





YESHIVA  
UNIVERSITY

LEVEL II

①

BELFER GRADUATE SCHOOL OF SCIENCE

2495 Amsterdam Avenue / New York, N.Y. 10033 / (212) 568-8400

FINAL REPORT

AD A101120

PIEZO-OPTICAL DETERMINATION OF DEFORMATION POTENTIALS  
RELEVANT TO TRANSPORT PROPERTIES CALCULATIONS OF  
MULTIVALLEY SEMICONDUCTORS

ONR CONTRACT NO / N00014-76-C-0481

15

11 14 AUG 78

24

DTIC FILE COPY

PRINCIPAL INVESTIGATOR

PROF / F.H. POLLAK

10

DTIC  
ELECTED  
JUL 8 1981  
S  
A

This document has been approved  
for public release and sale; its  
distribution is unlimited.

022

ABSTRACT

A piezospectroscopic investigation of the normalized wave-length-modulated absorption spectra of the phonon-assisted indirect exciton in Si (TO-phonon) and Ge (LA phonon) at 77°K has yielded values for the ratio of the electron-phonon to the hole-phonon matrix elements for the  $\Gamma$ -A (Si) and  $\Gamma$ -L (Ge) transitions.

7

UNCLASSIFIED  
DATE 12/10/2013  
BY SP-10/2013  
UNCLASSIFIED  
AUTHORITY 101-108

*Put in file*

Distribution/		
Availability Codes		
Dist. 1 or 2 or		
Special		
A		

## I. RESULTS OF WORK PERFORMED UNDER PRESENT CONTRACT

### A. Introduction .

An investigation of the stress-dependence of an indirect absorption process can yield information concerning the relative contributions of the phonon-assisted electron and hole scattering mechanisms to the absorption processes.<sup>1-4</sup> Once the relative coefficients are known a fit to the absorption coefficient can be made in order to determine the absolute values for the electron-phonon deformation potentials. These parameters are related to intervalley scattering mechanisms in multivalley semiconductors and hence are important in the calculations of the high field transport properties of these materials.<sup>5</sup>

In a multivalley indirect semiconductor absorption processes can proceed by two different scattering mechanisms involving electron-phonon and hole-phonon scattering processes. Measurements of only the absorption spectrum cannot sort out the contributions of these two different processes. However, in the case of Si it has been demonstrated that the two mechanisms are affected differently by the application of an uniaxial stress along different crystallographic directions.<sup>1-4</sup> This is due to the fact that the electron-photon interaction related to the two different scattering mechanisms occurs at different places in the Brillouin Zone and hence is affected in a different manner by the various stresses. The stress-dependence of the intensity of the indirect absorption process can be determined by utilizing the sensitive technique of wavelength-modulated transmission at 77°K.

We have investigated the stress-dependence of the normalized wavelength-modulated absorption (WMA) spectra of the phonon-assisted indirect exciton in Si (TO-phonon)<sup>6,7</sup> and Ge (LA-phonon)<sup>7</sup> at 77<sup>o</sup>K. These measurements have enabled us to obtain values for the ratio of the electron-phonon (EP) to hole-phonon (HP) scattering matrix elements for the  $\Gamma$ - $\Delta$  (Si) and  $\Gamma$ -L (Ge) transitions. For Si<sup>6,7</sup>  $EP_{TO}/HP_{TO} = 1.4$  while in Ge<sup>7</sup>  $EP_{LA}/HP_{LA} = 0.16$ .

### B. Theoretical Framework

It can be shown that the absorption coefficient for an indirect exciton absorption process can be written as:<sup>8</sup>

$$\alpha(\omega) = \frac{Ve^2}{\eta_m^2 c \omega} \left( \frac{2M}{\hbar^2} \right) \sum_{\ell} \sum_{\neq} |C^{\pm}(c,v;\ell)|^2 \times \sum [\hbar\omega - E_g + \frac{R}{\hbar^2} \pm \omega_{\ell}(\vec{Q})]^{\frac{1}{2}} \times |\bar{\psi}_{c,v}^n(0)|^2 \quad (1)$$

where  $\eta$  is the real part of the refractive index,  $M = m_e^* + m_h^*$ ,  $E_g$  is the indirect gap,  $R$  is the ground state exciton energy,  $n$  is the exciton series index and  $\hbar\omega_{\ell}(\vec{Q})$  is the energy of the  $\ell^{\text{th}}$  phonon of wave-vector  $\vec{Q}$ .

The quantity  $C(c,v;\ell)$  is the matrix element for the indirect transition from the valence band state  $\psi_{v,k}$  to the conduction band state  $\psi_{c,k}$ , accompanied by the creation (+) or annihilation (-) of a phonon of wave-vector  $\vec{Q}$  belonging to the  $\ell^{\text{th}}$  phonon and can be written as:

$$\begin{aligned}
& \sum_i \frac{\langle \psi_{v,k} | \hat{e} \cdot \vec{p} | \psi_{i,k} \rangle \langle \psi_{i,k} | \mathcal{H}_e^{\pm}(Q) | \psi_{c,k'} \rangle}{E_c(k') - E_i(k) \pm \hbar \omega_e(Q)} \\
& + \frac{\langle \psi_{c,k'} | \hat{e} \cdot \vec{p} | \psi_{i,k'} \rangle \langle \psi_{i,k'} | \mathcal{H}_e^{\pm}(Q) | \psi_{v,k} \rangle}{E_v(k) - E_i(k') \mp \hbar \omega_e(Q)}
\end{aligned} \tag{2}$$

where  $i$  represents the intermediate state. The quantity  $\psi^n(\vec{r})$  is a solution to the effective mass Hamiltonian [Eq. (52) in Ref. (8)].

