3. METHODOLOGY

For Laue symmetries other than triclinic, there are restrictions on the allowed S_{hkl} terms and, as a practical matter, additional equivalences from symmetry-forced reflection overlaps for trigonal and tetragonal Laue symmetries.

Monoclinic (2/m, b axis unique; others similar, nine coefficients):

$$\Gamma^2_{sL} = S_{400}h^4 + S_{040}k^4 + S_{004}l^4 + 3S_{202}h^2l^2 + 3(S_{220}h^2k^2 + S_{022}k^2l^2) + 2(S_{301}h^3l + S_{103}hl^3) + 4S_{121}hk^2l. \quad (3.3.34)$$

Orthorhombic (mmm, six coefficients):

$$\Gamma^2_{sL} = S_{400}h^4 + S_{040}k^4 + S_{004}l^4 + 3(S_{220}h^2k^2 + S_{202}h^2l^2 + S_{022}k^2l^2). \quad (3.3.35)$$

Tetragonal (4/m, five coefficients):

$$\Gamma^2_{sL} = S_{400}(h^4 + k^4) + S_{004}l^4 + 3S_{220}h^2k^2 + 3S_{202}(h^2l^2 + k^2l^2) + 2S_{310}(h^3k - hk^3). \quad (3.3.36)$$

The last coefficient (S_{310}) cannot normally be determined owing to exact reflection overlaps. Thus, equation (3.3.37) is normally used for both 4/m and 4/mmm Laue symmetries:

Tetragonal (4/mmm, four coefficients):

$$\Gamma^2_{sL} = S_{400}(h^4 + k^4) + S_{004}l^4 + 3S_{220}h^2k^2 + 3S_{202}(h^2l^2 + k^2l^2). \quad (3.3.37)$$

Trigonal ($\bar{3}$, rhombohedral setting, five coefficients):

$$\Gamma^2_{sL} = S_{400}(h^4 + k^4 + l^4) + 3S_{220}(h^2k^2 + h^2l^2 + k^2l^2) + 2S_{310}(h^3k + k^3l + hl^3) + 2S_{130}(h^3l + kl^3 + hl^3) + 4S_{211}(h^2kl + hk^2l + hkl^2). \quad (3.3.38)$$

The pair of coefficients S_{310} and S_{130} cannot normally be independently determined owing to exact reflection overlaps. Thus, equation (3.3.39) is normally used for both rhombohedral symmetries:

Trigonal ($\bar{3}m$, rhombohedral setting, four coefficients):

$$\Gamma^2_{sL} = S_{400}(h^4 + k^4 + l^4) + 3S_{220}(h^2k^2 + h^2l^2 + k^2l^2) + 2S_{310}(h^3k + k^3l + hl^3 + h^3l + kl^3 + hl^3) + 4S_{211}(h^2kl + hk^2l + hkl^2). \quad (3.3.39)$$

Trigonal ($\bar{3}$, five coefficients):

$$\Gamma^2_{sL} = S_{400}(h^4 + k^4 + 2h^3k + 2hk^3 + 3h^2k^2) + S_{004}l^4 + 3S_{202}(h^2l^2 + k^2l^2 + hkl^2) + S_{301}(2h^3l - 2k^3l - 6hk^2l) + 4S_{211}(h^2kl + hk^2l). \quad (3.3.40)$$

The coefficient S_{301} cannot normally be independently determined owing to exact reflection overlaps. Thus, equation (3.3.42) is normally used for $\bar{3}$ Laue symmetry.

Trigonal ($\bar{3}m1$, four coefficients):

$$\Gamma^2_{sL} = S_{400}(h^4 + k^4 + 2h^3k + 2hk^3 + 3h^2k^2) + S_{004}l^4 + 3S_{202}(h^2l^2 + k^2l^2 + hkl^2) + S_{301}(3h^2kl - 3hk^2l + 2h^3l - 2k^3l). \quad (3.3.41)$$

The coefficient S_{301} cannot normally be independently determined due to exact reflection overlaps. Thus, equation (3.3.43) is normally used for $\bar{3}m1$ Laue symmetry.

