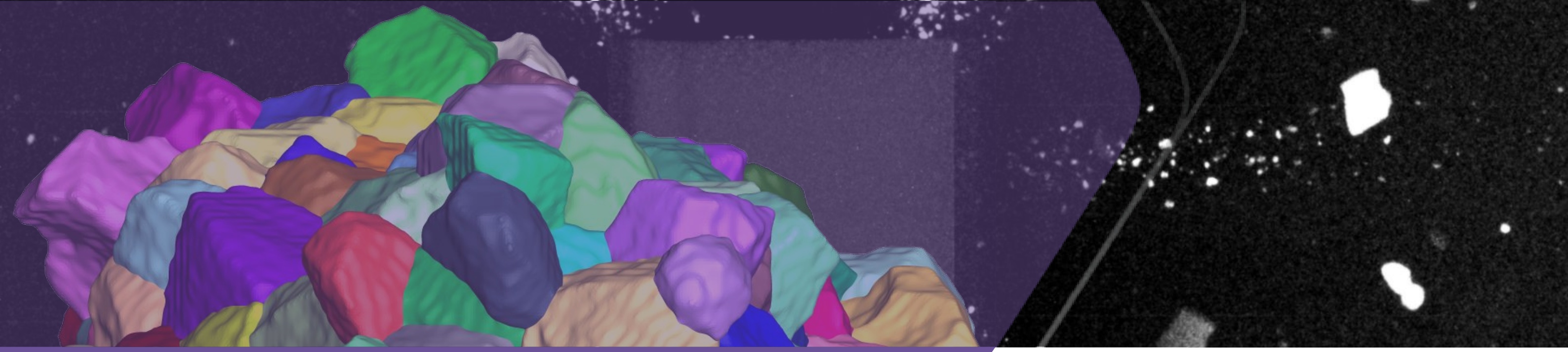

GrainMapper3D *Application Note*

Mapping many facets of quartz

Quartz and Dauphiné twinning

Quartz (SiO_2) is one of the most abundant minerals in Earth's crust and is found in nearly all rocks of igneous, metamorphic, and sedimentary origin. It also precipitates from hydrothermal fluids passing through open spaces in subsurface rocks, allowing formation of well-developed crystals like those in Figure 1.

Quartz is one of many minerals that develops twinning, or symmetrical intergrowths. One of its most common twin types grows according to the Dauphiné Law but is rarely observed by the unaided eye. The Dauphiné twin has impacted quartz's technological role in society for nearly a century because it disrupts the mineral's piezoelectricity, a property that makes quartz an ideal resonator in oscillator circuits. Quartz is found in everyday electronics, such as clocks, radios, computers, and cellphones. In the oscillator-plate industry, Dauphiné twin removal has been intensely investigated for engineering purposes. In contrast, twins have become a useful tool to reconstruct geological processes.

Dauphiné twins in 3D

Until now, studies of Dauphiné twins have required destructive analysis like acid etching or EBSD to see them, restricting observations of their complex morphologies to two dimensions. Figure 1 shows a cluster of hydrothermal quartz crystals that each contain a Dauphiné twin, which was measured and characterized in 3D by lab-based DCT [1]. Indexing crystal faces, whose *hkil* are determined from DCT data, verifies the Dauphiné Law, which transposes positive r $\{10\bar{1}1\}$ and negative z $\{01\bar{1}1\}$ rhombohedral forms. This is seen in Figure 1 as a "swap" of r and z planes across the curved twin boundary where it intersects an external rhombohedral face. The top and

