**06.7–1**     ACCURATE THERMAL PARAMETERS OF LI7H and LI7D
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The neutron structure factors of Li7H and Li7D were mea-
sured at 300K, 160K and 93K (Li7H) or 83K (Li7D) on the
high flux reactor of the ILL (Grenoble) using the 4 cir-
cle diffractometer D9 with $\lambda$ = 0.5465 Å.

The crystals were thermally treated and annealed to avoid
the Li excess and strong primary extinction. The diffi-
culties encountered in the course of these experiments
were twofold : the high reactivity of the compounds and
their weak diffracted intensities. The hygroscopic sam-
ples were protected from the atmosphere in special quartz
containers sealed under vacuum. This protection enabled
us to perform all the measurements with only one single
crystal for each compound. A visual inspection method was
worked out and used to select the reflections included
in the structure refinements; the simple averaging of all
measured equivalents produced less satisfactory results.

The selected data were analysed by two methods :
1) The isotropic thermal parameters are refined together
with the scale factor and the extinction parameters using
a conventional least squares fitting program.

2) The iterative Fourier method of Vahvaselkä A. &
Kurki-Suonio K. (1975, Phys. Fenn. 10, 87-99) was used,
whereby the thermal parameters and the scale factor were
varied until $\Delta\rho_0(0) - \Delta\rho_0(dr)$ was minimum at the atomic
centers.
The extinction corrections obtained by standard least-
square refinements were applied before using the itera-
tive Fourier procedure. The comparison of both methods
yields two significant results :

1) When including reflections with increasingly higher
sin $\theta/\lambda$, the thermal parameters were reaching their
asymptotic limits much earlier in the iterative Fourier
method compared to the normal least-squares fitting.

2) The usual correlation problems of a least-squares
fitting procedure were circumvented in the iterative
Fourier approach.

The final results of both methods are similar. However,
the applied least-square procedure is different from the
usual treatment in that :

1) Correlation effects are reduced by selective inclusion
of reflections (visual inspection and non-systematic
averaging).

2) The quality of fit is improved by cutting out the noi-
sy high angle data (sin $\theta/\lambda$ threshold).

Inclusion of the weak reflections in the standard least-
squares procedure increases the correlation effects and
is therefore less efficient than the iterative Fourier
method.

The thermal parameters obtained by Calder R.S., Cochran
W., Griffiths D. and Löwde R.D. ((1962) J. phys. Chem.
Solids., 23, 621-632) for LiH (Li natural) agree quite
well with the ones obtained in the present analysis for
Li7H. The extrapolated values at 0°K are in good agree-
ment with the values obtained from the Debye-temperatu-
res.

The present work is a part of an X-N analysis of Li7H
and Li7D.

**06.7–2**     SELECTIVE ENHANCEMENT OF DIFFERENT ELECTRON
POPULATIONS BY ELECTRON-POSITRON ATTRACTION. APPLICATION
TO ZINC. By S. Daniuk, G. Kontrym-Sznajd, A. Rubaszek
and H. Stachowiak., Institute for Low Temperature and
Structure Research, Polish Academy of Sciences, Wrocław,
Poland; J. Mayers, P.A. Walters and R.N. West, School of
Mathematics and Physics, University of East Anglia,
Norwich, England.

In principle positron annihilation could give information
about electron distribution both in momentum space and
in real space. But while the Fermi surface as seen by
positrons is not affected by electron-positron attraction
(EPA) it is not so with other annihilation characteris-
tics. Several theories have been proposed for determining
the influence of EPA on the annihilation rate for differ-
ent electronic states. The best known EPA theory has been
proposed by Kahana (Phys. Rev. (1963) 129,1622). But while
EPA in an electron gas is relatively easy to treat, it
is not so with real metals, in particular transition met-
als. The approach to EPA used in this work is essentially
a Thomas-Fermi type approximation; the influence of EPA
at a given point in the lattice is considered to be the
same as in an electron gas of density equal to the elec-
tron density in this particular point in the absence of
the positron. This approach is an extension of the idea
proposed by Bonderup et al. (Phys. Rev. (1979) B20, 883).
The method was applied to the two-dimensional angular
correlation data obtained at Norwich for zinc (Mayers et
al., in Positron Annihilation, ed. by R.R. Hasiguti and
K. Fujiwara, Japan Institute of Metals, Sendai 1979).
Such measurements give one-dimensional integrals of the
electron density in momentum space (as seen by positrons).
The Kahana approach was used for obtaining the enhance-
ment factors $\varepsilon(E_{n\bar{k}}, \rho)$ as functions of the energy $E_{n\bar{k}}$
(with regard to the Fermi energy) of the electronic state
$n\bar{k}$ and the density $\rho$ of the electron gas.
The amplitude of annihilation of the $n\bar{k}$ state with emis-
sion of two photons of total momentum $\bar{p}$ was computed
from the formula:

$$A(\bar{p},\bar{k},n) \sim \int \sqrt{\varepsilon\left[E_{n\bar{k}}, \rho(\bar{r})\right]}\ \psi_{n\bar{k}}(\bar{r})\psi_+(\bar{r})\ e^{-i\bar{p}\bar{r}}\ d\bar{r} \quad , \quad (1)$$

where $\psi_{n\bar{k}}(\bar{r})$, $\psi_+(\bar{r})$ are the electron and positron wave
functions respectively.
The application of this formalism to zinc is not trivial
because from the point of view of positron annihilation
Zn is a transition metal. Such a treatment of the en-
hancement resulted in improving the agreement between
theoretical predictions and experimental data by a fac-
tor of about three in comparison with the independent
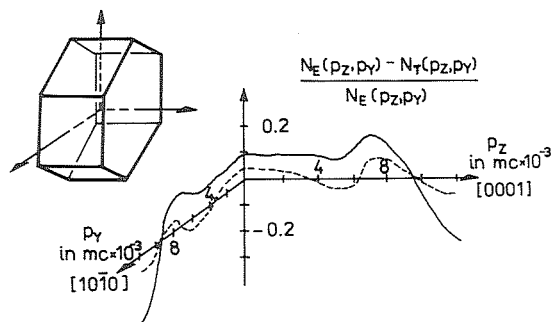particle model in the whole momentum range.



Fig. 1. Relative differences (along two axes) between
experimental data $N_E$ and theoretical predictions $N_T$
(full curve-according to the independent particle model,
dashed curve-as obtained from Eq. (1)). $N_E$ and $N_T$ are ob-
tained by integrating the electron density along straight
lines pointed in the $[11\bar{2}0]$ direction.