PHYSICAL REVIEW B VOLUME 9, NUMBER 6 15 MARCH 1974

Local-mode frequencies due to isoelectronic impurities in zinc-blende-type crystals

D. N. Talwar* and Bal K. Agrawal
Department of Physics, University of Allahabad, Allahabad-211002, India

(Received 10 August 1973)

The localized mode frequencies for a number of isoelectronic impurity atoms in II-VI and III-V compounds have been calculated in the mass-defect approximation by the Green's-function method. The results of a seven-parameter second-neighbor-ionic (SNI) model for the host lattice have been employed for computing the high-frequency lattice Green's function. The calculated local-mode frequencies are seen to be in strikingly good agreement with the experimental values. Thus the isoelectronic impurities in zinc-blende-type crystals discussed in the present article behave very nearly as mass defects.

I. INTRODUCTION

A small concentration of substitutional impurities in crystalline lattices may give rise to exceptional (local, gap, or resonance) vibrational modes. A wide variety of experimental techniques, viz., the impurity-induced infrared absorption, Raman spectroscopy, specific-heat measurements, Mössbauer effect, neutron scattering, tunneling between the superconductors, and the temperature dependence of the relaxation time for spin flips (for paramagnetic impurities) have been used to study the exceptional vibrational modes in ionic crystals, in polar and homopolar semiconductors and in metals. The most thoroughly studied experimental method for investigating the dynamical properties of imperfect crystals is the impurity-induced infrared absorption. A second powerful tool that has been drawing much interest these days is Raman spectroscopy.

In diatomic systems such as ionic crystals or polar semiconductors of the zinc-blende structure, the substitutional impurities occupy sites of cubic symmetry. If the substitutional atom is light enough compared to the mass of the host-lattice atom, or is coupled much more strongly to the neighboring atoms than the atom it replaces, one observes the localized or bound states. The frequencies of the localized states lie outside the range of the allowed phonon frequencies of the host crystal. The displacement amplitudes of the atoms in these modes decay faster than exponentially with increasing distance from the impurity site. If there exists a gap in the frequency spectrum of the crystal, the localized vibration modes appearing in the gap region are named as gap modes. There is, in fact, no fundamental distinction between a localized mode and a gap mode.

A number of experimental studies have shown the occurrence of the local modes. The first evidence for the appearance of the localized modes was furnished by Schaefer[1] who observed peaks in the absorption spectrum in the far-infrared region due to *U* centers (H^- ions) in alkali halides. Later, the localized modes were also detected owing to other light impurities such as boron[2] and carbon[3] in silicon. More recently, the list has grown to include the localized modes due to a number of substitutional impurities in II-VI and III-V semiconductors.[4] A theoretical calculation of the localized mode (LM) frequencies in some III-V semiconductors has been made by Krishnamurthy and Haridasan[5] using a simple molecular model. Recently an elementary phonomenological linear diatomic-chain model[6] has been applied to predict the LM frequencies due to substitutional impurities in various systems.

The above approximate calculations suggest that the mass-defect approximation is quite valid and the effects of force-constant changes caused by the impurities on the LM frequencies in II-VI and III-V compounds are not significant. Another technique, i.e., the well-known Green's-function method for estimating the LM frequencies is more realistic in comparison to the molecular or the phenomenological linear diatomic-chain models as the former method takes into account the effects of the entire phonon spectrum of the lattice. Thus in the Green's-function method we require a detailed knowledge of the frequencies and the polarization vectors of normal modes in the pure crystal. In a recent paper, Gaur *et al.*[7] have calculated the LM frequencies in a number of II-VI and III-V compounds using a Green's-function technique in the mass-defect approximation. In order to estimate the LM frequencies these authors have used the results for the eigenfrequencies and eigenvectors of the phonon states as obtained by a four-parameter rigid-ion model (RIM).[8] Although the values of the LM frequencies as obtained by Gaur *et al.*[7] are in reasonable agreement with the experimental values, there still exists certain discrepancies, probably due to the use of a simplified lattice-dynamical model.

