Model dielectric constants of Si and Ge

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A method is described for calculation of the real (ϵ_1) and imaginary parts (ϵ_2) of the dielectric function of Si and Ge at energies below and above the fundamental absorption edge, in which the model is based on the Kramers-Kronig transformation and strongly connected with the electronic energy-band structure of the medium. A complete set of the critical points (CP's) are considered in this study. This model reveals distinct structures at energies of the E_0, $E_0 + \Delta_0$ [three-dimensional (3D) M_0], E_1, $E_1 + \Delta_1$ (3D M_1 or 2D M_0), E_2 [a mixture of damped harmonic oscillator (DHO) and 2D M_2], E'_1, and E'_0 (triplet) CP's (DHO). The indirect-band-gap transitions also play an important part in the spectral dependence of ϵ_2 of Si. Results are in satisfactory agreement with the experimental information over the entire range of photon energies. The strength and broadening parameters at energies of each CP are obtained and discussed.

I. INTRODUCTION

Studies of the optical properties of solids have proved to be a powerful tool in our understanding of the electronic energy-band structures of these solids.[1] The dielectric function, $\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$, is known to describe the optical properties of the medium at all photon energies $E = \hbar\omega$. Real and imaginary parts of this dielectric function are connected by the Kramers-Kronig (KK) relations:

$$\epsilon_1(\omega) = 1 + \frac{2}{\pi} \int_0^\infty \frac{\omega' \epsilon_2(\omega')}{(\omega')^2 - \omega^2} d\omega' ,$$

$$\epsilon_2(\omega) = -\frac{2}{\pi} \int_0^\infty \frac{\omega' \epsilon_1(\omega')}{(\omega')^2 - \omega^2} d\omega' .$$

Spectroscopic ellipsometry is an excellent technique with which to investigate the optical response of semiconductors.[2-20] Recently, Aspnes and Studna[4] have studied optical properties of Si and Ge by spectroscopic ellipsometry. They reported room-temperature pseudodielectric-function data and related optical constants of Si and Ge for energies E from 1.5 to 6.0 eV. Viña et al.[7] also studied the temperature dependence of the dielectric function of Ge in the temperature range between 100 and 850 K by spectroscopic ellipsometry ($E = 1.25-5.6$ eV). They obtained broadening parameters, amplitudes, and phase angles for the E_1, $E_1 + \Delta_1$, E'_0, and E_2 critical points (CP's). They also found a decrease of the excitonic interaction with increasing temperature. More recently, Lautenschlager et al.[19] measured the dielectric function of Si by ellipsometry in the (1.7–5.7)-eV photon-energy range. They obtained the parameters of the E'_0, E_1, E_2, and E'_1 CP's at temperatures between 30 and 820 K. However, these spectral-dependence data seem to have one disadvantage with respect to theoretical modeling: they are not expressed as continuous analytic functions of the photon energies.

In this paper we present a method for calculation of the spectral dependence of the dielectric constants, $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$, of Si and Ge based on a simplified model of the energy-band structures of the materials. This model covers the optical response of Si and Ge over the entire range of photon energies. In Sec. II we present a brief review of material properties of Si and Ge with particular emphasis on their electronic energy-band structures. This information will be used to build a theoretical model in the next section. We describe in Sec. III the details of our model, which is based on the KK transformation and includes the E_0, $E_0 + \Delta_0$, E_1, $E_1 + \Delta_1$, E_2, E'_1, and E'_0 (triplet) gaps as the main dispersion mechanisms. The effects of indirect-band-gap transitions, which will play an important part in the analysis of the ϵ_2 spectrum (Si), are also discussed. In Sec. IV we show the fits with our model to the experimental data of Si and Ge reported by Philipp and Ehrenreich (Ref. 21) and Aspnes and Studna (Ref. 4). Finally, in Sec. V the conclusions obtained in this study are briefly summarized.

II. ENERGY-GAP ARGUMENT

Si and Ge have been the subject of considerable research and device-development activities. A wide variety of calculations[22-56] and experiments[57-103] have given detailed information about their electronic energy-band structures. We reproduce in Fig. 1 the energy-band structures of Si and Ge along two lines of high symmetry from the center to the boundary of the first Brillouin zone (BZ) (see, e.g., Refs. 33 and 35). The electronic states are labeled using the notation for the representations of the single group of the diamond structure.[104] The locations of several interband transitions are included in the figure. These are the transitions which may play an important part in the analysis of ϵ_1 and ϵ_2 spectra. We also list in Tables I and II indirect-band-gap and CP energies of the main structure present in the optical spectra of Si (Table I) and Ge (Table II) at 300 K taken from the literature reported.

FIG. 1. Electronic energy-band structures of Si and Ge along two symmetry directions, including locations of several interband transitions.

The fundamental absorption edge of Si corresponds to indirect transitions from the highest valence band at the Γ point to the lowest conduction band near X (i.e., $\Gamma_{25'}^v \rightarrow \Delta_1^c$). The conduction band Γ_{15}^c appears to be lower in energy than $\Gamma_{2'}^c$. This ordering of the conduction bands is in direct contrast to those of Ge and zinc-blende materials (such as GaAs and InP). The spin-orbit interaction splits Γ_{15}^c into Γ_6^c and Γ_8^c (double-group notation; splitting energy Δ_0'), and $\Gamma_{25'}^v$ into Γ_8^v and Γ_7^v (double-group notation; splitting energy Δ_0). The corresponding transitions at or near $\mathbf{k}=0$ (Γ) are, respectively, labeled E_0' [$\Gamma_{25'}^v(\Gamma_8^v) \rightarrow \Gamma_{15}^c(\Gamma_6^c)$], $E_0'+\Delta_0'$ [$\Gamma_{25'}^v(\Gamma_8^v) \rightarrow \Gamma_{15}^c(\Gamma_8^c)$], $E_0'+\Delta_0$ [$\Gamma_{25'}^v(\Gamma_7^v) \rightarrow \Gamma_{15}^c(\Gamma_6^c)$; dipole forbidden], $E_0'+\Delta_0'+\Delta_0$ [$\Gamma_{25'}^v(\Gamma_7^v) \rightarrow \Gamma_{15}^c(\Gamma_8^c)$], E_0 [$\Gamma_{25'}^v(\Gamma_8^v) \rightarrow \Gamma_{2'}^c(\Gamma_6^c)$], and $E_0+\Delta_0$ [$\Gamma_{25'}^v(\Gamma_7^v) \rightarrow \Gamma_{2'}^c(\Gamma_6^c)$]. The splitting energies Δ_0 and Δ_0' of Si are, however, very small[103] and are not taken into consideration in the present analysis. The lowest direct band gap of Si is the E_0' edge. It is not easy to measure the E_0 and $E_0+\Delta_0$ edges of Si because of their exceedingly weak structures in this material.[98]

The E_1 and $E_1+\Delta_1$ transitions in Si take place along the $\langle 111 \rangle$ directions (Λ) of the BZ [E_1, $\Lambda_3^v(\Lambda_{4,5}^v) \rightarrow \Lambda_1^c(\Lambda_6^c)$; $E_1+\Delta_1$, $\Lambda_3^v(\Lambda_6^v) \rightarrow \Lambda_1^c(\Lambda_6^c)$].[29,32−34,38,39,48,49] The spin-orbit-splitting energy Δ_1, like Δ_0 and Δ_0', of Si is extremely small,[103] and thus no clear observations relating to it have been reported. The E_1 transitions in Si are nearly degenerate with the E_0' transitions, and therefore the most attention has been given to these complicated E_1-edge structures [(3.1–3.4)-eV region].[59,60,63,64] The edge labeled E_1' results from transitions in the Λ directions of the BZ, $\Lambda_3^v \rightarrow \Lambda_3^c$, and is well separated in energy from other CP's (see Table I).

