13–15 October 1998
AsCA'98 Third Conference of the Asian Crystallographic Association. Bangi, Selangor, Malaysia. [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]

30 November–4 December 1998
Fall 1998 Meeting of the Materials Research Society. Boston, Massachusetts, USA. [Contact: Materials Research Society, 9800 McKnight Road, Pittsburgh, PA 15237, USA. Tel: 1 (412) 367 3004; Fax: 1 (412) 367 4373; E-mail: info@mrs.org; Info: http://www.mrs.org].

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 14217, USA. Tel: 1 (716) 856 9600; Fax: 1 (715) 852 4846; Info: http://www.hwi.buffalo.edu/aca].

Regional Reports

A Report on the ICDD March 1997 Annual Meeting: Invited talks and the Poster Session

Hideo Toraya,
Ceramics research Laboratory, Nagoya Institute of Technology, Asahigaoka, Tajimi 507, Japan

The ICDD Annual Meeting was held on March 19 and 20, 1997 at its Headquarters in Newtown Square, Pennsylvania. Four speakers were invited to present talks at the Meeting, namely Professor R. Allmann of Philipps-Universität, Germany; Professor J. Fiala of SKODA Research Ltd., the Czech Republic; and Professor Shao-Fan Lin of Nankai University, China. A poster session was also held, and the theme of the session was “Materials Characterization by X-ray Analysis Techniques.” There were a total of eight posters displayed outside the conference rooms during the entire meeting. The posters were of high quality in both contents and appearance, with very nice photographs displayed. The following are abstracts of the invited talks and posters presented, they are arranged in alphabetical order by author’s names.

Invited Papers

A Proposal for Cross-references between the Databases PDF and ICSD

(Rudolf Allmann, Institut fr Mineralogie, Phillips-Universität, D-35032 Marburg, Germany)

The Power Diffraction File (PDF) contains about 46,000 inorganic compounds in 1996 (including about 12,000 intermetallic phases). They are mostly indexed, and often include the corresponding space groups. But the information whether the structure is known or not is not given for many compounds. On the other hand, the Inorganic Crystal Structure Database (ICSD, edited by Fachinformationszentrum, Karlsruhe and Gmelin-Institut, Frankfurt/Main, Germany) contains about 43,000 inorganic structures in 1996 (excluding intermetallics). These data can be taken as continuation of the inorganic part of the Structure Reports (SR, part A), which were left off in 1990 (for organic part in 1985). The last volume of SR is a valuable index for nearly all structures solved until 1990. But ICSD is more informative than SR, because all available coordinates are recorded. Even most of the deposited data on (anisotropic) displacement factors together with their standard deviations can be found in ICSD.

ICSD includes the somewhat outdated program LAZY PULVERIX for the calculation of powder patterns from the recorded structural data. The program MicroPowder (Materials Data, Inc.) with its much better graphical possibilities is able to read the ICSD data too. Another easily manageable program for this purpose is PowderCell (Dr. Nolze, Bundesanstalt für Materialforschung, Berlin, Germany). A comparison of such calculated powder patterns with observed ones...
would be greatly facilitated, if a reference to the correspond-
ing PDF entry would be included in the ICSD file and, vice 
versa, PDF would gain a hint of known structure. As such a 
reference the citation of the ICSD entry number would be 
sufficient.

For certain important minerals, a number of structure 
determinations have been done for a series of different tem-
peratures, pressures, or solid solutions. In an equivalence list 
of minerals in ICSD and PDF, which has been checked by 
the author, only one ICSD entry is cited for each mineral 
with the lowest R-value at normal temperature and pressure 
(about 1,200 equivalent minerals until now).

Several minerals with known structures are missing in 
PDF. If these powder patterns are not measured (they often 
are), they should be calculated and included in PDF. Several 
structures of mineral solids solutions were determined but in 
PDF they are often missing. The handling of intermediate 
members of mineral solid solution series could improve the 
PDF. For a reliable quantitative phase analysis the knowl-
edge of many members of all involved solid solution series is 
indispensable. The author could initiate the correction of 
ICSD (e.g., errors in the handling of last digits or in the 
calculation of bond angles). In the normal presentation of the 
ICSD data on screen the original data on CD-ROM are 
rounded. To get the full information, the data should be ed-
xported as COLEDIT-file. This is the format used by the ab-
stractors of ICSD to add a new entries in to ICSD.

The ICSD-remark has two meanings: firstly, the struc-
ture is known, and secondly it is the reference to a complete 
structure determination, sufficient to get a calculated pattern. 
In such a calculation it is easy to include a texture simulation 
too (e.g., the March-Dollase model). So the texture of the 
observed pattern can be estimated.