If we consider the case of, for example, TO-phonon assisted transitions in silicon then the intermediate state is  $\Gamma_{15,c}$  or  $\Delta_{5,v}$ , the valence band is at  $\Gamma_{25',v}$  and the conduction band minimum is at  $\Delta_{1,c}$ . Equation (2) takes the form:<sup>1-4,6</sup>

$$\begin{aligned}
\alpha(\omega) \sim & \left[ \frac{\langle \Gamma_{25',c} | \hat{e} \cdot \vec{p} | \Gamma_{15,c} \rangle \langle \Gamma_{15,c} | \mathcal{H}_{TO}(\Delta_1) | \Delta_{1,c} \rangle}{E(\Delta_{1,c}) - E(\Gamma_{15,c}) + \hbar \omega_{TO}} \right] \\
& + \left[ \frac{\langle \Delta_{1,c} | \hat{e} \cdot \vec{p} | \Delta_{5,v} \rangle \langle \Delta_{5,v} | \mathcal{H}_{TO}(\Delta_5) | \Gamma_{25',v} \rangle}{E(\Gamma_{25',v}) - E(\Delta_{5,v}) - \hbar \omega_{TO}} \right]^2
\end{aligned} \tag{3}$$

The first term in Eq. (3) is related to scattering of an electron by a TO phonon while the second term corresponds to hole scattering. These two processes are shown schematically in Fig. 1. In an unstressed crystal it is not possible to differentiate between the relative contribution of these two processes to the absorption coefficient. It is of interest to be able to make this distinction

for the purposes of obtaining the deformation potentials for both electron and hole scattering.

### C. Experimental Approach

The transmitted intensity can be written as:

$$I_T = I_0 (1-R)^2 e^{-\alpha t} \quad (4)$$

where  $I_0$  is the incident intensity,  $R$  the reflectivity,  $\alpha$  is the absorption coefficient and  $t$  is the thickness of the sample. Taking the wave-length derivative of Eq. (4) one obtains ( $I_0$  and  $R$  are not  $\lambda$  - dependent in the region of the indirect exciton of silicon):

$$\frac{dI_T}{d\lambda} = - I_0 (1-R)^2 e^{-\alpha t} \left[ -t \frac{d\alpha}{d\lambda} \right] \quad (5)$$

and hence dividing Eq. (5) by Eq. (4) one obtains the normalized derivative:

$$\frac{dI_T/I_T}{d\lambda} = -t \frac{d\alpha}{d\lambda} = -t \left[ \frac{(\hbar\omega)^2}{12398} \frac{d\alpha}{d(\hbar\omega)} \right] \quad (6)$$

where  $d\alpha/d(\hbar\omega)$  is the quantity of interest.

Light from a quartz-iodine source is passed through a 1/4 meter Jarell-Ash monochromator. The exit mirror is connected to a General Scanning Corp. Model 320 optical scanner which modulates the output wavelength at 530 cps (freq.  $\Omega_1$ ). The light incident on the monochromator is chopped at 200 cps (freq.  $\Omega_2$ ). After the light leaves

the monochromator it is focused onto the sample, (typical dimension 2mm x 2mm x 20mm) which is mounted in a stress frame. The entire stress apparatus is immersed in a glass liquid nitrogen dewar.

Mounted on the stress frame in the proximity of the sample is a heater and Lake Shore Cryotronic TG-100-P/M Silicon Temperature sensor. The output of the heater and temperature sensor are connected to a Lake Shore Cryotronic Model DTC-500 Precision Temperature indicator/controller. In this manner excellent temperature stability can be obtained for long periods of time. After the light passes through the sample it is focused onto a PbS detector. Thus the PbS detector sees two signals, one at frequency  $\Omega_1$  (wavelength-modulated signal  $dI_T/d\lambda$  and one at frequency  $\Omega_2$  (chopped light which is proportional to the dc intensity,  $I_T$ ).

The output of the PbS detector is passed through an Ithaco 3152 Voltage Controlled Amplifier. The signal from the Ithaco Amplifier is detected by two lock-in amplifier, one at freq.  $\Omega_1$  and the second at freq.  $\Omega_2$ .

The dc output signal from the  $\Omega_2$  lock-in is fed into a differential operational amplifier so that the output of the differential op-amp is the difference between the  $\Omega_2$  lock-in signal and a reference voltage. This difference voltage is then detected by the Ithaco amplifier and controls the gain of the amplifier. In this manner the quantity  $I_T$  is kept at a constant value.

Since  $I_T$  is being kept constant as a function of wavelength the  $\Omega_1$  lock-in reads the normalized derivative signal  $(dI_T/d\lambda)I_T$ . The output from lock-in  $\Omega_1$  is recorded by a strip-chart recorder with

wavelength marker. The quantity  $(dI_T/d\lambda)I_T \sim d\alpha/d(\hbar\omega)$  is then measured in the region of the indirect exciton for different values of  $X$  and polarization  $\parallel$  and  $\perp$  to  $X$ .

#### D. Results

##### 1. Silicon

We have measured the stress-dependence of the amplitude of the normalized wavelength-modulated absorption (WMA) spectra of the TO-phonon assisted indirect exciton of silicon at 77°K for stress  $\vec{X}$  along [001] and [111]<sup>6,7</sup>. These measurements have enabled us to obtain the first value for the ratio of the  $EP_{TO}$  to  $HP_{TO}$  scattering matrix elements in this material<sup>6,7</sup>. Although Laude et al<sup>2</sup> have reported a value for this parameter based on a study of the stress-dependence of WMA they did not measure the normalized spectra and in addition used an incorrect expression for the relative contributions of the two processes<sup>9</sup>. The stress-dependence of recombination radiation<sup>3</sup> and WMA (at low stresses)<sup>4</sup> of the free exciton have recently been investigated. However, since both these works employed only  $\vec{X} \parallel [001]$  it was not possible to deduce a unique number for the  $EP_{TO}$  to  $HP_{TO}$  ratio. A rough estimate of this parameter has been made by Smith and McGill<sup>10</sup> based on a comparison of their calculations with the experimental results of Ref. 2.

In silicon the TO-phonon assisted indirect exciton is at 1.21 eV at 77°K and occurs between the  $\Gamma$  valence band maxima and the  $A_1$  conduction band minima. For this transition the intermediate state can be either the  $\Gamma_{15,c}$  conduction or the  $\Delta_{5,v}$  valence band. Application of uniaxial stress  $\vec{X}$  along [111] splits the doubly degenerate

valence band maxima into two levels ( $v_1$  and  $v_2$ ) but does not destroy the equivalence of the conduction band minima and hence two peaks ( $A_1$  and  $A_2$ ) are observed<sup>2,11</sup>. For  $\vec{X}||[001]$  both valence band degeneracies and conduction band equivalences are removed and four transitions ( $B_1 - B_4$ ) are possible<sup>1-4,6,11</sup>. The schematic representation of the effects in silicon are shown in Fig. 1 of Ref. 2. We have calculated the correct theoretical expression for the intensities of these transitions including the stress-dependent wavefunction mixing<sup>2</sup> between the  $v_1$  band and the spin-orbit split state  $v_3$ . Comparison with experiment has yielded a value for the ratio of the  $EP_{TO}$  to  $HP_{TO}$  scattering strengths.

