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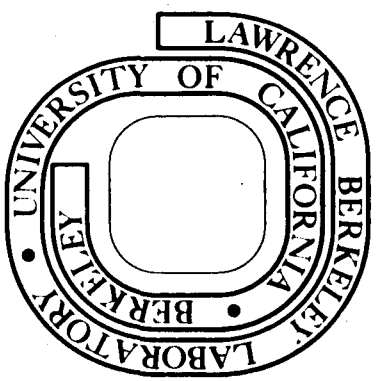

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High Resolution Band Structure and the E_2 Peak in Ge*

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Abstract

We find evidence that the E_2 optical peak in Ge arises from transitions in a well-defined, limited region inside the Brillouin zone. This conclusion is compatible with the recent experimental results of Aspnes. The region of interest is not on symmetry lines, but it is close to the (3/4, 1/4, 1/4) special point determined by Chadi and Cohen. The calculated modulated reflectivity, density of states, and interband masses are in good agreement with experiment.

Recently Aspnes[1] has proposed that the E_2 reflectivity peak, the most prominent peak, in Ge appears to arise from a localized region in the Brillouin zone (BZ) in apparent contradiction to previous theoretical calculations.[2,3,4,5,6] By using a non-local pseudopotential scheme, we are able to determine that the interband transitions of interest arise from a specific BZ region; these conclusions are not at variance with the experimental results. Analysis of the calculated reflectivity reveals that the E_2 peak arises from a well defined, limited region inside the BZ which

is not along lines of high symmetry. This region lies near the special point (3/4, 1/4, 1/4) determined by Chadi and Cohen.[8,9] These results are consistent with previous theoretical calculations and with Aspnes' suggestion that the observed structure can arise from a set of equivalent critical points. We also obtain an interband mass for the E_2 region in reasonably good accord with the experimentally determined value.

In addition, our non-local pseudopotential calculation yields a derivative reflectivity spectrum and density of states in excellent agreement with experiments on modulated reflectivity, X-ray photoemission spectroscopy (XPS), and ultraviolet photoemission spectroscopy (UPS).

The band structure was calculated using the Empirical Pseudopotential Method (EPM) which has been discussed extensively elsewhere.[7,10] For the atomic pseudopotential we took a non-local pseudopotential of the form,

$$V_{NL}(r) = V_L(r) + A_2 f(r) \mathcal{P}_2 \qquad (1)$$

where $V_L(r)$ is the usual local atomic pseudopotential, f(r) is given by $f(r) = \exp(-r^2/R^2)$, and $\mathcal{P}_2$ projects out the $\ell = 2$ angular momentum component.

This non-local pseudopotential is quite similar to the one used recently by Phillips and Pandey.[11] It has been noted by them, and elsewhere[12] that such a non-local d-well potential is necessary to obtain agreement with both the optical reflectivity and the density of states as determined by experiment. However, unlike the Phillips-Pandey calculation we have not used a square well for f(r), but rather a gaussian well. The gaussian

well probably resembles more closely the true potential, and is computationally simpler. As can be noted in Table 1, we obtain comparable agreement with experimentally known transitions. The local form factors used were those of Phillips and Pandey with minor modification,[13] and the gaussian well radius, R, (i.e. the 1/e value) was also chosen to coincide with their square well radius. For the well height we have used $A_2 = 0.55$ Ryd.

Once the band structure has been obtained the imaginary part of the dielectric function, $\epsilon_2(\omega)$, is calculated using the Gilat-Raubenheimer technique.[14] The real part of the dielectric function, $\epsilon_1(\omega)$, can then be calculated by the Kramers-Krönig dispersion relations, and a reflectivity, $R(\omega)$ obtained.