X-ray Power Diffraction Study of Superconducting Oxides 
and Related Materials, Problems and Perspective

(E. V. Antipov, S. N. Putilin, R. V. Shpanchenko, A. V. 
Mironov, A. M. Abakumov and O. G. D'yachenko, Department of 
Chemistry, Moscow State University, Moscow 119899, Russia)

X-ray powder diffraction patterns of different supercon-
ducting Cu-based mixed oxides and related phases were pre-
pared in the frame of the ICDD Grant-in-Aid (APS 91-05). 
The main families of the studied compounds are Hg-, Bi-, 
and Pb-based, 123, 223, T* phases, different double perovs-
kites, oxhyalides. Several important problems, caused by 
specific features of these materials, embarrass a preparation 
of their high-quality XRD patterns.

XRD patterns of the high members of the 
HgBa2Ca12n-1Cu2n+2O2n+4+ superconductors have incom-
mensurate modulated crystal structures due to cooperative 
atomic displacements in the layers, resulted from the mis-
match between rock salt (BiO double layer) and perovskite 
(containing CuO2 layer) blocks and accompanied by an in-
sertion of the extra oxygen atoms in the first block of type. It 
leads to the appearance of satellite reflections, which can not 
be indexed by three Miller indices and demands the applica-
tion of the 3+d dimensional crystallography. In particular, 
four studied samples were indexed using four Miller indexes. 
Satellite reflections can not be withdrawn from consideration 
because the intensities of the strongest ones are as high as 
6–8%.

Low temperature (350 °C) preparation conditions of su-
perconducting Cu-based oxyfluorides (e.g., YBa2Cu3O6.6F2 
and Sr2Cu(OF)4+δ) and mechanisms of their synthesis result 
in strong broadening of reflections on XRD patterns, and, 
moreover, the disappearance of hkl intensities with l0 for the 
former compound. Several important groups of supercon-
ducting compounds are absent in the Data Base up to now 
and their XRD patterns have to be done and included.

Application of the PDF in Surface and Interface Engineering 

(J. Fiala, SKODA Research Ltd., 31600 Plzen, Czech Republic)

The principle of the phenomena of epitaxy, endotaxy, 
and topotaxy consists in structural coherence relations in sol-
ids. To be able to make use of these effects and to control 
them, we need an instrument for each recognition and quan-
tification of the structural coherence. To this end, the 
JCPDS-International center for Diffraction Data Powder Di-
fraction File, containing currently information on some 
63500 crystalline substances, maybe used to advantage. 
Electron density is a superposition of plane waves, 
\[\exp(-2\pi i(h* + k*l))\]. These harmonic components have wave-
lengths equal to the interplanar distances \(d_{hkl}\) and amplitudes 
proportional to the (square roots of) intensities \(I_{hkl}\) of the 
individual reflections. The greater the amplitude of the given 
harmonic, the greater is the part of the electron density of the 
crystal contained in this harmonic. The \(d, l\)-data deposited 
in the Power Diffraction File bear information on 3D-
structure in a form which is extremely well suited to the 
recognition of the possible topotactical relations between two 
materials under consideration. Intensive lines with the same 
(or nearly the same) \(d\)-values in the diffraction patterns of the 
two crystals indicate that a significant part of their (elec-
tronic) structure is coherent; the sets of planes with common 
\(d\)-values—when properly oriented—effectuate the topotacti-
cal concretion of crystals across their interface. The more the 
common \(d\)-values and the larger the corresponding \(l\)-values, 
the greater will be the probability of the topotactical rela-
tions.

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Structure Determining of Organic Crystals from Powder Diffraction Data by the Combined Use of Molecular Mechanics

(Yunde Xiao, Jun Zhao, Longxin Shen, Xinkai Yao, Jinping Zhang, Shaofan Lin and Weidong Zhang, Central Laboratory, Nan-
determination of unit-cell parameters (indexing) and possible
termination consists of four major steps: (1) the
structure determination from powder diffraction data is to
be prepared in the form of single crystals with sufficient size
and quality for conventional single crystal X-ray diffraction
studies. In such cases, the structural information can be ex-
ttracted from powder diffraction data. The major problem in
the structure determination from powder diffraction data is to
obtain a good starting structure model. A purpose of the
present paper is to provide the method based on the com-
bined use of molecular mechanics for the structure determi-
ation of organic crystals. A full procedure for structure de-
termination consists of four major steps: (1) the
determination of unit-cell parameters (indexing) and possible
space groups(s), (2) the energy minimization by molecular
mechanics to give the atomic coordinates of molecule, (3)
the conversion of the molecular coordinates into crystallo-
graphic coordinates by the Patterson method, (4) the refine-
ment of the structure by the Rietveld method.