The four-parameter RIM, though, gives an exact account of the long-wavelength optical phonons, but discrepancies up to ~ 50% for the acoustic-mode frequencies are seen to exist when compared with the observed values at the Brillouin-zone boundary.[9] On the other hand, a seven-parameter second-neighbor-ionic (SNI) model of Banerjee and Varshni[10] gives a much better agreement with the neutron data of GaAs, GaP, CuCl,[10] ZnSe, InSb,[11] CuI, and ZnS[12] and the errors in the transverse-acoustic-mode frequencies are reduced to ~ 10%. Also, the model has been seen to be quite successful in explaining the thermodynamical properties of various II-VI and III-V semiconductors[10,13] and the impurity-induced infrared absorption due to beryllium substitutional impurities in cadmium telluride.[14] Furthermore, since the application of the shell model and its various ramifications for discussing the lattice dynamics have been questioned on basic grounds,[15] it is worthwhile to rely on the simple but more physically meaningful seven-parameter SNI model[10] in the calculation of the vibrational properties of perfect or imperfect zinc-blende-type crystals. We find that the calculated local-mode frequencies in the mass-defect approximation with the use of SNI model are in very good agreement with the experimental values.

The present paper is devoted to study the lattice vibrations of isoelectronic impurities[16] in zinc-blende-type semiconductor compounds. We have restricted ourselves to the study of these impurities with the simple reason that they are expected to incur small changes in the atomic interactions.[17] A Green's-function method in the mass-defect approximation has been employed to calculate the local-mode frequencies. In the calculation we have used the eigenamplitudes and the eigenfrequencies of the normal modes of the perfect crystals obtained earlier by incorporating the SNI lattice-dynamical model (as described in Sec. II). Explicit calculations have been performed for the different isoelectronic impurities in CdTe, ZnTe, ZnSe, ZnS, InSb, InP, InAs, GaAs, GaSb, and GaP. The calculated LM frequencies have been compared with the experimental results and with those obtained earlier in a four-parameter RIM. A somewhat better agreement than that obtained by Gaur *et al.*[7] has been observed in almost all the cases.

II. LATTICE DYNAMICS

Most of the II-VI and III-V semiconductor compounds exhibit the zinc-blende crystal structure with point group (T_d) symmetry. The dynamics of these compounds has widely been studies using both phenomenological shell[18–20] and rigid-ion models.[8–12] The shell model, which had previously been proved to be very successful for studying the lattice dynamics of alkali halides, is not the best that can be chosen for the zinc-blende-type crystals. It contains far too many disposable parameters, some of them have very little physical significance. The unique evaluation of those parameters can be made only if extreme restrictions are placed on the model. It is evident from the fact that a somewhat simpler six-parameter shell model fails to give even an approximate phonon dispersion relation for ZnS,[20] particularly with the available data on the optical modes, and thus the model have been questioned on basic grounds.[15] This example intends to indicate the unsuitability of the shell model for predicting phonon frequencies in zinc-blende-type crystals particularly for those for which little experimental data are known. The rigid-ion model, on the other hand, does not suffer from the defect to the same extent. A four-parameter RIM has been applied to ZnS by Vetelino *et al.*[9] and somewhat better agreement than that provided by the shell model was obtained. Vetelino *et al.*[9] evaluated the involved four-parameters from the elastic constants and the zone-center phonon frequencies. A seven-parameter SNI model of Banerjee and Varshni[10] provides better agreement with the neutron data for GaAs, GaP, CuCl,[10] InSb, ZnSe,[11] CuI, and ZnS.[12] In the present model, the involved lattice-dynamical-model parameters have been evaluated utilizing the zone-center (Γ) and zone-boundary frequencies at the critical point (X) as an input, while the three elastic constants c_{11}, c_{12}, and c_{44} are used only as constraints on the values of the parameters. If one insists on the values of the elastic constants (see Velelino *et al.*[9]), the resulting agreement with the zone-boundary phonon frequencies will be rather poor. Also in many cases, of course, the zone-boundary phonon frequencies are more accurately known than the elastic constants and provide a better basis for the evaluation of the parameters. In the absence of optical data (as is the case with a few systems), we have follow reliable theoretical approaches (described in Secs. IIA and IIB to get an approximate estimation of the optical- and acoustic-zone-boundary phonon frequencies so as to evaluate the model parameters.

