

and Arbeitsgemeinschaft für Kristallographie. Dr H. E. Göbel was the Organizing Committee Chairman and Dr J. Visser was the Programme Committee Chairman. Approximately 220 participants from 24 countries took part in the activities. During the meeting a commercial exhibition was organized, showing recent developments in hardware and software in the field of X-ray studies. More than twenty companies, including Siemens, Philips, Seifert, Enraf-Nonius, Stoe and Nicolet, took part. Demonstrations and a workshop concerning the JCPDS-ICDD powder diffraction file and other crystallographic databases were perfectly prepared.

The two and a half days scientific programme was opened by an honorary lecture by Professor H. Jagodzinski on 'The Role of Munich for X-ray Powder Crystallography and the History of X-ray Powder Diffraction'. It was followed by 16 main lectures dedicated to areas of general interest: 'X-ray Diffraction Profiles Due to Real Polycrystals' by P. Klimanek, 'Quo Vadis Quantitative Powder Diffraction Analysis' by J. Fiala, 'Crystal Structure Analysis and Refinement by the Two-Step Method' by G. Will, 'Neutron Powder Diffraction and Oxide Superconductors' by A. W. Hewat, 'Applied Crystallography in Advanced Ceramics' by R. L. Snyder, 'New Instrumentation in Powder Diffraction' by J. Ihringer, 'New Detectors in X-ray Diffraction' by P. Tucker, 'Energy Dispersive XRPD at High Pressure' by L. Gerward, 'Glory and Misery of the Structure Analysis of Thin Polycrystalline Films' by V. Valvoda, 'Characterization of Epitaxial Thin Films by X-ray Diffraction' by A. Segmüller, 'Powder Diffraction Using Synchrotron Radiation' by M. Hart, 'X-ray Absorption and Reflection in Materials Science' by B. Lengeler, 'Preferred Orientation in Powder Diffraction' by H.-J. Bunge, 'X-ray Stress Analysis' by J. M. Sprauel, 'On the Use of Rietveld Refinements for Structural Studies' by P.-E. Werner, 'Indexing of Powder Diffraction Patterns' by D. Louër. 54 other oral contributions and 120 posters were also presented.

It is difficult to mention all the lectures which were of the greatest interest, but some of them have to be pointed out. Among these, a contribution by A. W. Hewat describing one of the most exciting applications of high-resolution neutron diffraction ever performed, the HRTEM photos presented by H. Budin showing the sinusoidal orientation of unit cells in the Bi-based superconductors and a talk given by J. Schneider demonstrating even anharmonic temperature factor

analysis which can be carried out in combination with the X-ray and neutron Rietveld method. Real structure was one of the main fields of the conference. Lectures on texture by H.-J. Bunge, inhomogeneity by P. Klimanek and V. Valvoda were also the center of interest. Surface roughness was discussed in some papers (N. Masciocchi, B. Lengeler). B. Greenberg described the new QPD system developed in Philips Laboratories designed in connection with real structure problems.

The high level of the meeting should be maintained during EPDIC 2, which will take place on the campus of the University of Twente, the Netherlands, from 30 July to 1 August 1992.

KAREL HUML  
ECC Chairman

## Crystallographers

*J. Appl. Cryst.* (1991), **24**, 1080–1081

*This section is intended to be a series of short paragraphs dealing with the activities of crystallographers, such as their changes of position, promotions, assumption of significant new duties, honours, etc. Items for inclusion, subject to the approval of the Editorial Board, should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England).*

### F. L. Hirshfeld 1927–1991

Fred Hirshfeld arrived at the Weizmann Institute in 1951 armed with a Master's degree in mathematics from Columbia, a sharp mind and a deep faith in the precepts of Torah Judaism. All these were to remain with him until his untimely passing, from the ravages of a rapidly developing cancer, in May 1991. Coupled to these intellectual assets were some very human qualities – an ability to tolerate and accept people whose views on many subjects were very different from his own, and a willingness to help others that ranged from the critical review of manuscripts *in statu nascendi* to knuckling down to details of organizing meetings, summer schools and committees.