Molecular mechanics employs empirical potentials
(force field) to calculate accurately the energy and structure
of molecule. It is widely used in computer chemistry. The
molecular mechanics energy expression can be written as:

$$E_{\text{total}} = E_{\text{bond}} + E_{\text{angle}} + E_{\text{dihedral}} + E_{\text{vdw}} + E_{\text{electrostatic}} + \ldots$$

The functional form of force fields and the parameters have much
effect for the special application. Here, we selected Alliger
force field. The generated energy minimization configuration
by molecular mechanics is regarded as a rigid structure. Then
the relative coordinates of atoms in molecule can be identi-
\ndied, and converted into crystallographic coordinates. There-
fore, the crude crystal structure is obtained. As an example of
application, the crystal structure of ethyl hydrazedicarboxy-
late has been determined by using the present procedure.

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Poster Session

X-ray Diffraction Study of PtSi Thin Films

(Tom Blanton and Chris Hoople, Eastman Kodak Company,
Imaging Research and Advanced Development, Rochester,
New York 14650-2106)

Silicide Shottky barrier diodes (SBD) on p-type silicon
(Si) have been utilized for detecting infrared radiation. This
technology is promising in terms of manufacturability due to
its excellent compatibility with existing Si integrated device
technology. Platinum silicide (PtSi) on p-type Si has been
shown to provide useful SBD for detection of infrared radia-
tion up to 5.5 microns (down to 1820 cm$^{-1}$). In this type of
device, the typical PtSi thickness is less than 50 A, which is
considered an ultrathin film. During SBD fabrication, Pt is
deposited on the Si wafer and then annealed to form PtSi.
From a production perspective, it is important to be able to
determine phase purity, planar orientation, crystallite size,
and film thickness. X-ray diffraction (XRD) methods have
been developed so that these parameters can be measured.

Test Data for the Calculation of Powder Patterns for Inter-
metallic Phases

(L. D. Calvert, a 1) P. L. Wallace, b 2) T. C. Huang, c 3) J. A. Kaduk, d
J. N. Dann, e 5) M. H. Mueller, f 6) and A. C. Roberts, g 7) 1) Deceased; 2)
Los Alamos National Laboratory, P. O. Box 1663, MS E500, Los
Alamos, NM 87545, USA; 3) 6584 Radko Drive, San Jose, CA
95119-1924, USA; 4) Amoco Research Center, Mail Code F-9,
P.O. Box 3011, Naperville, IL 60566-7011, USA; 5) OSRAM SYL-
VANIA Inc., Hawes Street, Towanda, PA 18848-0504, USA; 6)
Deceased; 7) Geological Survey of Canada, 762-601 Booth Street,
Ottawa, Ontario, Canada K1A 0E8.

Powder diffraction patterns are often calculated from
structural parameters to assist in the identification of materi-
als. To ensure that powder pattern calculations are correct, it
is useful to have data to test the computer program doing the
calculations. This paper contains test data for each of the
crystallographic point groups and 63 of the 230 space
groups. An important feature of the data is that many tests
involve two high-symmetry structures (sodium and magne-
sium) that are set in successively lower-symmetry space
groups. Thus, the calculated powder intensities for sodium,
for example, are identical whatever the setting is. Though the
data were chosen to be especially useful for the calculation
of the powder patterns of metals and intermetallic com-
ounds, the data have wider utility.

Powder Diffraction at the NSLS

(D. E. Cox1) and P. W. Stephens,2) 1) Physics Dept.,
Brookhaven National Laboratory, Upton, NY 11973, USA and 2) Physics Dept.,
State University of New York, Stony Brook, NY
11794, USA and National Synchrotron Light Source, Brookhaven
National Laboratory, Upton, NY 11973, USA)

Powder diffraction at the National Synchrotron Light
Source is easy to do—and easier to arrange than commonly
supposed! By contacting the appropriate beamline person-
nel, informal arrangements can usually be made for feasibility
studies or short experiments, including ‘mail-order’ service
in some cases. For longer experiments, several days beam
time can be requested by completing a General User Pro-
posal. Proprietary work can also be carried out, subject to
full-cost recovery charges specified by the NSLS. Among the
many diffractometers at the NSLS available for powder dif-
fraction studies, the three most frequently used are the fol-
lowing (spokespersons are listed in parentheses): X3B1 (P.
W. Stephens), X7A (D. E. Cox), X7B (J. C. Hanson), and
X12A (D. P. Siddons—under construction). The above dif-
fractometers provide many options for data collection, and
can be used in a wide variety of configurations depending on
the requirements of the experiment. For highest resolution
and peak-to-background discrimination, a crystal analyzer is
mounted in the diffracted beam, and for more rapid data