Shown in Fig. 2 is the normalized WMA spectrum of the TO-phonon assisted indirect exciton in silicon at 77<sup>o</sup>K for  $X = 0$ . Also plotted in Fig. 2 is the spectrum for  $X = 3.51 \times 10^9$  dyn-cm<sup>-2</sup> along [001] for the electric field vector of the light,  $\vec{E}$ , polarized parallel ( $||$ ) and perpendicular ( $\perp$ ) to the stress axis. Similar results have been observed for  $\vec{X}||[111]$  where only two peaks,  $A_1$  and  $A_2$ , are observed.

It has been shown that the lineshape of the derivative absorption spectrum of the indirect exciton in silicon can be fitted by an expression of the form<sup>12</sup>

$$\frac{d\alpha}{d(\hbar\omega)} \sim F(\omega) \quad (7)$$

where  $\alpha$  is the absorption coefficient. The function  $F(\omega)$  is given by

$$F(W) = [(W^2 + 1)^{\frac{1}{2}} + W]^{\frac{1}{2}} / [W^2 + 1]^{\frac{1}{2}} \quad (8)$$

where  $W = [(\hbar\omega - \hbar\omega_{\text{exciton}})/\Gamma]$  and  $\Gamma$  is the broadening parameter.

By appropriate subtraction of the background we have been able to fit the lineshapes of the various peaks to this form and hence obtain a quantitative determination of the amplitude of the modulated exciton spectra. In Fig. 3 we have plotted the experimental values (solid line) of the  $B_1^{\parallel}$  peak of Fig. 2 and the theoretical fit (dashed line) from Eq. (7). There is good agreement in the lineshapes. Similar results have been obtained for the other B peaks as well as the A structures. In order to obtain a measure of integrated intensity,  $d\alpha$ , we have multiplied the value of  $d\alpha/d(\hbar\omega)$  by the broadening parameter  $\Gamma$ .

Listed in Table I are the experimentally determined relative and actual (in parenthesis) values of  $[d\alpha/d(\hbar\omega)] \times \Gamma$  for the various B and A peaks at the indicated stresses for  $\vec{E} \parallel \vec{X}$  and  $\vec{E} \perp \vec{X}$ . Similar results have been obtained at several other applied stresses for both stress directions.

The general theoretical expression for the intensities of the excitonic lines in the optical spectra, corresponding to TO-phonon-assisted indirect transitions between the  $\Gamma_{25',v}$  valence and  $\Delta_{1,c}$  conduction bands via  $\Gamma_{15,c}$  conduction and  $\Delta_{5,v}$  valence band intermediate states, can be written as being proportional to:

$$\begin{aligned}
 \rho = & \left| \frac{\langle \Gamma_{25',v} | \hat{e} \cdot \vec{p} | \Gamma_{15,c} \rangle \langle \Gamma_{15,c} | \mathcal{H}_{TO} | \Delta_{1,c} \rangle}{E(\Gamma_{15,c}) - E(\Delta_{1,c})} + \right. \\
 & \left. \frac{\langle \Gamma_{25',v} | \mathcal{H}_{TO} | \Delta_{5,v} \rangle \langle \Delta_{5,v} | \hat{e} \cdot \vec{p} | \Delta_{1,c} \rangle}{E(\Gamma_{25',v}) - E(\Delta_{5,v})} \right|^2
 \end{aligned}$$

where  $\hat{e}$  is the unit polarization vector of the incident electric field,  $\vec{p}$  is the linear momentum of the electron and  $\mathcal{H}_{TO}$  is the Hamiltonian for the electron (hole)-phonon interaction. Using the stress-dependent eigenfunctions for the  $v_1$  and  $v_2$  valence bands given in Ref. 2 and the appropriate selection rules for the photon and TO-phonon transitions<sup>1-4</sup> we have calculated the theoretical expressions for the intensities of the B and A transitions for  $\vec{E} \parallel \vec{X}$  and  $\vec{E} \perp \vec{X}$ . These are listed in Table II. The terms  $\eta_1^j$  represent the contribution of the stress-induced mixing between the  $v_1$  and  $v_3$  bands<sup>13</sup>, an effect which has not been taken into account in Refs. 3 and 4<sup>14</sup>. We have neglected the small splitting (0.29 meV) due to the mass anisotropy of the exciton<sup>4</sup>. The fact that the ratio  $U_{TO}/V_{TO}$  is real<sup>4,10</sup> has enabled us to write these theoretical expressions in the simplified form given in Table II.

Comparison of the theoretical expressions of Table II and the experimental values listed in Table I enables the ratio of  $U_{TO}/V_{TO}$  to be determined. The value of  $B_4^\perp/B_2^\perp = 4$  yields that  $U_{TO}/V_{TO} = 1$  or  $-\frac{1}{3}$ . The above ambiguity is resolved by an examination of the  $A_2^\parallel/A_1^\parallel$  ratio, for which the agreement between experiment and theory is good

only for  $U_{TO}/V_{TO} = 1$ . Using this value of the ratio we have calculated the relative theoretical values listed in Table I. There is in general good agreement between experiment and theory. Not only can comparisons be made between peak intensities of a given polarization but between the same peak for the two observed polarizations, thus eliminating any effects due to different line broadenings. For example, the theoretical ratio of  $A_2^\perp/A_2^\parallel = 1.34$  is in good agreement with the experimental ratio of  $(0.112/0.086) = 1.3$ . Similar correspondences are found for  $A_1^\perp/A_1^\parallel$  and  $B_4^\perp/B_4^\parallel$ . We find, however, that any ratio of intensities that involves  $\tau_1^0$  or  $\tau_2^0$  does not yield as good an agreement with theory.

From the value of  $U_{TO}/V_{TO} = 1$  and the ratios of the photon matrix elements  $(\langle \Delta_{5,v}^x | p_x | \Delta_{1,c} \rangle / \langle \Gamma_{15,c}^y | p_x | \Gamma_{15,c}^y \rangle) = 1.06$  and energy denominators  $\{ [E(\Gamma_{15,c}^y) - E(\Delta_{1,c})] / [E(\Gamma_{25,v}^y) - E(\Delta_{5,v})] = 1.3 \}$  obtained from a  $\vec{k} \cdot \vec{p}$  band structure calculation we have<sup>15</sup> determined the value of 1.4 for the ratio of the  $EP_{TO}$  ( $\langle \Gamma_{15,c}^z | p_y | \Delta_{1,c} \rangle$ ) to  $HP_{TO}$  ( $\langle \Gamma_{25,v}^z | p_y | \Delta_{5,v} \rangle$ ) scattering matrix elements.