Hirshfeld soon showed his mettle in Rehovoth. His abilities as a constructive critic led Gerhard Schmidt to include him as a co-author on Schmidt's first paper on intramolecular overcrowding [*J. Chem. Soc.* (1954), pp. 3288–3294], even though he had made no experimental contribution to the work described – but his participation was an essential factor in the development and description of the then-novel ideas. Moreover, despite his theoretical bent and background, Hirshfeld became an active experimentalist in Schmidt's early exploitation of the advantages of liquid-

N<sub>2</sub> low temperatures in crystal structure analysis [*J. Chem. Phys.* (1957), **26**, 923–929].

Hirshfeld really found his metier in the field of electron density studies. Here he was a pioneer, as shown by a long series of careful studies involving both experimental measurements and theoretical analyses. The term 'deformation density' dates from this period. One of Hirshfeld's last papers was a review (*Electron Density Distributions in Molecules*) in *Crystallogr. Rev.* [(1991), **2**, 169–201] which he was able to see just before he died. This was an area, with its combination of the need for careful definition of objectives, accurate and exacting experimental measurement and deep theoretical analysis, which admirably suited Hirshfeld's personality.

Despite his concentration on electron density studies, other characteristic, and still quoted, papers appeared from time to time in the crystallographic literature. An early and noteworthy contribution was his definition of the Cheshire groups [*Acta Cryst.* (1968), **A24**, 301–311], the groups of minimal symmetry needed for determining possible molecular arrangements from a real-space comparison of observed and calculated structure factors. The elegance of this work was typical of Hirshfeld's approach, even if its current practical importance has been diminished by our present plethora of computing power. This was followed by discussion, together with Dov Rabinovich [*Acta Cryst.* (1973), **A29**, 510–513], of whether reflections with intensities measured as negative should be included in least-squares analyses. Another relates to the relative vibration amplitudes of pairs of atoms along the vector joining them. Hirshfeld's criterion [*Acta Cryst.* (1976), **A32**, 239–244] that this value should be less than 10 pm<sup>2</sup> in a rigid molecule is often applied as a test of intramolecular rigidity, while deviation from this norm gives information about internal vibrations and disorder.

Hirshfeld was an active participant in the life of the crystallographic community. He was Chairman of the Israel Crystallographic Society in 1973, an organizer of the Bat-Sheva Seminar on Electron Density Mapping in Molecules and Crystals held in Rehovoth in 1977 and Editor of the Report (*Isr. J. Chem.* (1977), **16**, 87–231], a member of the Editorial Board of *Isr. J. Chem.* for a number of years in the 1970's, a member of the Organizing Committee of ECM-7 (Jerusalem, 1982) (and displayed hitherto unknown talents as graphics designer of the Book of Abstracts), a member of the Commission on Crystallographic Data of the

IUCr from 1966 to 1975 and of the Commission on Charge, Spin and Momentum Densities from 1984 to 1990.

He leaves a wife, Rachel, five children and 21 grandchildren. He straddled two worlds without being embarrassed by the contradictions between them. I end with the traditional Hebrew saying 'May his memory be blessed'.

FRANK HERBSTEIN

Dr L. J. DeLucas, Center for Macromolecular Crystallography, University of Alabama at Birmingham, Alabama, USA, will fly as a payload specialist on the first US Microgravity Laboratory (USML-1) mission, which is a 13 day Spacelab mission scheduled for flight aboard the Space Shuttle in June 1992.

Professor S. C. Harrison, Biochemistry Department, and Professor D. C. Wiley, Biochemistry and Molecular Biology Department, both of Harvard University, Cambridge, Massachusetts, USA, and Mrs J. S. Richardson, Biochemistry Department, Duke University, Durham, North Carolina, USA, are amongst the 60 newly elected members of the US National Academy of Sciences.

Professor R. E. Newnham, Alcoa Professor of Solid State Science, Materials Research Laboratory, Pennsylvania State University, University Park, Pennsylvania, USA, has been awarded the John Jeppson Medal and Award of the American Ceramic Society for distinguished, creative and inspiring contributions to ceramic science, technology and education in the area of electronic ceramic materials.

Professor C. O. Pabo, Molecular Biology Department, Johns Hopkins Medical School, Baltimore, Maryland, USA, is the recipient of the Protein Society's 1991 Young Investigator Award. This award recognizes his research towards understanding the molecular details of protein-DNA interactions and his contributions to the field of protein/peptide design.

Professor J. M. Thomas, The Director of the Royal Institution, London, has received a Knighthood.

## International Union of Crystallography

*J. Appl. Cryst.* (1991). **24**, 1081-1082

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