddenly active provides a possible elegant way to reconcile the picture of the twin-forming process with the practical existence of a critical resolved shear stress [4]. The adoption of a single critical resolved shear stress for twinning has been challenged [17] because the differential stress necessary to produce twinning is dependent upon grain size [1] and strain (calcite hardens once twinned) [18]. Further experimental work has thus been devoted to better constraining the stress conditions for twinning, including estimates of the value of the macroscopic (empirical) critical resolved shear stress and its variation with grain size [1] and strain [18]. Recent calcite twin-based paleopiezometric studies take into account the dependence of the critical resolved shear stress on these parameters ([6,12]).

Considering the long-lasting investigations on deformation twinning in calcite, and the remaining questions under debate (i.e., the existence of a real or apparent critical resolved shear stress, twins as strain or stress indicators, and twin morphology as a paleothermometer), it was highly stimulating to try to demonstrate the recent advances on the topic by gathering both review papers and contributions reporting original developments and applications.

The review paper by Lacombe et al. [19] is the cornerstone of the Special Issue. It is a follow-up of the review papers by [20–22] and provides an overview of the recent progress on the understanding of the formation of calcite twins, their measurement, and their use as tectonic markers and as a stress-strain gauge. The paper summarizes our current knowledge on twin nucleation and growth, and critically discusses the concept of critical resolved shear stress. Calcite twin measurement techniques are presented together with their pros and cons. The classical use of calcite twin morphology as a geothermometer is critically discussed. Inversion techniques allowing for the use of calcite twins as indicators of orientations and/or magnitudes of stress and strain are summarized, and the benefits for paleo-tectonic studies are illustrated through several examples. Finally, the paper addresses the successful combination of calcite twinning paleopiezometry with the mechanical analysis of fractures and stylolite roughness paleopiezometry.

Three papers within the volume deal with paleopiezometry or with the reconstruction of regional paleostress orientations from calcite twins. Rutter et al. [23] use electron backscatter diffraction (EBSD) to determine the orientation of mechanically twinned grains in Carrara marble experimentally deformed to a small strain at room temperature and at a moderate confining pressure. Although the thickness of the deformation twins was mostly too small to permit a determination of their orientation by EBSD, the authors have measured their orientations by calculating possible twin orientations from the host grain orientation, and then comparing calculated traces to the observed twin traces. The validity of the Turner and Weiss method for principal stress orientations was confirmed, particularly when based on a calculation of the resolved shear stress. The authors show that methods of paleopiezometry based on twinned volume fraction must be rejected. They further explore a practical paleopiezometric approach based on twin density and find that twin density correlates positively with resolved shear stress. However, the intrinsic variability of the results imposes a limit on the achievable accuracy of this approach.

In their study, Parlangeau et al. [24] have deformed samples of Carrara marble in uniaxial compression and at low temperature. The experiments were monitored in situ using a Scanning Electron Microscope and a deformation analysis was performed at regular intervals via image correlation. The authors show that twinning occurs as a result of an accumulation of strain visible before the appearance of the first twinned plane, followed by a densification and a progressive thickening of the twin lamellae. Fracturing only appears in a late stage as a precursor to the collapse of the sample. The application of the Calcite Stress Inversion Technique [6] to the twinned planes formed during the experiment shows a good consistency with the applied macroscopic stress. The Schmid factors extracted from this analysis are correlated to the loading curves. For crystals of about 200 μm in diameter, the critical resolved shear stress value falls in the range 6.75–8.25 MPa. These new results help improve our knowledge of the variation of the critical resolved shear stress for twinning in calcite as a function of grain size.

The last stress paper reports a regional application of an improved version of the calcite twin inversion technique by Shan et al. [8]. Starting from the established model that during the Mesozoic era NE to NNE-trending folds overprinted E−W-trending folds to form the Longshan dome in the central South China continent, Zheng et al. [25] performed a paleostress analysis using calcite twins to test this model and to provide new constraints on the process of reworking the continent. The paleostress reconstruction from limestone samples collected on the flanks of the dome allowed for the identification of several states of stress, either related to layer-parallel shortening or not. The authors propose a challenging complex deformation sequence where NE to NNE-trending folds predate E−W-trending folds. The ~ N−S regional compression responsible for the former folds may have a more profound effect than previously thought.

