

Bibliography

- Avilov, A., Kuligin, K., Nicolopoulos, S., Nickolskiy, M., Boulhaya, K., Portillo, J., Lepeshov, G., Sobolev, B., Collette, J. P., Martin, N., Robins, A. C. and Fischione, P. (2007). Precession technique and electron diffractometry as new tools for crystal structure and chemical bonding determination. *Ultramicroscopy*, 107, pp. 431-444.
- Barnard, J. S., Eggeman, A. S., Sharpe, J., White, T. A. and Midgley, P. A. (2010). Dislocation electron tomography and precession electron diffraction – minimizing the effects of dynamical interactions in real and reciprocal space. *Philosophical Magazine*, 90, pp. 4711-4730.
- Berg, B. S., Hansen, V., Midgley, P. A., and Gjønnnes, J. (1998). Measurement of three-dimensional intensity data in electron diffraction by the precession technique. *Ultramicroscopy*, 74, pp. 147-157.
- Bird, D. M. and Saunders, M. (1992). Sensitivity and accuracy of CBED pattern matching. *Ultramicroscopy*, 45, pp. 241-251.
- Birkel, C. S., Mugnaioli, E., Gorelik, T., Kolb, U., Panthofer, M. and Tremel, W. (2010). Solution synthesis of a new thermoelectric Zn_{1+x}Sb nanophase and its structure determination using automated electron diffraction tomography. *Journal of the American Chemical Society*, 132, pp. 9881-9889.
- Bithell, E. G., Merrill, C. A. and Midgley, P. A. (2010). Reconstruction strategies for structure solution using precession electron diffraction data from hybrid inorganic-organic framework materials. *Journal of Physics: Conference Series*, 241, 012025.
- Blackman, M. (1936). On the intensities of electron diffraction rings. *Proceedings of the Royal Society of London A*, 173, pp. 68-82.
- Buerger, M. J. (1964). *The precession method*. New York, Wiley.

- Burla, M. C, Caliendo, R., Camalli, M., Carrozzini, B., Cascarano, G. L., De Caro, L., Giovacazzo, C., Polidori, G., Siliqi, D. and Spagna, R. (2007). IL MILIONE: a suite of programs for crystal structure solution of proteins. *Journal of Applied Crystallography*, 40, pp609-613.
- Buxton, B. F., Loveluck, J. E. and Steeds, J. W. (1977). Bloch waves and their corresponding atomic and molecular orbitals in high energy electron diffraction. *Philosophical Magazine*. A, 38, pp. 259-278.
- Boulahya, K., Ruiz-Gonzalez, L., Parras, M., Gonzalez-Calbet, J. M., Nickolsky, M. S. and Nicolopoulos, S. (2007). Ab initio determination of heavy oxide perovskite related structures from precession electron diffraction data. *Ultramicroscopy*, 107, pp. 445-452.
- Ciston, J., Deng, B., Marks, L. D., Own, C. S. and Sinkler, W. (2008). A quantitative analysis of the cone-angle dependence in precession electron diffraction. *Ultramicroscopy*, 108, pp. 514-522.
- Cochrane, W. (1955). Relations between the phases of structure factors. *Acta Crystallographica*, 8, pp473-478.
- Coelho, A. A. (2007). A charge-flipping algorithm incorporating the tangent formula for solving difficult structures. *Acta Crystallographica*, A63, pp 400-406.
- Crewe, A. V. and Wall, J. (1970). A scanning microscope with 5Å resolution. *Journal of Molecular Biology*, 48, pp. 375-393.
- Denysenko, D., Gryzwa, M., Tonigold, M., Streppel, B., Krkljus, I., Hirscher, M., Mugnaioli, E., Kolb, U., Hanss, J. and Volkmer, D. (2011). Elucidating gating effects for hydrogen sorption in MFU-4-type triazolate-based metal-organic frameworks featuring different pore sizes. *Chemistry – A European Journal*, 17, pp. 1837-1848.
- Dorset, D. L. (2006). The crystal structure of ZSM-10, a powder X-ray and electron diffraction study. *Zeitschrift für Kristallographie*, 221, pp 260-265
- Dorset, D. L., Gilmore, C. L., Jorda, J. L. and Nicolopoulos, S. (2007). Direct electron crystallographic determination of zeolite zonal structures. *Ultramicroscopy*, 107, pp. 462-473.
- Eades, J. A. (1980). Zone-axis patterns formed by a new double rocking technique. *Ultramicroscopy*, 5, pp. 71-74.
- Eggeman, A. S., White, T. A. and Midgley, P. A. (2009). Symmetry modified charge flipping. *Acta Crystallographica* A65, pp. 120-127.