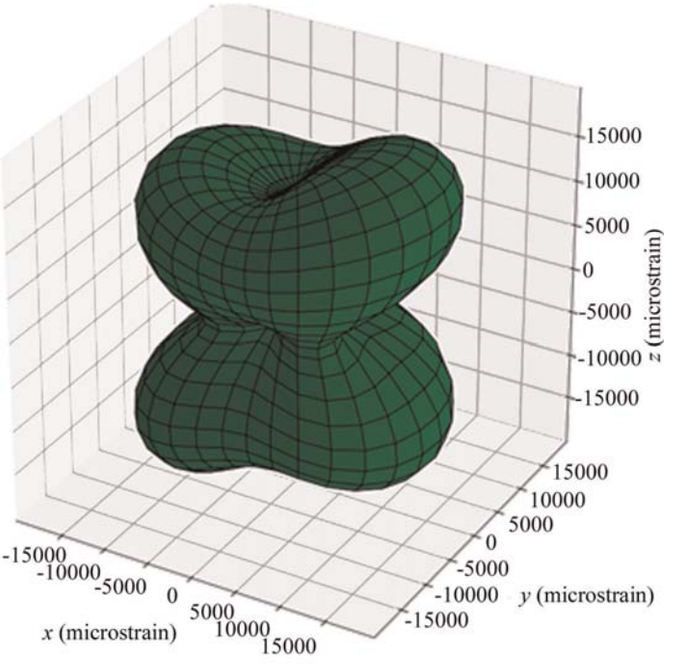

Figure 3.3.4
Microstrain surface for sodium parahydroxybenzoate multiplied by 10^6.

Trigonal ($\bar{3}1m$, four coefficients):

$$\Gamma^2_{sL} = S_{400}(h^4 + k^4 + 2h^3k + 2hk^3 + 3h^2k^2) + S_{004}l^4 + 3S_{202}(h^2l^2 + k^2l^2 + hkl^2) + 4S_{211}(h^2kl + hk^2l). \quad (3.3.42)$$

Hexagonal (6/m and 6/mmm, three coefficients):

$$\Gamma^2_{sL} = S_{400}(h^4 + k^4 + 2h^3k + 2hk^3 + 3h^2k^2) + S_{004}l^4 + 3S_{202}(h^2l^2 + k^2l^2 + hkl^2). \quad (3.3.43)$$

Cubic ($m\bar{3}$ and $m\bar{3}m$, two coefficients):

$$\Gamma^2_{sL} = S_{400}(h^4 + k^4 + l^4) + 3S_{220}(h^2k^2 + h^2l^2 + k^2l^2). \quad (3.3.44)$$

These equations can be used with the refined values of the coefficients to produce a surface representing the extent of the microstrain in reciprocal space. The surface resulting from Stephens' (1999) analysis of powder diffraction data from sodium parahydroxybenzoate is shown Fig. 3.3.4. At the present time, the connection between the elastic properties and defects with these microstrain surface models is unclear. Some aspects of this for cubic and hexagonal systems are discussed in Chapter 5.1.

References

Avdeev, M., Jorgensen, J., Short, S. & Von Dreele, R. B. (2007). *On the numerical corrections of time-of-flight neutron powder diffraction data. J. Appl. Cryst.* **40**, 710–715.
Buras, B. & Holas, A. (1968). *Nukleonika*, **13**, 591–620.
Caglioti, G., Paoletti, A. & Ricci, F. P. (1958). *Choice of collimators for a crystal spectrometer for neutron diffraction. Nucl. Instrum.* **3**, 223–228.
Carpenter, J. M., Lander, G. H. & Windsor, C. G. (1984). *Instrumentation at pulsed neutron sources. Rev. Sci. Instrum.* **55**, 1019–1043.
Cheary, R. W. & Coelho, A. A. (1998*a*). *Axial divergence in a conventional X-ray powder diffractometer. I. Theoretical foundations. J. Appl. Cryst.* **31**, 851–861.
Cheary, R. W. & Coelho, A. A. (1998*b*). *Axial divergence in a conventional X-ray powder diffractometer. II. Realization and evalua-*