The more pronounced structure found in the region higher in energy than E_1 is labeled E_2. The nature of the E_2 transitions in Si is more complicated, since it does not correspond to a single, well-defined CP. In fact, the pre-

TABLE I. Energies of indirect-band-gap (E_g^{id}) and critical points in Si at 300 K (in eV).

E_g^{id}	E_0'	E_1	E_0	$E_0+\Delta_0$	E_2	E_1'
1.1117[a]						
1.124[b]						
	3.281[c]	3.360[c]				
	3.294[d]	3.412[d]				
		3.38[e]			4.4[e]	
	3.32[f]	3.38[f]	4.06[f]	4.13[f]	4.31[f]	
					4.49[f]	
	3.320[g]	3.396[g]			4.270[g]	5.317[g]
					4.492[g]	
	3.330[h]	3.40[h]				
	3.34[i]	3.41[i]				
	3.5[j]	3.7[j]			4.5[j]	
		3.38[k]			4.4[k]	
					4.303[l]	

[a]Reference 57.
[b]Reference 58.
[c]Reference 59.
[d]Reference 60.
[e]Reference 61.
[f]Reference 62.
[g]Reference 19.
[h]Reference 63.
[i]Reference 64.
[j]Reference 65.
[k]Reference 66.
[l]Reference 67.

TABLE II. Energies of indirect-band-gap (E_g^{id}) and critical points in Ge at 300 K (in eV).

E_g^{id}	E_0	$E_0+\Delta_0$	E_1	$E_1+\Delta_1$	E_0'	$E_0'+\Delta_0'$	$E_0'+\Delta_0'+\Delta_0$	E_2	E_1'
0.6657[a]									
	0.802[b]								
	0.798[c]	1.09[c]							
	0.80[d]	1.09[d]							
	0.796[e]	1.092[e]	2.09[e]	2.26[e]					
			2.12[f]	2.34[f]	3.13[f]	3.32[f]		4.42[f]	
			2.065[g]	2.266[g]					
			2.087[g]	3.291[g]					
			2.09[h]	2.29[h]				4.35[h]	
			2.105[i]	2.303[i]					
			2.126[i]	2.332[i]					
			2.107[j]	2.303[j]					
			2.11[k]	2.31[k]				4.44[k]	
			2.111[l]	2.298[l]	3.110[l]			4.368[l]	
			2.115[m]	2.325[m]					
			2.12[n]	2.32[n]	2.80[n]	2.93[n]			
			2.15[o]	2.35[o]					
					2.92[p]				
					2.983[q]	3.169[q]	3.470[q]		
									5.80[r]

[a]Reference 57.   [g]Reference 72.   [m]Reference 76.
[b]Reference 68.   [h]Reference 73.   [n]Reference 77.
[c]Reference 69.   [i]Reference 74.   [o]Reference 78.
[d]Reference 70.   [j]Reference 75.   [p]Reference 79.
[e]Reference 71.   [k]Reference 61.   [q]Reference 80.
[f]Reference 62.   [l]Reference 7.   [r]Present work.

cise low-field electroreflectance analysis[91] revealed that the E_2 structure consists of three CP's, $E_2(1)$, $E_2(2)$, and $E_2(3)$, of type M_1, M_1, and M_2, respectively. It was concluded that this is due to an accidental coincidence of the M_1 saddle point in the $\langle 110 \rangle$ directions ($\Sigma_2^v \rightarrow \Sigma_3^c$) and an M_2 saddle point near X ($\Delta_5^v \rightarrow \Delta_1^c$).

The energy-band structure of Ge is essentially the same as that of Si because both materials have the same crystal structure (i.e., diamond lattice). However, the conduction-band ordering at the Γ point of Ge is quite different from that of Si (but is the same as those of zinc-blende, III-V materials), as mentioned above.

The Ge crystal is an indirect-band-gap semiconductor. The lowest indirect-absorption edge of Ge corresponds to transitions from the highest valence band at the Γ point ($\Gamma_{25'}^v$) to the lowest conduction band at or near L (L_1 or Λ_1). As in the zinc-blende materials, the lowest direct-band-gap transitions in Ge occur in the center of the BZ [E_0: $\Gamma_{25'}^v(\Gamma_8^v) \rightarrow \Gamma_{2'}^c(\Gamma_6^c)$]. The E_1 edge results from transitions in the Λ directions of the BZ. The next prominent structure, E_2, is attributed to an accidental coincidence of an M_1 saddle point at X and an M_2 saddle point in the Σ directions.[30,31,39] This structure is also believed to originate mainly from a region in the Γ-X-U-L plane near $\mathbf{k}=(2\pi/a)(\frac{3}{4},\frac{1}{4},\frac{1}{4})$.[49,105] More recently, it is attributed to a small region centered at $\mathbf{k}=(2\pi/a)(0.77, 0.29, 0.16)$.[106] The Δ_0, Δ_0', and Δ_1 spin-orbit splittings of Ge are considerably larger than those of Si,[103] and thus the splitting-related transitions have been experimentally observed (see Table I).

III. THEORETICAL EXPRESSION

The joint-density-of-states functions $J_{cv}(\omega)$ can be related to the optical constant $\epsilon_2(\omega)$ as follows:

$$\epsilon_2(\omega)=\frac{4\hbar^2 e^2}{\pi m^2 \omega^2}\,|\,\langle c\,|\,p\,|\,v\,\rangle\,|^2\,J_{cv}(\omega)\;, \qquad (1)$$

where $\langle\,|\,p\,|\,\rangle$ is the momentum matrix element for v (valence) $\rightarrow c$ (conduction) transitions. In the following we try to obtain the model dielectric functions for the CP's of various transition energies (E_0, $E_0+\Delta_0$, E_1, $E_1+\Delta_1$, E_2, E_1', etc.). The effects of indirect-band-gap transitions which will take an important part in the analysis of the ϵ_2 spectrum (Si) are also discussed briefly.