- Eggeman, A. S., White, T. A. and Midgley, P. A. (2010). Is precession electron diffraction kinematical? Part II: A practical method to determine the optimum precession angle. *Ultramicroscopy*, 110, pp 771-777.
- Giacovazzo, C. (1998). *Direct phasing in crystallography: Fundamentals and applications*. Oxford Science Publications.
- Gerchberg, R. W. and Saxton, W. O (1972). A practical algorithm for the determination of phase relationships from image and diffraction plane pictures. *Optik*, 35, pp 237-246.
- Gemmi, M., Zou, X. D., Hovmöller, S., Migliori, A., Vennström, M. and Andersson, Y. (2002). Structure of Ti_2P solved by three-dimensional electron diffraction data collected with the precession technique and high-resolution electron microscopy. *Acta Crystallographica A* 59, pp. 117-126.
- Gilmore, C. J., Bricogne, G. and Bannister, C. (1990). A multisolution method of phase determination by combined maximization of entropy and Likelihood II: Application to small molecules. *Acta Crystallographica A* 46, pp. 297-308.
- Gilmore, C. J., Dong, W. and Dorset, D. L. (2007), Solving the crystal structures of zeolites using electron diffraction data. 1. The use of potential-density histograms. *Acta Crystallographica A* 64, pp 284-294.
- Gjønnnes, K. (1997). On the integration of electron diffraction intensities in the Vincent-Midgley precession technique. *Ultramicroscopy*, 69, pp. 1-11.
- Gjønnnes, J., Hansen, V., Berg, B. S., Runde, P., Cheng, Y. F., Gjønnnes, K., Dorset, D. L. and Gilmore, C. J. (1998). Structure model for the phase Al_mFe derived from three-dimensional electron diffraction intensity data collected by a precession technique. Comparison with convergent-beam diffraction. *Acta Crystallographica A* 54, pp. 306-319.
- Hadermann, J., Abakumov, A. M., Tsirlin, A. A., Filonenko, V. P., Tan, H., Verbeek, J., Gemmi, M., Antipov, E. V. and Rosser, H. (2010). Direct space structure solution from precession electron diffraction data: resolving heavy and light scatterers in $\text{Pb}_{13}\text{Mn}_9\text{O}_{25}$. *Ultramicroscopy*, 110, pp. 881-890.
- Hadermann, J., Abakumov, A. M., Turner, S., Hafideddine, Z., Khasanova, N. R., Antipov, E. V. and Van Tendeloo, G. (2011). Solving the structure of Li ion battery materials with precession electron diffraction: application to $\text{Li}_2\text{CoPO}_4\text{F}$. *Chemistry of Materials*, doi:10.1201/cm201257b.

