

11.4-4 TRANSVERSAL CORRELATIONS AND TRANS-LATIONAL SYMMETRY IN QUASI-LOWDIMENSIONAL AN-HARMONIC CRYSTALS. By V.K.Pershin and I.S. Gersht. Ural Polytechnical Institute, 620002 Sverdlovsk-2, USSR.

Long-range order in the system of weakly interacting chains and the structure of layered crystal type is investigated at the pseudo-harmonic approximation of the selfconsistent phonon field technique. The influence of the weak interchain and interplanar interaction on the convergence of mean-square deviations from the equilibrium position in the chain  $\langle u_c^2 \rangle$  and in the layer  $\langle u_l^2 \rangle$  is considered. The result is  $\langle u_c^2 \rangle \sim kT(\Phi_{lc})^{-1/2}$ ,  $\langle u_l^2 \rangle \sim -kT \ln \Phi_{ll}$  where  $\Phi_{lc}$  and  $\Phi_{ll}$  are the transversal force constants between the chains and layers. For the case of central forces it is shown that  $\Phi_{ll}^h = 0$  at the harmonic approximation and the account of the interaction anharmonism leads to  $\Phi_{ll}^{anh} \neq 0$ . Thus, long-range order  $\langle u_l^2 \rangle^h \rightarrow \infty$  is not possible in the quasi-lowdimensional system of harmonic oscillators in spite of the fact that the inter-chain and interplanar potential is not suggested to be equal to zero. The mean-square deviation convergence in such crystals (i.e. the long-range translational symmetry) is provided with the transversal correlations between the neighbouring chains  $\langle u_c^2 \rangle \sim kT(\Phi_{lc}^{anh})^{-1/2}$  and the layers  $\langle u_l^2 \rangle \sim -kT \ln \Phi_{ll}^{anh}$ , respectively. These correlations are due to the anharmonism of the interpartial interaction.

11.4-5 X-RAY EVIDENCE OF DIRECT GENERATION OF NON-EQUILIBRIUM PHONONS IN QUARTZ BY INFRARED RADIATION. By L. D. CHAPMAN, S. M. HSIEH, and R. COLELLA. Purdue University, Physics Department, West Lafayette, Indiana, 47907, U.S.A.

Quartz is a suitable crystal for generation of non-equilibrium phonons. It has a strong absorption band centered at about 9.3  $\mu$ , due to one of the TO phonons at  $K=0$ . The light of a CO<sub>2</sub> laser has several lines around 10  $\mu$ , and is strongly absorbed in quartz, which is an indication of favorable conditions for phonon generation. Quartz is a polar crystal, and is expected to respond to electromagnetic stimulation. Non-equilibrium TO phonons have been resonantly excited by means of a 15KW Q-switched CO<sub>2</sub> laser, with a repetition rate of 10KHz and pulse duration of 200 nsecs. The crystal was cut in the form of a thin slab perpendicular to the c-axis and cooled to 77°K. Monochromatic Cu-K $\alpha$  radiation ( $\lambda = 1.54\text{\AA}$ ) was used. The region around (004) in K-space was explored because the (004) reflection is absent and only optical phonons with  $K = 0$  can contribute diffuse intensity in that region. A time resolved counting technique was used, with a resolution time of 500 nsecs. To avoid problems associated with noise generated by the laser, the experiment was repeated with the laser beam blocked, and the counting rate was subtracted out. The effect can also be seen at the zone boundary, which can only result from anharmonic decay of high frequency phonons with  $K = 0$ . It has been verified that the effect is visible only when the polarization vector of the laser beam has a non-zero component along the scattering vector of the x-rays, as expected.

11.4-6 EXPERIMENTAL EVIDENCE OF PHASE EXCITATIONS IN SOLIDS BY X-RAY DIFFRACTION. By L. D. CHAPMAN AND R. COLELLA, Purdue University, Physics Department, West Lafayette, Indiana, 47907, U.S.A.

While ordinary Bragg reflections vary with temperature according to the usual Debye-Waller factor, it is not clear what should be the temperature dependence of satellite reflections generated by Charge Density Waves (CDW's). The existence of phasons<sup>1</sup> would drastically alter their temperature dependence without affecting Bragg reflections. A phason is a thermal instability in the phase of a CDW. Phasons are the analog of phonons, in the sense that a phason is a thermal instability in the lattice position of an atom. Phasons play the same role for CDW satellites as phonons do for Bragg reflections. However, phasons are much more effective in attenuating intensities of diffraction spots than phonons. We have investigated the temperature dependence of six first order satellites in TaS<sub>2</sub>, in the incommensurate T<sub>1</sub> phase ( $T > 80^\circ\text{C}$ ). Three satellites were close to the (010) reflection, the other three were close to the (030). It was found that their temperature dependence was much stronger than that of the (030). More importantly, it was found that all satellites had the same temperature dependence on a semi-logarithmic plot of intensity vs. temperature, with K<sup>2</sup> values ranging from 2.5 to 46  $\text{\AA}^{-2}$  (K = scattering vector). We interpret this result, theoretically predicted in ref. 1, as the signature of a Phason Temperature Factor:  $e^{-CT}$ , with  $C = 1.8 \times 10^{-3} \text{K}^{-1}$ . At 90°C this factor attenuates all first order satellites by a factor of 4.

1) A. W. Overhauser, Phys. Rev. B3, 3173 (1971).

11.4-7 MULTIPHONON DIFFUSE X-RAY SCATTERING FROM SPHALERITE STRUCTURE MATERIALS. John S. Reid, Department of Natural Philosophy, The University, Aberdeen, AB9 2UE, Scotland.

It has been known since the work of Waller that the total harmonic scattering of X-rays by all phonon processes can be written as a multiple summation over the real and the reciprocal lattices. Although the total scattering has traditionally been expanded as a power series in multiphonon processes, it was shown by Reid & Smith in 1970 (J. Phys. C 3, 1513-1526) that the total scattering cross-section could be evaluated for the NaCl structure by a computer that was then considered large but which would now be regarded as modest. The technique is extended here to the sphalerite structure and results will be presented for the representative materials GaAs, CdTe, CuI and SiC showing the variation of scatter with scattering vector and with temperature. These results illustrate that even at room temperature the multiphonon scattering may be comparable to the single phonon scattering for quite modest scattering vector. The eigendata used is that produced by the current generation of lattice dynamical models.

The program is written in Fortran 77 in a modular form that lends itself to adaptation to other structures. Routines are included to handle the zero-phonon contribution. Attention has been given to efficient calculation and internal checks. It is intended that the program will be published through the CPC library.