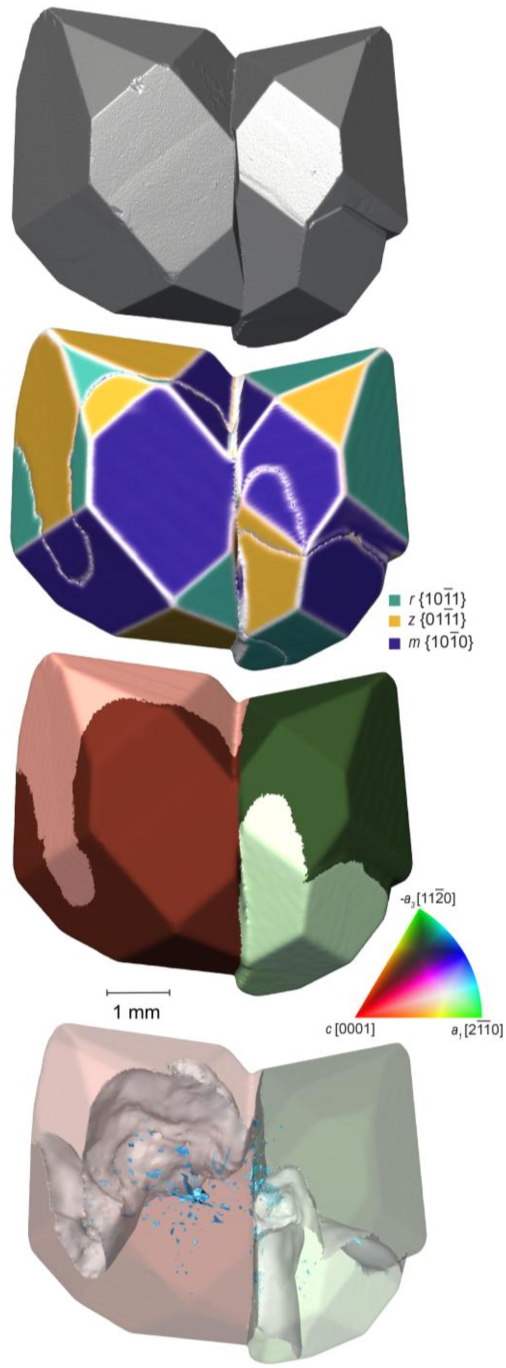

Figure 1. Correlative maps of quartz obtained by combining lab-based diffraction contrast tomography (DCT) and absorption contrast tomography (ACT). From top to bottom: Crystal facets (gray) are observed by ACT. The hkil families are then assigned to crystal faces, which belong to rhombohedral (r, z) and prism (m) forms. The IPF map shows crystal orientations; Dauphiné twin domains are separated by curved boundaries in each crystal. Distributions of fluid (blue) and solid (black) inclusions are viewed with respect to twin and grain boundaries.

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bottom twin domains in each crystal, as seen in the inverse pole figure (IPF) map, are related by a 180° rotation about the quartz *c*-axis [001] and share the same handedness. This rotation disrupts quartz's piezoelectric effect by reversing the polarity of the *a*=X electrical axes.

Correlating boundaries and inclusions

Lab-based DCT combined with ACT allows one to explore qualitative and quantitative 3D relationships between twin or grain boundaries and features inside crystals, such as mineral and fluid inclusions. In Figure 1, there is no observed spatial relationship between twin boundaries and planar arrays of fluid inclusions. However, there is spatial correlation between grain boundaries and fluid inclusions, and between each crystal center and positions of solid inclusions. Such information can help elucidate origins of twinning and inclusions, which has implications for the estimated temperature-pressure conditions of parent hydro-thermal fluids and the burial history of host rocks [1].

