INFLUENCE OF DEFORMATION POTENTIAL ELECTRON-PHONON INTERACTION ON THE OPTICAL TRANSITIONS AND INTERVALLEY SCATTERING IN III-V-SEMICONDUCTORS

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We discuss the relationship between deformation potential intervalley scattering and the shifts and broadenings of interband critical points (CPs) with temperature and present ellipsometric data for the temperature dependence of the E_1-CPs of InAs, GaP, and GaSb.

Semiconductors exhibit large shifts and lifetime broadenings of interband CPs with temperature, which are mainly due to the deformation potential-type electron-phonon interaction. Such shifts and broadenings for an electron state $|\vec{k}n>$ can be written as [1]

$$\Delta E_{\vec{k}n} - i\Gamma_{\vec{k}n} = \left\langle < \vec{k}n|H_2|\vec{k}n > + \sum_{\vec{k}'n'} \frac{| < \vec{k}'n'|H_1|\vec{k}n > |^2}{E_{\vec{k}n} - E_{\vec{k}'n'} + i\eta} \right\rangle_{th.ave.} \tag{1}$$

to second order in phonon displacement, with H_1 and H_2 being the first two contributions from the Taylor expansion of the electron-atom potential [2]. The two terms are known as Debye-Waller and self-energy, respectively.

We define the deformation potential constant $D(\vec{q}, j, \vec{k}, n, n')$, which couples the electron states $|\vec{k}+\vec{q}, n'>$ and $|\vec{k}n>$ through a phonon $|\vec{q}j>$, through the expression [3]

$$\left|\left\langle \vec{k}+\vec{q}n'|H_1|\vec{k}n\right\rangle\right| = D(\vec{q}, j, \vec{k}, n, n')u_{\vec{q}j}\sqrt{N_{\vec{q}j} + \frac{1}{2} \pm \frac{1}{2}} \qquad \text{with} \quad u^2_{\vec{q}j} = \frac{\hbar^2}{2ME_{\vec{q}j}}, \tag{2}$$

where M is the mass of the primitive cell, $E_{\vec{q}j}$ the energy of the phonon mode and $N_{\vec{q}j}$ the Bose-Einstein factor. The plus (minus) sign stands for phonon absorption (emission). In this definition, we have included the overlap factor between the final and initial electron states and phonon-polarization dependences in the D.

We use the overlap valence shell model [4,5] and empirical local pseudopotentials (EPM) [6,7] to calculate the phonon and electron states. The calculated [8] D's for the coupling between the lowest conduction band at Γ and those at L (L_1) and at X (X_1 and X_3) for zincblende-type semiconductors are given in Table 1. We find X_1 to be the lowest conduction band state at X (with the anion at the origin). This may not be the case for GaSb as suggested recently by self-consistent

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Table 1: Calculated intervalley scattering deformation potentials (in eV/Å). The references for the pseudopotential form factors and phonon models used are given in columns 2 and 3.

Material	EPM	Phonons	$D_{\Gamma L}$		$D_{\Gamma X_1}$		$D_{\Gamma X_3}$	
			LA	LO	LA	LO	LA	LO
GaAs	[6]	[5]	3.0	0.5	0	3.5	3.2	0
GaSb	[6]	[5]	2.8	2.7	0	4.5	2.5	0
InSb	[7]	[4]	4.3	1.1	0	4.9	3.3	0
InP	[6]	[4]	1.6	3.0	2.3	0	0	3.7
InAs	[6]	[4]	2.5	1.4	3.2	0	0	2.8
GaP	[6]	[5]	1.2	1.0	1.5	0	0	1.2

calculations [9]. These D's enter into the strengths of indirect transitions and are also important for hot-carrier phenomena [10]. The values given in the table agree reasonably with those in the literature [11]. The D's do not dependend critically on the pseudopotential form factors used, but some models permute the roles of LA and LO phonons at X for GaAs and InSb, where both atoms have similar masses. The prediction of phonon eigenvectors by empirical models remains an open question [12].

