06.1-01 GAMMA-RAY DIFFRACTOMETERS FOR QUANTITATIVE CHARGE DENSITY ANALYSIS. By F. Ross and W. Yelon, Research Reactor Facility, University of Missouri, Columbia, Mo. 65211.

Valence electron distributions in crystalline solids are considerably more diffuse than are the corresponding distributions of core electrons. For this reason, most of the Bragg diffraction information from the valence electrons occurs at low scattering angles. These reflections are frequently among the largest intensities measured in a conventional x-ray diffraction experiment as well. Because of extinction, absorption, detector linearity, source fluctuations and other intensity-dependent forms of error, the low-angle intense reflections suffer a reduction in reliability. This reduction is usually of the order of 2-5% of F^2 which, for atoms of $Z>10$, exceeds the total valence diffraction contribution in most structure factors.

We have attempted to remove a large fraction of this error by measuring all low-angle data ($\sin\theta/\lambda$ <0.5) with a gamma-ray diffractometer. This dramatically decreases extinction and absorption effects and the increased penetration permits construction of low-temperature instrumentation using aluminum rather than beryllium. The gamma-ray source can be counted directly to determine absolute structure factors which provides an additional important constraint for charge density modeling. We have analyzed electron distributions in several compounds using x-ray and neutron diffraction and the University of Missouri Gamma-Ray Spectrometer(MUGS). The results of these X,N,γ experiments and the design of a longer wavelength source (0.2 instead of 0.120Å for MUGS) suitable for use with a modified picker diffractometer will be discussed.

06.1-02 THE MODULATION X-RAY DIFFRACTION METHOD TO INVESTIGATE THE MICROSCOPIC STRUCTURAL CHANGES AS INDUCED BY AN EXTERNAL ELECTRIC FIELD (GaAs). By Isao Fujimoto, Broadcasting Science Research Laboratories of Nippon Hoso Kyokai, 1-10-11, Kinuta, Setagaya-ku, Tokyo 157, Japan.

The microscopic structural changes induced by an external field such as ionic displacement and redistribution of bonding electrons are important for understanding of dielectric, optical and electronic properties of crystals. However, direct detection of such structural changes by means of X-ray diffraction has been impossible, because the changes in diffracted intensity are too small to be measured by the conventional method. For this end, the present author developed a method "modulation X-ray diffraction" and observed such microscopic structural changes in $LiNbO_3$ and $LiTaO_3$, which are responsible for the electrooptic effect.[3] The purpose of this paper is to report its application to study of chemical bond of GaAs and to demonstrate its capability.

In this method, an alternating electric field (square waves) is applied to the specimen crystal. The diffracted intensities of X rays changes depending on the two alternating states, and the small intensity difference between the two states can be obtained by the synchronized detection. The long-term drift of the measurement system such as those of the intensities of the incident X rays and of electronic instruments can be eliminated so as to allow us to measure the small intensity change with a high accuracy by taking the measurement time sufficiently long. The measurement was automatically controlled with use of a microcomputer. For GaAs, the electric field with frequencies of more than 300 Hz and strengths of up to 80 kV/cm was applied in <111> and <100> directions, and the small changes of 0.01~0.3% in integrated intensity of the diffracted X rays were measured for hhh(h=$\pm$1,$\pm$2,---,$\pm$7) and h00(h=$\pm$2,$\pm$4) reflections using $AgK\alpha_1$ and $MoK\alpha_1$ radiations. In order to avoid strain effects, highly perfect crystals were used. In the analysis of the results, the dynamical formula was used for the integrated intensities.

The displacement of As ions relative to Ga ion framework was determined by measuring the intensity changes for higher order reflections which arises predominantly from the core electrons. By the least squares analysis, the displacement was found to be 7.2×10^{-5}Å in the direction opposite to the external field, i.e., As ion is negatively charged, contrary to most of the results obtained by many other authors. Using the simple theory of dielectrics, the effective charge of the Ga ion was found to be +1.1e.

The displacement of the bond charge was studied using the 222 and $\bar{2}\bar{2}\bar{2}$ reflections. Their structure factors are given by the scattering factor of bonding electrons, f_b, and the difference $(f+f'+if")_{Ga-As}$ in scattering factor between the Ga and As ions. The intensity changes due to the electric field can be determined by the four factors, $(f+f'+if")_{Ga-As}$, f_b, the displacements of the ions and bonding electrons. Using the value of the ionic displacement mentioned above, the three remaining factors were determined by measuring the intensity ratios, $I(222)/I(\bar{2}\bar{2}\bar{2})$, as well as the intensity changes for the two wavelengths, $AgK\alpha_1$ and $MoK\alpha_1$, and the following results were obtained:[1] (1) The bond charge is about 0.6 times of that of Ge. This reflect the ionicity of the chemical bond of GaAs. (2) The displacement of the bond charge is considerably smaller than expected from the simplified point bond charge theory. Therefore, the theory needs some improvement such as taking into account of the spatial distribution of bonding electrons.

Metal-semiconductor contact (Schottky barrier) of Al-GaAs was studied by the similar method, and a strong electric field was detected for the first time.

From these observations, the capability of the modulation X-ray diffraction method may be understood.

06.1-03 GAMMA-RAY SCATTERING - AN ALTERNATIVE TO RADIOGRAPHY? By M. J. Cooper and A. R. Rollason, Department of Physics, University of Warwick, Coventry CV4 7AL, U.K.

The sensitivity of photoelectric absorption to variations in composition is offset by the inevitable averaging through the sample in shadow radiography. If an equally sensitive scattering method is available the signal can be associated with a specific volume of the sample. The use of elastic gamma ray scattering, normalised by the accompanying inelastic Compton scattered intensity has been suggested by Puumalainen, Olkkonen and Sikanen (J. Appl. Radiation and Isotopes, 1977, 28, 785). In the present work ^{241}Am gamma radiation, together with conventional Compton scattering apparatus, has been used to investigate the potential sensitivity of the method for studying variations in composition in a range of solids.