- Harker, D. and Kasper, J. S. (1948). Phases of Fourier coefficients directly from crystal diffraction data. *Acta Crystallographica*, 1, pp. 70-75.
- Holmestad, R., Birkeland, C. R., Marthinsen, K., Høier, R. and Zuo, J. M. (1999). Use of quantitative convergent-beam electron diffraction in materials science. *Microscopy Research and Techniques*, 46, pp. 130-145.
- Hovmöller, S., Zou, X. D. and Weirich, T. E. (2002), Crystal structure determination from EM images and electron diffraction patterns. *Advances in Imaging and Electron Physics*, 123, pp. 257-289.
- Ishizuka, K. (2001). Hremresearch website (<http://www.hremresearch.com/>)
- Jacob, D., Cordier, P., Morniroli, J. P. and Schertl, H. P. (2009). Application of precession electron diffraction to the characterization of (021) twinning in pseudo-hexagonal coesite. *American Mineralogist*, 94, pp. 684-692.
- Jacob, D. and Cordier, P. (2010). A precession electron diffraction study of alpha, beta and Dauphine twin in quartz. *Ultramicroscopy*, 110, pp. 1166-1177.
- Ji, G., Morniroli, J. P., Auchterlonie, G. J., Drennan, J. and Jacob, D. (2009). An efficient approach to characterize pseudo-merohedral twins by precession electron diffraction: application to the LaGaO_3 perovskite. *Ultramicroscopy*, 109, pp. 1282-1294.
- Karle, J. and Hauptmann, H. (1950). The phases and magnitudes of structure factors. *Acta Crystallographica*, 3, pp 181-187
- Kirkland, E. (1998). *Advanced computing in electron microscopy*. New York, Plenum.
- Kilaas, R., Marks, L. D. and Own, C. S. (2005). EDM 1.0: electron direct methods. *Ultramicroscopy*, 102, pp. 233-237.
- Klein, H. and David, J. (2010), The quality of precession electron diffraction data is higher than necessary for structure solution of unknown crystalline phases. *Acta Crystallographica*, A67, pp.297-302.
- Krakow, W. and Howland, L. A. (1976). A method for producing hollow cone illumination electronically in the conventional transmission microscope. *Ultramicroscopy*, 2, pp. 53-67.
- Kolb, U., Gorelick, T. and Otten, M. (2008). Towards automated diffraction tomography. Part II- Cell parameter determination. *Ultramicroscopy*, 108, pp. 763-772

- Kverneland, A., Hansen, V., Vincent, R., Gjønnes, K. and Gjønnes, J. (2006). Structure analysis of embedded nano-sized particles by precession electron diffraction. η' precipitate in an Al-Zn-Mg alloy as example. *Ultramicroscopy*, 106, pp. 492-502.
- Lawson, F. (1967). Tin oxide Sn_2O_3 . *Nature*, 215, pp. 955-956.
- Marks, L. D., Sinkler, W. and Landree E. (1999). A feasible set approach to the crystallographic phase problem. *Acta Crystallographica*, A55, pp. 601-612.
- McCallam, B. C. and Rodenburg, J. M. (1993). Error analysis of crystalline ptychography in the STEM mode. *Ultramicroscopy*, 52, pp. 85-99.
- McCusker, L. B. (1991). Zeolite crystallography. Structure determination in the absence of conventional single-crystal data. *Acta Crystallographica* A47, pp 297-313.
- Midgley, P. A. and Vincent, R. (1991). Electron Crystallography of LaAlO_3 . *Electron microscopy and Analysis*, 1991, pp. 371-374.
- Midgley, P. A., Saunders, M. and Vincent R. (1995). Fourier reconstruction from coherent convergent beam electron diffraction patterns. *Institute of Physics Conference Series*, 147, pp. 145-148
- Midgley, P. A., Sleight, M. E. and Vincent, R. (1996). The structure of metastable Au-Sn phase determined by convergent beam electron diffraction. *Journal of Solid State Chemistry*, 124, pp. 132-142.
- Midgley, P. A., Sleight, M. E., Saunders, M and Vincent, R.(1998). Measurement of Debye-Waller factors by electron precession. *Ultramicroscopy*, 75, pp. 61-67.
- Moeck, P., Rouvimov, S., Rauch, Nicolopoulos, S. (2009). Structural fingerprinting of nanocrystals: advantages of precession electron diffraction, automated crystallite orientation and phase maps. *Materials Research Society Symposium Proceedings*, 1184, GG03-07.
- Moeck, P., Rouvimov, S., Rauch, E. F., Veron, M., Kirmse, H., Hausler, I., Neumann, W., Bultreys, D., Maniette, Y. and Nicolopoulos, S. (2011). High spatial resolution semi-automatic crystallite orientation and phase mapping of nanocrystals in transmission electron microscopes. *Crystal Research and Technology*, 46, pp. 589-606.
- Morniroli, J. P. and Redjaimia, A, (2007). Electron precession microdiffraction as a useful tool for the identification of the space group. *Journal of Microscopy*, 227, pp 157-171.