The same method can be used to calculate the self-energies of band gaps due to electron-phonon interaction. The thermal average for the shifts and broadenings in equation (1) gives a factor of $N_{\vec{q}j}+\frac{1}{2}$, as both emission and absorption are possible. Therefore, the self-energy term can be written in terms of deformation potential constants as

$$\Delta E_{\vec{k}n}(T)_{SE} - i\Gamma_{\vec{k}n}(T) = \sum_{\vec{q}jn'} \frac{D^2(\vec{q},j,\vec{k},n,n')u^2_{\vec{q}j}}{E_{\vec{k}n} - E_{\vec{k}+\vec{q},n'} + i\eta} \left(N_{\vec{q}j}+\frac{1}{2}\right) \cdot 2 \qquad (3)$$

The shifts and broadenings can be obtained ellipsometrically [13] by measuring the temperature dependence of the dielectric function $<\epsilon>$. Figure 1 shows the imaginary part of $<\epsilon>$ for GaP, InAs, and GaSb at different temperatures. With increasing temperature, the CP's broaden and shift to lower energies. By fitting the third numerical derivatives of our spectra with a Lorentzian lineshape [13], we find the CP energies and broadenings (Figure 2).

The shifts of the E_1-CP with temperature are shown in figure 3 for the three materials. The solid lines are the results of the calculation outlined above, with Debye-Waller term and thermal expansion effects included [8,11], and are in good agreement with the experimental results. Therefore, we believe that the deformation potential formulation gives a good description of shifts of interband CP's with temperature.

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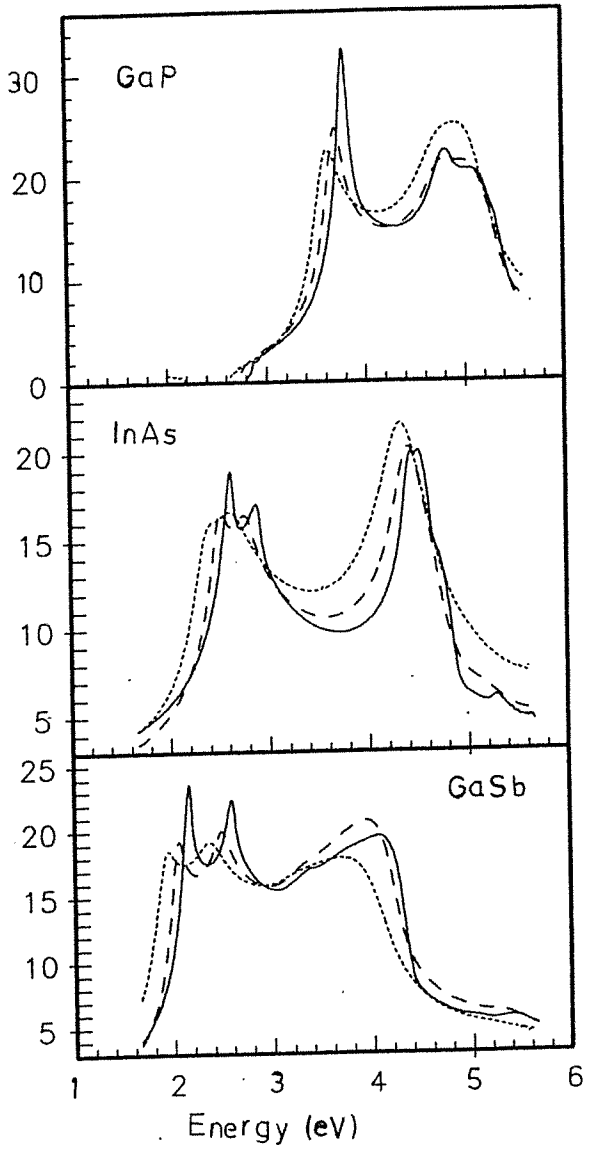


Figure 1: Imaginary part of the pseudodielectric function versus energy (in eV) at 10 K (solid line), 300 K (dashed line) and 500 K (dotted line) for GaP (top), InAs, and GaSb (bottom).

Figure 2: Imaginary part of the third numerical derivative of InAs in the E_1-CP region at 10 K (x). The dashed line is a fit with a Lorentzian lineshape, the solid line is the real part of the fit. The arrows give the positions of the E_1 and $E_1 + \Delta_1$-CP's.

