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addenda and errata

Density functional calculations of polysynthetic Brazil twinning in α-quartz. Corrigenda and addenda

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Two corrections and a number of additions are made to the article by Grimmer & Delley [*Acta Cryst.* (2012), A**68**, 359–365].

In §2 of Grimmer & Delley (2012), conventions standard in crystallography were used to describe the structures of laevorotatory and dextrorotatory α-quartz: for laevorotatory quartz the standard description used by the Inorganic Crystal Structure Database (ICSD) was followed, where Si is at position 3*a* (*t*, 0, 1/3), O at 6*c* (*x*, *y*, *z*) of space group $P3_121$ (No. 152); for dextrorotatory quartz the standard description proposed by Parthé & Gelato (1984) was followed, where Si is at position 3*a* ($-t$, 0, $-1/3$), O at 6*c* ($-x$, $-y$, $-z$) of space group $P3_221$ (No. 154). According to the description of the positions given in *International Tables for Crystallography* (2005), the origin of both space groups is chosen at the intersection of a threefold screw axis with a twofold axis in the [110] direction. The authors were not aware that these conventions are not compatible with the standard conventions of mineralogy, where the planes of the major rhombohedron *r* are denoted by $\{10\bar{1}1\}$ and the planes of the minor rhombohedron *z* by $\{01\bar{1}1\}$. In fact, with the crystallographic conventions described above, it is the other way round, as can be seen by comparing the structure data used by Grimmer & Delley (2012) with Table 1 of Donnay & Le Page (1978). It follows that Figs. 2, 3 and Tables 2–6 refer to polysynthetic twins with composition plane *r*, Fig. 4 and Table 7 to twins with composition plane *z*. Corresponding changes have to be made also in the text.

One of the individuals on the two sides of the composition plane of a Brazil twin boundary is laevorotatory, the other dextrorotatory. In §2 we considered the case where the fractional coordinates of the atom positions of the dextrorotatory quartz are obtained from those of the laevorotatory quartz by an inversion $\bar{1}$ not at the origin but at $\mathbf{v} = \delta\mathbf{B}$, which corresponds to a translation of the dextrorotatory quartz by $2\mathbf{v}$. In Table 2 the sign of $Y = 2\delta$ is wrong. Consider model 1 of Table 2, for which the oxygen tetrahedra crossing the composition plane are undistorted. This is the case if the dextrorotatory quartz is shifted by $-0.4395\mathbf{B} = -0.4395(\mathbf{a} + \mathbf{b})$ with respect to the laevorotatory quartz. Equivalently, the laevorotatory quartz can be shifted by $0.4395\mathbf{B} = 0.4395(\mathbf{a} + \mathbf{b})$ with respect to the dextrorotatory quartz. In the following we shall discuss how this result is connected with the displacement vector **R** of Phakey (1969) and with the fault vector **f** of Lang (1967).

Phakey (1969) described the structure of α-quartz using a coordinate system with the same *c* axis as Grimmer & Delley (2012) and axes $\mathbf{a}_1 = -\mathbf{a}$, $\mathbf{a}_2 = -\mathbf{b}$, $\mathbf{a}_3 = \mathbf{a} + \mathbf{b}$. In §5.1 he considers a Brazil twin boundary with composition plane $r(\bar{1}101)$ and states that displacing the right-handed (*i.e.* laevorotatory) structure by $\mathbf{R} = -0.442(\mathbf{a}_1 + \mathbf{a}_2) = 0.442(\mathbf{a} + \mathbf{b})$ with respect to the left-handed (*i.e.* dextrorotatory) structure brings the oxygens with bindings across the boundary into complete register, which means that the oxygen tetrahedra crossing the composition plane are undistorted. This agrees with the corrected result of Grimmer & Delley (2012), considering that the slight differences of the shift vectors in the two models are due to slightly different choices of the structure parameters.

Phakey (1969) considers in §§5.2 and 5.3 also the two other possible orientations of the composition plane belonging to the major rhombohedron *r*. The displacement of the right-handed structure that brings the oxygens with bindings across the boundary into complete register is $\mathbf{R} = 0.442\mathbf{a}_2 - 1/3\mathbf{c}$ for $(10\bar{1}1)$ and $\mathbf{R} = 0.442\mathbf{a}_1 + 1/3\mathbf{c}$ for $(0\bar{1}11)$. The three orientations considered by Phakey (1969) correspond to the three cases shown in Table 1 of Grimmer & Delley (2012).

The fault vector **f**, as defined by Lang (1967), is closely related to the displacement vector **R** of Phakey (1969). Lang (1967) states on page 834 'When the composition plane (of a Brazil twin) contains a twofold axis, it is structurally reasonable to place the Bravais lattice origin on that twofold axis, on both sides of the twin boundary.' Whereas Phakey (1969) chooses coordinates for which the origin lies at the intersection of a threefold screw axis and a twofold axis $\mathbf{a}_3$ in $(\bar{1}101)$, the proposal of Lang (1967) corresponds to using the origin at the intersection of a threefold screw axis with a twofold axis $\mathbf{a}_1$ for $(0\bar{1}11)$, a twofold axis $\mathbf{a}_2$ for $(10\bar{1}1)$ and a twofold axis $\mathbf{a}_3$ for $(\bar{1}101)$. The advantage of using three different coordinate systems is that the three composition planes $r\{10\bar{1}1\}$ considered by Phakey give rise to fault vectors $\mathbf{f} = 0.442\mathbf{a}_1$ for $(0\bar{1}11)$, $\mathbf{f} = 0.442\mathbf{a}_2$ for $(10\bar{1}1)$ and $\mathbf{f} = 0.442\mathbf{a}_3$ for $(\bar{1}101)$, which make the equivalence of the three cases evident. Investigating Brazil twin boundaries with composition plane *r* by means of X-ray topography, Lang (1967) obtained $|\mathbf{f}| \simeq 0.4a$, Lang & Miuscov (1969) $|\mathbf{f}| = (0.42 \pm 0.02)a$. Lang (1972) mentions an unpublished model of the structure of Brazil twin boundaries with composition plane *r* that involves very little distortion of the normal bond lengths and angles, which predicts $\mathbf{f} \simeq 0.44\mathbf{a}$. He states that this vector **f** produces values of $|\mathbf{g} \cdot \mathbf{f}|$ that account well for the observed boundary visibilities in X-ray topography with diffraction vector **g**. Comparing his model result for **f** with $\mathbf{f} = 0.4395\mathbf{a}_3$ for model 1 of Grimmer & Delley (2012) and with $\mathbf{f} = 0.442\mathbf{a}_3$ for the model of Phakey (1969) we conclude that the three models are essentially the same.

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