In Figure 1 the experimental and theoretical modulated reflectivity is given for Ge, and as can be observed, the agreement is excellent. In Table 2 identification of the important reflectivity structure is tabulated. Since we have not included spin-orbit interactions in our calculations, the usual E_1 doublet does not appear in the theoretical reflectivity in Figure 1. We also have not included exciton effects which accentuates the experimental E_1 doublet. It is interesting to note that the usual $\Lambda_3 - \Lambda_1$ critical point has been effectively displaced to $L_3' - L_1$ in our calculation. Hence, no $L_3' - L_1$ M_o critical point exists. It is possible, however, that the usual $L_3' - L_1$ M_o critical point can be reinstated with a small change in the potentials and the experimental situation has yet to be clearly resolved.[15]

The E_o' structure near 3.3 eV comes from a $\Delta_5 - \Delta_1$ M_1 critical point. While the $\Gamma_{25}' - \Gamma_{15}$ M_o critical point occurs at this energy, it occupies a small volume and does not contribute significantly to this feature. This is the usual case in band structure calculations; however, experimentally it is possible that exciton effects could enhance the $\Gamma_{25}' - \Gamma_{15}$ transition.

In analyzing the E_2 peak we find that it originates from a specific region of the Γ-X-U-L plane. Figure 2 indicates the energy contours of interest in this region. This very flat plateau region has large dipole matrix elements and because it is not a point of high symmetry there are 48 equivalent regions in the full Brillouin zone making up a large volume. Further, we find no critical point along Σ, and as noted elsewhere[5,6,10] the $X_4 - X_1$ critical point is of little consequence due to its small volume. Such a plateau feature has been noted before in zincblende compounds[6] and Ge[3], where it usually, but not always, is accompanied by a Σ critical point.

The plateau itself, consists of a nearly, if not completely, degenerate $M_1 - M_2$ pair of critical points, and while it is not a "localized" region in the sense of a critical point at a symmetry point, it is still a well-defined and limited region. The dipole matrix elements and energy difference of bands 4 and 5 are nearly constant over the entire plateau. And as will be mentioned in more detail below, the interband mass in this region is also nearly constant. Finally it has been noted that the E_2 peak in the $\epsilon_2(\omega)$ appears to arise from just such a combination,[15] and Aspnes has

determined that at least one interband mass component should be negative in this region.[1] Both of these results are compatible with our calculations.

The E_1' structure in our theoretical modulated reflectivity comes from an $L_3' - L_1$ critical point, and, again, no doublet occurs in the theory due to the absence of spin-orbit interactions.

In order to compare the interband masses as experimentally determined by Aspnes to our resulting band structure, we have calculated some interband masses from the following expression:

$$\frac{m}{m_{ij}} = \frac{2\hbar^2}{m} \sum_{\ell}{}' \left(\frac{P_{j\ell}^2}{E_j - E_\ell} - \frac{P_{i\ell}^2}{E_i - E_\ell} \right) \tag{2}$$

where m_{ij} is a measure of the interband mass size for the ith and jth bands, and $P_{i\ell}$ is the gradient matrix element. We have calculated m_{45} for several points in the plateau region with a range of 0.09m to 0.11m, with the latter value closer to the center of the region. Our results for the interband masses are compared with the experimental results of Aspnes in Table III, and the results are in reasonably good agreement.

Finally we note a possible relationship between the plateau region and the special point (3/4, 1/4, 1/4) of Chadi and Cohen, who have developed a scheme for evaluating sums over wave vector in the Brillouin zone of a periodic function.[8] They have found that by choosing special points in k-space, rapid convergence of the sum can be achieved (e.g. for charge density calculations).

In particular, if we have

$$f = \sum_{\underset{\sim}{k}} g(\underset{\sim}{k}) \tag{3}$$

they have shown that the best two point approximation which can be made is

$$f \cong \frac{1}{4} g(\underset{\sim}{k}_1) + \frac{3}{4} g(\underset{\sim}{k}_2) \tag{4}$$

where $\underset{\sim}{k}_1 = (1/4,\ 1/4,\ 1/4)$ and $\underset{\sim}{k}_2 = (3/4,\ 1/4,\ 1/4)$. It is interesting that such a two point $\epsilon_2(\omega)$ would pick up a contribution to the E_1 and E_1' peaks from k_1 and a contribution to the E_2 peak from k_2. Of course, it is just these peaks which dominate the structure. This would seem to indicate such a scheme might be applicable in evaluating the sum over wave vector needed for dielectric function calculations; further investigations are under way.

In conclusion we have found a specific limited region in the Brillouin zone giving rise to the E_2 structure in the optical spectrum in accordance with the results of Aspnes. Further by using a non-local pseudopotential scheme we are able to obtain excellent agreement with the experimental reflectivity and density of states, and fairly good agreement with the measured interband masses. We have also noted the possibility of applying the Chadi-Cohen special point scheme to evaluating the dielectric function.

