**Generation of a twin law matrix from a 180° (or other angle) rotation about either [hkl] or the normal to (hkl).**

There are a number of ways to do this. I chose to use the Rodrigues formula [1-4] applied in Cartesian space, but it could also be done using the methodology described by Sands [5]. In Cartesian space we take the direct axis vector [hkl] or the reciprocal lattice vector hkl, orthogonalize the chosen vector, and then convert it to a unit vector.

Orthogonalization can be carried out for the covariant vector [hkl] (we’ll call it **h**), as the product **Lh**, while the contravariant vector hkl (we’ll call it ***h***)may be orthogonalized as the product **U*h*** [6].

In the International Tables for X-ray Crystallography, Volume B, Shmueli, in a derivation of general rotations in non-orthogonal systems, Shmueli [1] states:

“If all the vectors are referred to a Cartesian basis, that is three orthogonal unit vectors, the direct and reciprocal metric tensors reduce to a unit tensor, there is no difference between covariant and contravariant quantities, and equation (1.1.4.31) reduces to

*Rij* = *kikj*(1 - cos *θ*) + *δij* cos *θ* + *eipjkp* sin *θ*, (1.1.4.32)

where all the indices have been taken as subscripts, but the summation convention is still observed. The relative simplicity of (1.1.4.32), as compared to (1.1.4.31), often justifies the transformation of all the vector quantities to a Cartesian basis. This is certainly the case for any extensive calculation in which covariances of the structural parameters are not considered.”

For a twin law involving a 180° rotation, equation (1.1.4.32) simplifies, with the last term on the right dropping out when sin 180° = 0. Then we have:

*Rij* = *kikj*(1 - cos *θ*) + *δij* cos *θ* (1.1.4.32-S)

And then, when *i* = *j*, *Rii* = 2*ki*2 -1, and when *i* = *j*, *Rij* = 2*kikj* [2].

In terms of Sands’ chapter 4 [5], *R* in the above equation is the Cartesian rotation matrix, and thus corresponds to *R’* in Sands’ equation (4-41), page 102. To get the twin law matrix, we need to apply equation (4-41), substituting ITX’s *R* in place of *R’* in (4-41):

(4-41) where **F** is contragredient to **G** (that is, **F = G-1**).

In Sands, **G** transforms the covariant basis vectors and **F** transforms the contravariant coordinates. In the language and discussion of Rollett’s Computing Methods in Crystallography, those matrices will be U and L, respectively, and we may write

**R = LT R’ U**

Note that this is all is Sands [5,7] in a different way:

On page 14 he reminds us that:

“The full implications of the distinction between covariance and contravariance will become apparent in the development of transformation properties in Chapter 3. Only in cartesian coordinate systems does **ai** = **ai** for i = l, 2, 3.”

Sands’ equation Equation 4-42 is:



So, in Omega2, I determine a twin law matrix using equation 4-42, page 102. That gives me the Cartesian transformation matrix R’, and then I can get it in crystal space using 4-41, just on p. 102 above 4-42. The symmetric R’ matrix, as described in the first part of this memo, will be: (2u12 – 1, 2u1u2, 2u1u3 / 2u2u1,2u22 – 1, 2u2u3 / 2u3u1, 2u3u2,2u32 – 1).

Equation 4-42 simplifies for a 180° rotation in Cartesian space, to:

*Rij* = *uiuj*+ (*δij* - *uiuj*) cos *θ*

Which is identical to equation (1.1.4.32-S) derived earlier!

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[1] Shmueli, U. (2010). International Tables for Crystallography, Vol. B. Reciprocal space in crystallography. 2nd online edition; edited by U. Shmueli, Chapter 1.1, pp. 2–9. Chester: International Union of Crystallography.

[2] Rodrigues, O. (1840). J. Math. Pures Appl. 1(5), 380–440. Ref 1 does not refer to this as the Rodrigues formula, but that would have been proper!

[3] Three-Dimensional Rotation Matrices: <http://scipp.ucsc.edu/~haber/ph216/rotation_12.pdf> This is a very clear introduction to the subject, and to the Rodrigues formula.

[4]Morawiec, A. Acta Cryst. (2016). On representing rotations by Rodrigues parameters in non-orthonormal reference systems, **A72**, 548–556.

[5] Sands, D. E. Vectors and Tensors in Crystallography, New York: Addison-Wesley, 1982, Chapter 4.

[6] Rollett, J. S. Computing Methods In Crystallography, Oxford: Pergamon Press, 1965, Chapter 3.

[7] Reference 5, Chapter 1.