In SNI model the seven lattice-dynamical-model parameters α, β, μ_1, μ_2, λ_1, λ_2 and χ are related with the three second-order elastic constants by the following relations:

$$2ac_{11} = 0.1255\chi + \alpha + 4(\mu_1 + \mu_2) , \tag{1}$$

$$2ac_{12} = -1.324\chi + 2\beta - \alpha - 2(\lambda_1 + \lambda_2) + 2(\mu_1 + \mu_2) , \tag{2}$$

and

$$2ac_{44} = -0.063\chi + \alpha + 2(\lambda_1 + \lambda_2) + 2(\mu_1 + \mu_2) - 2a\,\frac{A^2}{B} , \tag{3}$$

with

$$2a\,\frac{A^2}{B} = \frac{(1.2595\chi - \beta)^2}{\alpha - \frac{1}{6}\pi\chi} .$$

Four of the model parameters α, χ, μ_1 and μ_2 may be independently evaluated from the zone-center and zone-boundary phonon energies at the critical point (X) by the relations

$$\alpha = \frac{m^*}{12}\left[\omega^2_{\mathrm{LO}(\Gamma)} + 2\omega^2_{\mathrm{TO}(\Gamma)}\right] , \tag{4}$$

$$\chi = \frac{m^*}{2\pi}\left[\omega^2_{\mathrm{LO}(\Gamma)} - \omega^2_{\mathrm{TO}(\Gamma)}\right] , \tag{5}$$

$$\mu_1 = \tfrac{1}{4}\left[\tfrac{1}{4} m_1 \omega^2_{\mathrm{LO}(X)} - \alpha - 0.541\,25\chi\right] , \tag{6}$$

and

$$\mu_2 = \tfrac{1}{4}\left[\tfrac{1}{4} m_2 \omega^2_{\mathrm{LA}(X)} - \alpha - 0.541\,25\chi\right] , \tag{7}$$

with $m^* = m_1 m_2/(m_1 + m_2)$ ($m_1 < m_2$).

Using these values of the calculated parameters approximate values of β and $(\lambda_1 + \lambda_2)$ are calculated from their relations with the elastic constants [Eqs. (1)-(3)]. The value of the parameter β is varied slightly in a way to get the values of the parameters λ_1 and λ_2 independently from their relations with the zone-boundary phonon energies such that they satisfactorily reproduce the zone-boundary TO(X), TA(X) phonon energies

$$\lambda_1 = \tfrac{1}{8} m_1\left[\tfrac{1}{2}(\omega^2_{\mathrm{TO}(X)} + \omega^2_{\mathrm{TA}(X)}) + \{\tfrac{1}{4}(\omega^2_{\mathrm{TO}(X)} - \omega^2_{\mathrm{TA}(X)})^2 - (4\beta - 5.335\chi)^2/m_1 m_2\}^{1/2} - (4/m_1)(\alpha + 2\mu_1 - 0.27\chi)\right] \tag{8}$$

and

$$\lambda_2 = \tfrac{1}{8} m_2\left[\tfrac{1}{2}(\omega^2_{\mathrm{TO}(X)} + \omega^2_{\mathrm{TA}(X)}) - \{\tfrac{1}{4}(\omega^2_{\mathrm{TO}(X)} - \omega^2_{\mathrm{TA}(X)})^2 - (4\beta - 5.335\chi)^2/m_1 m_2\}^{1/2} - (4/m_2)(\alpha + 2\mu_2 - 0.27\chi)\right] . \tag{9}$$

We have followed the procedure as described above for the systems where detailed data of phonons from inelastic neutron scattering are available,[11,12] in order to calculate the phonon dispersion throughout the Brillouin zone.

