High-Resolution Band Structure and the E_2 Peak in Ge†

James R. Chelikowsky* and Marvin L. Cohen
Department of Physics, University of California, Berkeley, California 94720, and
Inorganic Materials Research Division, Lawrence Berkeley Laboratory, Berkeley, California 94720
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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 $(\frac{3}{4},\frac{1}{4},\frac{1}{4})$ 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.[2-6] By using a nonlocal 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 $(\frac{3}{4},\frac{1}{4},\frac{1}{4})$ determined by Chadi and Cohen.[7,8] These results are consistent with previous theoretical calculations and with Aspnes's 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 nonlocal pseudopotential calculation yields a derivative reflectivity spectrum and density of states in excellent agreement with experiments on modulated reflectivity, x-ray photoemission spectroscopy, and ultraviolet photoemission spectroscopy.

The band structure was calculated using the empirical pseudopotential method which has been discussed extensively elsewhere.[9,10] For the atomic pseudopotential we took a nonlocal pseudopotential of the form

$$V_{\mathrm{NL}}(\vec{\mathbf{r}}) = V_{\mathrm{L}}(r) + A_2 f(r)\mathcal{O}_2, \tag{1}$$

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

This nonlocal 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 nonlocal 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. Furthermore, 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 $A_2 = 0.55$ Ry.

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-Kronig dispersion relations, and a reflectivity $R(\omega)$ obtained.

In Fig. 1 the experimental and theoretical modulated reflectivity is given for Ge, and, as can be

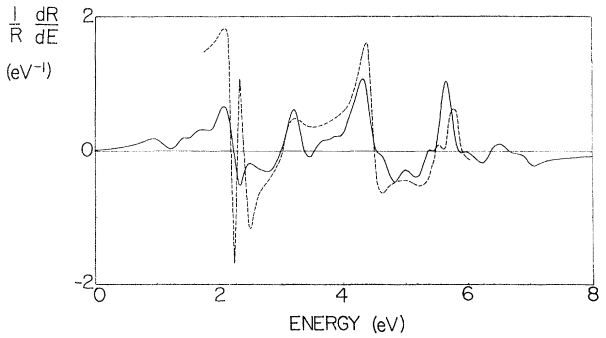

FIG. 1. A comparison of theoretical (solid line) and experimental (dashed line) modulated reflectivity for Ge. (The experimental results are from Ref. 15.)

TABLE I. Theoretical and experimental reflectivity structure at 5°K (from Ref. 15), and their identifications, including the location in the Brillouin zone, energy, and symmetry of the calculated critical points.

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	Δ_5-Δ_1(0.1,0.,0.)	M_1	3.25
		Γ_{25}'-Γ_{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	--	Δ_5-Δ_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.

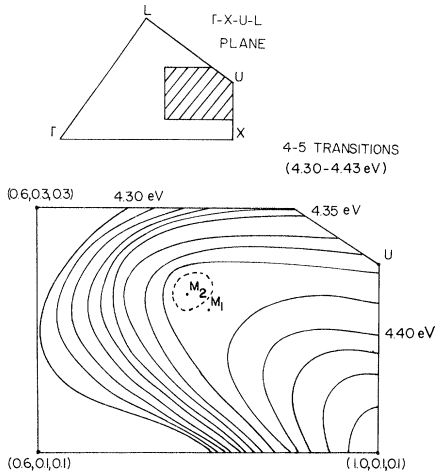

FIG. 2. Energy contours for the 4-5 transitions for the region of the Brillouin zone which contributes to the E_2 peak. The part of the Γ-X-U-L plane displayed is indicated by the shaded region. The contours are drawn in 0.01-eV steps, except around the M_2 critical point where a characteristic contour is indicated by the dashed line. (Contours below 4.30 eV and above 4.43 eV are not included.)

observed, the agreement is excellent. In Table I 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 Fig. 1. We also have not included exciton effects which accentuate the experimental E_1 doublet. It is interesting to note that the usual Λ_3-Λ_1 critical point has been effectively displaced to L_3'-L_1 in our calculation. Hence, no L_3'-L_1M_0 critical point exists. It is possible, however, that the usual L_3'-L_1M_0 critical point can be reinstated with a small change in the potentials, and the experimental situation has yet to be clearly resolved.[16]

The E_0' structure near 3.3 eV comes from a Δ_5-Δ_1M_1 critical point. While the Γ_{25}'-$\Gamma_{15}M_0$ 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 Γ_{25}'-Γ_{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 24 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 because of its small volume. Such a plateau feature has been noted before in zinc-blende 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 $\epsilon_2(\omega)$ 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 because of the absence of spin-orbit interactions.

