

**15.4-05** X-RAY DICHOISM AND POLARIZED ANOMALOUS SCATTERING. David H. Templeton and Lieselotte K. Templeton, Materials and Molecular Research Division, Lawrence Berkeley Laboratory and Department of Chemistry, University of California, Berkeley, California 94720 U.S.A.

Linearly polarized synchrotron radiation has been used to observe X-ray dichroism in both the Kossel structure and the EXAFS spectra of crystals containing vanadyl, uranyl, or bromate ions. A consequence of dichroism is that both the real and imaginary parts of the anomalous scattering depend on polarization direction and molecular orientation (Acta Cryst. (1980) A36, 237). The general case is very complicated to analyze. In a cubic crystal, where there can be no macroscopic dichroism, the beams propagate with a single absorption parameter and no birefringence, yet the polarization of the scattering factor affects the magnitude of the structure factor. At the  $L_3$  absorption edge of uranium the values of  $f'$  and  $f''$  each differ by up to 2.3 electrons according to the polarization geometry. These effects have been measured in diffraction experiments with cubic sodium uranyl acetate. Similar data for cubic sodium bromate are under analysis. These effects will occur even in experiments with unpolarized X-rays because of the polarization dependence of ordinary scattering. They complicate the use of anomalous scattering, near absorption edges, to determine diffraction phases. This work used the facilities of the Stanford Synchrotron Radiation Laboratory and was supported by the National Science Foundation (Grant CHE-7919532) in cooperation with the U.S. Department of Energy.

**15.5-01** AN X-RAY ENERGY-DISPERSIVE DIFFRACTOMETER FOR SYNCHROTRON RADIATION. By J. Staun Olsen, E. Buras<sup>x</sup>, and S. Steenstrup, Physical Laboratory II, University of Copenhagen, and L. Gerward, Laboratory of Applied Physics III, Technical University of Denmark, Lyngby, Denmark.

The availability of dedicated or partly dedicated x-ray synchrotron radiation sources has called for the development of instruments making full use of the specific features of synchrotron radiation. The paper describes a new white-beam energy-dispersive diffractometer built for HASYLAB in Hamburg, FRG, using the radiation from the storage ring DORIS. The following features are discussed:

Horizontal or vertical scattering plane, collimators, sample environment, remote control of goniometer, data acquisition, energy-sensitive detectors using small-area and large-area detector crystals, modes of operation, powder and single crystal diffraction.

The high intensity of the synchrotron radiation is important in high-pressure work, where the beam has to penetrate the material of the pressure cell, and the sample volume is extremely small. The energy-dispersive method is particularly advantageous because of the fixed geometry and the simultaneous recording of all the reflections. Moreover, the use of a spectrum extending to short wavelengths reduces the absorption in the cell and the sample. Examples will be given from a high-pressure study of  $\text{YbH}_2$  using a diamond anvil cell.

The energy-dispersive method is also suitable for high-temperature work. Structural changes can be studied simultaneously with changing sample temperature. Examples will be given from a study of  $\text{Y}_2\text{O}_3$  in the temperature range from room temperature to 1900 °C.

<sup>x</sup>) Also Risø National Laboratory, Roskilde, Denmark.

**15.5-02** THERMAL-VIBRATION EFFECT ON X-RAY INTEGRATED INTENSITIES NEAR K-ABSORPTION EDGES. - DETERMINATION OF THE TEMPERATURE FACTORS IN CuI AND GaSb. By B. Morlon<sup>+</sup>, T. Fukamachi<sup>++</sup>, S. Hosoya<sup>++</sup>, + Laboratoire Diélectriques, Faculté des Sciences, Dijon, France ++ Institute for Solid State Physics, University of Tokyo, Roppongi, Minato-ku, Tokyo 106, Japan.

A general analysis of the influence of the temperature factors  $B_j$  on the opposite reflections  $H$  and  $\bar{H}$ , near an absorption edge in non-centrosymmetric crystals has been given by the present authors (Acta. Cryst. 1979, A 35, 714-717). In this experimental part, an energy dispersive diffractometry has been carried out in the vicinity of the Cu and Ga K-absorption edges for the CuI and GaSb crystals. The experimental energy dependences of the integrated intensities  $I_{555}(\omega)$  and  $I_{\bar{555}}(\omega)$  and of their ratio  $r_5(\omega)$  are given. It is shown that the opposite faces (111) and ( $\bar{1}\bar{1}\bar{1}$ ) behave differently in X-Ray intensity near an absorption edge. The temperature factors are determined ( $B_I=2.0\text{\AA}^2$ ;  $B_{Cu}=3.3\text{\AA}^2$ ;  $B_{Ga}=0.9\text{\AA}^2$ ;  $B_{Sb}=0.4\text{\AA}^2$ ) in the case of CuI and GaSb, by fitting the experimental integrated intensities with those calculated for the mosaic case. The numerical calculations were carried out by using the experimental fine structure of scattering factors for the Cu and Ga atoms.

This anomalous scattering effect could give a method for determining the temperature factors in non-centrosymmetric structures. With synchrotron radiation more accurate measurements can be made on temperature factors using this present technique.