For the systems where little experimental data for zone-boundary phonon energies are available, we have followed the following theoretical approaches to get an approximate estimation.

A. Optical- and acoustic-phonon energies

An approximate estimation of the longitudinal-optical and -acoustical phonon energies at the critical point (X) can be made by plotting values of these phonons already known, either from the neutron scattering or by Raman scattering experiments, as a function of $(2ac_{11}m_1)^{1/2}$ and $(2ac_{11}/m_2)^{1/2}$ for various compounds having zinc-blende crystal structure (see Figs. 1 and 2 of Ref. 21). Both of these curves are approximately linear. The calculated values of $(2ac_{11}/m_1)^{1/2}$ and $(2ac_{11}/m_2)^{1/2}$ ($m_1 < m_2$) for the systems under study, in turn, give the longitudinal-optical and -acoustical phonon energies. Our theoretically calculated values for the LO(X) phonon energies are in reasonably good agreement with those obtained by second-order Raman scattering infrared absorption and other optical measurements wherever available. For the case of ZnTe and InP, our calculated values for the LO(X) phonon energies are surprisingly in good agreement with the values obtained by Irwin and LaCombe[22] and by Alfray and Borscherds,[23] while interpreting the second-order Raman spectrum of ZnTe and InP, respectively, in terms of four LO, TO, LA, and TA critical-point phonons.

B. Acoustical-phonon energies

The dispersion relations of GaAs,[18,24] GaP,[19] InSb,[25] InP[23] (acoustical branches only), ZnSe,[26] and ZnS[27] have been carefully studied by neutron scattering techniques. By plotting the dispersion of acoustical phonons for the [100] direction for any one of these compounds, the slopes of the dispersion curves near $\vec{q} = 0$ can be extrapolated to the zone boundary at X to give the "linear-limit" values. These linear-limit energies can be calculated from the experimentally determined elastic constants by the relations[28]

$$[L, \omega_{\mathrm{LA}(X)}] = (c_{11}/\rho)^{1/2}(2ca)^{-1} , \tag{10}$$

and

$$[L, \omega_{\mathrm{TA}(X)}] = (c_{44}/\rho)^{1/2}(2ca)^{-1} , \tag{11}$$

where ρ is the crystal density and $2a$ is the lattice constant; $[L, \omega_{\mathrm{LA}(X)}]$ and $[L, \omega_{\mathrm{TA}(X)}]$ are the "linear-limit" longitudinal- and transverse-acoustical-phonon energies at the critical point (X).

The acoustic-phonon energies can be correlated to the above linear-limiting values as

$$\omega_{\mathrm{LA}(X)} = c_1[L, \omega_{\mathrm{LA}(X)}] \tag{12}$$

and

$$\omega_{\mathrm{TA}(X)} = c_2[L, \omega_{\mathrm{TA}(X)}] , \tag{13}$$

where c_1 and c_2 are the unknown constants having positive values less than unity. These constants have been evaluated from the known dispersion curves for the acoustical-phonon energies and are taken to be the same for other similar type of compounds. It is found that the LA(X) phonon energies calculated in this manner and by the procedure as described in Sec. II A are very similar to the optical data wherever available. The same is also true for the case of TA(*X*) phonon energies.[21]

With the help of Brout sum rule,[29] the value of energy for the TO(*X*) phonon can be calculated using optical data for the energies at the center of the Brillouin zone and the calculated values of the energies for LO(*X*), LA(*X*), and TA(*X*) phonons. For the systems where detailed inelastic-neutron-scattering data are not available, the involved lattice-dynamical-model parameters and thus the lattice dynamics throughout the Brillouin zone were calculated in a manner as described in our earlier paper.[21]