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

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

		Interband Masses	
Transition	Mass Component (field [110])	Expt. Value[a] (in m_e)	Theor. Value[b] (m_{ij})
E_0	μ_{hh}, $\hat{e}[1\bar{1}0]$	0.0366±0.013	0.022
$E_0+\Delta_0$	μ_{so}	0.0269	
E_1	μ_T	0.045±0.004	0.050[d]
$E_1+\Delta_1$	μ_T	0.042±0.005	
E_0'	μ, $\hat{e}[001]$	0.034±0.005	0.047[c]
$E_0'+\Delta_0'$	μ, $\hat{e}[1\bar{1}0]$	0.048±0.009	
$E_0'+\Delta_0'+\Delta_0$	μ, $\hat{e}[001]$	0.062±0.006	
E_2	μ_T(?)	0.139±0.015	0.11[d]

[a]See Ref. 1.
[b]Spin-orbit interactions have not been included.
[c]The E_0' interband mass is from $\Gamma_{25}'-\Gamma_{15}$.
[d]Transverse mass component.

pression:

$$\frac{m}{m_{ij}}=\frac{2\hbar^2}{m}\sum_l{}'\left(\frac{P_{jl}{}^2}{E_j-E_l}-\frac{P_{il}{}^2}{E_i-E_l}\right), \tag{2}$$

where m_{ij} is a measure of the interband mass size for the ith and jth bands, and P_{il} 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 II, and the results are in reasonably good agreement.

Finally we note a possible relationship between the plateau region and the special point $(\frac{3}{4},\frac{1}{4},\frac{1}{4})$ of Chadi and Cohen, who have developed a scheme for evaluating sums over wave vector in the Brillouin zone of a periodic function.[7] 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

$$f=\sum_{\vec{k}} g(\vec{k}), \tag{3}$$

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

$$f\cong\tfrac{1}{4}g(\vec{k}_1)+\tfrac{3}{4}g(\vec{k}_2), \tag{4}$$

where $\vec{k}_1=(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ and $\vec{k}_2=(\frac{3}{4},\frac{1}{4},\frac{1}{4})$. 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 $\vec{k}_1$ and a contribution to the E_2 peak from $\vec{k}_2$. Of course, it is just these peaks which dominate the structure. This would seem to indicate that 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 nonlocal 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.

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Interaction between Magnons and Magnetic Excitons in $TbAl_2$

H.-G. Purwins,* J. G. Houmann, and P. Bak
Danish Atomic Energy Commission Research Establishment Risø, Roskilde, Denmark

and

E. Walker
Département Physique de la Matière Condensée, Université de Genève, Genève, Switzerland
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Inelastic neutron-scattering measurements of acoustic magnons are reported for ferromagnetic $TbAl_2$ between 4.2 and 80 K for wave-vector transfers of 0.00 and 0.10 $Å^{-1}$. Above 35 K we observe a double-peak structure in the scattered neutron intensity which is theoretically interpreted in terms of an interaction between the magnon and a magnetic exciton excited from an almost unpopulated state. This is the first observation of an interaction of this kind.

Magnetic substances in which the crystalline electric field and the exchange energies are of the same order of magnitude have many interesting features.[1] In particular it has been pointed out[2] that in the paramagnetic region excitations from the ground state can interact with excitations from almost unpopulated excited magnetic states. These interactions can lead to splittings of the magnetic exciton branches which can in principle be observed by inelastic neutron scattering. We show in the present paper that a splitting of the same nature can occur also in the ordered phase. In this case a magnon interacts with an exciton associated with a transition between higher-lying magnetic states. We report the experimental observation and theoretical interpretation of this magnon-exciton interaction.

The sample was a single crystal of $TbAl_2$ produced by the Czochralski method.[3] $TbAl_2$ has the cubic $MgCu_2$ structure[4] and orders ferromagnetically below 105 K.[5,6] The easy and hard directions of magnetization are $\langle 111\rangle$ and $\langle 100\rangle$, respectively, and the magnetic moment observed from low-temperature magnetization measurements has the free-ion value of $9\mu_B$.[6] The magnon dispersion relations for both the acoustic and optic branches at 4.2 K have been reported recently, and a spin-wave energy gap of 1.7 ± 0.1 meV has been observed. An isotropic Heisenberg exchange seems to account satisfactorily for the data which have so far been obtained.[7,8]

The neutron inelastic scattering experiment was performed on a triple-axis spectrometer at the DR 3 reactor at Risø. The constant-q mode of operation was used. In order to eliminate possible spurious peaks, all the scans were carried out for at least two different values of fixed scattered-neutron wave vector in the range 1.5 to 2.1 $Å^{-1}$. Some typical experimental results are shown in Fig. 1. We observe a well-defined magnon peak at 1.58 ± 0.05 meV at 4.2 K. At 39 K we

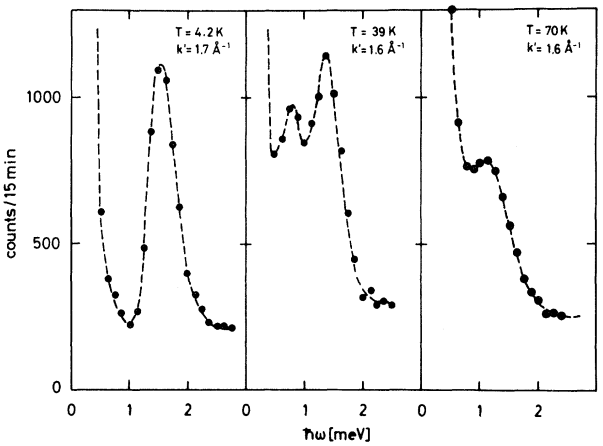

FIG. 1. Neutron intensity measured at the (111) reciprocal lattice point corresponding to $q = 0$. k' is the wave vector of the scattered neutrons and $\hbar\omega$ the energy transfer from the neutrons.