06.7–1 ACCURATE THERMAL PARAMETERS OF LI7H and LI7D BY NEUTRON DIFFRACTION. J.P. VIDAL, G. VIDAL-VALAT, Groupe de Dynamique des Phases Condensées (LA 233) U.S.T.L. - 34060 Montpellier Cedex, and W.F. KUHS, Institut Laüe Langevin, 156X - 38042 Grenoble Cedex, France.

The neutron structure factors of Li7H and Li7D were measured at 300K, 160K and 93K (Li7H) or 83K (Li7D) on the high flux reactor of the ILL (Grenoble) using the 4 circle diffractometer D9 with λ = 0.5465 Å.

The crystals were thermally treated and annealed to avoid the Li excess and strong primary extinction. The difficulties encountered in the course of these experiments were twofold : the high reactivity of the compounds and their weak diffracted intensities. The hygroscopic samples 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 $\Delta\rho_o(0) - \Delta\rho_o(dr)$ was minimum at the atomic centers.
The extinction corrections obtained by standard least-square refinements were applied before using the iterative Fourier procedure. The comparison of both methods yields two significant results :

1) When including reflections with increasingly higher sin θ/λ, 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 noisy high angle data (sin θ/λ 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 agreement with the values obtained from the Debye-temperatures.

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 characteristics. Several theories have been proposed for determining the influence of EPA on the annihilation rate for different 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 metals. 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 electron 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 enhancement 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 ρ of the electron gas.
The amplitude of annihilation of the $n\bar{k}$ state with emission of two photons of total momentum $\bar{p}$ was computed from the formula:

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

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 enhancement resulted in improving the agreement between theoretical predictions and experimental data by a factor of about three in comparison with the independent particle model in the whole momentum range.

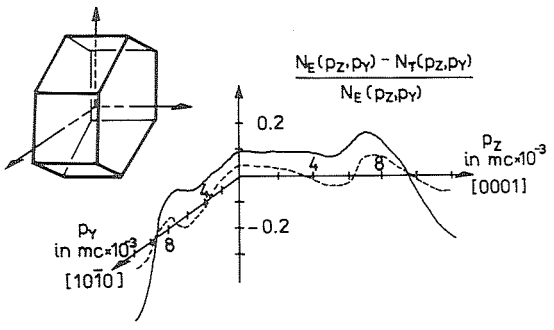

Fig. 1. Relative differences (along two axes) between experimental data N_E and theoretical predictions N_T (full curve-according to the independent particle model, dashed curve-as obtained from Eq. (1)). N_E and N_T are obtained by integrating the electron density along straight lines pointed in the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