Acknowledgement

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Table Captions

Table I. Comparison of theoretical and experimental transitions for Ge. Spin-orbit interactions have been subtracted out from the experimental values.

Table II. Theoretical and experimental reflectivity structure at $5^{\circ}K$ (from Ref. 20), and their identifications, including the location in the Brillouin zone, energy and symmetry of the calculated critical points.

Table III. Comparison of the theoretical inteband mass, m_{ij}, from Eq. (2), with the experimental values. Absolute values are tabulated, and the notation is from Ref. 1.

Figure Captions

Figure 1. A comparison of theoretical (solid line) and experimental (dotted line) modulated reflectivity for Ge. (The experimental results are from Ref. 20.)

Figure 2. Energy contours for the 4-5 transitions for the region of the Brillouin zone which contributes to the E_2 peak. The part of the Γ-X-U-L plane displayed is indicated by the shaded region. The contours are drawn in 0.01 eV steps. (Contours below 4.30 eV and above 4.43 eV are not included.)

Table I.

Transition	Experiment (eV)	Theory (eV)
$\Gamma_1 - \Gamma_{25}'$	12.6 ± 0.3^a, 12.8 ± 0.4^b	12.56
$L_2' - \Gamma_{25}'$	10.6 ± 0.4^a, 10.5 ± 0.4^b	10.30
$L_1 - \Gamma_{25}'$	7.7 ± 0.2^a, 7.4 ± 0.2^b	7.52
$\Sigma_1^{min} - \Gamma_{25}'$	4.5 ± 0.2^a, 4.5 ± 0.3^b	4.55
$L_3' - \Gamma_{25}'$	1.4 ± 0.2^c	1.44
$\Gamma_{25}' - \Gamma_2'$	0.98^d	0.99
$\Gamma_{25}' - \Gamma_{15}$	3.24^e	3.25
$\Gamma_{25}' - L_1$	0.87^f	0.85
$\Gamma_{25}' - X_1$	1.2^g	1.25
$\Gamma_{25}' - L_3$	4.3^c	4.30

a) See Ref. 16 (UPS).
b) See Ref. 21 (XPS).
c) See Ref. 17.
d) See Ref. 22.
e) See Ref. 18.
f) See Ref. 19.
g) See Ref. 5.

Table II.

Reflectivity Structure (eV)		Associated Critical Points Location in Zone	Symmetry	Critical Point Energy (eV)
Theory	Experiment			
2.28	2.22[a] 2.42	$L_3'-L_1$ (0.5,0.5,0.5)	M_1	2.28
3.25	3.20	$\Delta_5-\Delta_1$(0.1,0.,0.)	M_1	3.25
		$\Gamma_{25}'-\Gamma_{15}$ (0.,0.,0.)	M_0	3.25
4.50	4.49	Bands (4-5) Near (0.75,.25,.25)	M_1-M_2	4.38
5.03	5.01	Vol. (4-5) near (.7,.25,.1)	--	--
5.38	--	$\Delta_5-\Delta_2'$ (.5,0.,0.)	M_1	5.35
5.78	5.65[a] 5.88	$L_3'-L_3$ (.5,.5,.5)	M_1	5.73

a) Spin-orbit splitting.

Table III.

Interband Masses

Transition	Mass Component (field [110])	Expt. Value[a] (in m_e)	Theor. Value[b] (m_{ij})
E_o	μ_{hh}, $\hat{e}[1\bar{1}0]$	0.0366±0.013	0.022
$E_o+\Delta_o$	μ_{so}	0.0269	
E_1	μ_T	0.045±0.004	0.050
$E_1+\Delta_1$	μ_T	0.042±0.005	
E_o'	μ, $\hat{e}[001]$	0.034±0.005	0.047[c]
$E_o'+\Delta_o'$	μ, $\hat{e}[1\bar{1}0]$	0.048±0.009	
$E_o'+\Delta_o'+\Delta_o$	μ, $\hat{e}[001]$	0.062±0.006	
E_2	μ_T(?)	0.139±0.015	0.11

a) See Ref. 1.
b) Spin-orbit interactions have not been included.
c) The E_o' interband mass is from $\Gamma_{25}'-\Gamma_{15}$.