A. E_0 and $E_0+\Delta_0$ transitions

The E_0 and $E_0+\Delta_0$ transitions in the diamond- and zinc-blende-type semiconductors occur in the center of the BZ (Γ). These transitions are of the three-dimensional (3D) M_0 CP's. Assuming the bands are parabolic, we obtain the contribution of these gaps to $\epsilon_2(\omega)$ and $\epsilon_1(\omega)$ (Ref. 107):

$$\epsilon_2(\omega)=[\,A/(\hbar\omega)^2][(\hbar\omega-E_0)^{0.5}H(\chi_0-1)$$
$$+\tfrac{1}{2}(\hbar\omega-E_0-\Delta_0)^{0.5}H(\chi_{s.o.}-1)]\;, \qquad (2)$$

$$\epsilon_1(\omega) = AE_0^{-1.5}[f(\chi_0) + \tfrac{1}{2}[E_0/(E_0+\Delta_0)]^{1.5}f(\chi_{s.o.})] \ , \tag{3}$$

with

$$A = \tfrac{4}{3}(\tfrac{3}{2}m^*)^{1.5}P^2 \ , \tag{4}$$

$$f(\chi_0) = \chi_0^{-2}[2 - (1+\chi_0)^{0.5} - (1-\chi_0)^{0.5}H(1-\chi_0)] \ , \tag{5a}$$

$$f(\chi_{s.o.}) = \chi_{s.o.}^{-2}[2 - (1+\chi_{s.o.})^{0.5}$$
$$- (1-\chi_{s.o.})^{0.5}H(1-\chi_{s.o.})] \ , \tag{5b}$$

$$\chi_0 = \hbar\omega/E_0 \ , \tag{6a}$$

$$\chi_{s.o.} = \hbar\omega/(E_0+\Delta_0) \ , \tag{6b}$$

and

$$H(y) = \begin{cases} 1 & \text{for } y \geq 0 \\ 0 & \text{for } y < 0 \ . \end{cases} \tag{7}$$

In Eq. (4), m^* is the combined density-of-states mass and P^2 is the squared momentum matrix element.

As we will see later, the strength of the E_0 and $E_0+\Delta_0$ transitions in Ge is very weak. This is due to the small density of states associated with these transitions (i.e., due to the small effective mass of the $\Gamma_{2'}$ conduction band). However, we can clearly see the $E_0/(E_0+\Delta_0)$ structures in the optical spectrum of Ge in the region very close to the fundamental absorption edge.[68-71,108]

The $E_0/(E_0+\Delta_0)$ structures in Si, on the other hand, appear in spectrum between the dominant E_1 and E_2 structures.[63,98] As a result, its exceedingly weak nature would be completely covered with them. Because of this reason, we shall not take into account the contribution of these transitions in the $\epsilon(\omega)$ spectra of Si.

B. E_1 and $E_1+\Delta_1$ transitions

Band-structure calculations and some experimental work indicated that the E_1 and $E_1+\Delta_1$ transitions take place along the $\langle 111 \rangle$ directions (Λ) of the BZ. These CP's are of the 3D M_1 type and occur in the region near 3.4 eV (E_1) for Si and near 2.1 eV (E_1) and 2.3 eV ($E_1+\Delta_1$) for Ge. The contributions to $\epsilon_2(\omega)$ of this type are[107]

$$\epsilon_2(\omega) = \begin{cases} \pi\chi_1^{-2}[B_1 - B_{11}(E_1-\hbar\omega)^{0.5}] & (\hbar\omega < E_1) \ , \\ \pi B_1\chi_1^{-2} & (\hbar\omega \geq E_1) \end{cases} \tag{8}$$

for the E_1 transitions, and

$$\epsilon_2(\omega) = \begin{cases} \pi\chi_{1s}^{-2}[B_2 - B_{21}(E_1+\Delta_1-\hbar\omega)^{0.5}] & (\hbar\omega < E_1+\Delta_1), \\ \pi B_2\chi_{1s}^{-2} & (\hbar\omega \geq E_1+\Delta_1) \end{cases} \tag{9}$$

for the $E_1+\Delta_1$ transitions, where

$$\chi_1 = \hbar\omega/E_1 \ , \tag{10a}$$

$$\chi_{1s} = \hbar\omega/(E_1+\Delta_1) \ . \tag{10b}$$

In Eqs. (8) and (9), the B's are the strength parameters. Since the M_1 CP longitudinal effective mass is much larger than its transverse counterparts, one can treat these 3D M_1 CP's as two-dimensional (2D) minima M_0. The contribution to $\epsilon_2(\omega)$ of this type of 2D minima is given by

$$\epsilon_2(\omega) = \pi[B_1\chi_1^{-2}H(\chi_1-1) + B_2\chi_{1s}^{-2}H(\chi_{1s}-1)] \ , \tag{11}$$

where the H's are functions defined by Eq. (7).

The contribution of the E_1 and $E_1+\Delta_1$ transitions to $\epsilon_1(\omega)$ can be calculated from Eq. (11) by using the KK transformation. The result is

$$\epsilon_1(\omega) = -B_1\chi_1^{-2}\ln(1-\chi_1^2) - B_2\chi_{1s}^{-2}\ln(1-\chi_{1s}^2) \ . \tag{12}$$

The first and second term on the right-hand side of Eq. (12), respectively, correspond to the E_1- and $(E_1+\Delta_1)$-gap contributions.

C. E_2 transitions

The E_2 structure appears in the region near 4.3 eV for Si and near 4.4 eV for Ge. As mentioned in Sec. II, the nature of the E_2 transitions is more complicated: it does not correspond to a single, well-defined CP. The structure in Si had been tried to be characterized by a one-dimensional (1D) maximum,[109] a mixture of a 2D M_1 and a 2D M_2,[19] or a mixture of a 3D M_1 and a 3D M_2 CP.[63,91] The E_2 structure in Ge could be fitted using either a 3D M_2 or a mixture of a 2D M_1 and a 2D M_2 CP.[7]

Here we shall characterize the E_2 structure as that of a damped harmonic oscillator (DHO). This oscillator gives

$$\epsilon_2(\omega) = C\chi_2\gamma/[(1-\chi_2^2)^2 + \chi_2^2\gamma^2] \ , \tag{13}$$

$$\epsilon_1(\omega) = C(1-\chi_2^2)/[(1-\chi_2^2)^2 + \chi_2^2\gamma^2] \ , \tag{14}$$

with

$$\chi_2 = \hbar\omega/E_2 \ , \tag{15}$$

where C and γ are, respectively, the strength and damping parameters of the oscillator.

The DHO model provides a Lorentzian-like line shape (see Figs. 2 and 3), and in the limit $\gamma \to 0$ the ϵ_2 spectrum exhibits a divergence at $\hbar\omega = E_2$. We can also regard the E_2 gap as the CP of 2D M_1 type. The contribution to ϵ_2 of this type is

$$\epsilon_2(\omega) = \pi\chi_2^{-2}(D_1\ln|1-\chi_2| - D_2) \ , \tag{16}$$

where the D's are the strength parameters. Equation (16) exhibits a divergence at $\chi_2 = 1.0$ (i.e., $\hbar\omega = E_2$), and its spectrum very much resembles that of the DHO model when we take into account the damping effect in the equation. Therefore, we can say that the DHO is a different representation of the broadened 2D M_1 CP. It is also interesting to point out[110] that variation of CP anisotropy parameters from three to two dimensions changes the density-of-states functions from M_1 and M_2 CP's (3D) to M_1 (2D). This simply means that the 2D M_1 CP originates from the 3D M_1 and M_2 CP's.

