

is somewhat exaggerated (instead of the expected physical nearly-Gaussian shape), and the diameter of the atom appears to be smaller than usual. This result underlines the qualitative nature of the density calculated.

4. Conclusion

Although the present algorithm can be developed further by incorporation of more prior knowledge in the form of additional constraints, it has also in its present form very impressive features compared with the ordinary Fourier transform: with X-ray data or in cases where it is known from the physics of an experiment that the resulting scattering densities have to be positive, it can be guaranteed by the use of the program MEED. The Maximum-Entropy algorithm is less influenced by missing reflections of an incomplete dataset. An important possibility is that of using different types of information together in a single calculation of a scattering density: a first set of reflections with known structure factor $F = |F| \exp(i\Phi)$; a second set of reflections with the phase determined with a remaining ambiguity, $\Phi_{\pm} = \Psi_{\sigma} \pm \Delta$; a third set of reflections with only the intensity $|F|^2$ known; and a fourth set of groups of overlapping reflections in a powder diffraction pattern, where only the sum of intensities $\sum m_i |F_i|^2$ is known for each group! The ordinary Fourier transformation can only use the first set and has to omit the others, while a MEM calculation can now use all four sets in the form of constraint functions of different type, which contribute to the total constraint sum C . This additional information used improves the calculated density considerably.

New versions of the original MEED program have been presented; they have been improved in several ways: MEED for strictly positive densities, MEND for neutron data, where also negative scattering densities may occur, and MEEDCAB with the new "ambiguous phase" A-constraints

implemented. These programs run on common desktop computers, are freely available, and offer important help to crystallographers in *ab initio* structure determination, especially if only powder data is available.

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Calendar of Meetings

Donald R. Petersen
Greenleaf Associates
6210 Siebert Street
Midland, MI 48640-2724

16–19 June 1998

Twentieth Annual Symposium on Applied Surface Analysis and Tenth Annual Symposium of the Pacific Northwest Chapter of the American Vacuum Society. Richland, Washington, USA. [Contact: Ms. Bonnie Williams, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Post Office Box 999, Richland, WA 99352. Tel: 1 (509) 376 1518; Fax: 1 (509) 376 5106; E-mail: bj_williams@pnl.gov; Info: <http://www.vacuum.org/surfanal98.html>].

20–25 June 1998

Tenth International Symposium on Molecular Recognition and Inclusion. Warsaw, Poland. [Contact: Kinga Suwinska, Symposium Secretary, Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, PL-01 224 Warsaw, Poland. Tel: 48 (22) 632 7343; Fax: 48 (22) 632 5276; E-mail: ismri-10@ichf.edu.pl or klatrat@ichf.edu.pl; Info: <http://www.iucr.ac.uk/cww-top/ismri-10.html>].

5–10 July 1998

Twelfth International Zeolite Conference. Baltimore, Maryland, USA. [Contact: D. H. Olson, Department of Chemical Engineering, 311A Towne Building, University of Pennsylvania, Philadelphia, PA 19104. Tel: 1 (215) 573 4201; Fax: 1 (215) 573 2093; E-mail: dholson@seas.upenn.edu].

18–23 July 1998

ACA'98 American Crystallographic Association Annual Meeting. Arlington, Virginia, USA. [Contact: T. A. Vanderah, National Institute of Standards and Technology, Ceramics Division, Building 223, Room A256, Gaithersburg, MD 20899, USA. Tel: 1 (301) 975 5785; Fax: 1 (301) 990 8729; E-mail: terrell@credit.nist.gov or V. L. Karen, NIST, Materials Science and Engineering Laboratory, Materials Building Room, A215, Gaithersburg, MD 20899, USA. Tel: 1 (301) 975 6255; E-mail: karen@tiber.nist.gov; Info: <http://www.hwi.buffalo.edu/aca/>].

26–31 July 1998

Twelfth International Conference on Crystal Growth, held concurrently with the Tenth International Conference on Vapor Growth and Epitaxy. Jerusalem, Israel. [Contact: ICCG 12, c/o International Travel & Congresses, Ltd., 9 Rothschild Boulevard, Post Office Box 29313, Tel Aviv 61292, Israel. Tel: 972 (3) 510 2538; Fax: 972 (3) 516 0604; E-mail: 100264.2432@CompuServe.com; Info: <http://www.technion.ac.il/~iccg12/>].

3–7 August 1998

47th Annual Denver X-ray Conference. Colorado Springs, Colorado, USA. [Contact: Linda Shertz, International Centre for Diffraction Data, 12 Campus Boulevard, Newtown Square, PA 19073-3273, USA. Tel: 1 (610) 325 9814; Fax: 1 (610) 325 9823; E-mail: dxc@ICDD.com; Info: <http://www.dxcicdd.com/>].