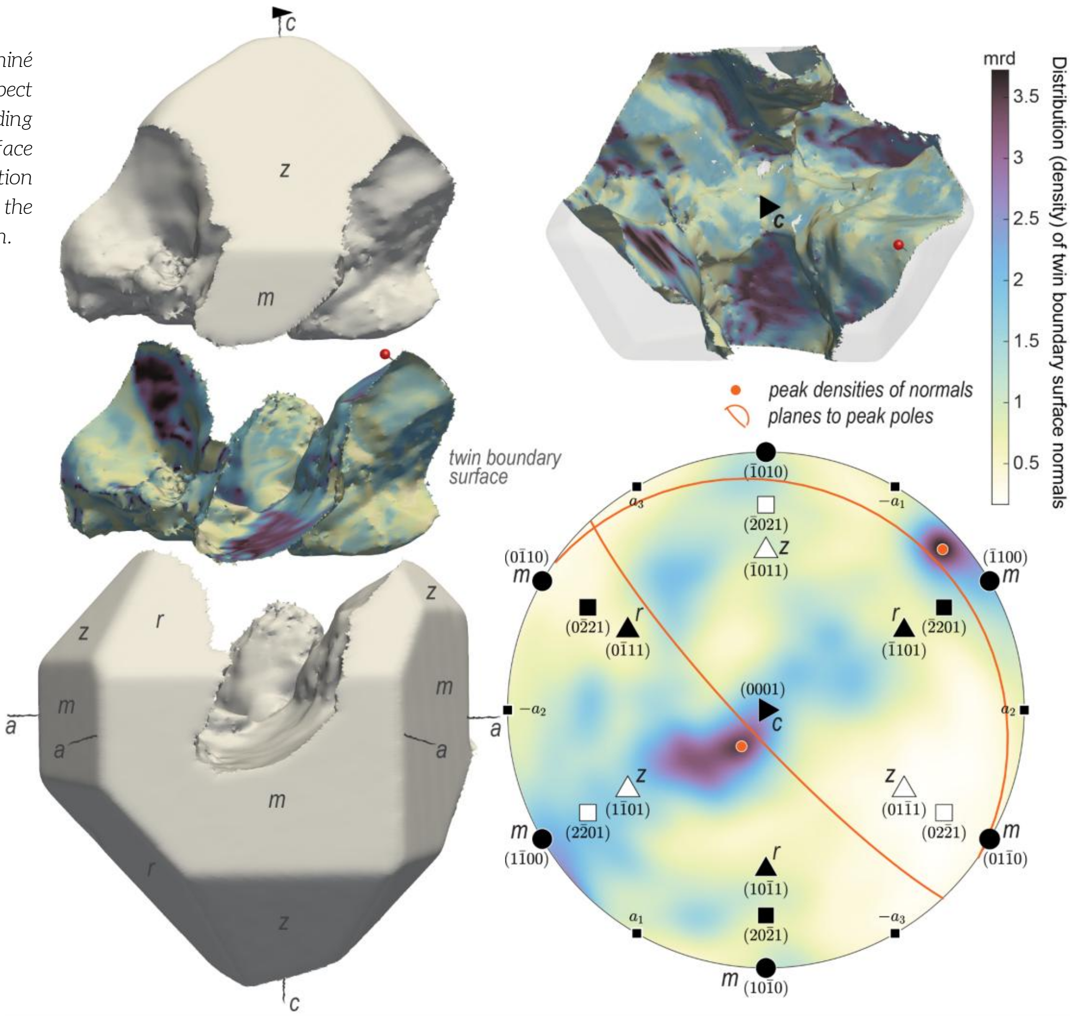
Orientations of the twin boundary

The 3D reconstruction of twin domains and their boundaries in Figure 2 allows the distribution of boundary surface normals to be mapped with respect to quartz crystallography. Measurement of twin boundary orientation complements qualitative observations and shows the boundary prefers to parallel crystallographic directions the twin domains share, being the *c*-axis [001] and *a*-axial plane, as well as the twin composition plane $\{10\bar{1}0\}$ [1].

References:

[1] *With author permission, this Application Note distributes modified material from Barbee, Pankhurst, Bachmann, Oddershede, & Sun (2024). A sinusoidal twin boundary harmonizes with the elastic anisotropy of quartz. Preprint published at Research Square. doi.org/10.21203/rs.3.rs-3949818/v1 This work is openly licensed via CC BY 4.0. Authors own the copyright © 2024.*

Figure 2. Orientations of a Dauphiné twin boundary are mapped with respect to quartz crystallography and according to the distribution of boundary surface normals. The stereographic projection shows boundary orientations from the perspective of the bottom twin domain.



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