06.X-07 THE MEASUREMENT OF X-RAY ATTENUATION COEFFICIENTS IN THE 5 TO 100 keV RANGE. By L. Gerward, Laboratory of Applied Physics III, Technical University of Denmark, DK-2800 Lyngby, Denmark.

Standard X-ray crystallography covers the energy range from 5 to 25 keV, making use of commonly available characteristic lines. However, the use of white-beam diffraction techniques, in particular in connection with synchrotron radiation sources, has called for the extension of the upper energy limit to about 100 keV. Attenuation coefficients determined in this extended energy range should be of great value also in dosimetry, fluorescence-analysis, microanalysis etc.

The value of the attenuation coefficient changes by several orders of magnitude within the energy range considered here, in particular when all the elements of the periodic table are taken into account. Thus there is no universal method for measuring X-ray attenuation coefficients, and a number of precautions have to be taken. The paper discusses briefly the following problems:

The use of characteristic lines and white X-rays, such as Bremsstrahlung or synchrotron radiation; crystal monochromatization and collimation and the effect of harmonics; specimen and specimen handling; determination of specimen thickness; X-ray detectors; stability problems; scattering contributions, in particular Bragg scattering and thermal diffuse scattering in crystalline specimens.

06.X-08 SURVEY OF RESULTS ON OXALIC ACID DIHYDRATE. By Philip Coppens, Chemistry Department, State University of New York at Buffalo, Buffalo, N. Y. 14214, USA.

Results of studies performed under the oxalic acid project of the Commission on Charge, Spin and Momentum densities will be compared. They include several X-ray and neutron analyses and at least two different theoretical calculations. Special emphasis will be placed on the comparison of thermal parameters, deformation electron densities and derived physical properties such as net atomic and molecular charges and the dipole moment of the water molecule in the crystal.

06.X-09 ON THE DATA BANK PROJECT FOR CHARGE, SPIN AND MOMENTUM DENSITY DATA. By H.Burzlaff and A. Hountas, Institut für Angewandte Physik, Lehrstuhl für Kristallographie, Universität Erlangen-Nürnberg, Germany, Fed. Rep.

Since the middle of the last year the installation of a data bank for charge, spin and momentum density data was started following a suggestion of M. LEHMANN. The data bank project is supported by the FIZ Karlsruhe, Germany, Fed. Rep. It will contain all papers that give informations on compounds investigated with respect to the properties mentioned above. In detail the data bank will consist of

(i) a data file referring to the papers and their subjects
(ii) a data file with structure factor lists provided by the authors,
(iii) a set of service programs for handling the informations.

The present state of the project and the facilities of the data bank will be discussed.

06.X-10 CHARGE AND MOMENTUM DENSITY STUDIES IN SINGLE CRYSTALS. By J.R. Schneider, Hahn-Meitner-Institut für Kernforschung, Berlin, FRG

Crystalline copper provides a testing ground for the theoretical understanding of the electronic structure of metals involving d-bands. The energy band dispersions E vs $\vec{k}$ were studied by means of angle-resolved photoemission spectroscopy (Thiry, Chandesris, Lecante, Guillot, Pinchaux & Pétroff, Phys.Rev.Lett.(1979)43, 82). A recent self-consistent bandstructure calculation by Bagayoko, Laurent, Singhal & Callaway (Phys. Lett.(1980)76A, 187)provides E vs $\vec{k}$, Compton profiles and structure factors (Bagayoko (1980) private comm.) and, thus, allows an experimental test to be made both of the bandstructure and the groundstate wave functions. On the basis of absolute structure factors measured by means of γ-ray diffractometry and Compton profiles from γ-ray scattering experiments, the contribution of charge and momentum density studies to the understanding of the electronic structure of solids will be discussed. The emphasis is on the necessary accuracy and resolution in Bragg- and Compton scattering experiments. A comparison is

made with the results of investigations of the angular correlation of positron annihilation radiation (Berko, Proc. 5th Int. Conf. Positron Annihilation, Japan 1979, 8A-II-3).

Considerable progress in the field of charge and momentum density studies is expected once Synchrotron radiation and instrumentation adapted to its properties is in use. A 5-circle diffractometer installed at HASYLAB (Hamburg) will be described. The first Compton profile measurements performed at LURE (Paris) on Be metal (Loupias, Petiau, Issolah & Schneider, M., phys. stat. sol. b102 (1980) 79) will be compared with recent γ-ray and X-ray measurements. In the near future it will still be difficult to extend the photon Compton scattering technique to thin film studies. Here high energy electron Compton scattering may become a useful tool, provided the problem of radiation damage can be solved. Another possibility is to explore the interaction of fast ions with thin foils which leads to radiative electron capture (Spindler, Betz & Bell, J. Phys. B 10 (1977), 1561). Again radiation damage limits the range of applications and further cross-section studies are necessary.

06.X-11 ANALYSIS OF THE ELECTRONIC STRUCTURE BASED ON DIFFRACTION AND COMPTON SCATTERING MEASUREMENTS. EXAMPLES: Be AND Li_3N.
By N.K. Hansen, Hahn-Meitner-Institut für Kernforschung, Berlin, FRG

We wish to discuss how combined information from diffraction and Compton scattering experiments may be used to obtain a better understanding of chemical bonding in solids. Two examples will be presented: Be, a metal, and Li_3N, a fast ionic conductor.

For Be the most recent X-ray structure factor measurements (Larsen & Hansen, to be published) are in disagreement with P.J. Brown's previous measurements (Phil.Mag.(1972)26,1377). The earlier data were interpreted as indicating a predominant sp_z hybridization, whereas the new data show only a very small deviation from superimposed free atom densities. On the other hand, the Compton profiles for Be can certainly not be described by free atoms. In order to obtain reasonable agreement with the Compton profiles, we must start from another model (e.g. a free electron gas) or go through a procedure which includes explicitly corrections for solid state effects on the atomic model. We have constructed a simple renormalised free atom model for the 1-electron wave functions which does give rise to some of the right trends both for the structure factors as well as for the Compton profiles, but which certainly does not exhaust the available information.

Li_3N will be used to demonstrate how effects of short and long range interactions can be separated in the Fourier transform of the Compton profile, and how sensitive it is to the nonbonding interactions in this crystal. The analysis supports the conclusions based on NQR and X-ray diffraction results: The bonding in Li_3N is basicly ionic with evidence of considerable distortion of the N^{3-} ion due to wave function overlap with neighbouring ions. It was important for the understanding of the electronic structure that various theoretical models at different levels of sophistication were available, including a recent self-consistent pseudopotential calculation (Kerker, MPI, Stuttgart, to be published).

06.X-12 X-RAY DIFFRACTION STUDIES OF SURFACES AND INTERFACES.
By P. Eisenberger, Bell Laboratories, Murray Hill, NJ 07974, U.S.A.

Using glancing angle Bragg diffraction including the use of total external reflection, one has enough sensitivity with modern high powered X-ray sources to study monolayer structures or buried thin interfaces. Results on reconstructed Ge(100) and on the Aℓ/GaAs interface will be discussed.