We found that the E_2 structures in some III-V compounds (such as InSb, GaAs, GaP, and $Al_xGa_{1-x}As$)

(Refs. 107 and 111) can be well fitted by the DHO model. However, unfortunately the structures in semiconductors of group IV (Si and Ge) are not reasonably fitted only by the DHO. We find that the best result is obtained with a mixture of the DHO and a 2D maxima (M_2).

The contribution of the 2D M_2 CP to $\epsilon_2(\omega)$ is written as

$$\epsilon_2(\omega) = \begin{cases} \pi F \chi_2^{-2} & (\hbar\omega \leq E_2), \\ 0 & (\hbar\omega > E_2), \end{cases} \tag{17}$$

where F is the strength of the 2D M_2 CP.

The conduction and valence bands reducing to infinitely small energies implied by Eq. (17) should be nonphysical. Because of this reason, we now modify the model by taking into account a low-energy cutoff at the energy E_{cl}. This modification provides

$$\epsilon_2(\omega) = \pi F \chi_2^{-2} H(\chi_{cl} - 1), \tag{18}$$

with

$$\chi_{cl} = \hbar\omega/E_{cl}. \tag{19}$$

The KK transformation of Eq. (18) gives

$$\epsilon_1(\omega) = -F\chi_2^{-2}\ln\left|\frac{1-\chi_{cl}^2}{1-\chi_2^2}\right|. \tag{20}$$

In Figs. 2 and 3, respectively, we show the line shapes of the E_2-gap contribution to $\epsilon(\omega)$ for Si and Ge. The dashed lines correspond to the DHO [ϵ_2, Eq. (13); ϵ_1, Eq. (14)], and the solid lines are the results of a mixture of the DHO and 2D M_2 CP [ϵ_2, Eq. (18); ϵ_1, Eq. (20)]. The numerical parameters used in the calculations are listed in Table III. Here, the low-energy cutoff E_{cl} in Eqs. (18)–(20) is assumed to be the same value as E_1 (i.e.,

FIG. 3. Line shapes of the E_2-gap contribution to $\epsilon(\omega)$ for Ge. The dashed lines correspond to the DHO [ϵ_2, Eq. (13); ϵ_1, Eq. (14)]. The solid lines are the results of a mixture of the DHO and 2D M_2 CP [ϵ_2, Eq. (18); ϵ_1, Eq. (20)].

TABLE III. Parameters used in the calculation of $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$.

Parameter	Material	
	Si	Ge
E_0 (eV)		0.80
$E_0 + \Delta_0$ (eV)		1.09
A (eV$^{1.5}$)		2.70
E_1 (eV)	3.38	2.11
$E_1 + \Delta_1$ (eV)		2.30
B_1	5.22	3.79
B_{11} (eV$^{-0.5}$)	7.47	5.08
B_2		3.29
B_{21} (eV$^{-0.5}$)		7.35
$\Gamma[E_1/(E_1+\Delta_1)]$ (eV)	0.05	0.07
E_2 (eV)	4.27	4.35
C	3.01	2.51
γ	0.127	0.109
F	3.51	0.23
$\Gamma(E_2)$ (eV)	0.04	0.04
E_a (eV)[a]	5.32	5.80
C_a	0.21	0.51
γ_a	0.089	0.156
E_b (eV)[b]		3.30
C_b		0.91
γ_b		0.140
E_c (eV)[b]		3.80
C_c		1.33
γ_c		0.133
E_g^{id} (eV)	1.12	
D	0.89	
$\epsilon_{1\infty}$	1.8	2.7

[a]This energy corresponds to the E_1' gap (see Tables I and II).
[b]These take account of the [E_0' (triplet)]-gap contribution.

FIG. 2. Line shapes of the E_2-gap contribution to $\epsilon(\omega)$ for Si. The dashed lines correspond to the DHO [ϵ_2, Eq. (13); ϵ_1, Eq. (14)]. The solid lines are the results of a mixture of the DHO and 2D M_2 CP [ϵ_2, Eq. (18); ϵ_1, Eq. (20)].

$E_{cl} = E_1$). An addition of the 2D M_1 component to the DHO one increases optical density (ϵ_2) in the low-energy region and produces a new structure in ϵ_1 in the region close to E_{cl}. As we will see in the next section, a considerably larger strength of the 2D M_2 CP is required for Si to achieve a fit with experimental data.

D. E_1', E_0', $E_0' + \Delta_0'$, and $E_0' + \Delta_0' + \Delta_0$ transitions

The E_1' transitions are seen in optical spectra near 5.3 eV for Si and near 5.8 eV for Ge. Their structures could be characterized by the 2D M_1 saddle point[19] or the 3D M_1 (or M_2) CP.[63] For Si the E_0' structure lies very close to the E_1 region.[59,60,63,64] The E_0' triplet (E_0', $E_0' + \Delta_0'$, and $E_0' + \Delta_0' + \Delta_0$) in Ge, on the other hand, appears in the energy region between the dominant E_1 and E_2 structures. They were treated either as a 2D M_0 (room temperature) (Ref. 19) or a 3D M_0 CP.[60,63,64] In previous works,[107,111,112] no attention had been paid to the E_1' and E_0' (triplet) transitions in analyses of optical constants of semiconductors (GaSb, InAs, GaP, etc.). This is because they are too weak to be dominant in optical spectra.[113] For completeness, we shall take into account these transitions, but for simplicity we assume their nature to be as the following DHO's:[114]

$$\epsilon_2(\omega) = \sum_i C_i \chi_i \gamma_i / [(1 - \chi_i^2)^2 + \chi_i^2 \gamma_i^2] , \qquad (21)$$

$$\epsilon_1(\omega) = \sum_i C_i (1 - \chi_i^2) / [(1 - \chi_i^2)^2 + \chi_i^2 \gamma_i^2] , \qquad (22)$$

with

$$\chi_i = \hbar\omega / E_i , \qquad (23)$$

where the E_i's are the energies of corresponding oscillators.

E. Indirect-band-gap transitions

Si and Ge are indirect-band-gap semiconductors. The lowest indirect band gap of Si is ~ 1.1 eV and that of Ge is ~ 0.8 eV. The transition mechanism at the indirect band gap, E_g^{id}, is expressed by a second-order process in the perturbation. Using the result of the perturbation calculation, we can write the contribution of the indirect optical transitions to $\epsilon_2(\omega)$ as

$$\epsilon_2(\omega) = \frac{G}{(\hbar\omega)^2} (\hbar\omega - E_g^{id} \pm \hbar\omega_q)^2 H(1 - \chi_g) , \qquad (24)$$

with

$$\chi_g = (E_g^{id} \pm \hbar\omega_q) / \hbar\omega , \qquad (25)$$

where G is the direct-transition strength parameter, $\hbar\omega_q$ is the phonon energy taking part in the indirect transitions, and H is a function defined by Eq. (7).