- Morniroli, J. P., Redjaimia, A. and Nicolopoulos, S. (2007). Contribution of electron precession to the identification of the space group from microdiffraction patterns. *Ultramicroscopy*, 107, pp. 514-522.
- Morniroli, J. P., Houdellier, F., Roucau, C., Puiggali, J., Gestì, S. and Redjaima, A. (2008). LACDIF, a new electron diffraction technique obtained with the LACBED configuration and a Cs corrector: comparison with precession electron diffraction. *Ultramicroscopy*, 109, pp. 758-765.
- Morniroli, J. P. and Ji, G. (2009). Identification of the kinematical forbidden reflections from precession electron diffraction. *Materials Research Society Symposium Proceedings*, 1184-GG01-03
- Morniroli, J. P., Stadelmann, P., Ji, G. and Nicolopoulos, S. (2009). The symmetry of precession electron diffraction patterns. *Journal of Microscopy*, 237, pp 511-515.
- Mugnaoli, E., Gorelick, T. and Kolb, U. (2009). “Ab initio” structure solution from electron diffraction data obtained by a combination of automated diffraction tomography and precession technique. *Ultramicroscopy*, 109, pp. 758-765.
- Nakashima, P. N. H. and Muddle, B. C. (2010) Differential convergent beam electron diffraction: experiment and theory. *Physical Review B*, 81, 115135.
- Nakashima, P. N. H., Smith, A. E., Etheridge, J. and Muddle, B. C. (2011). The bonding electron density in aluminium. *Science*, 331, pp. 1583-1586.
- Nicolopoulos, S. (2007) Nanomegas website (<http://www.nanomegas.com/>)
- Oszlányi, G. and Sütő, A. (2004). Ab initio structure solution by charge flipping. *Acta Crystallographica A*60, pp. 134-141.
- Oszlányi, G. and Sütő, A. (2005). Ab initio structure solution by charge flipping. *Acta Crystallographica A*61, pp. 147-152.
- Oszlányi, G. and Sütő, A. (2007). The charge flipping algorithm. *Acta Crystallographica A*64, pp. 123-134.
- Own, C. S. (2005). System design and verification of the precession electron diffraction technique. PhD thesis, Northwestern University, Evanston, IL, USA.
- a) Own, C. S., Sinkler, W and Marks, L. D. (2006). Rapid structure determination of a metal oxide from pseudo-kinematical electron diffraction data. *Ultramicroscopy*, 106, pp 114-122.

- b) Own, C. S., Marks, L. D. and Sinkler, W. (2006). Precession electron diffraction 1: multislice simulation. *Acta Crystallographica A* 62, pp. 434-443.
- Own, C. S., Sinkler, W. and Marks, L. D. (2007). Prospects for aberration corrected electron precession. *Ultramicroscopy*, 107, pp. 534-542.
- Palatinus, L. and Chapuis, G. (2007). SUPERFLIP - a computer program for the solution of crystal structures by charge flipping in arbitrary dimensions. *Journal of Applied Crystallography*, 40, pp 786-790.
- Rauch, E. F., Veron, M., Portillo, J., Bultreys, D., Maniette, Y. and Nicolopoulos, S. (2008), Automatic crystal orientation and phase mapping in TEM by precession diffraction. *Microscopy and Analysis*, 22(6), S5-S8.
- Rauch, E. F., Portillo, J., Nicolopoulos, S., Bultreys, D., Rouvimov, S. and Moeck, P. (2010). Automated nanocrystal orientation and phase mapping in the transmission electron microscope on the basis of precession electron diffraction. *Zeitschrift für Kristallographie*, 225, pp. 103-109.
- Rossouw, C. J., Maunders, C. J., Whitfield, H. J. and Etheridge, J. (2006). CBED contrast in the lower order Laue zone. *Ultramicroscopy*, 106, pp. 439-448.
- Saunders, M., Midgley, P.A., Vincent, R. and Steeds, J. (1996) Recent advances in quantitative convergent beam electron diffraction. *Journal of Electron Microscopy*, 45, pp. 11-18.
- Sayre, D. (1952). The squaring method: A new method for phase determination. *Acta Crystallographica*, 5, pp 60-65.
- Seko, A., Togo, A., Obo, F. and Tanake, I. (2008). Structure and stability of a homologous series of tin oxides. *Physical Review Letters*, 100, 045802.
- Sellar J.R., Imeson D. and Humphreys C. J. (1980). The critical-voltage effect in convergent-beam high-voltage electron diffraction. *Acta Crystallographica A* 36, pp. 686-696
- Sinkler, W., Marks, L. D., Edwards, D. D., Mason, T. O., Poeppelmeier, K. R., Hu, Z. and Jorgensen, J. D. (1998). Determination of oxygen atomic positions in a Ga-In-Sn-O ceramic using direct methods and electron diffraction. *Journal of Solid State Chemistry*, 136, pp. 145-149.
- Sinkler, W. and Marks, L. D. (1999). A simple channelling model for HREM contrast transfer under dynamical conditions. *Journal of Microscopy*, 194, pp. 112-123

