## 8. REFINEMENT OF STRUCTURAL PARAMETERS

where  $A_g = U_g^{\text{eff}}t$ , and  $J_0$  is the Bessel function of zero order. For a small gap, the intensity is proportional to  $|U^{\text{eff}}|^2$ . By many-beam calculations, Gjønnes & Bøe (1994) showed the integrated intensities to be less sensitive to dynamical interactions along the row than that indicated from the Bethe potentials, and that relative intensities are fairly independent of thickness. Coordinate refinement based on intensities from a few high-order Kossel-line segments appear to produce accuracies roughly one order of magnitude poorer than good single-crystal X-ray determination. This may suggest that if some form of three-dimensional intensity data could be collected in electron diffraction the same level of accuracies as with X-rays may be attainable – which, however, remains to be seen.

## References

8.1

- Anderson, E., Bai, Z., Bischof, C., Demmel, J., Dongarra, J., Du Croz, J., Greenbaum, A., Hammarling, S., McKenney, A., Ostrouchov, S. & Sorenson, D. (1992). *LAPACK user's* guide, 2nd ed. Philadelphia: SIAM Publications.
- Berger, J. O. & Wolpert, R. L. (1984). The likelihood principle. Hayward, CA: Institute of Mathematical Statistics.
- Boggs, P. T., Byrd, R. H., Donaldson, J. R. & Schnabel, R. B. (1989). ODRPACK – software for weighted orthogonal distance regression. ACM Trans. Math. Softw. 15, 348–364.
- Boggs, P. T., Byrd, R. H. & Schnabel, R. B. (1987). A stable and efficient algorithm for nonlinear orthogonal distance regression. SIAM J. Sci. Stat. Comput. 8, 1052–1078.
- Boggs, P. T. & Rogers, J. E. (1990). Orthogonal distance regression. Contemporary mathematics: statistical analysis of measurement error models and applications. Providence, RI: AMS.
- Box, G. E. P., Hunter, W. G. & Hunter, J. S. (1978). Statistics for experimenters: an introduction to design, data analysis and model building. New York: John Wiley.
- Box, G. E. P. & Tiao, G. C. (1973). Bayesian inference in statistical analysis. Reading, MA: Addison-Wesley.
- Bunch, D. S., Gay, D. M. & Welsch, R. E. (1993). Algorithm 717: subroutines for maximum likelihood and quasi-likelihood estimation of parameters in nonlinear regression models. ACM Trans. Math. Softw. 19, 109–130.
- Dennis, J. E. & Schnabel, R. B. (1983). Numerical methods for unconstrained optimization and nonlinear equations. Englewood Cliffs, NJ: Prentice Hall.
- Donaldson, J. R. & Schnabel, R. B. (1986). Computational experience with confidence regions and confidence intervals for nonlinear least squares. Computer science and statistics. Proceedings of the Seventeenth Symposium on the Interface, edited by D. M. Allen, pp. 83–91. New York: North-Holland.
- Draper, N. & Smith, H. (1981). Applied regression analysis. New York: John Wiley.
- Fedorov, V. V. (1972). *Theory of optimal experiments*, translated by W. J. Studden & E. M. Klimko. New York: Academic Press.
- Fuller, W. A. (1987). *Measurement error models*. New York: John Wiley & Sons.
- Heath, M. T. (1984). Numerical methods for large, sparse, linear least squares problems. SIAM J. Sci. Stat. Comput. 5, 497–513.
- Nash, S. & Sofer, A. (1995). Linear and nonlinear programming. New York: McGraw-Hill.
- Prince, E. (1994). Mathematical techniques in crystallography and materials science, 2nd ed. Berlin: Springer.

- Schwarzenbach, D., Abrahams, S. C., Flack, H. D., Prince, E. & Wilson, A. J. C. (1995). Statistical descriptors in crystallography. II. Report of a Working Group on Expression of Uncertainty in Measurement. Acta Cryst. A51, 565–569.
- Stewart, G. W. (1973). Introduction to matrix computations. New York: Academic Press.

8.2

- Belsley, D. A., Kuh, E. & Welsch, R. E. (1980). *Regression diagnostics*. New York: John Wiley.
- Box, G. E. P. & Tiao, G. C. (1973). Bayesian inference in statistical analysis. Reading, MA: Addison-Wesley.
- Collins, D. M. (1982). Electron density images from imperfect data by iterative entropy maximization. Nature (London), 298, 49–51.
- Collins, D. M. (1984). Scaling by entropy maximization. Acta Cryst. A40, 705-708.
- Hoaglin, D. C., Mosteller, M. & Tukey, J. W. (1983). Understanding robust and exploratory data analysis. New York: John Wiley.
- Huber, P. J. (1973). Robust regression: asymptotics, conjectures and Monte Carlo. Ann. Stat. 1, 799–821.
- Huber, P. J. (1981). Robust statistics. New York: John Wiley.
- Jaynes, E. T. (1979). Where do we stand on maximum entropy? The maximum entropy formalism, edited by R. D. Liven & M. Tribus, pp. 44-49. Cambridge, MA: Massachusetts Institute of Technology.
- Livesey, A. K. & Skilling, J. (1985). Maximum entropy theory. Acta Cryst. A41, 113–122.
- Nicholson, W. L., Prince, E., Buchanan, J. & Tucker, P. (1982). A robust/resistant technique for crystal structure refinement. Crystallographic statistics: progress and problems, edited by S. Rameseshan, M. F. Richardson & A. J. C. Wilson, pp. 220–263. Bangalore: Indian Academy of Sciences.
- Rietveld, H. M. (1969). A profile refinement method for nuclear and magnetic structures. J. Appl. Cryst. 2, 65-71.
- Shore, J. E. & Johnson, R. W. (1980). Axiomatic derivation of the principle of maximum entropy and the principle of minimum cross-entropy. IEEE Trans. Inf. Theory, IT-26, 26–37; correction: IT-29, 942–943.
- Tukey, J. W. (1974). Introduction to today's data analysis. Critical evaluation of chemical and physical structural information, edited by D. R. Lide & M. A. Paul, pp. 3-14. Washington: National Academy of Sciences.
- Wilson, A. J. C. (1976). Statistical bias in least-squares refinement. Acta Cryst. A32, 994–996.