The last two papers deal with strain analysis from calcite twins. The paper by Groshong [26] presents a personal account of the origin and development of the pioneering twinned-calcite strain gauge technique [27], its experimental verification, and its relationship to stress analysis. The method enables the calculation of the 3D deviatoric strain tensor based on five or more twin sets. A minimum of about 25 twin sets should provide a reasonably accurate result for the magnitude and orientation of the strain tensor. The experiments confirmed a magnitude accuracy of 1% strain over the range of 1–12% axial shortening. Samples with more than 40% negative expected values imply multiple or rotational deformation. If two deformations are at a high angle with respect to one another, the strain calculated from the positive and negative expected values separately provides a good estimate of both deformations.

Craddock et al. [28] present an application of Groshong's twinned-calcite strain gauge technique through a regional study in the foreland of the Alpine orogen. The authors have studied samples from the internal Alpine nappes northwestward across the Alps and Alpine foreland to the older extensional margin along the Atlantic coast in Ireland. Along the coast of Northern Ireland, twinned calcite has recorded a sub-horizontal SW-NE shortening strain with a vertical extension and no strain overprint. This sub-horizontal shortening is parallel to the margin of the opening of the Atlantic Ocean, and this penetrative fabric is only observed ~100 km inboard of the margin to the southeast. The strain regime related to the younger collisional Alpine orogeny is dominated by SE-NW sub-horizontal shortening preserved in limestones and calcite veins in France, Germany, and Britain. This layer-parallel shortening strain, preserved across the foreland in the plane of the Alpine thrust shortening (SE-NW), is compared with twinning strains from the frontal Jura Mountains, the Molasse basin, the Pre-Alp nappes, the Helvetic and Penninic nappes, and the internal Tauern window. The results highlight the record of a consistent Alpine orogenic strain up to ~1200 km northwest from the Alps.

This new collection of high-quality articles will hopefully show that it is worth making an effort to better understand how twins develop in calcite single grains and aggregates and how twinning accommodates internal strain during the progressive deformation of calcite-bearing rocks. One should keep in mind that in fold-and-thrust belts and sedimentary basins where limestones are deformed in the diagenetic domain, calcite twin analysis remains to date the most powerful and widely accepted paleopiezometric technique [29].

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References

1. Parlangeau, C.; Dimanov, A.; Lacombe, O.; Hallais, S.; Daniel, J.M. Uniaxial compression of calcite single crystals at room temperature: Insights into twinning activation and development. *Solid Earth* **2019**, *10*, 307–316. [CrossRef]
2. Schuster, R.; Habler, G.; Schafler, E.; Abart, R. Intragranular deformation mechanisms in calcite deformed by high-pressure torsion at room temperature. *Mineral. Petrol.* **2020**, *114*, 105–118. [CrossRef]
3. Schuster, R.; Schafler, E.; Schell, N.; Kunz, M.; Abart, R. Microstructure of calcite deformed by high-pressure torsion: An X-ray line profile study. *Tectonophysics* **2017**, *721*, 448–461. [CrossRef]
4. Covey-Crump, S.J.; Schofield, P.F.; Oliver, E.C. Using neutron diffraction to examine the onset of mechanical twinning in calcite rocks. *J. Struct. Geol.* **2017**, *100*, 77–97. [CrossRef]
5. Rybacki, E.; Evans, B.; Janssen, C.; Wirth, R.; Dresen, G. Influence of stress, temperature, and strain on calcite twins constrained by deformation experiments. *Tectonophysics* **2013**, *601*, 20–36. [CrossRef]
6. Parlangeau, C.; Lacombe, O.; Schueller, S.; Daniel, J.M. Inversion of calcite twin data for paleostress orientations and magnitudes: A new technique tested and calibrated on numerically-generated and natural data. *Tectonophysics* **2018**, *722*, 462–485. [CrossRef]
7. Yamaji, A. Generalized Hough transform for the stress inversion of calcite twin data. *J. Struct. Geol.* **2015**, *80*, 2–15. [CrossRef]
8. Shan, Y.; Zheng, J.; Liang, X. Inversion of polyphase calcite twin data for deviatoric stress tensors: 1. A novel numerical approach. *J. Struct. Geol.* **2019**, *128*, 103873. [CrossRef]
9. Amrouch, K.; Lacombe, O.; Bellahsen, N.; Daniel, J.M.; Callot, J.P. Stress and strain patterns, kinematics and deformation mechanisms in a basement-cored anticline: Sheep Mountain Anticline, Wyoming. *Tectonics* **2010**, *29*, TC1005. [CrossRef]

