Supplementary Information

Interfaces structure and stress of gypsum ($CaSO_4 \cdot 2H_2O$) penetration twins.

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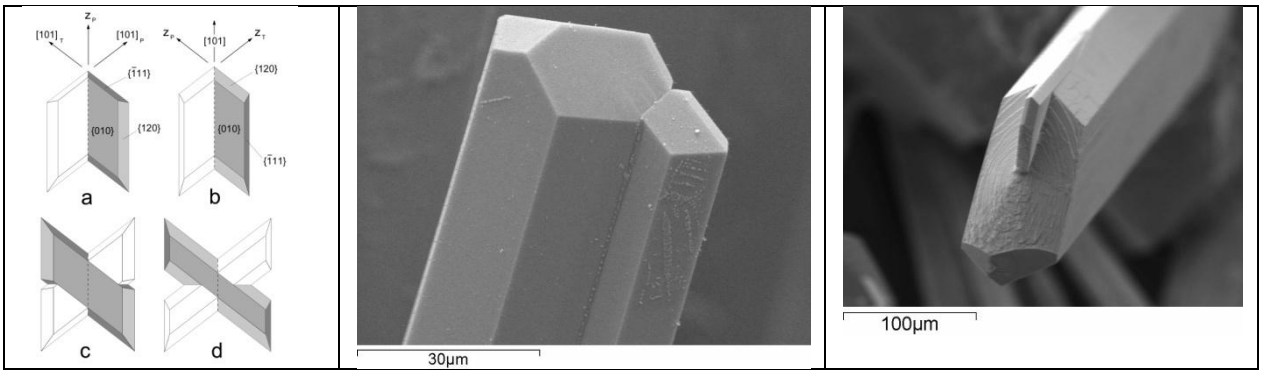
Twins



Left side : comparison between the morphological aspects of contact (a,b) and penetration (c,d) twins of gypsum crystal. In the contact twins the two individuals forming the aggregate share *only one surface*, i.e.: that of the original composition plane (OCP). In the penetration twins the two individuals share *more than one crystal surface*, since they encompass each other during growth.

a) and b) represent the 100 and the $\bar{1}01$ contact twins, respectively; c) and d) the corresponding penetration twins.

Centre: SEM image of the a 100 contact twin

Right side: SEM image of the a 100 penetration twin, where the encompassing is clearly visible.

Transformation matrix from the reference system by De Jong and Bouman, and the one used to describe the bi-crystal is:

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix}_{bi-crystal} = \begin{bmatrix} -0.974471 & 0 & 0.051058 \\ 1 & 0 & 2 \\ 0 & 1 & 0 \end{bmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{DeJong\ Bouman}$$

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Computer code and algorithms

When the 2D super-cell common to the P and T crystals has a large area it is required a huge amount of computer memory to construct a sufficiently tick slab. Constrained by the features of our hardware, we chose the accurate but large memory demanding algorithm and we limited the slab thickness. Doing so, the bulk properties are approached only in a quite limited region of each crystal as it can be seen in Fig. S1. This is not due to errors, but it is the real effect of the interactions of the surfaces of the twinned slabs with the interface between T and P crystals. The asymmetry of the perturbation of the equidistance d_{010} could be eliminated by still more stringent gradient and function tolerances, but this does not reduce the interactions between interfaces.

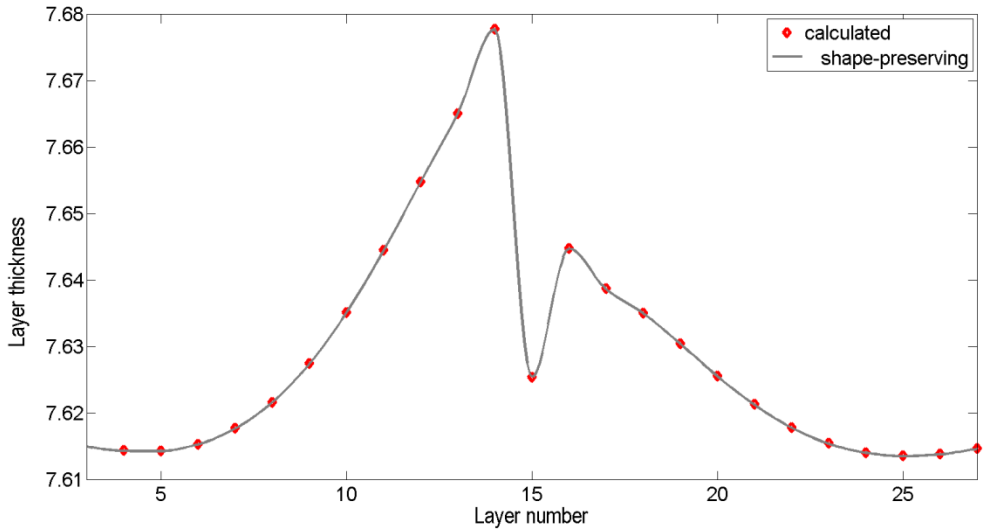

Fig. S1 Penetration twin $10\bar{1}$. The maximum perturbation of the equidistance d_{010} at the interface is about 0.06 Å. The bulk configuration is approached in a very limited volume of the two crystals (T and P) for the thinness of the slab.