06.3–1 MOMENTUM DISTRIBUTION IN NbO. By Y. Kubo, S. Wakoh and K. Schwarz*, University of Library and Information Science, Yatabe-machi, Ibaraki-ken, Japan and Technical University Vienna*, A-1060 Vienna, Austria.

A crystal structure of NbO can be considered as a NaCl structure with 25% vacancies on both sublattices, a situation which can be denoted by $Nb_{0.75}O_{0.75}$ (Fig.1). This compound has many interesting properties and an investigation of its electronic structures seems to be very important. In this report, a theoretical momentum distribution of electrons in NbO and that sampled by thermalized positrons are calculated by the APW method. The positron wave function at the ground state seems to be well described by 33 APW's with cubic harmonics upto ℓ=4. So far, there is no Compton profiles nor ACAR from NbO, only theoretical predictions will be discussed.

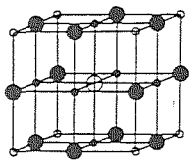

Fig.1: NbO defect structure: oxygen (small circles), niobium (large circles). The voids are shown as open circles (size corresponds to atom).

06.3–2 COMPTON AND BRAGG SCATTERING OF PHOTONS FROM METALS WITHIN THE OPW MODEL. By K. Mansikka, O. Aikala, and P. Soininen, Department of Physical Sciences, University of Turku, Turku, Finland.

Compton scattering and Bragg scattering of photons give valuable information about the electronic structure of different types of solids in the momentum and physical space, respectively. Then, the most interesting knowledge is obtained for the loosely bound conduction electrons. For example, directed Compton profiles are closely associated to the cross-sections of the Fermi-surface of a metal, whereas the elastic scattering factors, being Fourier-transforms of electron density, show in their behaviour integrated solid state effects. In the present work, we have investigated scattering properties of typical metals such as alkali metals, aluminium, magnesium, beryllium etc. by using the OPW Bloch states for the conduction electrons and the LCAO states for the core electrons. The numerical computations are based on the single OPW functions. The theoretical results for different quantities agree well with experimental data. Furthermore, the theoretical expressions for Compton profiles and elastic scattering factors can be presented in the closed forms suitable for computer calculations. (O. Aikala and K. Mansikka: Phys. Kondens. Mat. 14, 105 (1972); K. Berggren, S. Manninen, T-Paakkari, O. Aikala, and K. Mansikka: "Compton Scattering", McGraw-Hill, London (1977), p. 139; K. Mansikka, O. Aikala, and P. Soininen: Proc. 3rd Gen. Conf. Cond. Matter Div. of EPS, Lausanne, Switzerland (1983), p. 440.)

06.3–3 COMPTON PROFILE ANISOTROPIES IN HEXAGONAL BORON NITRIDE AND GRAPHITE. By R. Tyk, J. Felsteiner and I. Gertner, Department of Physics, Technion-Israel Institute of Technology, 32000 Haifa, Israel.

The Compton profiles of pyrolytic boron nitride and pyrolytic graphite have been measured in the directions of the c-axis ($J_{\parallel}$) and perpendicular to the c-axis ($J_{\perp}$) using 60 keV γ-rays of ^{241}Am. The anisotropy measured in boron nitride is found to be significantly smaller than that in graphite, particularly near zero momentum. This is consistent with the picture that boron nitride is a poorer conductor than graphite and the contribution to the Compton profile of the π-electrons in boron nitride is less anisotropic than in graphite.

We find $J_{\perp}(0) > J_{\parallel}(0)$ in both boron nitride and graphite, the same as in all previously known measurements of graphite. To our knowledge no other Compton anisotropy measurements of boron nitride have been reported. Our results disagree with the recent LCAO self-consistent field calculations of Dovesi et al. (Phys. Rev. B24, 4170 (1981)), who have obtained $J_{\perp}(0) < J_{\parallel}(0)$ for both hexagonal boron nitride and graphite.

06.3–4 ON THE ELECTRONIC STATE OF LITHIUM NITRIDE STUDIED BY COMPTON SCATTERING. By O. Aikala, Department of Physical Sciences, University of Turku, SF-20500 Turku 50, Finland.

The possible existence of the N3- ion in the fast ion conductor lithium nitride has been discussed recently in the literature. Schwarz and Schulz (Acta cryst. (1978) A 34, 999) have calculated numerical wave functions for N3- ion within the Watson sphere model with various Watson sphere radii. We have fitted these to STO's and using them and free ion wave functions of Li+ ion we have calculated the Compton profiles in the main directions of lithium nitride crystal. The local orbitals were orthogonalised symmetrically with the Fourier series method (Aikala, J. Phys. C (1983) 16, 2217) and the profiles were then calculated with the method presented by the author (Aikala, Phil. Mag. (1976) 33, 603). The obtained profiles and B-functions (Fourier transforms of Compton profiles) as well as anisotropies in these quantities agree qualitatively with the experimental data (P. Pattison and J. Schneider, Acta Cryst. (1980) A 30, 390). The profile values agree with the corresponding experimental ones better for larger Watson sphere radii ($\simeq$ 1.4 - 1.5 Å) but the anisotropies are better reproduced with smaller radii ($\simeq$ 1.2 - 1.3). It is concluded, that the ionic model (3 Li+, N3-) is valid for lithium nitride but the Watson sphere model is too crude to produce satisfactory wave functions for the N3- ion in the crystalline environment.