To make a survey of 24 576 frequencies, the translational vectors of the reciprocal space were divided into 16 equal parts that give rise to 4096 equally spaced points inside the first Brillouin zone. From the symmetry considerations of the Brillouin zone for the zinc-blende structure, one needs to know the frequencies only in the range

$$\vec{q}=\frac{\pi}{2a}\frac{1}{16}(q_x, q_y, q_z) ,$$

where the positive integers q_x, q_y, q_z satisfy the following inequalities

$$0 \leq q_x \leq q_y \leq q_z \leq 16$$

and

$$|q_x+q_y+q_z| \leq 24 .$$

There are 149 points defined by these numbers in this section and there are 48 such sections in the Brillouin zone.

III. LOCAL-MODE FREQUENCIES

The frequencies of the impurity modes (local, gap, or resonance) may be calculated by solving the equation

$$|D(z)| = |\overleftrightarrow{I}+\overleftrightarrow{g}(z)\overleftrightarrow{p}(\omega^2)| = 0 , \tag{14}$$

where $\overleftrightarrow{I}$ is the unit matrix; $\overleftrightarrow{p}(\omega^2)$ and $\overleftrightarrow{g}(z)$ are the perturbation and the lattice-Green's function matrices in the subspace of a single impurity, respectively.

In the mass-defect approximation the dimension of $D(z)$ is 3×3. The point-group symmetry of the impurity site in zinc-blende-type crystals is T_d and the symmetry modes that appear in the present problem are the infrared-active F_2 modes. For isotope defects, Eq. (14) reduces to

$$1-\epsilon(\kappa)\omega_L^2 g(\kappa)=0 , \tag{15}$$

where

$$\epsilon(\kappa)=\frac{m'(\kappa)-m(\kappa)}{m(\kappa)}$$

is the mass-change parameter. ω_L is the local-mode frequency, and the Green's-function matrix element $g(\kappa)$ is given by

$$g(\kappa)=\frac{1}{N}\sum_{\vec{q}}\sum_{s}\frac{|e_\alpha(\kappa|\vec{q},s)|^2}{\omega^2(\vec{q},s)-\omega_L^2} ,$$

where κ denotes one of the ions of the unit cell; $\omega(\vec{q},s)$ and $e_\alpha(\kappa|\vec{q},s)$ are the frequencies and the

TABLE I. Comparison of the observed and the calculated local-mode frequencies (cm^{-1}) due to various isoelectronic impurities in II-VI and III-V zinc-blende-type semiconductor compounds.

A. II-VI semiconductor compounds

Systems	Experimental	Lattice-dynamical calculations		Source of the experimental data
		SNI model	RI model (Ref. 7)	
*Cd*Te : Be	391	397	426	a
*Cd*Te : ^{24}Mg	249	238	266.3	a
CdTe : ^{25}Mg	245	232		a
*Cd*Te : ^{26}Mg	241	229		a
Cd*Te* : ^{32}S	249	265	···	a
Cd*Te* : ^{34}S	244	259	···	a
Cd*Te* : Se	170	173	172	a
*Zn*Te : Be	415	421	461.5	a
*Zn*Te : Al	313	356	274.5	a
Zn*Te* : S	269	263	266.5	a
*Zn*Se : Be	450	452	498	a
*Zn*Se : ^{24}Mg	352	365	317.2	a
*Zn*Se : ^{25}Mg	345	360	312	a
*Zn*Se : ^{26}Mg	334	347	306.6	a
*Zn*Se : Al	359	394	301.9	a
Zn*Se* : S	297	303	285.9	b
*Zn*S : Be	490	506	543	a
B. III-V semiconductor compounds				
*In*Sb : Ga	196	198	209.8	a
*In*Sb : Al	296	288.4	307	a
In*Sb* : P	293	302	···	a
In*Sb* : As	200	199	206.6	a
*In*P : ^{10}B	543.5	556	···	a, c
*In*P : ^{11}B	522.8	548	···	a, c
*In*As : Ga	240	243	244	a
In*As* : P	295	291	···	d
Ga*P* : ^{14}N	488	460	525.2	a
Ga*P* : ^{15}N	472	450	509	a
*Ga*P : Al	444.7	439	442.2	a
*Ga*P : ^{10}B	594	620	636.6	e
*Ga*P : ^{11}B	571	597	611.6	e
*Ga*Sb : Al	316.7	315	333	a
Ga*Sb* : P	324	328	327.3	a
Ga*Sb* : As	240	238	248	a
*Ga*As : ^{10}B	540	539	···	a
*Ga*As : ^{11}B	517	514.5	···	a
*Ga*As : Al	362	365	368.9	a
Ga*As* : P	355.4	358	351	f

