either high or low order Bragg reflections to extract either TFs or SFs. The analysis for the TFs shows that the variance of the results is of order 5 percent for the mean vibration amplitude which is readily explained by experimental errors and uncertainties. The accuracy of SFs obtained so far is in the order of a tenth of a percent. First results on bond charge density clearly reveal a covalent bond between Ni and Al atoms.

Charge, Spin & Momentum Density IV Magnetization & Momentum Densities

MS09.04.01 AB-INITIO QUANTUM MECHANICAL CALCULATIONS OF POLARISED NEUTRON DIFFRACTION: RESULTS IN TRANSITION METAL COMPLEXES. P.A. Reynolds, Research School of Chemistry, Australian National University, Canberra, ACT 0200, Australia

Metal-ligand bonding in metal complexes is poorly understood. Spin density is a fundamental property, it is much modified by bonding effects, and it has important chemical consequences. Consider the instability of triplet H_2 and the stability of singlet H_2. In certain magnetically simple cases in paramagnetic crystals we can estimate many Fourier components of the spin-density, with an accuracy of ca. 1%, by use of polarised neutron diffraction. *Covalence*, resulting in delocalisation of positive metal-centred spin density onto ligand atoms is particularly marked in our recent results on $[As(C_6H_5)_4][TcNCl_4]$ in which 26% of an ionic, technetium centred, $4d_{XY}^1$ spin density has been delocalised onto the chlorines' in-plane $3p_\pi$ orbitals. *Spin-polarisation*, due to electron-electron correlation, is also marked in the TcN bond. The nitrogen spin population is negative, -0.18 e. *Spin-orbit coupling* besides causing canting of the magnetisation, as in Cr(II) Tutton salt, can also cause large changes in the radial distribution of the spin density around the metal site, as in $CoCl_4^{2-}$.

Calculations must be able to duplicate these covalence, spin polarisation, and spin-orbit coupling effects. This requires a correlated relativistic wavefunction (example $CoCl_4^{2-}$). In some cases approximations such as the Unconstrained Hartree-Fock method may be appropriate in description of metal-ligand bonding, but other approximations such as the Restricted Hartree-Fock method never are (example $TcNCl_4^-$).

MS09.04.02 THE USE OF MAXIMUM ENTROPY IN THE INTERPRETATION OF MAGNETIZATION DENSITIES IN NITROXIDE COMPOUNDS. P. Schleger[1,2], A. Puig-Molina[1], E. Ressouche[1],O. Rutty[1], and J. Schweizer[1]. [1]Commissariat a l'Energie Atomique, Centre d'Etudes Nucleaires de Grenoble, Department de Recherche Fondamentale sur la Matière Condensè,17 rue des Martyrs, 38054 Grenoble Cedex 9, France; and [2]Institut Laue-Langevin, B.P. 156, 38042 Grenoble Cedex 9, France.

A maximum entropy method for the reconstruction of magnetization densities in both centric and acentric crystal structures will be presented which is not restricted to weak spin systems, and allows for the incorporation of relevant corrections such as extinction. Thus it is now possible for the first time to reconstruct, without the application of a model, the real space magnetization densities in essentially any physical system from polarized neutron diffraction experiments. This, for example, dramatically simplifies the interpretation process of data on non-centrosymmetric nitroxide free radicals.

MS09.04.03 MAGNETIZATION DENSITY PROFILES IN MAGNETIC MULTILAYERS. J A C Bland, Cavendish Laboratory, Madingley Road, Cambridge, CB3 OHE, UK

The capabilities of polarized neutron reflection (PNR) for directly determining the magnetic and non-magnetic structure in thin and ultrathin magnetic films and multilayers are reviewed. It is shown that the vector magnetization density profile can be obtained with atomic layer resolution in favourable cases and that the combination of structural and magnetic information provides decisive advantages. Estimates of the interface roughness and layer thicknesses can be accurately made and diffuse scattering measurements can be used to probe spin disorder at interfaces. The magnetisation profile across chemically homogeneous ultrathin films can be accurately measured and examples of recent measurements in both ultrathin Fe films and trilayer structures are given and compared with the results of conventional magnetometry measurements. Vector magnetometry measurements of the layer dependent magnetic moment orientations are shown to provide a powerful approach to the study of coupling behaviour in ferromagnetic (FM)/non-magnetic (NM)/FM trilayer structures. Finally the thickness dependent magnetic moment of epitaxial Cu/fcc Ni/Cu(001) structures with competing perpendicular and shape anisotropies is determined as a function of applied field and compared with the results of magnetometry measurements. A strong variation in moment is found which is reflected in the variation of the ratio of orbital and spin moments with thickness determined from X-ray circular dichroism (XMCD) experiments.

MS09.04.04 HIGH RESOLUTION COMPTON SCATTERING AS PROBE OF FERMIOLOGY AND ELECTRON CORRELATIONS. A. Bansil, Physics Dept., Northeastern Univ., Boston MA 02115, USA

In 1993, the I. U. Cryst. Commission on Charge, Spin, and Momentum Densities started a new project, "Fermiology of High-Tc Superconductors via High Resolution Synchrotron-based Compton Scattering Spectroscopy". Properly timed to exploit the rapid world-wide development of high resolution spectrometers, this project has generated vigorous activity. A substantial progress has been made in delineating the nature of electron states in simpler systems which serve as the foundation for understanding complex materials. Feasibility of determining Fermi surface radii via high resolution Compton has been demonstrated.[1] Careful comparisons between the measured and computed spectra in Li, Be, and LiMg[1-3] clearly reveal departures from the conventional one-particle local density approximation (LDA) picture of the ground state momentum density of the electron gas; work on a variety of other systems is in progress. Reconstruction of the full 3D density from a series of Compton profiles in Li is beginning to yield direct insight for the first time into the size of the momentum density break at the Fermi momentum in a metal.[3] Much work has been carried out by a number of groups in standardizing data handling procedures for synchrotron-based Compton data using Si as a target material. This talk provides an overview of the relevant work completed to date, and outlines areas of further study likely to prove fruitful in establishing high resolution Compton as a tool for investigating Fermiology related issues in wide range of materials.

[1] Y. Sakurai, et al., Phys. Rev. Letters 74, 2252(1995).
[2] K. Hamalainen, et al., Phys. Rev. B (1996).
[3] W. Schulke et al. (preprint).