Our results are consistent with the work of Alkeev et al<sup>3</sup> and Capizzi et al<sup>4</sup>, who both report a value of  $U_{TO}^2 / (U_{TO} + V_{TO})^2 \approx 0.25$  based on only a  $\vec{x} \parallel [001]$  study. As Table II indicates this stress direction does not allow a unique value for the  $U_{TO}/V_{TO}$  ratio to be established. Smith and McGill<sup>10</sup> suggest that  $U_{TO} \sim V_{TO}$  based on a comparison of their theoretical calculations with the experimental data of Ref. 2. However, since their model corresponds to only the  $\vec{x} \parallel [001]$  case their results cannot conclusively rule out the other possible value. Although Laude et al<sup>2</sup> have assumed a value of

$EP_{TO} = HP_{TO}$  in order to compare their experimental results with theory their conclusions are based on incorrect theoretical considerations <sup>9,13</sup>. Hence, we have reported the first correct, uniquely established number for this parameter <sup>6,7</sup>.

## 2. Germanium

We have investigated the stress-dependence of the amplitude of the normalized wavelength-modulated absorption (WMA) spectra of the phonon-assisted indirect exciton in Ge (LA phonon) at 77°K for stress  $\vec{X}$  along [001] and [111] <sup>7</sup>. From these measurements we have obtained values for the ratio of the EP to HP scattering matrix elements for the  $\Gamma$ -L indirect transition in Ge.

Shown in Fig. 4 is the normalized WMA spectrum of the LA-phonon assisted indirect exciton in Ge at 77°K for  $X = 0$  and  $3.73 \times 10^9$  dyn cm<sup>-2</sup> along [111] for the electric field vector of the light,  $\vec{E}$ , polarized parallel ( $\parallel$ ) and ( $\perp$ ) to  $\vec{X}$ .  $\vec{X} \parallel [111]$  splits both the valence and conduction bands and four transitions ( $A_1$ - $A_4$ ) are possible <sup>11</sup>. For  $\vec{X} \parallel [001]$  only the valence band is split and two peaks ( $B_1$  and  $B_2$ ) are observed <sup>11</sup>.

The lineshape of the WMA spectrum of the exciton can be fitted by Eq. (7). By appropriate subtraction of the background we have been able to fit the lineshapes of the various peaks to Eq. (7) and hence obtain a quantitative determination of the amplitudes of the spectra.

Listed in Table III are the theoretical expressions for the intensities of the stress-split LA-phonon assisted indirect exciton in Ge considering the intermediate state to be either the  $\Gamma_{2',c}$  conduction

band ( $U_{LA}$ ) or the  $L_{3',v}$  valence band ( $V_{LA}$ ) for  $\vec{X}||[111]$  and  $\vec{X}||[001]$  with  $\vec{E}||\vec{X}$  and  $\vec{E}\perp\vec{X}$ . The fact that the ratio  $V_{LA}/U_{LA}$  is real<sup>4</sup> has enabled us to write these theoretical expressions in the simplified form given in Table I. We have neglected (a) the stress-induced wave-function mixing with the spin-orbit split band<sup>6</sup> and (b) the valley-anisotropy splitting (1 meV)<sup>16</sup>.

Also listed in Table III are the experimentally determined relative and actual (in parentheses in units of  $\text{cm}^{-1}$ ) values of the quantity  $[d\alpha/d(\hbar\omega)] \times \Gamma$  in Ge for the various peaks for  $\vec{E}||\vec{X}$  and  $\vec{E}\perp\vec{X}$ . This quantity is a measure of the integrated intensity,  $d\alpha$ .

Comparison of the theoretical expressions of Table I with the experimental values enables the ratio  $V_{LA}/U_{LA}$  to be determined. The value of  $A_4^{\downarrow}/A_2^{\downarrow} = 2.15$  yields  $V_{LA}/U_{LA} = 0.6$  or  $-2.2$ . The above ambiguity is resolved by an examination of other ratios for which the agreement between experiment and theory is good only for  $V_{LA}/U_{LA} = 0.6$ . Using this value we have calculated the relative theoretical values listed in Table I. In general the agreement is quite good.

From a  $\vec{k}\cdot\vec{p}$  calculation for Ge<sup>15</sup> we obtain  $\langle \vec{X} | p_x | \Gamma_{2',c} \rangle / \langle L_{3',v}^{\vec{X}} | p_x | L_{1,c}^{(111)} \rangle = 1.03$ . Experimental values of the direct (0.880 eV), indirect (0.735 eV) and  $L_{1,c} - L_{3',v}$  (2.2 eV) gaps yields  $[E(\Gamma_{2',c}) - E(L_{1,c})] / [E(\Gamma_{25',v}) - E(L_{3',v})] = 0.1$ . Since  $V_{LA}/U_{LA} = 0.6$  the ratio of the  $EP_{LA}$  to  $HP_{LA}$  scattering matrix elements in Ge is 0.16. Thus, our results indicate that in Ge LA-phonon conduction band scattering is comparable to LA-phonon valence band scattering in spite of the large differences in energy denominators.