[a] Reference 4.

[b] O. Brafman, I. F. Chang, G. Lengyel, and S. S. Mitra, Phys. Rev. Lett. 19, 1120 (1967).

[c] R. C. Newman, F. Thompson, J. B. Mullin, and B. W. Straughan, Phys. Rev. Lett. A 33, 113 (1970).

[d] F. Oswald, Z. Naturforsch A 14, 374 (1959).

[e] W. Hayes, H. F. Macdonald, and C. T. Sennett, J. Phys. C 2, 1137 (1969).

[f] S. D. Smith, R. E. V. Chaddock, and A. R. Goodwin, in *Proceedings of the International Conference on the Physics of Semiconductors*, edited by E. Kanda (Academic of Japan, Kyoto, 1966), p. 67.

eigenvectors for the wave vector $\vec{q}$ in the polarization branch s for the host systems.

The eigenfrequencies and the corresponding eigenamplitudes of the normal modes, as calculated for a variety of II-VI and III-V compounds in the SNI model, have been used for the numerical estimation of the high-frequency Green's functions. A staggered-bin-averaging procedure is employed in the computer calculation of $g(\kappa)$. The quantities $|e_\alpha(\kappa|\vec{q}, s)|^2$ were first calculated and sorted by dividing the frequency into 60 equal bins. The resulting histograms were used to compute the real part of the Green's function following the method as suggested by Sievers *et al.*[30] Since the mesh points have finite size, the increment in the frequency is chosen in such a way that the spurious fluctuations appearing in the Green's function are minimum. For the present choice of 4096 points in the Brillouin zone, a value of 0.35 for the frequency increment in units of bin was found to be appropriate.

The local-mode frequencies due to various isoelectronic impurities in zinc-blende-type crystals have been computed in the mass-defect approximation using the above computed Green's functions. A representative list of II-VI and III-V semiconductor compounds examined so far is presented in Table I. We include in this table the experimentally observed local-mode frequencies and those calculated by the RIM and the SNI lattice dynamical models.

From Table I it may be noted that the calculated local-mode frequencies in mass-defect approximations using a SNI model are in somewhat better agreement with the experimental values than those of a four-parameter RIM. In fact, the discrepancies in most of the systems are of the order of ~ 5%. We may thus conclude that the isoelectronic impurities discussed in the present article behave very nearly as isotopic defects in zinc-blende-type crystals.

ACKNOWLEDGMENTS

The authors wish to express their sincere thanks to Professor A. Mitsuishi, Professor Vachaspati, Professor A. Grimm, Professor Y. P. Varshni, and Professor J. F. Vatelino for their interest in the present work. We are also thankful to Council of Scientific and Industrial Research and University Grants Commission, New Delhi, India for financial assistance. One of us (D. N. T.) is thankful to Dr. P. N. Ram for helpful discussions and to Dr. Harbhajan S. Randhawa for his kind hospitality during his visit to Indian Institute of Technology, Kanpur. All numerical calculations were performed on IBM 7044/1401 computers.

