MS–02.03.06 DIRECT METHODS FOR POWDER DIFFRACTION.
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The structure determination from powder diffraction data by an 'ab
initio' method like Direct Methods is greatly facilitated when as
many unique intensities as possible are known accurately. However,
powder patterns generally show a range in intensities from 1 to
1000, whereas single-crystal data are found in a much wider range.
Then overlap causes complications and, moreover, texture or
preferred orientation prevents the intensities to be correct.
Our procedure POWSIM employes for the reconstruction of intensities
a two step mechanism. In the first step the complete powder
diagram is used in a Rietveld-like procedure applied to the complete
diagram (J. Appl. Cryst., 1992, 25, 231), which proves to be an
improvement over Pawley's method (J. Appl. Cryst., 1981, 14, 357).
By minimizing the least-squares sum of the intensities and
background exactly, the fitting becomes independent of the initial
intensity and background values. Our results show that the intensities
refined with this new technique deviate less from the true intensity
values than those from the original Pawley method.
Any curve fitting procedure will never be able to unravel two peaks
at the same or nearly the same position. In order to attack this
problem, several relations from Direct Methods have been employed
to predict which overlapping reflections are strong and which are
weak. This information and the sum intensity of overlapping peaks,
which is determined correctly by the fitting procedure, can be used
to redistribute the intensities in each cluster of overlapping peaks (J.
Appl. Cryst.,1992, 25, 231). In this way a vast number of intensities
are determined accurately, each of them getting a reliability-index
for its accuracy, which is being used in the successive phasing
process (Z. Kristall., in the press).
At present fine-tuning of the Direct method is performed and
theoretical and practical work is carried out to include texture
corrections in the program system. The texture measurements are
done with a prototype of a diffractometer, developed in the Philips
Research Laboratories (Adv.X-Ray Anal, Vol 31 (1988), Plenum, 413).
Also structure determinations using the method will be presented.

PS–02.03.07 ELECTRON DISTRIBUTION IN GERMANIUM BY MAXIMUM
ENTROPY METHOD. By H.Ishibashi[*], K.Higashimine, S.Minamigawa
and K.Nakahigashi, Department of Materials Science, University of Osaka Prefecture, Japan.

A detailed electron density distribution in germanium was
examined from powder X-ray diffraction data. Ultrafine particles of Ge with average particle size less than $1 \mu m$ were
synthesized by a "hydrogen plasma-metal" reaction method(K.
Nakahigashi, H.Ishibashi, S. Minamigawa and M.Kogachi, Jpn.
J. Appl. Phys.,1992, 31, 2293-2298). Diffraction intensities
were measured by a step scanning with the sampling interval
of $0.02°$ in 2θ and accumulation time was 30 seconds for
every step. The scan range in 2θ was from $20°$ to $145°$ of
$CuK\alpha$ radiation with tube voltage and current of 50kV and
200mA. Integrated intensities were estimated by the computer
program WPPD (H.Toraya, J. Appl. Phys.,1986, 440-447). The
integrated intensities were converted to the structure factors by the ordinary least-squares refinement. By this analysis, we obtained the values of 11 independent structure
factors and one combined structure factor which was a pairs
of 333 and 511. The electron density distribution map was
drawn by the maximum entropy method (M.Sakata and M.Sato,
Acta Cryst.,1990, A42,263-270). A special feature for a
diamond structure reappeared well in the map for (110) plane.

However, the bonding electrons were not so clearly observed
because of the limited number of reflections measured. In
order to improve the map, an experiment using synchrotron
radiation is in progress. Results will be presented at the
meeting.

**PS–02.03.08 CHARGE-DENSITY ANALYSIS BY MEANS
OF GAMMA-RAY DIFFRACTION: NiF_2, FeF_2,
$SrTiO_3$.** By A.Palmer and W.Jauch, Hahn-Meitner-
Institut Berlin, Germany.

NiF_2 and FeF_2: Measurements of data sets up to
1.3 Å^{-1} at 295 and 15 K; contrast to MnF_2,
combination with neutron diffraction from the
identical samples gives no indication for a
polarization of the F-atoms in the antiferro-
magnetic phase; the population of 3d-orbitals,
derived from multipole-models agrees with the
expected crystal-field splitting in an
octahedral environment.

$SrTiO_3$: Data collection up to 1.6 Å^{-1} at room
temperature, at 5 K above the 107 K-structural
phase transition and at 50 K; determination of
the oxygen position in a single-domain sample;
anharmonic thermal motion at RT and
asphericities will be reported.

The maximum entropy method (MEM) has been
applied to NiF_2 and MnF_2 γ-ray data. It turned
out that the failure in mapping the charge-
density is not a consequence of insufficient
data quality, rather MEM maps are hardly
interpretable in the low-density region (Jauch,
W. and Palmer, A., Acta Cryst. A, 1993).

**PS–02.03.09   DIRECT INVESTIGATION OF ATOMIC THERMAL
VIBRATIONS OF BE METAL BY THE MAXIMUM ENTROPY METHOD.**
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Department of Physics, Science University of Tokyo,
Noda, Chiba 278 Japan and B.B.Iversen and F.K.Larsen,
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Aarhus C, Denmark.

The Maximum Entropy Method(MEM) applied to neutron
diffraction data directly yields the nuclear density
distribution, which is equivalent to the thermal smear-
ing function. The MEM procedure thus enables us to form
maps showing the atomic thermal vibrational features in
real space without using a structural model. The pur-
pose of this study is to examine this capability of the
MEM for the direct investigation of thermal vibrations
and Be was chosen as a test case.
Mean-square atomic displacement and antisymmetric
atomic vibrations in Be at room temperature have been
determined from short-wave length neutron data by
conventional analysis (Larsen,F.K., Lehmann,M.S. and
Merisalo,M., 1980, Acta Cryst., A36, 159-163). The
same data were treated by the MEM in the present study.
The resulting density distribution at the presumed
nuclear site in the basal and in the (100) plane of the
hcp structure are shown in Fig.1 (a) and (b), respec-
tively. In Fig.1(a) a characteristic triangular feature
is clearly visible. We interpret this as being caused
by 3rd order anharmonic vibrations in the basal plane.
In Fig.1(b) the nuclear density shows significant
deviation from the expected oblate shape from harmonic
vibrations. We interpret this feature as indicating a
significant quartic contribution in the potential