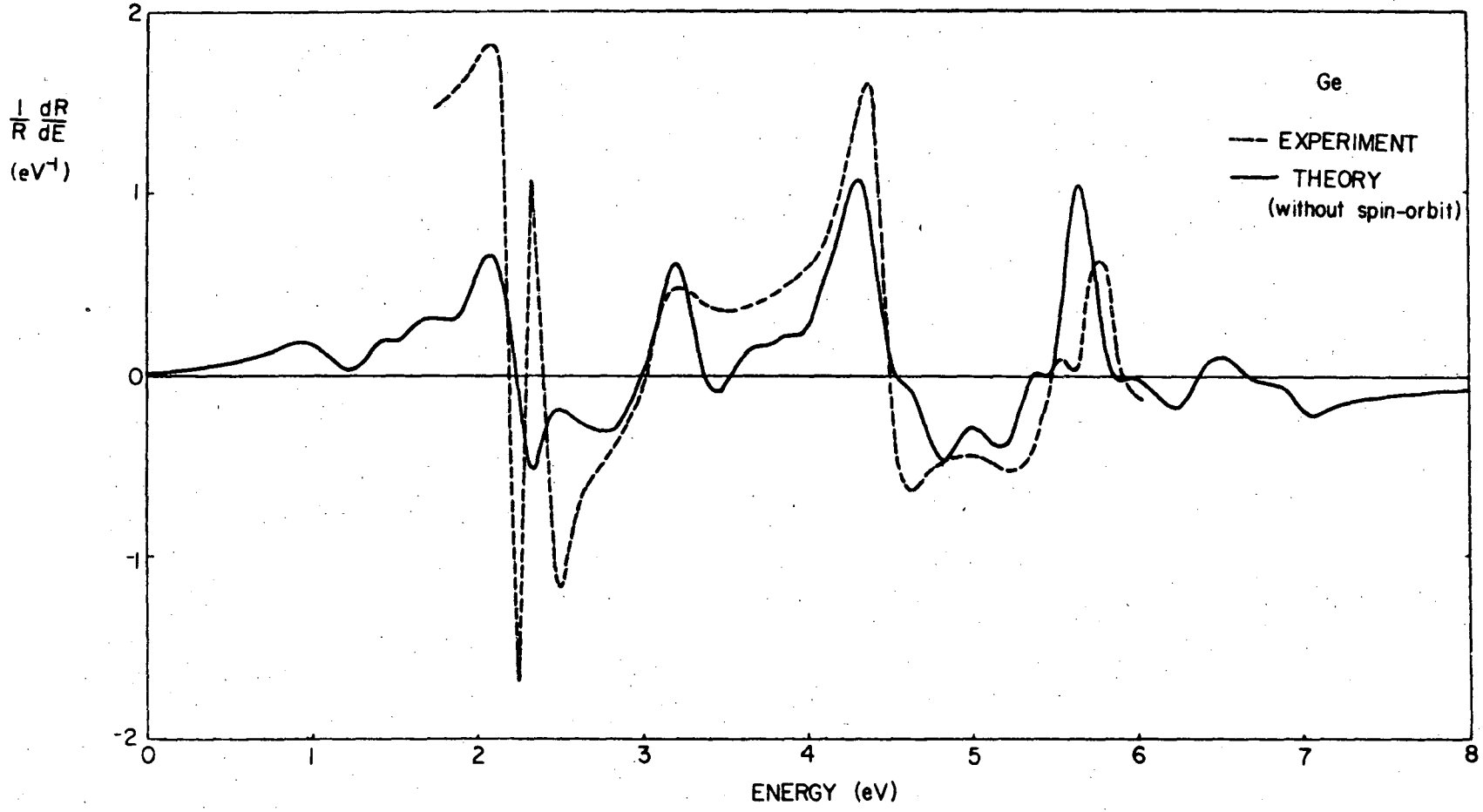
Ge
EXPERIMENT
THEORY
(without spin-orbit)
$\frac{1}{R}\frac{dR}{dE}$
(eV^{-1})
2
1
0
-1
-2
0
1
2
3
4
5
6
7
8
ENERGY (eV)