3–7 August 1998

International Centre for Diffraction Data, Fall Technical Meeting. Colorado Springs, Colorado, USA. Held concurrently with the 47th Annual Denver X-ray Conference. [Contact: Linda Shertz, International Centre for Diffraction Data, 12 Campus Boulevard, Newtown Square, PA 19073-3273, USA. Tel: 1 (610) 325 9814; Fax: 1 (610) 325 9823; E-mail: SHERTZ@ICDD.com; Info: <http://www.icdd.com/>].

10–14 August 1998

IMA'98 17th General Meeting of the International Mineralogical Association. Toronto, Ontario, Canada. The meeting will be centered on extensive scientific sessions, preceded and followed by field trips across Canada and the United States including important mineral locations, ore deposits, sites of impact craters, and classic petrologic locations. [Contact: IMA '98, Department of Geology, University of Toronto, Earth Sciences Centre, 22 Russell Street, Toronto, ON, Canada M5S 3B1. Tel: 1 (416) 946 3306; Fax: 1 (416) 978 3938; E-mail: ima98@quartz.geology.utoronto.ca; Info: <http://opal.geology.utoronto.ca:80/ima98/>].

16–20 August 1998

ECM-18 18th European Crystallographic Meeting. Praha, Czech Republic. The conference language is English, the site is the Czech Technical University. Celebrating the 50th anniversary of the IUCr. [Contact: Rádómir Kuzel, Conference Secretariat, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, 121 16 Praha 2, Czech Republic. Fax: 42 (2) 367 981; E-mail: kuzel@karlov.mff.cuni.cz; Info: <http://krystal.karlov.mff.cuni.cz/ecm/ecm.htm> or Jindrich Hasek, Conference Chairman, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovskeho nam. 2, 162 06 Praha 6, Czech Republic. Tel: 42 (2) 360 341 x390; Fax: 42 (2) 367 981; E-mail: hasek@imc.cas.cz; Info: <http://www-xray.fzu.cz/ecm/ecm.htm>].

21–22 August 1998

Can Crystal Structures Be Predicted? Dresden, Germany. An ECM-18 satellite meeting, held under the aegis of the Deutsche Akademie der Naturforscher Leopoldina. The conference language is English. Invited lectures and discussion. [Contact: Dr. Axel Nelles, Deutsche Akademie der Naturforscher Leopoldina, Postfach 11 05 43, D-06019 Halle (Saale), Germany. Tel: 49 (345) 202 5014; Fax: 49 (345) 202 1727; E-mail: nelles@leopoldina.uni-halle.de; Info: <http://www.phy.tu-dresden.de/leopoldina.html>].

22–25 August 1998

EPDIC-6 Sixth European Powder Diffraction Conference. Budapest, Hungary. [Contact: Prof. Tamás Ungár, Department of General Physics, Eötvös Loránd University, Múzeum krt 6–8, H-1008 Budapest, Hungary. Tel: 36 (1) 266 9833; Fax: 36 (1) 266 7927; E-mail: ungar@ludens.elte.hu; or epdic6@power.szfki.kfki.hu; Info: <http://www.kfki.hu/~epdic6/>].

9–11 September 1998

X-TOP 98 Fourth European Conference on High Resolution Diffraction and Topography. Durham, England, UK. [Contact: Prof. Brian Tanner, Department of Physics, University of Durham, South Road, Durham DH1 3LE, UK. Fax: 44 (191) 374 2111; E-mail: physics.chair@durham.ac.uk].

13–15 October 1998

AsCA'98 Third Conference of the Asian Crystallographic Association. Bangi, Selangor, Malaysia. [Contact: Prof. A. Hamid Othman, Jabatan Kimia, Universiti Kebangsaan Malaysia, 43600 Bangi, Selangor, Malaysia. Fax: 60 (3) 825 8828; E-mail: hamie@pkriscc.ukm.my; Info: <http://gandalf.otago.ac.nz:800/rweavers/asca/asca98.htm>].

25–30 October 1998

Rare Earths 98. Fremantle (near Perth), Australia. [Contact: Erica Jago, Materials Institute of Western Australia, 133 Salvado Road, Wembley, WA 6014, Australia. Tel: 61 (9) 387 9590; Fax: 61 (9) 383 9639; E-mail: re98@miwa.org.au; Info: <http://www.miwa.org.au/IREC98/>].

5–7 November 1998

Pittsburgh Diffraction Conference. Pittsburgh, Pennsylvania, USA.

30 November–4 December 1998

Fall Meeting of the Materials Research Society. Boston, Massachusetts, USA. [Contact: Materials Research Society, 506 Keystone Drive, Warrendale, PA 15086, USA. E-mail: info@mrs.org; Info: <http://www.mrs.org>].

5–9 April 1999

Spring Meeting of the Materials Research Society. San Francisco, California, USA. [Contact: Materials Research Society, 506 Keystone Drive, Warrendale, PA 15089, USA. E-mail: info@mrs.org; Info: <http://www.mrs.org>].

