06.3—9   EXPERIMENTAL AND THEORETICAL ANALYSIS OF
THE INTERIONIC INTERACTIONS IN CRYSTALLINE LiOH.
By E. Heuser-Hofmann and W. Weyrich, Faculty of Chemistry, University of Konstanz, Konstanz, Fed. Rep. of
Germany.

In order to study the electronic structure of the co-
valent bond in OH⁻, we have recently determined the com-
plete three-dimensional electron momentum density and
its Fourier transform (reciprocal form factor) in
single-crystal LiOH using Compton scattering of 241-Am
gamma-radiation. Apart from the strong anisotropy aris-
ing from the covalent bond in OH⁻, the data show the
influence of the interionic interactions in the crystal.

For the interpretation of these features we have applied
Löwdin's symmetrical orthogonalisation method to free-
ion wave functions in clusters of varying size with the
appropriate spatial arrangement of the crystal struc-
ture. Approximations to Wannier functions have been ob-
tained, from which we can analyse the nature of the
interionic interactions seen in the experimental data.

06.3—10   EXPERIMENTAL ELECTRON MOMENTUM DENSITIES IN
TWO-DIMENSIONAL SOLIDS. By G. Loupias and J. Chomilier,
Lab. de Cristallographie, U.P.M.C., 4 place Jussieu,
75230 Paris Cedex 05 and L.U.R.E., Bat 209C, 91405 Orsay
Cedex, France.

The Compton profile is a very good experi-
mental test for calculated wave functions because of its
preferential sensitivity to valence and conduction elec-
trons. The best resolution is obtained in the X-Ray ran-
ge with a crystal analysis of the scattered photons : the
Lure-DCI high resolution spectrometer was used for this
study (Loupias et al. Phys. Stat. Sol. b 102, 79 (1980)).
The insensitivity of this method to crystal defects ma-
kes it particularly suitable to understand the electron
behaviour in graphite intercalation compounds. The first
stage alkali compound is a sequence of successive alkali
and carbon layers. The crystallites are randomly oriented
in the basal plane but oriented along the $\vec{c}$ axis.

The simplest model for LiC_6, the rigid-band
model, assumes that the Li 2s electron is totally trans-
ferred to a graphite Π band. A recent pseudo-potential
calculation taking into account the valence band distor-
sion has been performed by Holzwarth and a Compton pro-
file has been derived.

The Compton profiles have been measured
with the same orientation of the scattering vector, for
LiC_6 and graphite. The experimental difference profile
allows us to conclude about the electron behaviour : its
excellent agreement with the last theory shows that it is
necessary to consider both the charge transfer and the
modification of the valence band in a so-called "Two di-
mensional" solid.

06.3—11   OFF-DIAGONAL MOMENTUM DENSITY OF Si
BY MEANS OF COHERENT COMPTON SCAT-
TERING. By W.Schülke, S.Mourikis, Institut für
Physik,Universität Dortmund,D-4600 Dortmund 50,
Fed.Rep. of Germany

As first pointed out by one of the authors (W.S,
Phys.Lett.1981,83A,451) the measurement of the
double differential cross section for inelastic
X-ray scattering, where the initial photon
state is the coherent superimposition of two
plane waves in the Bragg case of diffraction,
provides information about off-diagonal ele-
ments of the one particle density matrix in
momentum space. This information can be ob-
tained in the form of a one dimensional pro-
jection of the off-diagonal elements on the
scattering vector (so called correlation pro-
-files), where there exist certain intrinsic li-
mitations with respect to the momentum resolu-
tion of this information. These limitations are
discussed.
Then a method is presented, which utilizes in-
formation about the X-ray structure factor and
the dynamical theory of X-ray diffraction in
order to seperate correlation profiles from
Compton profiles, which both appear superim-
posed in the measured double differential
scattering cross section (DDSCS). By this means
experimental correlation profiles of Si-valence
electrons have been obtained by measuring
DDSCS's at different positions of the Si-crys-
tal within the Bragg reflection range utilizing
a double crystal setting with a highly asym-
metric cut first crystal. The solid state in-
formation made available by these measurements
is outlined.

06.3—12   MOMENTUM SPACE ELECTRON DENSITY OF Li
FROM DIRECTIONAL COMPTON PROFILES.
By W. Schülke, T. Langer, P. Lanzki, Institut
für Physik, Universität Dortmund, D-4600 Dort-
mund 50, Fed. Rep. of Germany.

With a momentum space resolution of 0.12 a.u.
10 directional Compton profiles (DCP's) of Li
have been measured by means of a focusing
crystal spectrometer with MoK_α-radiation
utilizing a linear position sensitive detector.
Effectively $5 \cdot 10^6$ counts have been accumulated
in one profile. By using Fourier transform (FT)
methods (Schülke, Phys.Stat.Sol.(b)1977,82,229;
Hansen et.al.,Z.Phys.1982,B22,675) the three-
dimensional momentum space electron density
$n(\vec{p})$ as well as the three dimensional occupa-
tion number density $n(\vec{k})$ of Bloch states have
been reconstructed from the DCP's. The recon-
structed $n(\vec{p})$ reveals well separated higher
momentum components (HMC's) near the N-point of
the Brillouin zone, whose amount could be fit-
ted to Fourier components of the Li-pseudo-
potential. The reconstructed $n(\vec{k})$ makes
possible an estimate of electron correlation
effects well separated from the influence of
HMC's. Supported by model calculation the Fermi
surface anisotropy of Li has been deduced from
the FT of DCP's to be

$$(k^F_{[110]} - k^F_{[100]})/\bar{k}^F = (1.7 \pm 0.3) \cdot 10^{-2}.$$

This is in good agreement with recent positron
annihilation data.