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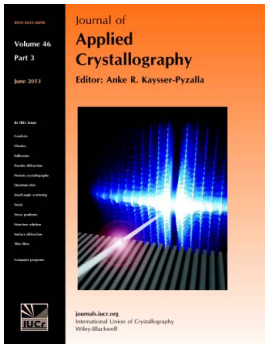

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# *Twiny*: from morphology to twin element and *vice versa*

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*Twiny* is a small Fortran program for identification or confirmation of the twin element from the morphological analysis of twins. It takes as input the twin element and computes the angle between corresponding [*uvw*] directions in two individuals of the twin: the result can be used by the investigator to confirm or invalidate the supposed twin element. *Twiny* also accepts as input the angle measured on the sample and computes all possible twin elements compatible with this angle: the result helps the investigator to identify the twin element before any attempt to unravel the diffraction pattern of a twin.

## 1. Introduction

Structure solution and refinement from diffraction data of a twinned sample requires that the measured pattern is unravelled to account for the contributions of the twinned individuals. In fact, the measured intensities from a twin are the weighted mean of the intensities from each individual, without phase relation (Catti & Ferraris, 1976). The weight factor is the fractional volume of the individuals, which enters as a parameter in the refinement strategy. For significant values of obliquity, only diffraction data at very low angles are overlapped and the integration software can easily separate the reciprocal lattices from each individual. In the case of twinning by merohedry, overlapping of diffraction patterns concerns the whole reciprocal lattice and there is no need to separate each contribution. In the case of twinning by reticular (pseudo)-merohedry with low or negligible obliquity (Nespolo & Ferraris, 2007), the flagging of overlapped *versus* non-overlapped diffraction patterns is preliminary to attempting a structure solution, but for that knowledge of the twin operation is necessary [for a detailed example, see Nespolo *et al.* (2000)]. Knowledge of the twin operation is also necessary to correctly describe the twin.

In the case of twins with a morphology sufficiently developed to identify a prominent direction [*uvw*], the possible twin element can be easily restricted to a small number of candidates once the angle ($\delta$ hereafter) between the corresponding [*uvw*] directions in the twinned individuals is measured. Also, if the twin element has been individuated, $\delta$ can be compared with a computed value and the twin element can thus be confirmed.

The software *Twiny* performs precisely these tasks and can be a useful companion in the preliminary stages of the study of a twinned sample, provided the cell parameters are known.

## 2. *Twiny*

The software is written in Fortran, with a graphical user interface in C++. The software accepts four options. Options 1 and 2 refer to the case of known twin elements; options 3 and 4 refer instead to the case of unknown twin elements but where the angle between the corresponding [*uvw*] directions in the twinned individuals is known.

(1) Reflection twin: the user enters the (*hkl*) Miller indices of the twin plane and the [*uvw*] indices of a prominent direction. *Twiny* calculates the angle $\delta$ between [*uvw*] in the two individuals related by (*hkl*).

(2) Rotation twin: the user enters the [$u'v'w'$] indices of the twin axis, the type of rotation (twofold, threefold, fourfold or sixfold) and the [*uvw*] indices of a prominent direction. *Twiny* calculates the angle $\delta$ between [*uvw*] in the two individuals related by [$u'v'w'$].

(3) Reflection twin: the user enters [*uvw*] indices of a prominent direction and the measured angle $\delta$ between [*uvw*] in the two individuals. *Twiny* estimates the possible twin planes leading to $\delta$.

(4) Rotation twin: the user enters [*uvw*] indices of a prominent direction, the measured angle $\delta$ between [*uvw*] in the two individuals and the type of rotation. *Twiny* estimates the possible twin axes leading to $\delta$.

### 2.1. Computation of the inter-direction angle for reflection twins

The algorithm is based on the mutual orthogonality of direct and reciprocal lattices. For the sake of brevity, we use the bra-ket notation and put row matrices in bra and column matrices in ket. According to *International Tables for Crystallography*, Vol. A, ch. 5 (Hahn, 2005), covariant quantities go in bra and contravariant go in ket. Vectors in direct and reciprocal space are thus written as $\langle \mathbf{abc} \mid uvw \rangle$ and $\langle hkl \mid \mathbf{a}^*\mathbf{b}^*\mathbf{c}^* \rangle$, respectively. The scalar product of the two vectors is $\langle hkl \mid \mathbf{a}^*\mathbf{b}^*\mathbf{c}^* \rangle \langle \mathbf{abc} \mid uvw \rangle = \langle hkl \mid \mathbf{I} \mid uvw \rangle = \langle hkl \mid uvw \rangle$, where $\mathbf{I}$ is the $3 \times 3$ identity matrix. The scalar product is, however, also expressed as $|\mathbf{r}_{uvw}||\mathbf{r}^*_{hkl}| \cos\varphi$, so that

