06. 3–5 MOMENTUM DENSITIES AND MOMENTUM SPACE PROPERTIES OF ATOMS AND IONS.* By W.M. Westgate, Alfredo M. Simas, and Vedene H. Smith, Jr., Department of Chemistry, Queen's University at Kingston, Kingston, Ontario, K7L 3N6, Canada.

The spherically averaged momentum densities, $\bar{\Pi}(p)$, for the ground states of the 92 atoms from hydrogen to uranium, and of 73 singly positive ions from helium to barium and from lutetium to radium, constructed from non-relativistic SCF wave functions, are examined. Pertinent correlations between the value of the momentum density at the origin, $\bar{\Pi}(0)$, and the electronic structure of the system are found and analyzed. From these investigations it is noted that the general shape of $\bar{\Pi}(p)$ of an atomic system is clearly determined by the orbitals of the outermost shell. Two distinct types of maxima that make $\bar{\Pi}(p)$ non-monotonic have been investigated: (i) a *primary* type, previously reported in the literature and which typically occurs for $p\varepsilon[.05,.60]\text{Å}^{-1}$, and (ii) a *secondary* type, generally very small and barely noticeable, which occurs for $p\varepsilon[0.7,1.5]\text{Å}^{-1}$. The results indicate that while maxima of the *primary* type result from occupied non-zero angular momentum orbitals of the outermost shell, maxima of the *secondary* type result from similar orbitals of the next inner shell.

In addition, the expectation values $\langle p^k \rangle$, $-2 \leq k \leq 4$, the characteristic momentum p* and distance r*, and the full relativistic kinetic energy $\langle T \rangle = \langle (m_e^2c^4 + p^2c^2)^{1/2} \rangle$ are computed and examined for the same systems. The periodic trends that are found to occur in many of these quantities are thoroughly examined. Subsequently, correlations are attempted between these and other chemical properties which display periodicity. Finally, an appraisal of the importance of momentum space studies to chemistry is presented.

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06. 3–6
DIRECTIONAL COMPTON PROFILES AND THE ELECTRON DENSITY DISTRIBUTION IN NICKEL

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Band structure calculations using various local approximations for the exchange-correlation potential predict Compton profile anisotropies which are too large. Recent measurements on thin single crystal slices of nickel along the [100], [110], [111] and [211] directions with $^{198}$Au 412 keV gamma radiation have revealed smaller anisotropies in the momentum density distribution than the band-structure calculation of Wang and Callaway. This is in accord with other measurements on V, Fe and Au using 412 keV gamma radiation. The current accuracy of the individual profiles has also highlighted the disagreement between the band-structure model and the absolute profile corrected for multiple scattering. The interpretation of the directional profiles in terms of the reciprocal form factors (B-functions) have revealed aspects of the density distribution which are not adequately described

06. 3–7 THREE DIMENSIONAL RECONSTRUCTION OF MOMENTUM DENSITY IN Ge, GaAs AND ZnSe BY USING DIRECTIONAL γ-RAY COMPTON PROFILES

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Abstract

In order to investigate systematically the electron structure of semiconductor Ge, GaAs and ZnSe, γ-ray Compton profiles of these single crystals along six directions ([100], [110], [111], [210], [211] and [221] for Ge and GaAs) were measured using 412 keV γ-rays from 120 Curie $^{198}$Au source and the pure Ge solid state detector at Rutherford Appleton Laboratory. Fourier transformed Compton profiles are compared with theoretical ones calculated by H. Nara et al (J. Phys. Soc. Jpn. 46, (1979), 77) using a pseudopotential. The three dimensional reconstruction of the reciprocal form factor and the momentum density distribution will be presented for Ge and GaAs. Similar experiments for ZnSe single crystals are now under way.

06. 3–8
DIRECTIONAL COMPTON PROFILES OF $Ni_3Ga$

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The [100] and [110] directional Compton profiles of $Ni_3Ga$ have been measured with $^{189}$Au, 412 keV, gamma radiation. The results are in good agreement with a recent symmetrised APW calculation by Kubo and Wakoh but are, as predicted, radically different from those found in the related positron annihilation one-dimensional angular correlation experiment. In the Compton difference profiles anisotropic contributions are found out to three atomic units of momenta whereas the positron differences are at lower momenta.

This highlights an advantage of gamma ray Compton scattering which can probe the localised d-like distribution whereas the positron, excluded from the core, only sees the s- or p-like band electrons.