06.X-4 COHERENT COMPTON SCATTERING: A USEFUL COMBINATION OF POSITION-SPACE AND MOMENTUM-SPACE INFORMATION. By W. Schülke, Institute of Physics, University of Dortmund, Fed. Republic of Germany

Conventional Compton scattering experiments yield information about the 3-D momentum space density of electrons, provided a sufficient number of directional Compton profiles are at hand for a 3-D reconstruction. X-ray diffraction will provide information about the position space density of electrons, if the phase problem can be solved. The density in one space is related, on the one hand, to diagonal elements of the one-particle density matrix in this very space, and on the other hand, to the space average of nondiagonal elements of the one-particle density matrix in the complementary space. It is shown that more detailed information about nondiagonal elements of the one-particle density matrix in momentum space $\Gamma(\vec{p}|\vec{p}\,')$, that is projections of $\Gamma(\vec{p}|\vec{p}+\vec{g})$ on the scattering vector, can be obtained by means of coherent Compton scattering, where the initial photon state is the standing wave field of a Bragg-reflection corresponding to the reciprocal lattice vector $\vec{g}$. Thus the spatial modulation of the initial photon state together with probing of momentum space via Compton scattering leads to phase information about momentum space wavefunction, which is the essential of nondiagonal density. The experimental procedure for obtaining $\Gamma(\vec{p}|\vec{p}+\vec{g})$ is shown, and results on Si are presented. Finally a means is discussed to get useful coherent Compton scattering results also for less perfect crystals.

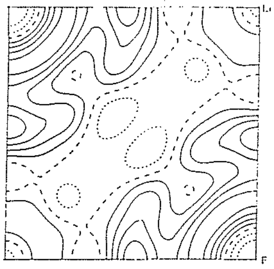
06.X-5 ELECTRON MOMENTUM SPECTROSCOPY OF ATOMS AND MOLECULES - SOME RECENT RESULTS. by E. Weigold, Institute for Atomic Studies, Flinders University, Bedford Park, 5042, Australia.

Electron momentum spectroscopy is based on the (e,2e) reaction, in which an electron of energy in the region of 1keV ionises a target atom or molecule. Two electrons are detected at polar angles of 45°. Variation of the relative azimuth enables the recoil momentum of the ion to be scanned. This is essentially the momentum of the knocked-out electron at the knockout instant, so a distribution of single-particle momentum is obtained for each resolved state of the ion. The momentum distribution is given very accurately and sensitively by the Hartree-Fock orbital of the target corresponding to the one-hole ion configuration. For atoms the momentum distribution is fully understood by including distortion due to electron-target scattering. The cross section for a particular ion state is proportional to the probability of finding the one-hole configuration in the ion state. This is the spectroscopic factor. It is a sensitive test of configuration interaction for ion states that result from the splitting of a one-hole state due to electron correlations. In general the Hartree-Fock calculation gives single-particle momentum distributions very accurately up to about 1 atomic unit of momentum. Exceptions occur for lone-pair orbitals where the variation method is insensitive. Configuration-interaction and Green's function calculations give spectroscopic factors that are only qualitatively correct.

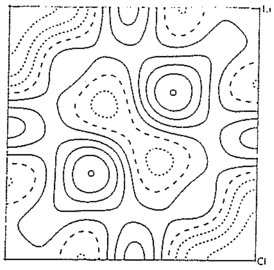
06.2-1 ATOM SIZE AND CHARGE IN ALKALI HALIDES. By J.A. Henderson and E.N. Maslen, Crystallography Centre, University of Western Australia.

The lowering of the potential energy due to overlap of atomic electron densities is an accurate approximation to the binding energies of the alkali halides. The kinetic energy gained because the electrons move in a higher electrostatic potential is offset by the reduction in potential energy due to polarisation of the electron density, including the two electron term.

It is widely believed that most of the polarisation energy is due to transfer of electrons from cation to anion. Experimental measurements of the electron density by X-ray diffraction indicates that the actual charge transfer depends quite strongly on the sizes of the atoms involved. Sections of the deformation densities calculated from the data for LiF by Merisalo & Inkinen (Ann. Acad. Sci. Fenn., 1962, AVI 207, 1-24) and for LiC*l* by Inkinen & Jarvinen (Phys. Kondens. Materie, 1968, 17, 372-382 are shown.



(100) plane LiF. Contour interval 0.025eÅ^{-3}



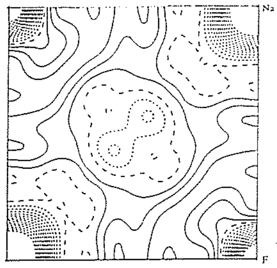
(100) plane LiCl. Contour interval 0.025eÅ^{-3}

The electron transfer from cation to anion, determined by the method of Hirshfeld (Theor. Chim. Acta 1977, 44, 129-138) is .13(1) and -.03(1) electrons for LiF and LiC*l* respectively. The reason why the charge transfer differs is indicated by the topography of the $\Delta\rho$ maps.

In LiF the electron density along the Li-Li vector is depleted, suggesting a repulsive interaction. The length of that vector (2.84 Å) is less than the nearest-neighbour Li-Li distance in lithium metal (3.11 Å). This is the predicted result of exchange when depletion resulting from overlap of electrons with parallel spins dominates. The LiF structure is stabilised by the attractive nearest neighbour Li-F interaction.

In LiC*l* the electron density along the Li-Li vector is enhanced, accounting for the reduced transfer of electrons from cation to anion. The Li-Li vector in this structure is more than twice the metal radius. The enhancement of density along that vector is also consistent with the effect of exchange, provided the concentration due to overlap of electrons with paired spins dominates.

The reasoning may be tested by applying it to the deformation density for NaF evaluated with the data of Sharma (Acta Cryst., 1974, A30 278-280). The electron density along the Na-Na vector is heavily depleted, as expected because the Na-Na distance of 3.27 Å is much shorter than that of 3.67 Å in sodium metal. The charge transfer from cation to anion in NaF of .54(1) electrons reflects the crowding of the sodium cations.



(100) plane NaF. Contour interval 0.05eÅ^{-3}

Thus the electronegativity of an atom is partly related to its size. Large metal atoms, such as the heavier alkali metals, are strongly electropositive. Such atoms diffuse valence shells, with large radii, and readily lose electrons by sharing due to exchange. Electron loss due to exchange depletion is low for fluorine. Electrons accumulate strongly near a fluorine atom because it is the smallest of the halogens.