The parabolic bands extending to infinite energies implied by Eq. (24) should also be nonphysical. We shall, therefore, modify the model in a manner similar to that mentioned in Sec. III C by taking into account a high-energy cutoff at the energy E_{ch}. This modification gives

$$\epsilon_2(\omega) = \frac{G}{(\hbar\omega)^2} (\hbar\omega - E_g^{id} \pm \hbar\omega_q)^2 H(1 - \chi_g) H(1 - \chi_{ch}) , \qquad (26)$$

with

$$\chi_{ch} = \hbar\omega / E_{ch} . \qquad (27)$$

Unfortunately, there has been no expression for the contribution of the indirect transitions to $\epsilon_1(\omega)$. Analytical expressions for this contribution from the KK transformation are also not yet available. We will, therefore, take into account the contribution of the indirect transitions only to $\epsilon_2(\omega)$, but not to $\epsilon_1(\omega)$.

IV. RESULTS AND DISCUSSION

The models given in Sec. III can be used to fit the experimental dispersion of ϵ_2 and ϵ_1 over most of the spectral range (0–6.0 eV). The experimental data of ϵ_1 in the transparency region are, however, usually somewhat smaller than those of our model (i.e., the sum of each contribution). In order to improve a fit, therefore, we shall consider an additional term, $\epsilon_{1\infty}$, to ϵ_1. This term is assumed to be nondispersive (i.e., constant).

A. Silicon

The fits with our model to the experimental ϵ_2 of Si are shown in Fig. 4. The experimental data are taken from Aspnes and Studna (Ref. 4). The solid line is obtained from the sum of Eqs. (8) (E_1 gap; 3D M_1 CP), (13) (E_2 gap; DHO), (18) (E_2 gap; 2D M_2 CP), (21) (E_1' gap; DHO), and (26) (indirect-band-gap transitions). The dashed line is from the sum of Eqs. (8), (13), (18), and (26) [*i.e., without taking account of Eq. (21)*]. The dotted line is the result of the sum of Eqs. (11) (E_1 gap; 2D M_0 CP), (13), (18), (21), and (26). We consider in Eq. (21) only one oscillator which corresponds to the E_1' transitions [i.e., $E_i (i = a) = E_1'$]. In Eq. (26) the high-energy cutoff E_{ch} is assumed to be $E_{ch} = E_1$. The numerical parameters of the fits used are listed in Table III.

The strength of the $E_0 / (E_0 + \Delta_0)$ transitions in Si is rather small,[98] and it can be seen to be successfully neglected here. It is also clear from the figure that the DHO model [Eq. (21)] interprets the E_1' structure (~ 5.3 eV) well. As discussed in Sec. III B, we are able to fit the E_1 CP structure with either the 3D [Eq. (8); solid line] or 2D model [Eq. (11); dotted line]. The 3D model explains the experimental lower-energy shoulder of this structure well. The fit in the (1–2)-eV region also becomes satisfactory when the indirect-band-gap contribution [Eq. (26)] is taken into account.

Figure 5 shows the fits with our model to the experimental ϵ_1 spectrum of Si. The theoretical curves are obtained from the sum of Eqs. (12) (E_1 gap; 2D M_0 CP), (14) (E_2 gap; DHO), (20) (E_2 gap; 2D M_2 CP), and (22) (E_1' gap; DHO). The nondispersive term, $\epsilon_{1\infty}$ (= 1.8), is also taken into consideration in this summation. The experimental data are taken below 1.5 eV from Philipp and Ehrenreich (Ref. 21; open circles) and those in the
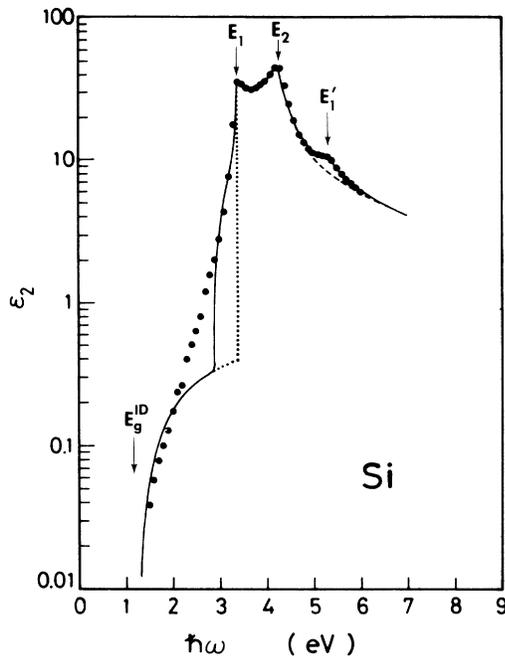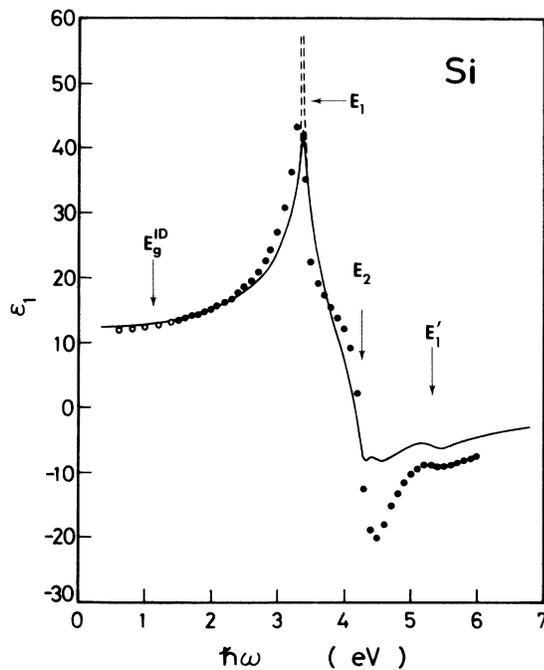
FIG. 4. ϵ_2 spectrum of Si. The solid line is obtained from the sum of Eqs. (8) (E_1 gap; 3D M_1 CP), (13) (E_2 gap; DHO), (18) (E_2 gap; 2D M_2 CP), (21) (E_1' gap; DHO), and (26) (indirect-band-gap transitions). The dashed line is taken by the sum of Eqs. (8), (13), (18), and (26) [i.e., without taking account of Eq. (21)]. The dotted line is the result of the sum of Eqs. (11) (E_1 gap; 2D M_0 CP), (13), (18), (21), and (26). The experimental data are taken from Ref. 4 (solid circles).

FIG. 5. ϵ_1 spectrum of Si. The theoretical curves are obtained from the sum of Eqs. (12) [E_1 gap; 2D M_0 CP, $\Gamma=0$ eV (dashed line) and $\Gamma=0.05$ eV (solid line)], (14) (E_2 gap; DHO), (20) (E_2 gap; 2D M_2 CP), and (22) (E_1' gap; DHO). The non-dispersive term, $\epsilon_{1\infty}$ ($=1.8$), is also taken into consideration in this summation. The experimental data are taken from Refs. 21 (open circles) and 4 (solid circles).