$$\varphi = \cos^{-1} \frac{hu + kv + lw}{\langle hkl \mid \mathbf{G}^* \mid hkl \rangle^{1/2} \langle uvw \mid \mathbf{G} \mid uvw \rangle^{1/2}}. \qquad (1)$$

Here $\mathbf{G}$ and $\mathbf{G}^*$ are the direct and reciprocal metric tensors, respectively, and $\varphi$ is the angle between [*uvw*] and [*hkl*]*. By construction, [*hkl*]* is perpendicular to (*hkl*) so that the angle between [*uvw*] and (*hkl*) is $\pi/2 - \varphi$ and $\delta = \pi - 2\varphi$.

### 2.2. Computation of the inter-direction angle for rotation twins

For twofold twins, a formula similar to that used for reflection twins can be adopted, taking into account that both directions [*uvw*] and [$u'v'w'$] are in direct space and that the angle between them is half the angle between [*uvw*] in the two individuals and is obtained from the scalar product of directions [*uvw*] and [$u'v'w'$]:

$$\varphi = \cos^{-1} \frac{\langle uvw \mid \mathbf{G} \mid u'v'w' \rangle^{1/2}}{\langle u'v'w' \mid \mathbf{G} \mid u'v'w' \rangle^{1/2} \langle uvw \mid \mathbf{G} \mid uvw \rangle^{1/2}}, \quad (2)$$

so that $\delta = 2\varphi$. This simple calculation does not apply for a higher degree rotation: a more general algorithm is thus necessary. Fig. 1 shows the scheme used to obtain $\delta$ for a general rotation. $[u'v'w']$ is the twin axis, and $[uvw]_{\rm I}$ and $[uvw]_{\rm II}$ are the corresponding directions in individuals I and II, respectively, both with period $r$. The following relations are obtained immediately from elementary trigonometry:

$$\begin{aligned} \mathrm{BC}^2 &= \mathrm{OB}^2 + \mathrm{OC}^2 - 2\mathrm{OB}\cdot\mathrm{OC}\cos\delta \\ &= 2r^2(1-\cos\delta) \quad \text{(law of cosines)}, \\ \mathrm{AB} &= \mathrm{AC} = r\sin\varphi, \\ \mathrm{BC} &= 2r\sin\varphi\sin\Psi/2, \\ 4r^2\sin^2\varphi\sin^2\Psi/2 &= 2r^2(1-\cos\delta), \\ \cos\delta &= 1 - 2\sin^2\varphi\sin^2\Psi/2, \end{aligned} \quad (3)$$

where $\varphi$ is obtained from equation (2) and $\psi$ is the angle corresponding to the twin operation. For a twofold rotation, equation (3) becomes $\cos\delta = 1 - 2\sin^2\varphi = \cos 2\varphi$, again giving $\delta = 2\varphi$.

### 2.3. Estimation of the twin plane from the measured angle

From the $[uvw]$ indices of the prominent direction and the measured angle, the twin plane can be estimated by making $(hkl)$ variable and calculating $\varphi$ from equation (1), $\delta$ being just $\pi - 2\varphi$. For a hexagonal setting the output gives Bravais–Miller indices even if in the input Miller indices are used. The solution is not necessarily unique, depending on the tolerance allowed on the difference between computed and measured values of $\delta$. To restrict the number of possible solutions, the exploration is made gradually: the tolerance starts at 0.5° and, if no solution is found, is increased by 0.5° up to 5°. For each value of the angular tolerance, the values of $h$, $k$ and $l$ span an interval $\leq|n|$, with $n$ starting at 2 and gradually increasing, if no solution is found, up to 20. This value may seem unreasonably high, but for rhombohedral lattices in a hexagonal setting the indices may easily take higher values than in other lattice systems. In any case, once a solution is found, the computation stops.