tion in a fundamental-parameter profile fitting procedure. J. Appl. Cryst. **31**, 862–868.
Cheary, R. W. & Coelho, A. (1992). *A fundamental parameters approach to X-ray line-profile fitting. J. Appl. Cryst.* **25**, 109–121.
Cheary, R. W., Coelho, A. A. & Cline, J. P. (2004). *Fundamental parameters line profile fitting in laboratory diffractometers. J. Res. Natl Inst. Stand. Technol.* **109**, 1–25.
Cole, I. & Windsor, C. G. (1980). *The lineshapes in pulsed neutron powder diffraction. Nucl. Instrum. Methods*, **171**, 107–113.
Cooper, M. J. & Sayer, J. P. (1975). *The asymmetry of neutron powder diffraction peaks. J. Appl. Cryst.* **8**, 615–618.
David, W. I. F. (1986). *Powder diffraction peak shapes. Parameterization of the pseudo-Voigt as a Voigt function. J. Appl. Cryst.* **19**, 63–64.
Finger, L. W., Cox, D. E. & Jephcoat, A. P. (1994). *A correction for powder diffraction peak asymmetry due to axial divergence. J. Appl. Cryst.* **27**, 892–900.
Glazer, A. M., Hidaka, M. & Bordas, J. (1978). *Energy-dispersive powder profile refinement using synchrotron radiation. J. Appl. Cryst.* **11**, 165–172.
Hastings, J. B., Thomlinson, W. & Cox, D. E. (1984). *Synchrotron X-ray powder diffraction. J. Appl. Cryst.* **17**, 85–95.
Howard, C. J. (1982). *The approximation of asymmetric neutron powder diffraction peaks by sums of Gaussians. J. Appl. Cryst.* **15**, 615–620.
Ikeda, S. & Carpenter, J. M. (1985). *Wide-energy-range, high-resolution measurements of neutron pulse shapes of polyethylene moderators. Nucl. Instrum. Methods Phys. Res. Sect. A*, **239**, 536–544.
Jorgensen, J. D., David, W. I. F. & Willis, B. T. M. (1992). *White-beam and time-of-flight neutron diffraction*. In *International Tables for Crystallography*, Vol. C, edited by A. J. C. Wilson. Dordrecht: Kluwer.
Jorgensen, J. D., Johnson, D. H., Mueller, M. H., Peterson, S. W., Worlton, J. G. & Von Dreele, R. B. (1978). *Profile analysis of pulsed-source neutron powder diffraction data*. Proceedings of the Conference on Diffraction Profile Analysis, Cracow 14–15 August 1978, pp. 20–22.
Jorgensen, J. D. & Rotella, F. J. (1982). *High-resolution time-of-flight powder diffractometer at the ZING-P″ pulsed neutron source. J. Appl. Cryst.* **15**, 27–34.
Laar, B. van & Yelon, W. B. (1984). *The peak in neutron powder diffraction. J. Appl. Cryst.* **17**, 47–54.
Malmros, G. & Thomas, J. O. (1977). *Least-squares structure refinement based on profile analysis of powder film intensity data measured on an automatic microdensitometer. J. Appl. Cryst.* **10**, 7–11.
Otto, J. W. (1997). *On the peak profiles in energy-dispersive powder X-ray diffraction with synchrotron radiation. J. Appl. Cryst.* **30**, 1008–1015.
Parrish, W. (1992). *Powder and related techniques: X-ray techniques*. In *International Tables for Crystallography*, Vol. C, edited by A. J. C. Wilson, ch. 2.3. Dordrecht: Kluwer.
Popa, N. C. (1998). *The (hkl) dependence of diffraction-line broadening caused by strain and size for all Laue groups in Rietveld refinement. J. Appl. Cryst.* **31**, 176–180.
Rietveld, H. M. (1967). *Line profiles of neutron powder-diffraction peaks for structure refinement. Acta Cryst.* **22**, 151–152.
Rietveld, H. M. (1969). *A profile refinement method for nuclear and magnetic structures. J. Appl. Cryst.* **2**, 65–71.
Robinson, R. A. & Carpenter, J. M. (1990). *On the use of switch functions in describing pulsed moderators*. Report LAUR 90-3125. Los Alamos National Laboratory, USA.
Stephens, P. W. (1999). *Phenomenological model of anisotropic peak broadening in powder diffraction. J. Appl. Cryst.* **32**, 281–289.
Thompson, P., Cox, D. E. & Hastings, J. B. (1987). *Rietveld refinement of Debye–Scherrer synchrotron X-ray data from Al_2O_3. J. Appl. Cryst.* **20**, 79–83.
Toby, B. H. & Von Dreele, R. B. (2013). *GSAS-II: the genesis of a modern open-source all-purpose crystallographic software package. J. Appl. Cryst.* **46**, 544–549.
Turberfield, K. C. (1970). *Time-of-flight neutron diffractometry*. In *Thermal Neutron Diffraction*, edited by B. T. M. Willis. Oxford University Press.
Von Dreele, R. B., Jorgensen, J. D. & Windsor, C. G. (1982). *Rietveld refinement with spallation neutron powder diffraction data. J. Appl. Cryst.* **15**, 581–589.
Wang, Y., Uchida, T., Von Dreele, R., Rivers, M. L., Nishiyama, N., Funakoshi, K., Nozawa, A. & Kaneko, H. (2004). *A new technique for angle-dispersive powder diffraction using an energy-dispersive setup and synchrotron radiation. J. Appl. Cryst.* **37**, 947–956.
Worlton, J. G., Jorgensen, J. D., Beyerlein, R. A. & Decker, D. L. (1976). *Multicomponent profile refinement of time-of-flight neutron diffraction data. Nucl. Instrum. Methods*, **137**, 331–337.
Young, R. A., Mackie, P. E. & von Dreele, R. B. (1977). *Application of the pattern-fitting structure-refinement method of X-ray powder diffractometer patterns. J. Appl. Cryst.* **10**, 262–269.
Young, R. A. & Wiles, D. B. (1982). *Profile shape functions in Rietveld refinements. J. Appl. Cryst.* **15**, 430–438.