11.4-1   HYDROSTATIC PRESSURE AND UNIAXIAL STRESS DEPENDENCE OF THE SILICON (222) X-RAY REFLECTION POWER. By U.Pietsch,Arbeitsgemeinschaft A(III)B(V)-Halbleiter, Karl-Marx-Universität, Leipzig, DDR.

For the interpretation of the silicon bond charge properties a moleculetheoretic model is introduced (Pietsch,phys.stat.sol.(b),120,183 (1983)). Both the total valence electron density and the bond charge, respectively, are constructed by superposition of diatomic molecule densities. Each molecule contains an individual overlap charge. The coefficients of the Gaussian like /s+sp₃> model wave functions are fitted to the known valence electron density of the solid state.
The bond charge amount depends on both the variation of the next neighbour distance ΔR and the changing of the bond angles $\Delta\Theta$, respectively.
The hydrostatic pressure dependence of the silicon (222) reflection power was published by D.R.Yoder-Short et.al.(Phys.Rev.Lett 149, 1438 (1982)). Using the above model the increased reflection power up to 10 GPa is described by the bond length dependence of the overlap charge. The coefficients of the model valence orbitals remain constant. The following decreasing of the (222) intensity up to the phase transition point at 12.5 GPa is interpreted by an increasing of the /s> portion at the model wave function.
After the precise determination of the internal strain parameter by H.D'Amour et. al.(J. Appl.Cryst. 15, 148 (1982)) and C.S.G. Cousins et. al.(J.Appl.Cryst. 15, 154(1982)) the analysis of the uniaxial strain dependence of the bond charge is of interest. The variation of the "forbidden" reflection powers for [001]and [011] stress are calculated with respect to the /p> portions of the model valence orbitals.For [001]stress, for instance, the (222) reflection intensity must decrease according to both the variation of the next neighbour distance and the changing of the bond angles, respectively. Neglecting the bond angle depended part a generally increased (222) reflection power will be found.
Therefore, these experiments would give a direct indication of the /p> like portions of the covalent bond in elemental semiconductors.

11.4-2   DEBYE-WALLER FACTORS OF SOME CRYSTALS WITH SIMPLE STRUCTURES. By D.B. Sirdeshmukh, Physica Department, Kakatiya University, Warangal - 506 009, India.

The Debye-Waller factor is no longer a mere correction factor for diffraction intensities. It has emerged as an independent solid state parameter capable of providing a wide range of information about the crystal.

This laboratory has on hand an extensive programme on the X-ray determination of Debye-Waller factors of crystals. Using a powder diffractometer, twenty crystals with NaCl structure, nine with CsCl structure and five with CaF₂ structure have been investigated so far. These include ionic crystals, refractory materials and rare earth compounds. The results are presented.

Apart from yielding values of amplitudes of vibrations and Debye temperatures, the Debye-Waller factors have provided interesting information regarding such aspects as the interatomic binding, the effect of mass ratio and electron environment on atomic vibration amplitudes and thermal defects in these crystals, some of which are discussed.

11.4-3   GENERALIZED VIRIAL APPROACH IN THE CRYSTALLINE STATE THEORY. By V.K.Pershin.Ural Polytechnical Institute,620002 Sverdlovsk,USSR

The infinite "linear" equations system

$$\sum_{i j \vec{p}} x^{si}_{\alpha j}(\vec{n},\vec{p})\ R^{ig}_{j \beta}(\vec{p},\vec{m}) = kT\delta_{sg}\,\delta_{\alpha\beta}\,\delta_{\vec{n}\vec{m}}\ ,$$

where $x^{si}_{\alpha j}(\vec{n},\vec{p}) = <u^s_\alpha(\vec{n})\ u^i_j(\vec{p})>$ and $R^{ig}_{j\beta}(\vec{p},\vec{m}) = <\partial^2 U/\partial u^i_j(\vec{p})\partial u^g_\beta(\vec{m})>$, is obtained at the pseudoharmonic approximation by use of the generalized form of the uniform distribution theorem as following

$$<u^s_\alpha(\vec{n})\partial U/\partial u^g_\beta(\vec{m})> = kT\delta_{sg}\,\delta_{\alpha\beta}\,\delta_{\vec{n}\vec{m}},$$

where $u^s_\alpha(\vec{n})$ is the displacement α-component of the particle s from the equilibrium position in the knot with the radius-vector $\vec{n}$;U is the potential crystal energy;T is the absolute temperature.On the basis of the correlations weakening theorem for threedimensional systems it is proved that this system has a single solution.It is shown that Kramer's rules are applicable for the solution of the virial equations system.The spectral theorem matrix formulation allowing to represent any pair correlation function in the dependence on the lattice force constants and to determine the contribution of each of them into the value of this function is given.The developed approach being a new mathematical version of the self-consistent field theory allows to investigate the structural dynamic crystal state without the analysis of the own vibration spectrum of the lattice and the integration over the k-space.