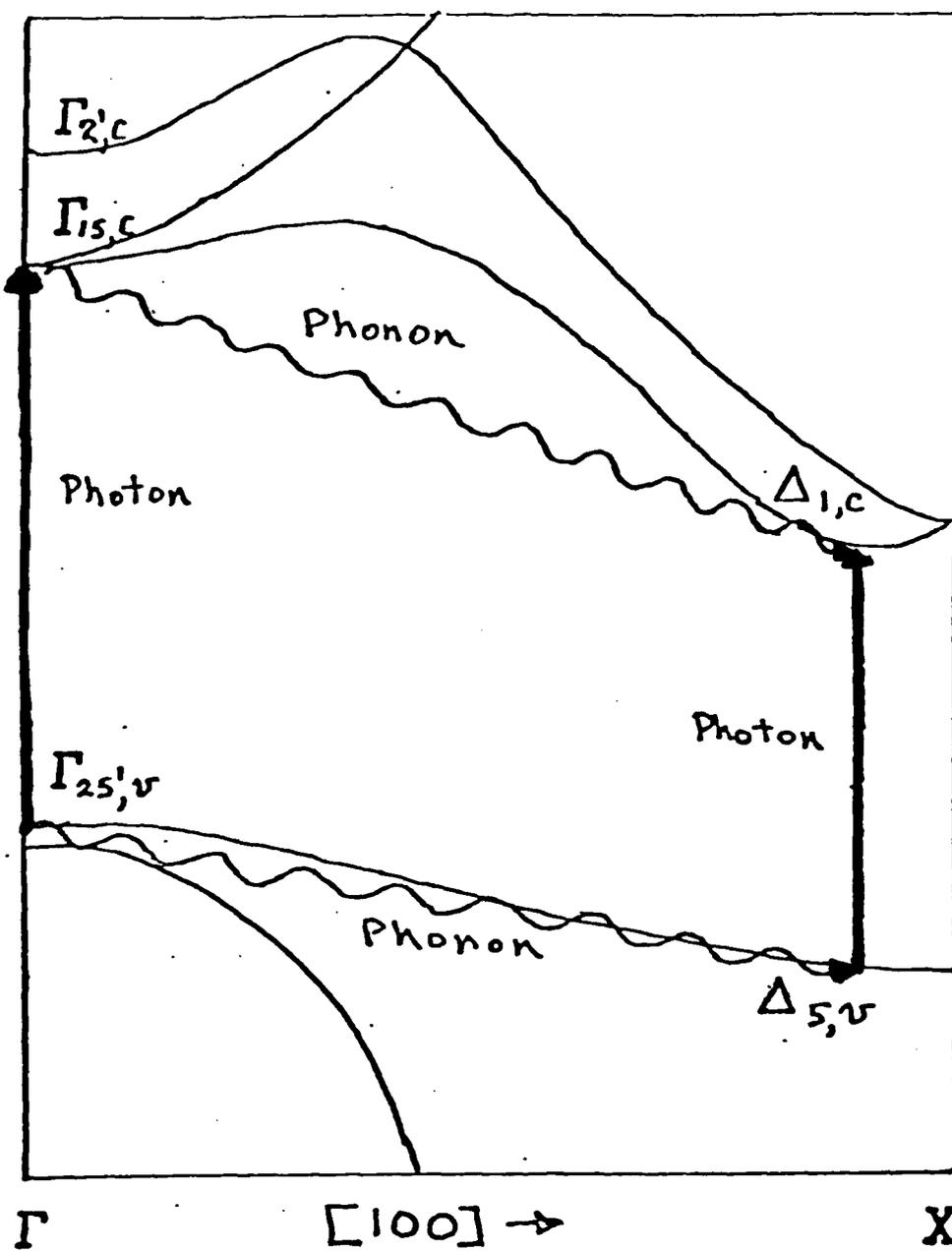


Fig. 1

Schematic representation of the electron and hole scattering mechanism which contribute to the TO-phonon assisted indirect transition absorption process in silicon.

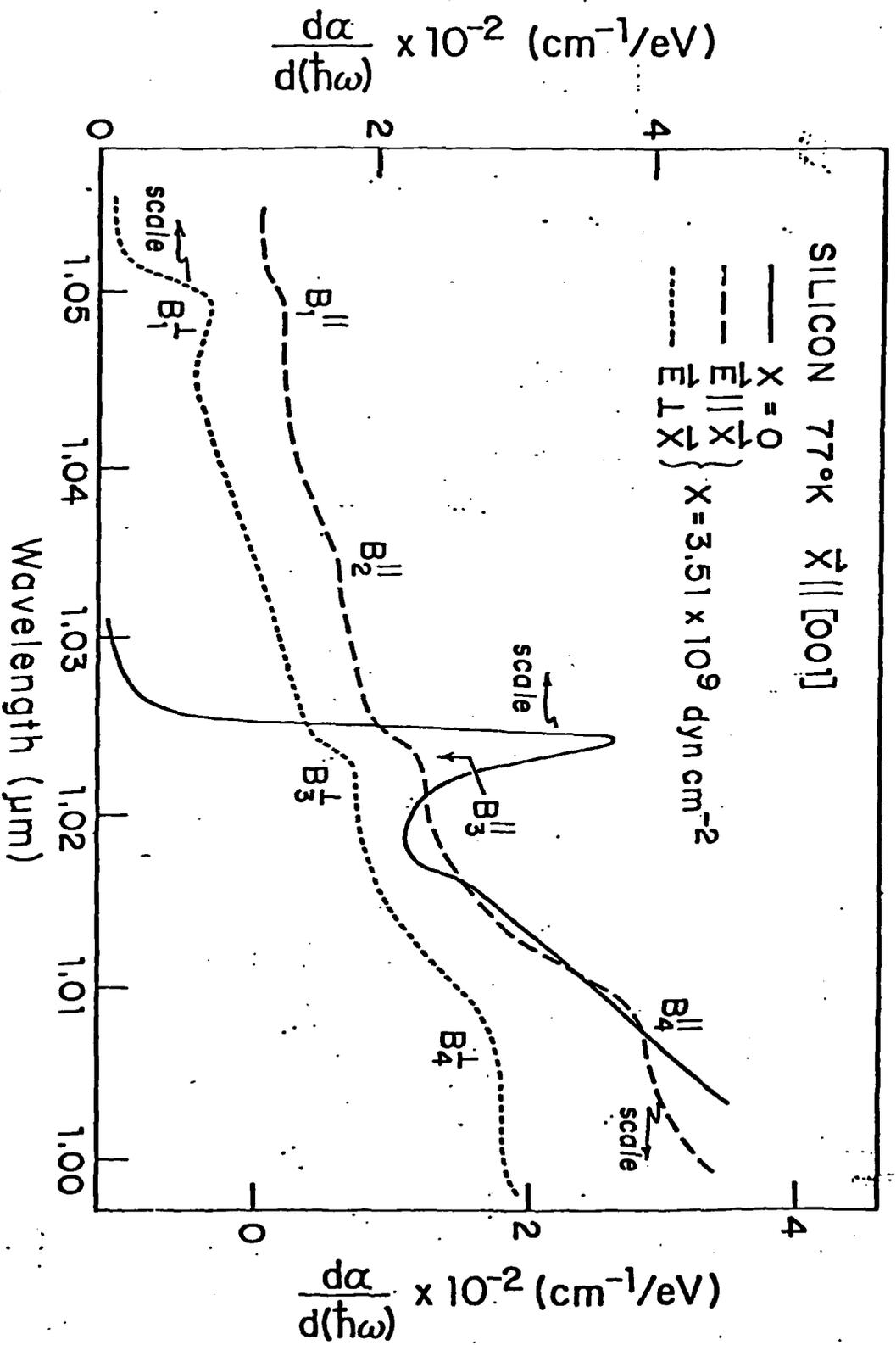


Fig. 2. Wavelength-modulated absorption spectra of the TO-phonon assisted indirect excitation of silicon at 77°K for  $X = 0$  and  $X = 3.51 \times 10^9 \text{ dyn cm}^{-2}$  along [001] for the electric field vector of the light  $\vec{E}$  polarized parallel and perpendicular to the stress axis.

