The rotation matrix, *W*, used in lattice_symmetry.h

The counterclockwise rotation of a vector **r** through a counterclockwise angle Φ about the normalized axis $\hat{\mathbf{t}}$ is treated geometrically, *e.g.*, by Goldstein (1980). Eq. 4-92 in that text gives the formula for the rotated vector,

$$\mathbf{r}' = \mathbf{r}\cos\Phi + \hat{\mathbf{t}}(\hat{\mathbf{t}}\cdot\mathbf{r})[1-\cos\Phi] + (\hat{\mathbf{t}}\times\mathbf{r})\sin\Phi \,. \qquad (1)$$

Note that Eq. 1 is for a rotating vector in a fixed laboratory frame. We want to express the rotation in the form of a matrix operator ***W*** (Fischer & Koch, 1996), such that $\mathbf{r}' = \boldsymbol{W}\mathbf{r}$. We expand the formula in (3×3) matrix notation and rearrange:

$$\mathbf{r}' = \left(\boldsymbol{I}\cos\Phi + \begin{bmatrix} \hat{t}_x^{\,2} & \hat{t}_x\hat{t}_y & \hat{t}_x\hat{t}_z \\ \hat{t}_x\hat{t}_y & \hat{t}_y^{\,2} & \hat{t}_y\hat{t}_z \\ \hat{t}_x\hat{t}_z & \hat{t}_y\hat{t}_z & \hat{t}_z^{\,2} \end{bmatrix} [1-\cos\Phi] + \begin{bmatrix} 0 & -\hat{t}_z & \hat{t}_y \\ \hat{t}_z & 0 & -\hat{t}_x \\ -\hat{t}_y & \hat{t}_x & 0 \end{bmatrix} \sin\Phi \right) \mathbf{r} \,. \qquad (2)$$

Eq. 2 is identical to one given in Boisen & Gibbs (1990). This can then be specialized for 2-fold rotations by taking Φ=180°, giving the matrix operator

$$\boldsymbol{W} = \begin{bmatrix} 2\hat{t}_x^{\,2}-1 & 2\hat{t}_x\hat{t}_y & 2\hat{t}_x\hat{t}_z \\ 2\hat{t}_x\hat{t}_y & 2\hat{t}_y^{\,2}-1 & 2\hat{t}_y\hat{t}_z \\ 2\hat{t}_x\hat{t}_z & 2\hat{t}_y\hat{t}_z & 2\hat{t}_z^{\,2}-1 \end{bmatrix} . \qquad (3)$$

It is stressed that ***W*** and $\hat{\mathbf{t}}$ are expressed in Cartesian laboratory coordinates rather than crystallographic coordinates.

References

Boisen, M. B. Jr & Gibbs, G. V. (1990). *Mathematical Crystallography, Reviews in Minerology*, Vol. 15 (revised edition). Washington, DC: Mineralogical Society of America.

Fischer, W. & Koch, E. (1996). In *International Tables for Crystallography, Volume A: Space-Group Symmetry*, 4th revised edition, Hahn, T., ed. Dordrecht: Kluwer Academic Publishers.

Goldstein, H. (1980). *Classical Mechanics*, 2nd edition. Reading, MA: Addison-Wesley, pp. 164-166.