- Sinkler, W. and Marks, L. D. (2010). Characteristics of precession electron diffraction intensities from dynamical simulations. *Zeitschrift für Kristallographie*, 225, pp. 47-55.
- Sleight, M. (1997). The use of convergent beam electron diffraction as a method for structure determination. PhD thesis, University of Bristol, UK.
- Smolin, Y. I. (1970). Determination of the crystal structure of erbium pyrogermanate, $\text{Er}_2\text{Ge}_2\text{O}_7$. *Soviet Physics – Crystallography*, 15, pp.36-37.
- Sperling, R., Amos, L. A. and Klug A. (1974). A study of the pairing interaction between protein subunits in the tobacco mosaic virus family by image reconstruction from electron micrographs. *Journal of Molecular Biology*, 92, pp. 541-558.
- Tabbarnor, M. A., Fox, A. G. and Fisher, R. M. (1990). An accurate reappraisal of the elemental form-factors and charge-density of copper. *Acta Crystallographica*, A46, pp. 165-170.
- Taftø, J. and Gjønnes, J. (1985). The intersecting Kikuchi line technique – Critical voltage at any voltage. *Ultramicroscopy*, 17, pp. 329-334.
- Taftø, J., Zhu, Y. and Wu, L. (1998). A new approach towards measuring structure factors and valence-electron distribution in crystals with large unit cells. *Acta Crystallographica*, A54, pp. 532-542.
- Tanaka, M., Saito, R., Ueno, K. and Harada, Y. (1980). Large-angle convergent beam electron diffraction. *Journal of Electron Microscopy*, 29, pp. 408-412.
- Tanaka, M., Takayoshi H., Terauchi M., Kondo Y., Ueno, K. and Harada, Y. (1984) Higher-Order Laue-Zone Diffraction Patterns Obtained by a Hollow-Cone Electron Beam. *Journal of Electron Microscopy*, 33, pp. 195-202.
- Terauchi, M., Tsuda, K., Kamimura, O., Tanaka, M., Kaneyama, T. and Honda, T. (1994) Observation of lattice fringes in convergent-beam electron diffraction patterns. *Ultramicroscopy*, 54, pp. 268-275.
- Van Dyck, D. and Op de Beek, M. (1995). A simple intuitive theory for electron diffraction. *Ultramicroscopy*, 64, pp. 99-107.
- Vincent, R., Bird, D. M. and Steeds, J. W. (1984). a, Structure of AuGeAs determined by convergent beam electron diffraction. I: Derivation of basic structure. *Philosophical Magazine A*, 50, 745-764. b, Structure of AuGeAs determined by convergent beam electron diffraction. II: Refinement of Structural Parameters. . *Philosophical Magazine A*, 50, pp. 765-786.