### 2.4. Estimation of the twin axis from the measured angle

The principle is exactly the same as for the estimation of the twin plane but equation (3) is used instead of equation (1). The user has to indicate the type of rotation. It may be necessary to repeat the calculation to find the correct twin element if the type of rotation is not necessarily known *a priori*. A result corresponding to too high indices of the twin axis may indicate that the type or rotation given by the user is not correct, although a numerical solution has been found.

### 2.5. Limits of the software

The software does not take as input the point group of the crystal but only the cell parameters. Planes or directions that are symmetry equivalent are therefore printed separately. The point group is not necessarily definitely confirmed before structure refinement; it is thus preferable not to impose symmetry restraints on calculation of the candidate twin elements.

In the very unlikely case of an index higher than 20 the software will fail to find the twin element and print a message saying that no twin element could be found.

The maximum tolerance on the measured angle is set to 5°; should the measurement be affected by a larger error, the result would be incorrect, or no twin element may be found.

## 3. Example

Figs. 2 and 3 show the graphical user interface for *Twiny* and present two examples taken from twins in quartz. In Fig. 2 the calculation of the angle between the [001] directions corresponding to the Japan/Verespatak twin occurring in $\alpha$- and $\beta$-quartz, both corresponding to $(11\bar{2}2)$, is presented. In Fig. 3 the estimation of the twin plane from the Belowda Beacon twin, with an angle of about 55° between the [001] directions, shows six planes all corresponding to the same angle;

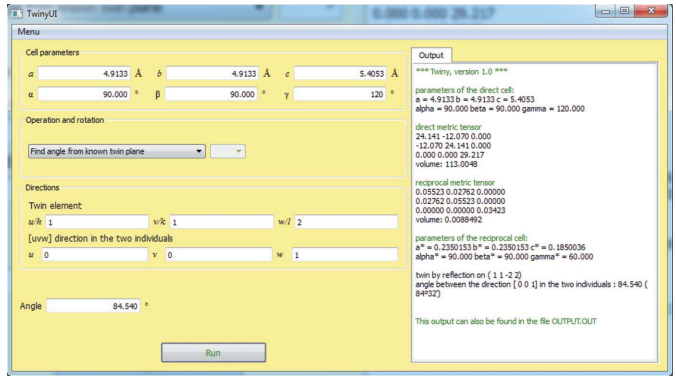


**Figure 2**
Screenshot showing the calculation of the angle between the [001] directions in two quartz crystals twinned according to the Japan/Verespatak law: twinning on $(11\bar{2}2)$.

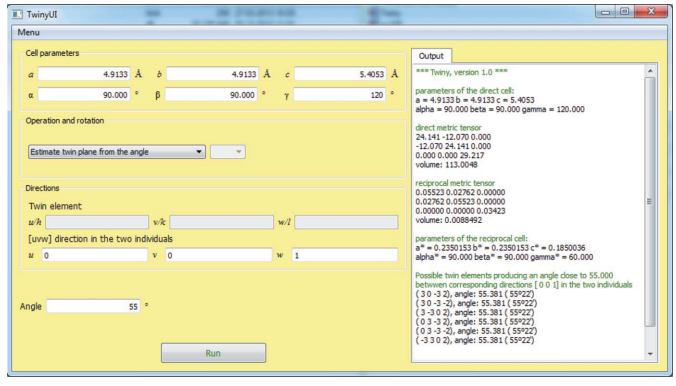


**Figure 3**
Screenshot showing the estimation of the twin plane for two twinned crystals of quartz making an angle of about 55° between the [001] directions, corresponding to the Belowda Beacon twin.

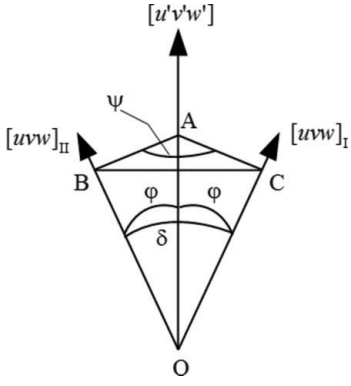


**Figure 1**
Derivation of the geometrical relations between quantities entering equation (3) used to compute the angle between corresponding directions in two twinned individuals for rotation twins.

these planes are all equivalent in the point group of quartz 321 [for further details about twins in quartz, see Frondel (1962)].

## 4. Software availability

*Twiny* is available for download from the CMR2 laboratory web site (http://www.crystallography.fr/Twiny) in three compilations for Windows, Linux and Macintosh.

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