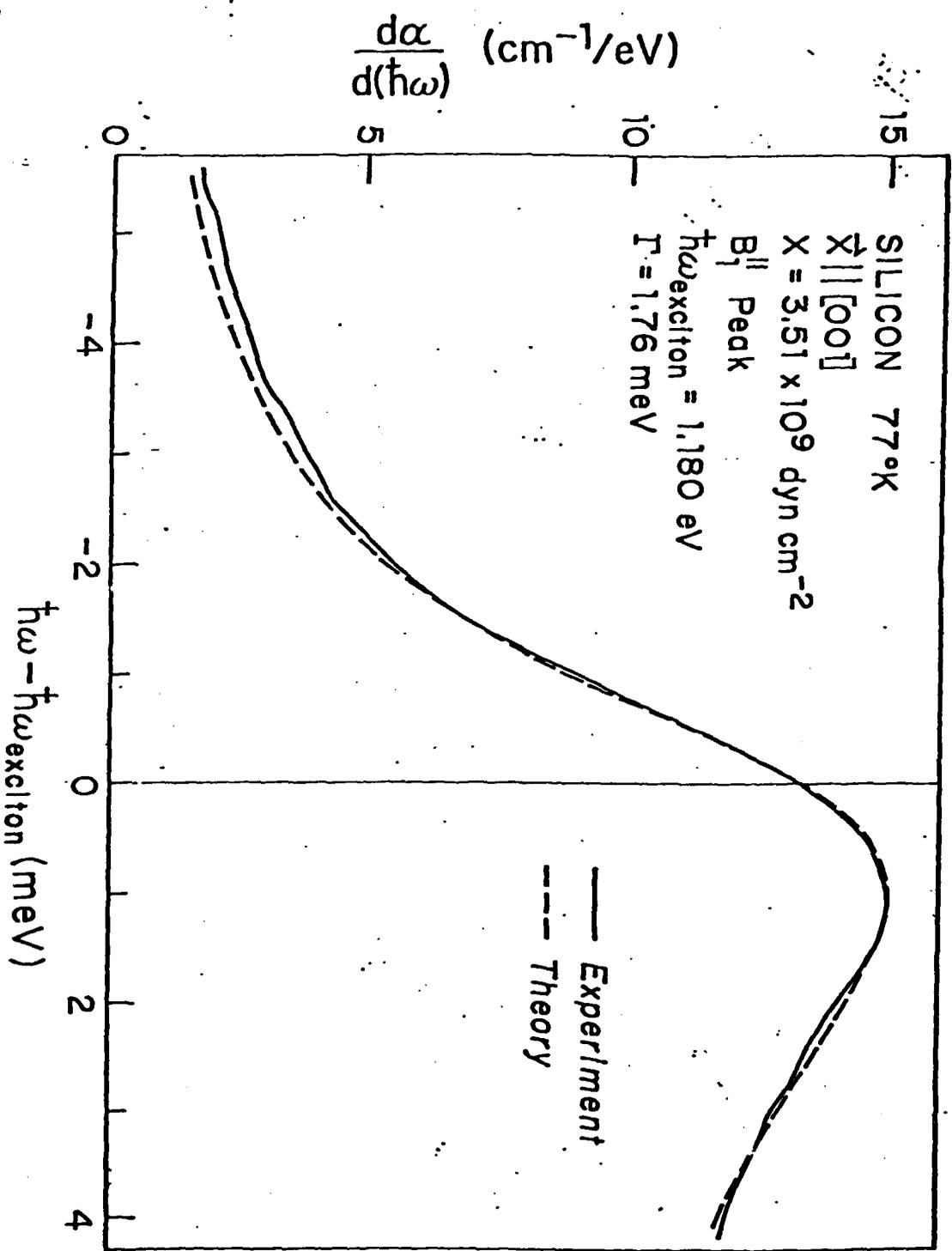


Fig. 3. Experimental values (solid line) of the wavelength-modulated absorption spectra of the  $B_1''$  peak of Fig. 1 after appropriate background subtraction and the theoretical fit (dashed line) obtained from Eq. (7).

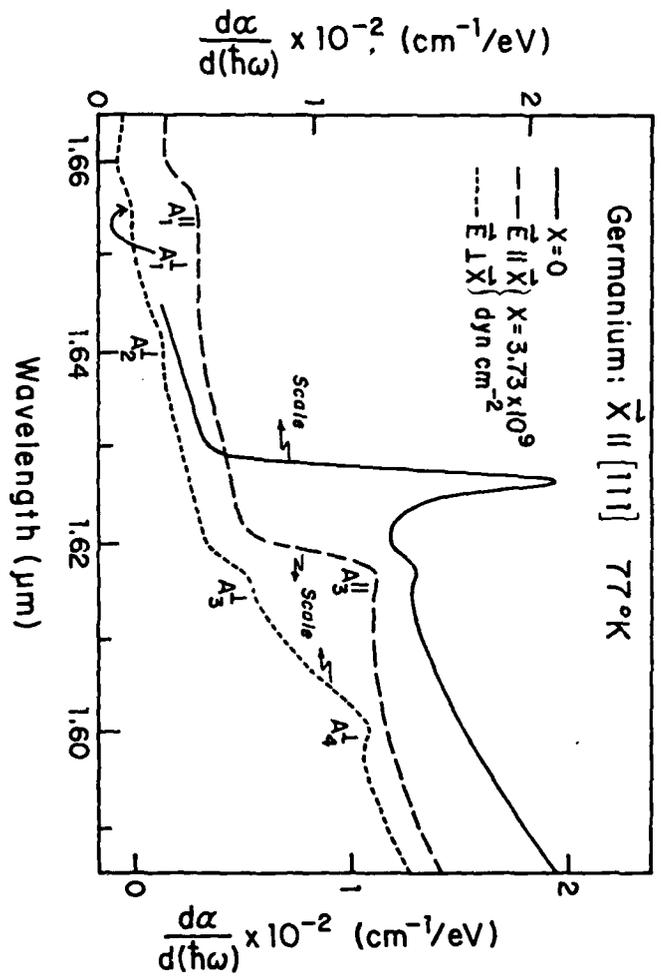


Fig. 4. Normalized RMA spectra of the LA-phonon assisted indirect exciton in Ge at 77°K for  $X = 0$  and  $3.73 \times 10^9 \text{ dyn cm}^{-2}$  along  $[111]$  for  $\vec{E} \parallel \vec{X}$  and  $\vec{E} \perp \vec{X}$ .

