06.3-01 INELASTIC X-RAY SCATTERING FROM Si AND Ge. By H. A. Rosenberg, V. F. Kerkenov, L. I. Kieschnikova, Phys. Dept., Institute of TRANSPORT Engineers, Irkutsk 664026, U.S.S.R.

Integrated over energy inelastic X-ray scattering cross sections $\sigma_{\text{TS}}$ were measured in perfect crystals Si and Ge along $<111>$ direction for $1.2 < \sin \theta < \sqrt{3}$ (region I) and $2/\sqrt{3} < \sin \theta < \sqrt{5}/2$ (region II). In region I, the measurements were done at temperatures ($T$) from 33 to 450K. In region II, the measurements were done at 5 temperatures ($T$) from 33 to 450K applying approximation $\sum_{\text{TS}} \sigma_{\text{TS}} \propto T^2$. The results were compared with the shell model calculations (J. P. Pirie & J. S. Reid, private communication).

After TDS subtraction from $\sigma_{\text{IS}}$, it is shown that in theoretical description of incoherent scattering process one may consider valence electrons in Si and Ge as electron gas. Thereby it is necessary to take account of the possibility of plasmon excitation in region I whereas in region II impulsive Waller-Bartree approximations of the total Compton scattering cross sections are both valid. Synchrotron-radiation opportunities on inelastic scattering measurements are discussed.

06.3-02 COMPTON SCATTERING OF X-RAY PHOTONS FROM STANDING WAVE FIELDS IN THE BRAGG-CASE OF DIFFRACTION. By W. Schulke and U. Bonse, Institut für Physik, Universität Dortmund, 4600 Dortmund 50, West Germany.

Theoretical calculations of the double differential cross section of inelastic X-ray scattering of photons from standing wave fields in the Bragg-case of diffraction are presented. Within the validity of the impulse approximation and with special arrangements of crystal orientation the measurements of the inelastic scattering cross section on X-ray Bragg-scattering single crystals should give information about the projection of the non-diagonal elements $\Gamma (p E p E) \frac{d^2 \sigma}{d p d E}$ of the momentum space one electron density matrix on the directions $\vec{k}_0 \cdot \vec{R}_\perp - \vec{k}_0$ and $\vec{k}_0 \cdot \vec{R}_\perp + \vec{k}_0$, respectively. $\vec{R}_\perp$ and $\vec{R}_\parallel$ are the constituting wave vectors of the Bragg-case standing wave field, $\vec{k}_0$ is the wave vector of the inelastically scattered wave, and $\vec{k}_\parallel$ is the reciprocal lattice vector of the Bragg-reflection. Since the structure factor $F_{\vec{k}_\parallel}$ is only the momentum space average of $\Gamma (p E p E) \frac{d^2 \sigma}{d p d E}$ the proposed novel measurements can yield a new insight into the electronic ground state of the crystal. Furthermore, first results of experimental Compton-profile measurements on Si in the Bragg-reflection position are presented and compared with the theory.

06.3-03 MOLECULAR WAVE FUNCTIONS IN MOMENTUM SPACE. By M. Baramazhi(1), H. Sarrazin(2), J. Navaza(2) and U. Zeeacari(1). Universitat Stuttgart, 7000 Stuttgart 80, W. Germany.効果X-Ray Scattering (X-RS) was carried out with a Siemens D5000 in the (333) Bragg-case of the Si(001) substrate. The results will be compared with theoretical calculations of the total Compton scattering cross section of the He atom in the momentum space as displayed in the work of M. Baramazhi(1) and J. Navaza(2). This is also a valuable check for the numerical solution of the Schrödinger equation in momentum space in a particular basis. The results will be compared with the recent theoretical calculations of the total Compton scattering cross section of the He atom in the momentum space.

Several mathematical techniques are presented, including standard fast Fourier-transform (FFT) techniques and numerical calculation of the involved convolutions. The results will be displayed and discussed. A useful application of the $p$-space calculation is the determination of the "best atomic wave functions" to be introduced in a LCAO procedure. As an example the results for $\text{H}_2$ are displayed. The above methods are extended to the $\text{H}_3$ molecule and preliminary results will be also presented.

06.3-04 CHARGE AND MOMENTUM DENSITY STUDY OF COPPER AND BERYLLIUM METAL. By N.K. Hansen, P. Pattison and J.R. Schneider, Nahn-Weihenst. Institut für Kernforschung, Berlin, FRG.

Absolute structure factors and directional Compton profiles determined from $\gamma$-ray scattering experiments on Cu single crystals provide the basis for a discussion of the electronic structure of this transition metal. Band structure calculations are available which allow a combined study of structure factors, Compton profiles and the energy band dispersions.

Until recently it was generally accepted that there was clear experimental evidence for a bonding interaction in Be metal through the tetrahedral holes in the h.c.p. lattice. The results of new neutron, x-ray and $\gamma$-ray diffraction experiments are in contradiction with the earlier conclusions. In the absence of a band structure calculation which provides both charge and momentum distributions, the experimental diffraction and Compton scattering data are discussed in terms of some simple solid state models.