---

*Council of Scientific and Industrial Research Fellow.

[1] G. Schaefer, J. Phys. Chem. Solids 12, 233 (1960).

[2] J. F. Angress, A. R. Goodwin, and S. D. Smith, Proc. Roy Soc. A 287, 64 (1965).

[3] R. C. Newman and J. B. Willis, J. Phys. Chem. Solids 26, 373 (1965).

[4] A. Mitsuishi and A. Manabe, Oyo Butsuri, 41, 7 (1972).

[5] N. Krishnamurthy and T. M. Haridasan, Ind. J. Pure and App. Phys. 7, 89 (1969).

[6] G. Lucovsky, M. H. Brodsky, and E. Burstein, Phys. Rev. B 2, 3295 (1970).

[7] S. P. Gaur, J. F. Vetelino, and S. S. Mitra, J. Phys. Chem. Solids, 32, 2737 (1971).

[8] A. K. Rajagopal and R. Srinivasan, Z. Phys. 158, 471 (1960).

[9] J. F. Vetelino, S. S. Mitra, and K. V. Namjoshi, Phys. Rev. B 2, 967 (1970); J. F. Vetelino and S. S. Mitra, Solid State Commun. 7, 1181 (1969); J. F. Vetelino, S. S. Mitra, O. Brafman, and T. C. Damen, Solid State Commun. 7, 1809 (1969).

[10] R. Banerjee and Y. P. Varshni, Can. J. Phys. 47, 451 (1969); J. Phys. Soc. Jap. 30, 1015 (1971); Solid State Commun. 10, 2801 (1971).

[11] D. N. Talwar and Bal K. Agrawal, Solid State Commun. 11, 1691 (1972).

[12] D. N. Talwar and Bal K. Agrawal, Phys. Status Solidi (to be published).

[13] D. N. Talwar and Bal K. Agrawal, Solid State Commun. (to be published).

[14] D. N. Talwar and Bal K. Agrawal, Phys. Rev. B (to be published).

[15] (a) W. Cochran, in *Lattice Dynamics*, edited by R. F. Wallis (Pergamon, New York, 1965), p. 75. (b) G. G. Dick, in Ref. 15(a), p. 159.

[16] Substituents belonging to the same column of the Periodic Table as their host atoms.

[17] A. Grimm, A. A. Maradudin, I. P. Ipatova, and A. V. Subashiev, J. Phys. Chem. Solids 33, 775 (1972).

[18] J. L. T. Waugh and G. Dolling, Phys. Rev. 132, 2410 (1963).

[19] J. L. Yarnell, J. L. Warren, R. G. Wenzel, and P. J. Dean, in Proceedings of the Conference on Inelastic Neutron Scattering, Copenhagen, Denmark, 1968 (unpublished).

[20] L. A. Feldkamp, G. Venktaraman, and J. S. King, Solid State Commun. 7, 1571 (1969).

[21] D. N. Talwar and Bal K. Agrawal, Phys. Rev. B 8, 693 (1973).

[22] J. C. Irwin and J. LaCombe, J. Appl. Phys. 41, 1444 (1970).

[23] G. F. Alfray and P. H. Borcherds, J. Phys. C 5, L275 (1972).

[24] G. Dolling and J. L. T. Waugh, in Ref. 15(a), p. 19.

[25] D. L. Price, J. M. Rowe, and R. M. Nicklow, Phys. Rev. B 3, 1268 (1971).

[26] B. Hennion, F. Moussa, G. Pepy, and K. Kunc, Phys. Lett. A 36, 376 (1971).

[27] J. Bergsma, Phys. Lett. A 32, 324 (1970).

[28] H. J. McSkimin, J. Appl. Phys. 24, 988 (1953).

[29] R. Brout, Phys. Rev. 113, 43 (1959).

[30] A. J. Sievers, A. A. Maradudin, and S. S. Jaswal, Phys. Rev. 138, A272 (1965).