(1.5–6.0)-eV range from Aspnes and Studna (Ref. 4; solid circles).

The theoretical ϵ_1 spectrum [Eq. (12)] exhibits a divergence at the E_1 edge.[107] It is well known that the optical transitions are strongly affected by a damping effect (i.e., a lifetime broadening). The damping effect can be easily introduced in Eq. (12) in a phenomenological manner by replacing ω by $\omega+i\,(\Gamma/\hbar)$. Variation of $\epsilon_1(\omega)$ for a particular choice of the damping energy Γ is shown in Fig. 5 by the dashed ($\Gamma=0$ eV) and solid lines ($\Gamma=0.05$ eV). As seen in the figure, the damping effect can decrease the strength of the E_1 structure and leads to a fact which is coincident with experimental verification. For the same reason, the value of $\Gamma=0.04$ eV is also taken into consideration in the calculation of Eq. (20). It can be recognized that our model explains the ϵ_1 spectrum of Si well, especially in the energy region below 4 eV.

An individual contribution to ϵ_2 of the E_1, E_2, E_1', and E_g^{id} transitions for Si is shown in Fig. 6. They are obtained from Eq. (8) for the E_1-gap contribution (3D M_1 CP), from Eqs. (13) (DHO) and (18) (2D M_2 CP) for the E_2-gap one, from Eq. (21) for the E_1'-gap one, and from Eq. (26) for the E_g^{id}-gap one. The sum of these contributions is shown by the bold line. The solid circles are the experimental data taken from Ref. 4.

The transitions at the E_g^{id} edge shown in Fig. 6 yield a continuous absorption spectrum characterized by a power law of $(\hbar\omega)^{-2}(\hbar\omega-E_g^{id})^2$. Because of the extremely low probability for indirect transitions, one can only expect to realize them experimentally below the direct threshold as a tail of the direct-absorption edge E_1 (also see Fig. 4). The E_g^{id} transitions may also occur at energies above $E_{ch}=E_1$. However, the ensuing E_1 and E_2 transitions can provide sufficient strength and thus take
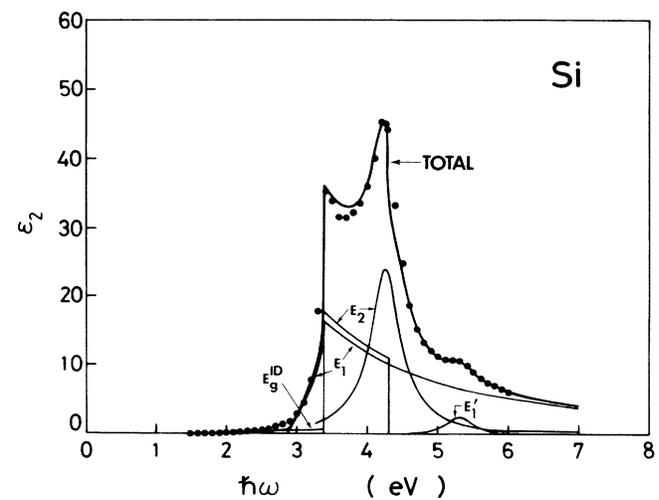

FIG. 6. Individual contribution to ϵ_2 of the E_1, E_2, E_1', and E_g^{id} transitions for Si. They are obtained from Eq. (8) for the E_1-gap contributions (3D M_1 CP), from Eqs. (13) (DHO) and (18) (2D M_2 CP) for the E_2-gap one, from Eq. (21) for the E_1'-gap one, and from Eq. (26) for the E_g^{id}-gap one. The sum of these contributions is shown by the bold line. The solid circles are the experimental data taken from Ref. 4.

over the indirect-band-gap oscillators present at above E_{ch}.

The E_1 gap is of the 3D M_1 (or 2D M_0) type. Hence, the line shape of the corresponding ϵ_2 spectrum should be characterized by a steep low-energy side and a broader high-energy side. This line shape is in good agreement with the experimental data. The strength parameter B_1 can be given analytically by[112]

$$B_1 = \frac{32\sqrt{3}}{9\omega_1}\left|\frac{a_B}{a_0}\right|,\qquad(28)$$

where a_B is the Bohr radius in Å, a_0 the lattice constant in Å, and ω_1 the E_1-gap energy in hartrees (27.2 eV). Equation (28) predicts $B_1 = 4.83$ at room temperature, while we obtained $B_1 = 5.22$ from the present analysis. The agreement is extremely good in view of the crudeness of the theory used. A notable difference between the calculated and experimental values of B_1 has, however, been found for InSb (Ref. 8) and GaP (Ref. 112), a fact that has been attributed to excitonic enhancement of the E_1 transitions.[75,115] Some calculations[63,116] also showed that the k-linear term for k perpendicular to $\langle 111 \rangle$ can significantly increase the strength of the E_1 structure.

The E_2 structure in Si can be fitted using a mixture of the DHO (broadened 2D M_1 CP) and the 2D M_2 CP. It is worth noting that the best-fit analyses of dielectric data in the E_2-structure region of group-(III–V) semiconductors required only the DHO contribution and no additional (2D M_2 CP) one.[107,111] As is clearly seen in Fig. 6, the 2D M_2 CP (E_2 structure) has a considerably large strength. The steep low-energy end of this contribution at E_1 is the result of the E_{cl} cutoff-energy modification. The strongest component in the ϵ_2 spectrum of Si is found to be the E_2-gap DHO. It is also recognized that the strength of the E_1' transitions is very weak.

B. Germanium

A comparison of our ϵ_2 model to the experimental data of Ge is shown in Fig. 7. The experimental data are taken below 1.5 eV from Philipp and Ehrenreich (Ref. 21; open circles) and those in the (1.5–6.0)-eV range from Aspnes and Studna (Ref. 4; solid circles). The solid line is taken by the sum of Eqs. (2) [$E_0/(E_0+\Delta_0)$ gaps; 3D M_0 CP's], (8) (E_1 gap; 3D M_1 CP), (9) ($E_1+\Delta_1$ gap; 3D M_1 CP), (13) (E_2 gap; DHO), (18) (E_2 gap; 2D M_2 CP), and (21) [E_1', E_0' (triplet); DHO]. The dashed line is obtained from the sum of Eqs. (2), (8), (9), (13), and (18) [i.e., without taking account of Eq. (21)]. The dotted line is the result of the sum of Eqs. (2), (11) [$E_1/(E_1+\Delta_1)$ gaps; 2D M_0CP's], (13), (18), and (21).

