06.X-05 PROGRESS REPORT ON THE I.U.Cr. X-RAY ATTENUATION PROJECT. By D.C. Creagh, Physics Department, Royal Military College, Duntroon, A.C.T., 2600, Australia

The importance of an accurate knowledge of the X-ray attenuation coefficients for the proper interpretation of data arising from X-ray diffraction experiments has been recognized for many years. Despite this, few systematic attempts have been made experimentally to determine values of the X-ray attenuation coefficients, and many of these experimental values have been in conflict with one another.

The Commission on Crystallographic Apparatus felt that a need existed to investigate the extent to which different experimental techniques for the measurement of X-ray attenuation coefficients contributed to the uncertainty in their measurement. A committee was formed to inaugurate a project to study the problem.

Participants in the project have been encouraged to use whatever techniques they considered best for the measurement of the X-ray attenuation coefficients, and a wide variety of configurations are currently in use. X-ray generators being used range from synchrotron radiation sources, through conventional and X-ray fluorescence sources, to radio-isotope sources. Various types of monochromators are being employed to select the energy of the incident photon. The energy selectivity of these monochromators, and their capacity for harmonic rejection, varies significantly from experiment to experiment. Detectors in use range from ion chambers, which have a high count rate capability but no energy selectivity, to solid state detectors, which have good energy selectivity but which can cope with only moderate beam intensities.

The design of a system for the determination of X-ray attenuation coefficients requires careful selection and integration of the foregoing components into the system. In this report comment will be made on the types of systems which can be devised to yield good X-ray attenuation data.

To eliminate difficulties which may arise from variations in the physical condition of specimens, participants in this project have received material originating from a common source and having well known physical properties. For instance, the first sets of specimens were prepared from high purity, low dislocation silicon single crystals. They were dispatched to the participants in special holders to minimize damage en route. Most participants have chosen geometries in which the incident beam falls normally onto the specimen surface. Some, however, have chosen to use techniques similar to those of Lawrence and Mathieson (1976, Acta Cryst. A32, 1002-1004) in which the specimen is tilted at an angle to the incident beam. A comparison of these results with those gained using the conventional technique will be given.

Also of importance to the success of X-ray attenuation measurements are the determination of specimen thickness and density, the use of measurements for a wide range of specimen thicknesses to establish that the Beer-Lambert Law does indeed apply, and the correct determination of system dead-time.

To summarize: in giving a report on the progress of the X-ray Attenuation Project suggestions will be made as to those experimental configurations which may best be used to determine X-ray attenuation coefficients. Criteria will also be given for the preparation of specimens for X-ray attenuation experiments.

06.X-06 MEASUREMENT OF X RAY ATTENUATION COEFFICIENTS FOR PHOTON ENERGIES IN THE RANGE 0.1 TO 5KeV. P. Dhez, ERA 719 and LURE-Université Paris Sud, Orsay(France)

In this energy range, photons can interact with several outer and inner shells of an atom; thus the classical behavior of the total attenuation cross section, well known in the hard X-ray region, does not apply here.

An atomic model with a non-coulombic potential, leading to centrifugal barrier effects, can explain the gross features appearing in an absorption spectrum: i.e. delayed onset and large single or double maxima. Elastic and inelastic cross-sections are small in this range; consequently attenuation measurements give the photoabsorption coefficient directly. Progress in the theory of inner shell photoionisation has recently been summarized (A. F. Starace. Appl. Opt. 19, 4051(1980)).

Synchrotron radiation sources emitting a continuum spectrum from I. R. to X rays allow continuous measurements over the 5 to 0.1KeV range and have been used extensively for about ten years. The advantage of the high intensities obtained from these sources over the whole range is sometimes counterbalanced by difficulties arising from higher orders and scattered light. The consequence of these difficulties is demonstrated by the large differences in total cross section ($\simeq 20\%$) measured in different experiments even for simple atoms like the rare gases.

Crystal spectrometers can be used from 5 to about 1KeV. For example a double beryl crystal system gives a resolution of 0.1eV at around 1KeV (M.H. Tuilier et al. Int. Conf. on X Ray Processes Stirling. Aug. 1980) . Grazing incidence spectrometers are commonly used from 0.1 to 0.28KeV(Carbon K edge) but the range to 1KeV, containing most of the K edges for the atoms involved in biological compounds, is more difficult to explore : Gratings must be used only a at very low grazing angles ($\simeq 1°$) and in ultra high vaccuum conditions ($\simeq 10^{-10}$torr) to avoid Carbon contamination; large 2d spacing organic crystals offer an alternative but they are rapidly destroyed by the intense synchrotron source ; metallic multilayers now under study may open new possibilities (R. P. Haelbich et al. App. Phys. Lett. 34, (3)184-(1979)) but only for low resolution studies such as EXAFS at least for the present.

Only rare gases (J. West et al. At. Data Nucl. Data Tables 22, 103(1978)) and mainly alkaline, transition metals or rare earths have been studied (B. Sonntag et al. Solid St. Commun. 7, 597(1969),(T. M. Zimkina et al Sov. Phys. Solid State 9, 1128(1967)) in both gas and solid phases. In some cases, spectra for the two phases are different, not only close to the ionization thresholds but also outside of this energy region ; molecular effects are also present. Thus absorption spectra for compounds cannot be deduced by summing atomic spectra of each component(F. C. Brown Chem. Phys. Lett. (54), 425(1978)) .

The present extensive development of synchrotron sources in several countries should encourage extensive work and should provide experimental absorption coefficients for many atoms. Such results are also neccesary to test new theoretical models currently being developped. A better understanding of the basic photoabsorption process in this range is also required for interpreting the data obtained in other fields such as biology, microlithography and plasma physics for fusion.