- Vincent, R. and Pretty, S. F. (1986). Phase analysis in the Ni-Ge-P system by electron diffraction. *Philosophical Magazine A*, 53, pp. 843-862.
- Vincent, R., Vine, W. J., Midgley, P. A., Spellward, P. and Steeds, J. W. (1993). Coherent overlapping LACBED patterns in 6H SiC. *Ultramicroscopy*, 50, pp. 365-376.
- Vincent R. and Exelby, D. R (1993). Structure of Al-Ge phase determined from large angle CBED patterns. *Philosophical Magazine B*, 68, pp. 513-528.
- Vincent, R. and Midgley, P. A. (1994). Double conical beam-rocking system for the measurement of integrated diffraction intensities. *Ultramicroscopy*, 53, pp. 271-282.
- Vine, W. J., Vincent, R., Spellward, P. and Steeds, J. W. (1992). Observation of phase contrast in convergent-beam electron diffraction patterns. *Ultramicroscopy*, 41, pp. 423-428.
- Weirich, T. E., Portillo, J., Cox, G., Hibst, H. and Nicolopoulos, S. (2006). Ab initio determination of the framework of the heavy metal oxide $\text{Cs}_x\text{Nb}_{2.54}\text{W}_{2.46}\text{O}_{14}$ from 100kV precession electron diffraction data. *Ultramicroscopy*, 106, pp. 164-175.
- White, T. A. (2009). Structure solution using precession electron diffraction and diffraction tomography. PhD thesis, University of Cambridge
- a) White, T. A, Eggeman, A. S. and Midgley, P. A. (2010). Is precession electron diffraction kinematical? Part I: 'Phase scrambling' multislice simulations. *Ultramicroscopy*, 110, pp.763-770.
- b) White, T. A., Moreno, M. S. and Midgley, P. A. (2010). Structure determination of the intermediate tin oxide Sn_3O_4 by precession electron diffraction. *Zeitschrift fur Krystallographie*, 225, pp. 56-66.
- Wilson, A. J. C. (1942). Determination of absolute from relative X-ray intensity data. *Nature*, 150, pp. 151-152.
- Wu, J. S. and Spence, J. C. H. (2002). Kinematic and dynamical CBED for solving thin organic films at low temperature; experimental tests with anthracene. *Acta Crystallographica*, A58, pp. 580-589.
- Wu, J. S., Spence, J. C. H, O'Keeffe, M. and Groy, T. L. (2004) Application of a modified Oszlanyi and Suto a initio charge-flipping algorithm to experimental data. *Acta Crystallographica*, A60, pp 326-330.

- Wu, J., Zhao, Y. S., Hu, H., Huang, J., Zuo, J. M. and Dravid, V. P. (2011). Construction of an organic crystal structural model based on combined electron and powder X-ray diffraction data and the charge flipping algorithm. *Ultramicroscopy*, 111, pp. 812-816.
- Xie, D. Baerlocher, C. and McCusker, L. B. (2008). Combining precession electron diffraction data with X-ray powder diffraction to facilitate structure solution. *Journal of Applied Crystallography*, 41, pp. 1115-1121.
- Zhou, Z. and Harris, K. D. M. (2008). Residue based charge-flipping: A new variant of an emerging algorithm for structure solution from X-ray diffraction data. *Journal of Physical Chemistry A*, 112, pp 4863-4868
- a) Zhang, D., Oleynikov, P., Hovmoller, S. and Zou X. (2010). Collecting 3D electron diffraction data by the rotation method. *Zeitschrift fur Kristallographie*, 225, 94-102.
- b) Zhang, D., Gruner, D., Oleynikov, P., Wan, W., Hovmoller, S. and Zou, X. (2010). Precession electron diffraction using a digital sampling method. *Ultramicroscopy*, 111, pp. 47-55.
- Zuo, J. M., and Spence, J. C. H (1991). Automated structure factor refinement from convergent-beam patterns. *Ultramicroscopy*, 35, pp. 185-196.
- Zuo, J. M., Kim, M., O'Keeffe, M. and Spence, J. C. H. (1999). Direct observation of d-orbital holes in Cu-Cu bonding in Cu₂O. *Nature*, 401, pp. 49-52.