As in Si, the indirect transitions (E_g^{id}) in Ge take part at below the onset of the direct-band-gap transitions which occurs at ~ 0.8 eV (E_0 gap). However, the energy separation between the E_g^{id} gap and the lowest direct band gap (E_0) for Ge is very small (~ 0.1 eV; see Table II) compared to that for Si (~ 2 eV; Table I). We can, therefore, successfully neglect the E_g^{id}-gap contribution for the case of Ge. [The $E_0/(E_0+\Delta_0)$-gap contribution
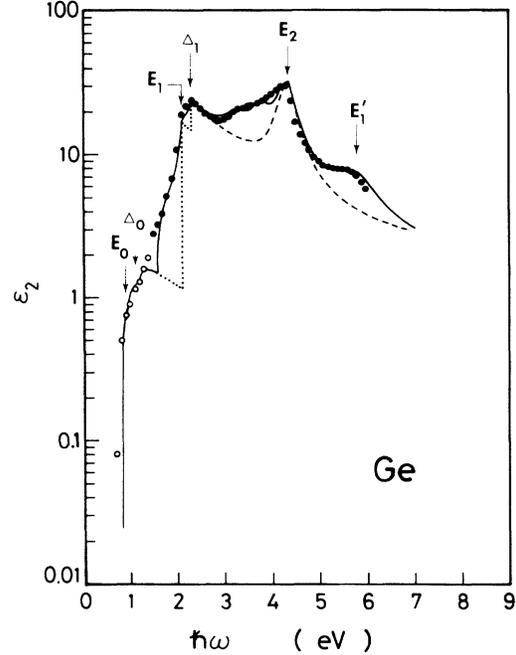

FIG. 7. ϵ_2 spectrum of Ge. The solid line is taken by the sum of Eqs. (2) [$E_0/(E_0+\Delta_0)$ gaps; 3D M_0 CP's], (8) (E_1 gap; 3D M_1 CP), (9) ($E_1+\Delta_1$ gap; 3D M_1 CP), (13) (E_2 gap; DHO), (18) (E_2 gap; 2D M_2 CP), and (21) [E_1', E_0' (triplet); DHO]. The dashed line is obtained from the sum of Eqs. (2), (8), (9), (13), and (18) [i.e., without taking account of Eq. (21)]. The dotted line is the result of the sum of Eqs. (2), (11) [$E_1/(E_1+\Delta_1)$ gaps; 2D M_0 CP's], (13), (18), and (21). The experimental data are taken from Refs. 21 (open circles) and 4 (solid circles).

can take over the weak E_g^{id}-gap one.] In fact, as shown in Fig. 7, we obtain a good fit with the experimental ϵ_2 spectrum in the fundamental absorption-edge region only by taking into account the $E_0/(E_0+\Delta_0)$-gap contribution [Eq. (2)].

We consider in Eq. (21) three DHO's: one corresponds to the E_1' transitions [$E_i(i=a)=E_1'$] and the remaining two take into account the E_0' (triplet) transitions [$E_i(i=b,c)$] (see Table III). A consideration of these components results in excellent agreement with the experimental ϵ_2 spectrum in the E_1'-edge region (~ 5.8 eV) and the region between 3 and 4.5 eV. The 3D M_1 terms [Eqs. (8) and (9)] and a mixture of the DHO and 2D M_2 terms [Eqs. (13) and (18)] also explain well the $E_1/(E_1+\Delta_1)$ and E_2 regions of the ϵ_2 spectrum, respectively. An excellent agreement can thus be achieved between our model (solid line) and the experimental data over a wide range of the photon energies.

The fits with our ϵ_1 model to the experimental data of Ge are shown in Fig. 8. The theoretical curves are obtained by the sum of Eqs. (3) [$E_0/(E_0+\Delta_0)$ gaps; 3D M_0], (12) [$E_1/(E_1+\Delta_1)$ gaps; 2D M_0], (14) (E_2 gap; DHO), (20) (E_2 gap; 2D M_2), and (22) [E_1', E_0' (triplet); DHO]. The nondispersive term, ϵ_∞ (=2.7), is also taken into consideration in this summation. The dashed line is obtained with $\Gamma=0$ eV [Eq. (12)] and $\Gamma=0.04$ eV [Eq. (20)], while the solid line is obtained with $\Gamma=0.07$ eV
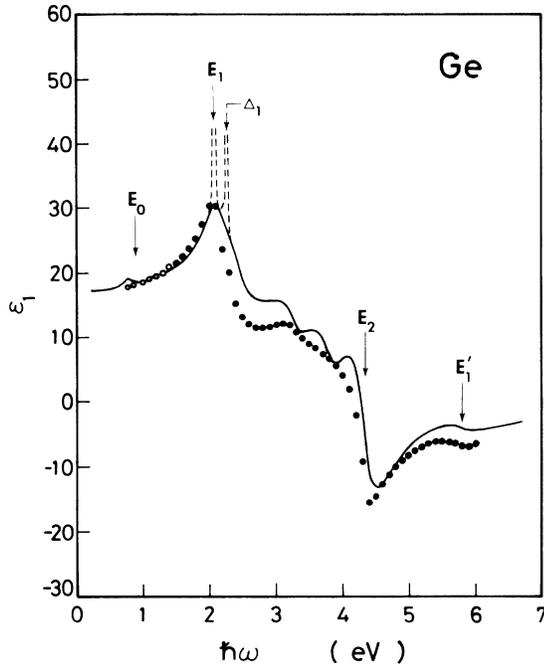
FIG. 8. ϵ_1 spectrum of Ge. The theoretical curves are obtained by the sum of Eqs. (3) $[E_0/(E_0+\Delta_0)$ gaps; 3D $M_0]$, (12) $[E_1/(E_1+\Delta_1)$ gaps; 2D M_0, $\Gamma=0$ eV (dashed line) and $\Gamma=0.07$ eV (solid line)] (14) $(E_2$ gap; DHO), (20) $(E_2$ gap; 2D $M_2)$, and (22) $[E_1'$, E_0' (triplet); DHO]. The nondispersive term, ϵ_∞ ($=2.7$), is also taken into consideration in this summation. The experimental data are taken from Refs. 21 (open circles) and 4 (solid circles).

FIG. 9. Individual contribution to ϵ_2 of the $E_0/(E_0+\Delta_0)$, $E_1/(E_1+\Delta_1)$, E_2, E_1', and E_0' (triplet) gaps for Ge. They are obtained from Eq. (2) for the $[E_0/(E_0+\Delta_0)$-gap contribution (3D M_0 CP), from Eq. (8) for the E_1-gap one (3D M_1 CP), from Eq. (9) for the $(E_1+\Delta_1)$-gap one (3D M_1 CP), from Eqs. (13) (DHO) and (17) (2D M_2 CP) for the E_2-gap one, and from Eq. (21) for the E_1'-gap (DHO) and $[E_0'$ (triplet)]-gap ones [DHO; marked by $(E_0'/\Delta_0'/\Delta_0)]$. The bold line in the figure is the sum of these contributions. The open and solid circles are the experimental data taken from Refs. 21 and 4, respectively.

[Eq. (12)] and $\Gamma=0.04$ eV [Eq. (20)]. The experimental data are taken from Refs. 21 (open circles) and 4 (solid circles).