FIGURE CAPTIONS

Fig. 1. Schematic representation of the electron and hole scattering mechanism which contribute to the TO-phonon assisted indirect transition absorption process in silicon.

Fig. 2. Wavelength-modulated absorption spectra of the TO-phonon assisted indirect exciton of silicon at 77°K for  $X = 0$  and  $X = 3.51 \times 10^9 \text{ dyn cm}^{-2}$  along [001] for the electric field vector of the light  $\vec{E}$  polarized parallel and perpendicular to the stress axis.

Fig. 3. Experimental values (solid line) of the wavelength-modulated absorption spectra of the  $B_1^{\parallel}$  peak of Fig. 1 after appropriate background subtraction and the theoretical fit (dashed line) obtained from Eq. (1).

Fig. 4. Normalized WMA spectra of the LA-phonon assisted indirect exciton in Ge at 77°K for  $X = 0$  and  $3.73 \times 10^9 \text{ dyn cm}^{-2}$  along [111] for  $\vec{E} \parallel \vec{X}$  and  $\vec{E} \perp \vec{X}$ .

TABLE I

Experimental and theoretical values of the intensities for the TO-phonon assisted indirect transitions in silicon. The relative and actual (in parentheses in units of  $\text{cm}^{-1}$ ) experimental values were obtained by multiplying  $d\alpha/d(\hbar\omega)$  by the broadening parameter  $\Gamma$ . The theoretical values were calculated from the expressions in Table II using  $U_{\text{TO}}/V_{\text{TO}} = 1$ .

$\vec{x} \parallel [001]$ ( $X = 3.51 \times 10^9$ $\text{dyn cm}^{-2}$ )	$\vec{E} \parallel \vec{x}$		$\vec{E} \perp \vec{x}$	
	EXP.	THEORY	EXP.	THEORY
$B_1$	3% (0.026)	3%	25% (0.139)	46%
$B_2$	16% (0.135)	17%	0 (0.00)	0
$B_3$	18% (0.156)	11%	12% (0.068)	18%
$B_4$	63% (0.551)	69%	63% (0.360)	36%

$\vec{x} \parallel [111]$ ( $X = 7.59 \times 10^9$ $\text{dyn cm}^{-2}$ )	$\vec{E} \parallel \vec{x}$		$\vec{E} \perp \vec{x}$	
	EXP.	THEORY	EXP.	THEORY
$A_1$	74% (0.244)	65%	44% (0.087)	45%
$A_2$	26% (0.086)	35%	56% (0.112)	55%

TABLE II

Theoretical expressions for the intensities of the TO-phonon assisted indirect transition in silicon as a function of stress for  $\vec{x} \parallel [001]$  and  $\vec{x} \parallel [111]$  and light polarized parallel and perpendicular to the stress axis. The quantities  $n_0, m_0, n_1, m_1, \delta E'_{001}$  and  $\delta E'_{111}$  are defined in Ref. 2.

$\vec{x} \parallel [001]$	$\vec{E} \parallel \vec{x}$	$\vec{E} \perp \vec{x}$
$B_1$	$\frac{1}{3} \eta_1^0 U_{TO}^2$	$\frac{2}{3} \eta_2^0 (U_{TO} + V_{TO})^2$
$B_2$	$U_{TO}^2$	0
$B_3$	$\frac{1}{3} \eta_1^0 (U_{TO} + V_{TO})^2$	$(\frac{1}{6} \eta_1^0 + \frac{2}{3} \eta_2^0) U_{TO}^2 + \frac{1}{6} \eta_1^0 (U_{TO} + V_{TO})^2$
$B_4$	$(U_{TO} + V_{TO})^2$	$\frac{1}{2} [V_{TO}^2 + (U_{TO} + V_{TO})^2]$
$\vec{x} \parallel [111]$	$\vec{E} \parallel \vec{x}$	$\vec{E} \perp \vec{x}$
$A_1$	$2 \eta_1^1 (U_{TO}^2 + U_{TO} V_{TO}) + \frac{2}{3} V_{TO}^2$	$\eta_2^1 (U_{TO}^2 + U_{TO} V_{TO}) + \frac{2}{3} V_{TO}^2$
$A_2$	$\frac{2}{3} (U_{TO}^2 + V_{TO}^2 + U_{TO} V_{TO})$	$\frac{1}{3} (5 V_{TO}^2 + 2 V_{TO}^2 + U_{TO} V_{TO})$

$$U_{TO} = \langle z | p_x | \Gamma_{15,c}^y \rangle \langle \Gamma_{15,c}^y | \kappa_{TO}^y | \Delta_{1,c}^{(001)} \rangle / [E(\Gamma_{15,c}) - E(\Delta_{1,c})]$$

$$V_{TO} = \langle z | \kappa_{TO}^y | \Delta_{5,v}^x \rangle \langle \Delta_{5,v}^x | p_x | \Delta_{1,c}^{(001)} \rangle / [E(\Gamma_{25',v}) - E(\Delta_{5,v})]$$

$$\eta_1^0 = [n_0(n_0 - m_0)]^{-1} [(n_0 - m_0) - (\delta E'_{001})]^2$$

$$\eta_2^0 = [n_0(n_0 - m_0)]^{-1} [\frac{1}{2} (n_0 - m_0) + (\delta E'_{001})]^2$$

$$\eta_1^1 = [n_1(n_1 - m_1)]^{-1} [(\delta E'_{111})^2 + \frac{1}{3} (n_1 - m_1)^2 + \frac{2}{3} \delta E'_{111} (n_1 - m_1)]$$

$$\eta_2^1 = [n_1(n_1 - m_1)]^{-1} [(\delta E'_{111})^2 + \frac{2}{3} (n_1 - m_1)^2 - \frac{2}{3} \delta E'_{111} (n_1 - m_1)]$$

Table III

Theoretical expression for the intensities of the LA-phonon assisted indirect transitions in Ge for  $\vec{X}||[111]$  and  $\vec{X}||[001]$  for  $\vec{E}||\vec{X}$  and  $\vec{E} \perp \vec{X}$ . Also listed are the experimental [relative and actual (in parentheses in units of  $\text{cm}^{-1}$ )] and theoretical ( $V_{\text{LA}}/U_{\text{LA}} = 0.6$ ) values of the intensities. For both stress directions  $X = 3.73 \times 10^9 \text{ dyn cm}^{-2}$ .