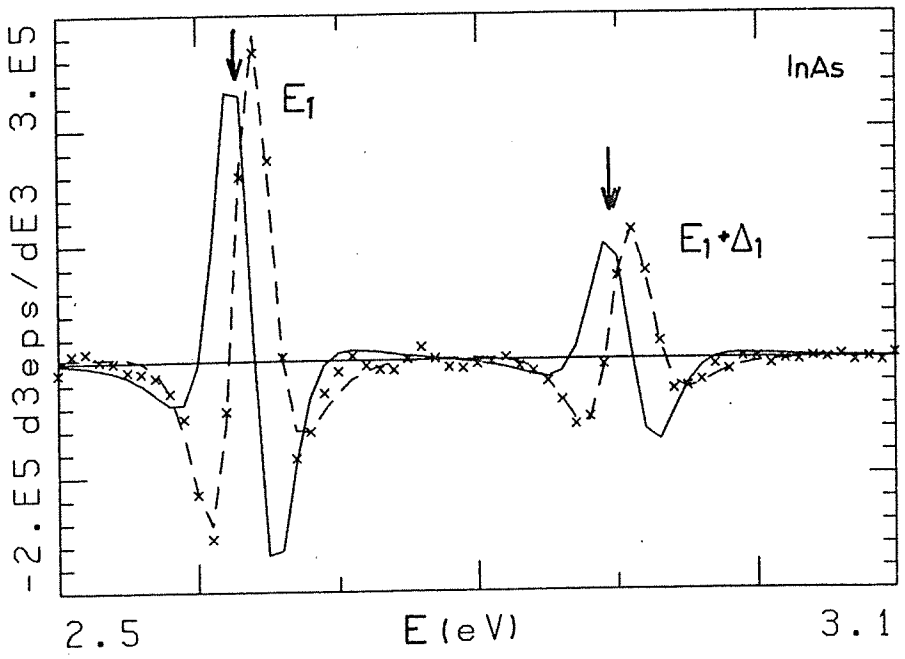
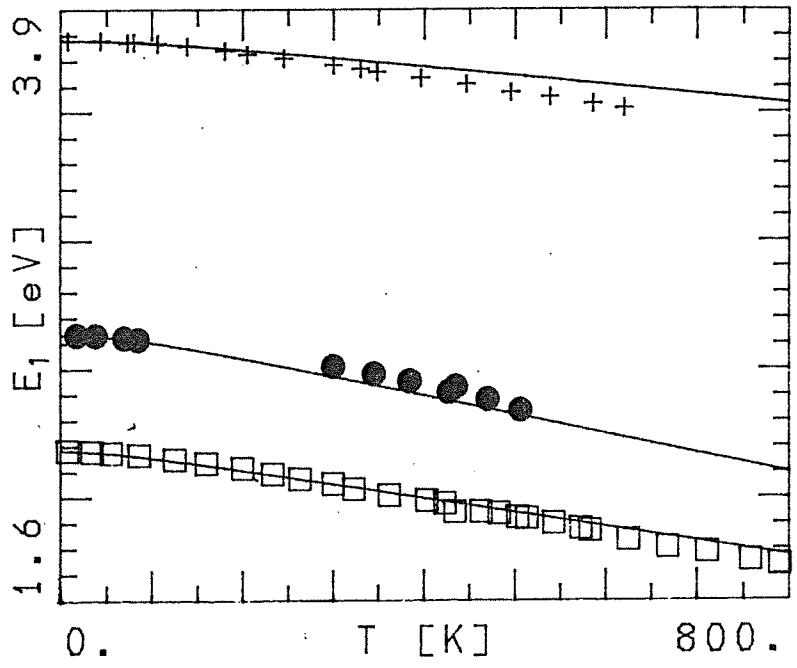


Figure 3: Shift of the E_1-CP energy with temperature for GaP (+), InAs (•), and GaSb (□). The solid lines give the results of the calculation for the shift as outlined in the text.



19th International Conference on

THE PHYSICS OF SEMICONDUCTORS

VOLUME 2

Warsaw, Poland
August 15-19, 1988

EDITOR: **W. ZAWADZKI**

Institute of Physics
Polish Academy of Sciences

Published by

Institute of Physics
Polish Academy of Sciences
02-668 Warsaw, Poland

19TH INTERNATIONAL CONFERENCE ON THE PHYSICS OF SEMICONDUCTORS

ISBN: 83-00-02465-4.

Printed in Wrocław by...
Wrocławska Drukarnia Naukowa – Zam. 2200/88 – 1400 – U-78