10. Lacombe, O.; Amrouch, K.; Mouthereau, F.; Dissez, L. Calcite twinning constraints on late Neogene stress patterns and deformation mechanisms in the active Zagros collision belt. *Geology* **2007**, *35*, 263–266. [CrossRef]
11. Zheng, J.; Shan, Y. Inversion of polyphase calcite-twin data for deviatoric stress tensors: 2. Application to the Huangling Dome, northern South China. *J. Struct. Geol.* **2020**, *138*, 104089. [CrossRef]
12. Beaudoin, N.; Koehn, D.; Lacombe, O.; Lecouty, A.; Billi, A.; Aharonov, E.; Parlangeau, C. Fingerprinting stress: Stylolite and calcite twinning paleopiezometry revealing the complexity of progressive stress patterns during folding. The case of the Monte Nero anticline in the Apennines, Italy. *Tectonics* **2016**, *35*, 1687–1712. [CrossRef]
13. Craddock, J.P.; Craddock, S.D.; Konstantinou, A.; Kylander-Clark, A.R.; Malone, D.H. Calcite twinning strain variations across the Proterozoic Grenville orogen and Keweenaw-Kapuskasing inverted foreland, USA and Canada. *Geosci. Front.* **2017**, *8*, 1357–1384. [CrossRef]
14. Jamison, W.R.; Spang, J. Use of calcite twin lamellae to infer differential stresses. *Geol. Soc. Am. Bull.* **1976**, *87*, 868–887. [CrossRef]
15. Ferrill, D.A. Critical re-evaluation of differential stress estimates from calcite twins in coarse-grained limestones. *Tectonophysics* **1998**, *285*, 77–86. [CrossRef]
16. Lacombe, O.; Laurent, P. Determination of deviatoric stress tensors based on inversion of calcite twin data from experimentally deformed monophase samples: Preliminary results. *Tectonophysics* **1996**, *255*, 189–202. [CrossRef]
17. de Bresser, J.; Spiers, C. Slip systems in calcite single crystals deformed at 300–800 °C. *J. Geophys. Res. Solid Earth* **1993**, *98*, 6397–6409. [CrossRef]
18. Laurent, P.; Kern, H.; Lacombe, O. Determination of deviatoric stress tensors based on inversion of calcite twin data from experimentally deformed monophase samples. Part II. Axial and triaxial stress experiments. *Tectonophysics* **2000**, *327*, 131–148. [CrossRef]
19. Lacombe, O.; Parlangeau, C.; Beaudoin, N.; Amrouch, K. Calcite twin formation, measurement and use as stress-strain indicators: A review of progress over the last decade. *Geosciences* **2021**, *11*, 445. [CrossRef]
20. Burkhard, M. Calcite twins, their geometry, appearance and significance as stress-strain markers and indicators of tectonic regime: A review. *J. Struct. Geol.* **1993**, *15*, 351–368. [CrossRef]
21. Lacombe, O. Comparison of paleostress magnitudes from calcite twins with contemporary stress magnitudes and frictional sliding criteria in the continental crust: Mechanical implications. *J. Struct. Geol.* **2007**, *29*, 86–99. [CrossRef]
22. Lacombe, O. Calcite twins, a tool for tectonic studies in thrust belts and stable orogenic forelands. *Oil Gas Sci. Technol.* **2010**, *65*, 809–838. [CrossRef]
23. Rutter, E.; Wallis, D.; Kosiorek, K. Application of Electron Backscatter Diffraction to Calcite-Twinning Paleopiezometry. *Geosciences* **2022**, *12*, 222. [CrossRef]
24. Parlangeau, C.; Dimanov, A.; Hallais, S. In-situ evolution of calcite twinning during uniaxial compression of Carrara marble at room temperature. *Geosciences* **2022**, *12*, 233. [CrossRef]
25. Zheng, J.; Shan, Y.; Hu, S. Palaeostress analysis of calcite twins from the Longshan Dome (central Hunan, South China): Mesozoic mega-fold superimposition in the reworked continent. *Geosciences* **2021**, *11*, 456. [CrossRef]
26. Groshong, R.H., Jr. Origin and application of the Twinned Calcite Strain Gauge. *Geosciences* **2021**, *11*, 296. [CrossRef]
27. Groshong, R.H., Jr. Experimental test of least-squares strain calculations using twinned calcite. *Geol. Soc. Am. Bull.* **1974**, *85*, 1855–1864. [CrossRef]
28. Craddock, J.P.; Ring, U.; Pfiffner, O.A. Deformation of the European Plate (58-0 Ma): Evidence from calcite twinning strains. *Geosciences* **2022**, *12*, 254. [CrossRef]
29. Beaudoin, N.; Lacombe, O. Recent and future trends in paleopiezometry in the diagenetic domain: Insights into the tectonic paleostress and burial depth history of fold-and-thrust belts and sedimentary basins. *J. Struct. Geol.* **2018**, *114*, 357–365. [CrossRef]