22–27 May 1999

ACA'99 American Crystallographic Association Annual Meeting. Buffalo, New York, USA. [Contact: Dr. G. David Smith, Hauptman-Woodward Institute, 73 High Street, Buffalo, NY 14203-1196, USA. Tel: 1 (716) 856 9600; Fax: 1 (716) 852 4846; E-mail: smith@hwi.buffalo.edu; Info: <http://www.hwi.buffalo.edu/aca>].

4–13 August 1999

18th IUCr General Assembly and International Congress of Crystallography. Glasgow, Scotland, UK. Satellite meetings in connection with the Congress will include: Synchrotron Radiation, Structural and Dynamic Aspects of Molecular and Ionic Solids Using Neutrons, Cambridge Crystallographic Database, and the Crystallographic Computing School. [Contact: Dr. C. J. Gilmore, Department of Chemistry, University of Glasgow, Glasgow G12 8QQ, UK. Tel: 44 (141) 339 8855, Fax: 44 (141) 330 4888; E-mail: iucr99@chem.gla.ac.uk or Prof. J. A. K. Howard, University of Durham, Department of Chemistry, South Road, Durham DH1 3LE, UK. Tel: 44 (191) 374 4647, Fax: 44 (191) 374 3745; E-mail: j.a.k.howard@durham.ac.uk; Info: <http://www.chem.gla.ac.uk/iucr99>].

29 November–3 December 1999

Fall Meeting of the Materials Research Society. Boston, Massachusetts, USA. [Contact: Materials Research Society, 506 Keystone Drive, Warrendale, PA 15086, USA. E-mail: info@mrs.org; Info: <http://www.mrs.org>].

Short Courses and Workshops

22–26 June 1998

Fifth Summer School on Neutron Scattering. Chalk River, Ontario, Canada. An introduction to the techniques of neutron scattering and their applications, a total of 18 lecture sessions and demonstration experiments, by Chalk River and visiting scientists. [Contact: Zin Tun, Neutron Program for Materials Research (NRC), Chalk River Laboratories, Chalk River, ON, Canada K0J 1J0. Tel: 1 (613) 584 8811; Fax: 1 (613) 584 4040; E-mail: zin.tun@nrc.ca; Info: <http://neutron.nrc.ca/SS98.htm>].

29 June–3 July 1998

Fourth Crystallographic Course: New Trends in Material Science—Powder Diffraction. La Laguna, Tenerife (Canary Islands), Spain. [Contact: Dr. Catalina Ruiz-Pérez, Department of Physics, University of La Laguna, 38204 La Laguna, Tenerife, Spain. Tel: 34 (22) 603 272; Fax: 34 (22) 603 684; E-mail: amg@iac.es].

5–16 July 1998

Seventh Annual ACA Summer Workshop on Crystallography. Athens, Georgia, USA. Fundamentals of structure determination using diffraction from single crystals. [Contact: Prof. Bi-Cheng Wang, Department of Biochemistry and Molecular Biology, University of Georgia, Athens, GA 30602, USA. Tel: 1 (706) 542 1747; Fax: 1 (706) 542 3077; E-mail: wang@BCL1.bmb.uga.edu; Info: <http://www.hwi.buffalo.edu/aca>].

1–5 August 1998

First SLS Workshop: Applications of Highly Brilliant and Coherent Synchrotron Radiation. Monte Verità, As-

cona, Switzerland. To bring together current and potential users of synchrotron radiation, particularly in applications involving highly brilliant and coherent radiation as will be supplied by the Swiss Light Source. [Contact: Prof. Bruno Reihl, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland. E-mail: bruno.reihl@psi.ch; Info: http://www1.psi.ch/www_sls_hn/slsf0304.html].

8–14 August 1998

Sixth Summer School on Neutron Scattering: Complementarity Between Neutron and Synchrotron X-ray Scattering. Lyceum Alpinum, Zuoz, Switzerland. [Contact: Renate Bercher, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland. Tel: 41 (56) 310 3402; Fax: 41 (56) 310 3131; E-mail: bercher@psi.ch; Info: http://www1.psi.ch/www_1ns_hn/welcome.html].

8–12 September 1998

XXVII Scuola: Diffattometria da materiali policristallini: recenti sviluppi delle tecniche di risoluzione e di raffinamento strutturale. Perugia, Italy. [Contact: Prof. Antonio Nunzi, Dipartimento di Scienze della Terra, Università di Perugia, Piazza dell'Università, 06100 Perugia, Italy. Tel: 39 (75) 585 3215 ext 2838; Fax: 39 (75) 585 3203; E-mail: dipsctnu@unipg.it; Info: <http://nunzi.sct.unipg.it>].

18–21 October 1998

Workshop on Modern Techniques in Structural Chemistry of Microcrystalline and Amorphous Compounds. Hünfeld (near Frankfurt/Main), Germany. The workshop will be held in the Bonifatius monastery located north of Fulda in the Rhön mountains. Hünfeld is accessible by car or