As discussed before, the smaller the damping energy in Eq. (12) gives the larger the E_1-peak value. The experimental value of ϵ_1 at the E_1 peak is 30.1 Calculation of Eq. (12) with $\Gamma=0.07$ eV (solid line) agrees well with this peak value. Equations (14) and (20) also interpret the peculiar line shape of the E_2 structure well [see (4–6)-eV spectrum region in Fig. 8].

An individual contribution to ϵ_2 of the $E_0/(E_0+\Delta_0)$, $E_1/(E_1+\Delta_1)$, E_2, E_1', and E_0' (triplet) gaps for Ge is shown in Fig. 9. They are obtained from Eq. (2) for the $E_0/(E_0+\Delta_0)$-gap contribution (3D M_0 CP), from Eq. (8) for the E_1-gap one (3D M_1 CP), from Eq. (9) for the $(E_1+\Delta_1)$-gap one (3D M_1 CP), from Eqs. (13) (DHO) and (17) (2D M_2 CP) for the E_2-gap one, from Eq. (21) for the E_1'-gap (DHO) and $[E_0'$ (triplet)]-gap ones [DHO; marked in the figure by $(E_0'/\Delta_0'/\Delta_0)]$. The bold line in the figure is the sum of these contributions. The open and solid circles are the experimental data taken from Refs. 21 and 4, respectively.

The $E_0/(E_0+\Delta_0)$ transitions yield a continuous $\epsilon_2(\omega)$ spectrum obeying the well-known $\frac{1}{2}$ power law [i.e., $\propto(\hbar\omega)^{-2}(\hbar\omega-E_0)^{0.5}]$. The transitions contribute strongly to the dispersion of $\epsilon_1(\omega)$ but not to its absolute value.[107,117,118]
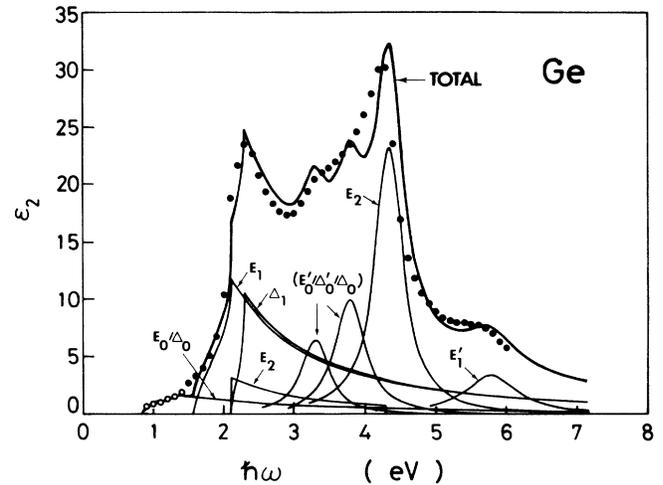
The strength of the E_1 and $E_1+\Delta_1$ transitions of diamond (zinc-blende) materials can be estimated with the simple expression[7–9,16,18,19]

$$B_1=44\frac{E_1+\Delta_1/3}{a_0E_1^2} , \tag{29a}$$

$$B_2=44\frac{E_1+2\Delta_1/3}{a_0(E_1+\Delta_1)^2} , \tag{29b}$$

where a_0 is the lattice constant in Å and E_1 and Δ_1 are in eV. This expression predicts $B_1=3.79$ and $B_2=3.29$. These values are used in the calculations of Eqs. (8)–(12). [The additional strength parameters B_{11} and B_{21} in Eqs. (8) and (9) are then determined from the best-fit procedures with the experimental ϵ_2 data (see Table III).] We can obtain good fits to the experimental ϵ_1 and ϵ_2 spectra using these predicted B_1 and B_2 values (Figs. 7 and 8).

The strength of the 2D M_2 (E_2-gap) contribution for Ge is very weak, compared to that for Si (see Figs. 6 and 9). As mentioned in Sec. II, the energy-band structure of Ge has a stronger resemblance to those of zinc-blende, III–V materials (such as GaAs and InAs) rather than to that of Si. The best-fit analyses of dielectric data in the E_2-structure region of such III–V semiconductors required no or negligibly small 2D M_2 contribution. A negligibly small or a weak strength of this contribution for Ge and some III–V semiconductors may come from their energy-band structures.

V. CONCLUSIONS

We have developed a method for calculation of the real (ϵ_1) and imaginary parts (ϵ_i) of the dielectric function of Si and Ge at energies below and above the fundamental absorption edge. This model is based on the Kramers-Kronig transformation and takes into account the effects of interband transitions at the E_0, $E_0 + \Delta_0$, E_1, $E_1 + \Delta_1$, E_2, E_1', and E_0' (triplet) CP's and indirect band gaps. The $E_0/(E_0 + \Delta_0)$ structures could be characterized by a 3D M_0 CP, the $E_1/(E_1 + \Delta_1)$ structures by a 3D M_1 (or 2D M_0) CP, the E_2 structure by a mixture of damped harmonic oscillator (DHO; a broadened 2D M_1 CP) and 2D M_2 CP, and the E_1' and E_0' (triplet) structures by the DHO's. The indirect transitions are assumed to provide a gradually increasing absorption spectrum expressed by a power law of $(\hbar\omega - E_g^{id})^2$ ($\hbar\omega$ is the photon energy, E_g^{id} the indirect band gap). Analyses are presented for these semiconductors, and results are in satisfactory agreement with the experimental data over the entire range of photon energies (0–6.0 eV). Line-shape analyses of ϵ_1 and ϵ_2 spectra yield information about the strength and broadening parameters of each CP. Dielectric-related optical constants, such as the refractive indices and the absorption coefficients, are easy to obtain from the present study in the form of practical functions. Since these expressions are purely analytical functions of the electronic energy-band parameters, the model would also be applicable to the analysis of some perturbation-induced effects of the optical constant (e.g., the pressure and temperature dependence of the refractive indices).

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[113]The band-structure calculation of Chelikowsky and Cohen (Ref. 52) for InP suggests four CP's in the (4.5–5.5)-eV energy region. Two of them correspond to transitions at the Γ point [$\Gamma_8^v \rightarrow \Gamma_7^c$ at 4.64 eV and $\Gamma_8^v \rightarrow \Gamma_8^c$ at 5.13 eV (Ref. 18)], and they are labeled E_0' and $E_0' + \Delta_0'$. In earlier work (Ref. 62), these transitions were attributed to an E_2 CP. The E_2 transitions occur in the region near the E_0' and $E_0' + \Delta_0'$ CP's, but their strength is weaker than that of the E_0' and $E_0' + \Delta_0'$ transitions. Thus, it is worth noting that in InP the strength of the E_0' and $E_0' + \Delta_0'$ transitions is relatively strong and dominant enough in optical spectra (see, e.g., Ref. 18).

[114]The E_0' (triplet) CP's would have a 3D M_0 character. We also treated their structures in Ge as the 3D M_0 type [i.e., Eqs. (2) and (3)]. However, this treatment led to a poorer fit with the experimental data than that using the DHO. This fact may be due to the multitude of possible CP's in the E_0' spectral region, which may give rise to an averaging over several CP's.

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