$\vec{X}  [111]$	$\vec{E}    \vec{X}$	THEORY	EXP	$\vec{E} \perp \vec{X}$	THEORY	EXP
A <sub>1</sub>	$\frac{2}{3} U_{\text{LA}}^2$	12%	16% (0.054)	$\frac{1}{6} (U_{\text{LA}}^2 + 2 U_{\text{LA}} V_{\text{LA}} + V_{\text{LA}}^2)$	8%	6% (0.013)
A <sub>2</sub>	0	0	0	$\frac{1}{2} (U_{\text{LA}}^2 + 2 U_{\text{LA}} V_{\text{LA}} + V_{\text{LA}}^2)$	23%	24% (0.054)
A <sub>3</sub>	$2 (U_{\text{LA}}^2 + \frac{16}{9} U_{\text{LA}} V_{\text{LA}} + \frac{22}{27} V_{\text{LA}}^2)$	85%	84% (0.279)	$\frac{1}{2} U_{\text{LA}}^2 + \frac{5}{9} U_{\text{LA}} V_{\text{LA}} + \frac{19}{54} V_{\text{LA}}^2$	18%	17% (0.038)
A <sub>4</sub>	0	0	0	$\frac{3}{2} U_{\text{LA}}^2 + \frac{5}{3} U_{\text{LA}} V_{\text{LA}} + \frac{41}{54} V_{\text{LA}}^2$	51%	53% (0.116)

$\vec{X}  [001]$	$\vec{E}    \vec{X}$	THEORY	EXP	$\vec{E} \perp \vec{X}$	THEORY	EXP
B <sub>1</sub>	$\frac{4}{3} (2U_{\text{LA}}^2 + \frac{8}{3} U_{\text{LA}} V_{\text{LA}} + V_{\text{LA}}^2)$	98%	100% (0.133)	$\frac{2}{3} (U_{\text{LA}}^2 + \frac{4}{3} U_{\text{LA}} V_{\text{LA}} + V_{\text{LA}}^2)$	26%	25% (0.038)
B <sub>2</sub>	$\frac{4}{9} V_{\text{LA}}^2$	2%	0 (0.00)	$2 (U_{\text{LA}}^2 + \frac{4}{3} U_{\text{LA}} V_{\text{LA}} + \frac{5}{9} V_{\text{LA}}^2)$	74%	75% (0.113)

$$U_{\text{LA}} = \langle \bar{\alpha} | p_x | \Gamma_{2',c} \rangle \langle \Gamma_{2',c} | g_{\text{LA}} | L_{1,c}^{(111)} \rangle / [E(\Gamma_{2',c}) - E(L_{1,c})]$$

$$V_{\text{LA}} = \langle \bar{\alpha} | g_{\text{LA}} | L_{3',v} \rangle \langle \Gamma_{3',v} | p_x | L_{1,c}^{(111)} \rangle / [E(\Gamma_{25',v}) - E(L_{3',v})]$$

$$\bar{\alpha} = \frac{1}{\sqrt{2}} (\alpha - \gamma)$$

$$p_x = \frac{1}{\sqrt{2}} (p_x - p_y)$$

## REFERENCES

1. E. Erlbach, Phys. Rev. 150, 767 (1966).
2. L. D. Laude, F.H. Pollak and M. Cardona, Phys. Rev. B3, 2623 (1971).
3. N.V. Alkeev, A.S. Kaminskii and Ya. E. Pokrovskii, Sov. Phys. Solid State 18, 410 (1976).
4. M. Capizzi, J.C. Merle, P. Fiorini and A. Frova, Solid State Comm. 24, 451 (1977).
5. See, for example, W. Fawcett, A.D. Boardman and S. Swain, J. Phys. Chem. Solids 31, 1963 (1970).
6. F.H. Pollak, A. Feldblum, H.D. Park and P.E. Vanier, to be published in Solid State Comm.
7. F.H. Pollak, A. Feldblum, H.D. Park and P.E. Vanier, to be presented at the 14th Int. Conf. on the Physics of Semiconductors, Edinburgh, 1978.
8. J.O. Dimmock in Semiconductors and Semimetals, ed. by R.K. Willardson and A.C. Beer (Academic Press, N.Y., 1967), Vol. 3, p. 296.
9. In Ref. 2 [Eq. (B1)] the intensity was incorrectly calculated to be proportional to the sum of the squares of the two contributions instead of the square of the two sums.
10. D.L. Smith and T.C. McGill, Phys. Rev. B14, 2448 (1976).
11. I. Balslev, Phys. Rev. 143, 636 (1966).
12. M. Cardona in Modulation Spectroscopy (Academic Press, N.Y., 1969) p. 111; B. Batz in Semiconductors and Semimetals, ed. by R.K. Willardson and A.C. Beer (Academic Press, N.Y., 1972), Vol. 9, p. 331.
13. The expressions for  $\eta_i^1$  in Ref. 2 are incorrect.
14. If the stress-induced coupling between  $v_1$  and  $v_3$  is neglected then  $\eta_i^j = 1$  and the expressions in Table II for  $\vec{x} \parallel [001]$  are in agreement with those of Ref. 3.

15. M. Cardona and F.H. Pollak, Phys. Rev. 142, 530 (1966).

M. Capizzi, F. Evangelisti, A. Frova and P. Valfre in  
Proc. 13th Int. Conf. on the Physics of Semiconductors,  
Rome, 1976 (Tipografia Marves, 1976) p. 857.

END

DATE  
FILMED

7-81

DTIC