Fig. 1

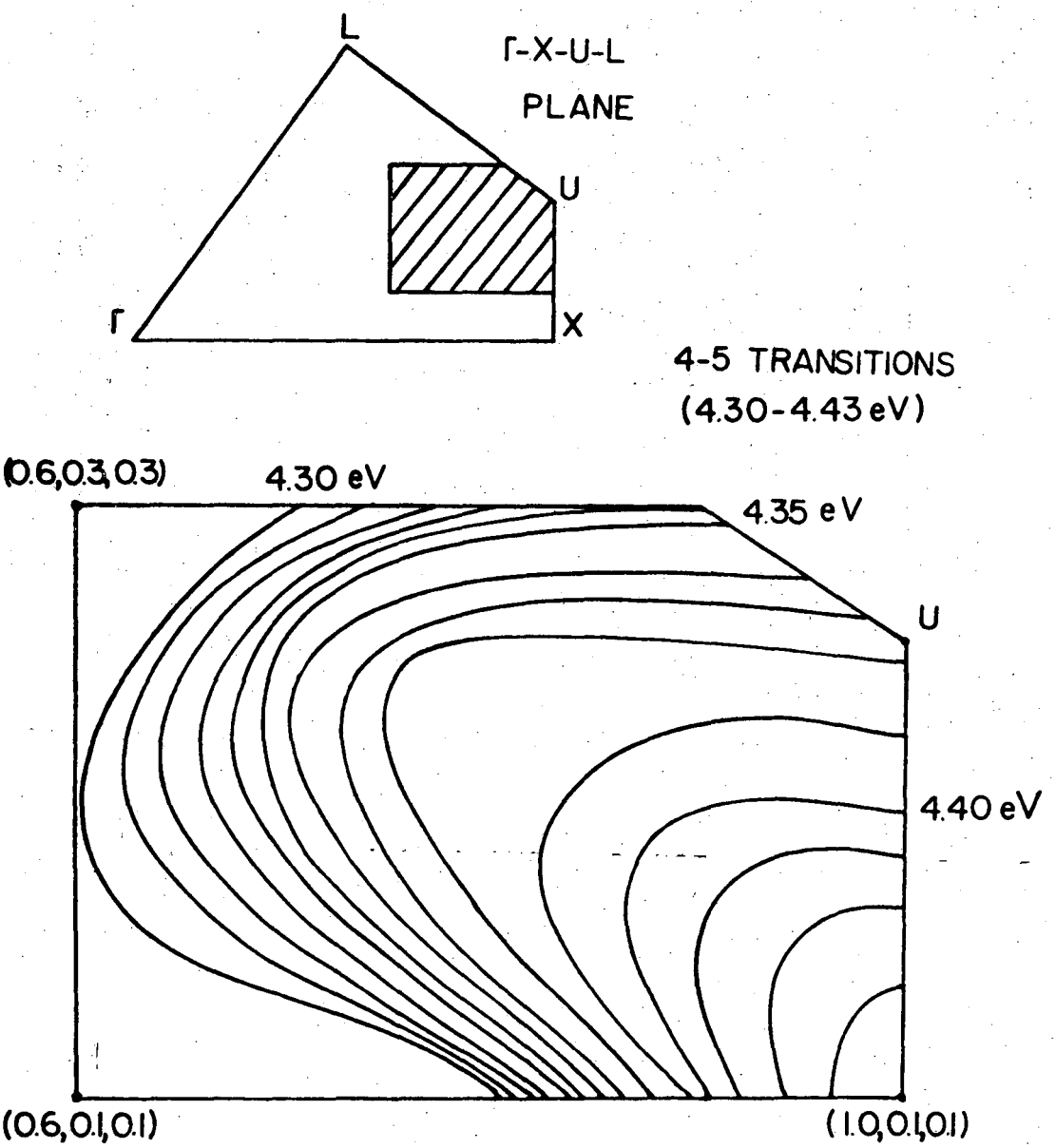
L
Γ-X-U-L
PLANE
U
Γ
X
4-5 TRANSITIONS
(4.30-4.43 eV)
(0.6,0.3,0.3)
4.30 eV
4.35 eV
U
4.40 eV
(0.6,0.1,0.1)
(1.0,0.1,0.1)

Fig. 2

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