11. REAL AND IDEAL CRYSTALS

11.4-4 TRANSVERSE CORRELATIONS AND TRANSLATIONAL SYMMETRY IN QUASI-LOWDIMENSIONAL ANHARMONIC CRYSTALS. By V. K. Pecharsky and I. S. Gersht. Ural Polytechnical Institute, 620002 Sverdlovsk-2, U.S.S.R.

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 self-consistent 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 \( \langle u^2 \rangle \) and in the layer \( \langle u^2 \rangle \) is considered. The result is \( \langle u^2 \rangle \sim kT(\Phi - \langle \Phi \rangle) / \langle \Phi \rangle - kT \ln(\Phi / \langle \Phi \rangle) \), where \( \Phi_0 \) and \( \Phi_{1.1} \) are the transversal force constants between the chains and layers. For the case of central forces it is shown that \( \Phi = 0 \) at the harmonic approximation and the account of the interaction anharmonism leads to \( \Phi_{1.1} \neq 0 \). Thus, long-range order \( \langle u^2 \rangle \rightarrow \infty \) is possible in the quasi-low-dimensional system of harmonic oscillators in spite of the fact that the harmonic decay 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 neighboring chains \( \langle u^2 \rangle \sim kT \ln\left(\Phi_{1.1} / \Phi_{1.0} \right) \) and the layers \( \langle u^2 \rangle \sim kT \ln\left(\Phi_{1.0} / \Phi_{1.1} \right) \), respectively. These correlations are due to the anharmonism of the interpartial interaction.

11.4-5 \( \sigma \)-RAY EVIDENCE OF DIRECT GENERATION OF NON-EQUILIBRIUM PHONONS IN QUARTZ BY INFRARED RADIATION. By L. D. Chapman, S. M. Hsieh, and R. Coella. 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 T0 phonons at \( K = 0 \). The light of a \( \text{CO}_2 \) 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 T0 phonons have been resonantly excited by means of a 15kHz Q-switched \( \text{CO}_2 \) laser, with a repetition rate of 10kHz and pulse duration of 200 nanoseconds. The crystal was cut in the form of a thin slab perpendicular to the c-axis and cooled to 77K. Nonresonant Cu-K\( \alpha \) radiation (\( \lambda = 1.54\) \( \AA \)) 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 300 nanoseconds. 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 the combination 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 \( \sigma \)-rays, as expected.

11.4-6 EXPERIMENTAL EVIDENCE OF PHASE EXCITATIONS IN SOLIDS BY \( \sigma \)-RAY DIFFRACTION. By L. D. Chapman and R. Coella, 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 phonons would drastically alter their temperature dependence without affecting Bragg reflections. A phonon is a thermal instability in the phase of a CDW. Phonons are the analog of phonons, in the sense that a phonon is a thermal instability in the lattice position of an atom. Phonons play the same role for CDW satellites as phonons do for Bragg reflections. However, phonons are much more effective in attenuating intensities of diffraction spots than phonons. We have investigated the temperature dependence of six first order satellites in \( \text{Te}_3\), in the incommensurate T-phase (\( T > 80^\circ \)). Three satellites were close to the (010) reflection, the other three were close to the (010). 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 \( K^2 \) values ranging from 2.5 to 46 \( \text{A}^{-2} \) (\( K = \text{scattering vector} \)). We interpret this result, theoretically predicted in ref. 119, as the signature of a Phase Temperature Factor: \( I(004) \sim K^2 \), with \( K = 0.8x10^{-1}/K \). At 90°C this factor attenuates all first order satellites by a factor of 4.

11.4-7 MULTIPHONON DIFFUSE \( \sigma \)-RAY SCATTERING FROM SPHALERITE STRUCTURE MATERIALS. John J. 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 \( \sigma \)-rays by all phonon processes can be written as a multiple summation over the real and reciprocal lattices. Although the total scattering has traditionally been expanded as a power series in multiphonon processes, it was shown by Waller & Smith in 1970 (J. Phys. C 3, 1513-1526) that the total scattering cross-section could be evaluated for the \( \text{NaCl} \) 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, \( \text{CdTe} \), 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 algorithm used is that produced by the current generation of lattice dynamical models.