06.3-01 INELASTIC X-RAY SCATTERING FROM Si AND Ge. Yu.A.Rosenberg, V.F.Karpenko, L.I.Kleschinsky, Phys. Dept., Institute of Transports Engineers, Irkutsk 664028, U.S.S.R.

Integrated over energy inelastic X-ray scattering cross sections σ_{IS} were measured in perfect crystals Si and Ge along <111> direction for $\frac{\sqrt{3}}{8a} \leq \frac{\sin\theta}{\lambda} \leq \frac{\sqrt{3}}{4a}$ (region I) and $\frac{3\sqrt{3}}{4a} \leq \frac{\sin\theta}{\lambda} \leq \frac{5\sqrt{3}}{4a}$ (region II), where "a" is the lattice parameter. Single phonon scattering cross sections σ^{1}_{TDS} were appreciated theoretically using rigid ion model and the known phonon dispersion curves. The contribution of multiphonon processes in region II was determined from measurements σ_{IS} at 5 temperatures (from 83 to 450K) applying approximation $\sum_{i=2} \sigma^{i}_{TDS} \propto T^2$. Resulted σ_{TDS} were compared with the shell model calculations (J.D.Pirie & J.S.Reid(1979) private communication).

After TDS subtraction from σ_{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 Impulse as Waller-Hartree 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. Schülke 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-diffracting single crystals should give information about the projection of the non-diagonal elements $\Gamma(\vec{p}|\vec{p}+\vec{g}_h)$ of the momentum space one electron density matrix on the directions $\vec{Q}_o=\vec{K}_o-\vec{K}'$ and $\vec{Q}_h=\vec{K}_h-\vec{K}'$, respectively. $\vec{K}_o$ and $\vec{K}_h$ are the constituting wave vectors of the Bragg-case standing wave field, $\vec{K}'$ is the wave vector of the inelastically scattered wave, and $\vec{g}_h$ is the reciprocal lattice vector of the Bragg-reflection.
Since the structure factor F_h is only the momentum space average of $\Gamma(\vec{p}|\vec{p}+\vec{g}_h)$ the proposed novel measurements can yield 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. Defranceschi(1), M. Sarrazin(2), J. Navaza(2) and G. Tsoucaris(2)(1) ENSJF, 1 rue M. Arnoux, 92120 Montrouge, (2) Lab. Physique, Centre Pharmaceutique, 92290 Chatenay-Malabry, France.

Momentum-Space calculations exhibit two kinds of advantages over position space : First, the numerical solution of Hartree-Fock equation is feasible without expansion of the wave functions in a particular basis. Equations exhibit only one avoidable singularity even for the multicenter case. This is clear from the general form of the Schrödinger equation in momentum p-space for one particle.

$$\Phi^{(1)}(\vec{p}) = \frac{V \otimes \Phi^{(o)}}{\frac{p^2}{2} - E} = \frac{1}{\frac{p^2}{2} - E} \int V(\vec{q})\, \Phi^{(o)}(\vec{p}-\vec{q})\, d^3q$$

with ; $\Phi^{(o)}(\vec{p})$: zero approximation wave function
$\Phi^{(1)}(\vec{p})$: first approximation wave function
$V(\vec{p})$: Fourier transform of the potential $v(\vec{r})$

Several mathematical techniques are presented, including standard fast Fourier-transform (FFT) techniques and numerical calculation of the involved convolutions. Second, momentum representation contributes in an original way to a better understanding of several physical problems arising in quantum chemistry. The two-body density matrix involving the electronic correlation are examined in both position and momentum space. 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 H_2 are displayed. The above methods are extended to the 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, Hahn-Meitner-Institut für Kernforschung, Berlin, FRG

Absolute structure factors and directional Compton profiles determined from γ-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 γ-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.