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Electric-dipole transitions between group-III acceptor states in uniaxially compressed Ge

T H Wang and S T Yen

Department of Electronics Engineering and Institute of Electronics, National Chiao Tung University, 1001 Ta-Hsueh Road, Hsinchu, Taiwan 30050, Republic of China

E-mail: styen@cc.nctu.edu.tw

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Abstract

We study the electric-dipole transitions between group-III acceptor states in Ge under stress along the [001] crystallographic direction in the effective mass approximation. We systematically investigate the cases of zero stress, infinitesimal stress, and finite stress including the low-stress and the high-stress regions. Our results show quantitative agreement with experimental data at zero stress and at infinitesimal stress. The relative intensities of infinitesimal-stress-induced components of transitions from the $1\Gamma_8^+$ state to the $n\Gamma_8^-$ states do not correlate significantly with the species of acceptors except for the transition to the $1\Gamma_8^-$ state. The oscillator strengths of some transitions are susceptible to the stress in the low-stress region ($<$0.3 kbar), and could be zero at a specific stress. The behaviours of the stress dependence of oscillator strengths for different transition lines are explained in terms of the compositions of the wavefunctions and the dipole matrix elements. In the high-stress region ($\gtrsim$3 kbar), the ground state is s-like, and only the transitions to the p-like states can have non-negligible oscillator strengths. The photon absorbed (emitted) and associated with each electric-dipole transition between the s-like and the p-like states is polarized either parallel or perpendicular to the stress direction. We also calculate the absorption spectra for Ge:Ga at liquid-helium temperature. The results are in good agreement with experiment.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The problem of impurities in semiconductors was extensively studied experimentally [1] and theoretically [2] in the 1960s and 1970s. Recently, research on shallow impurities in semiconductors has regained considerable interest, because the system is a promising candidate for a simple and coherent terahertz radiation source [3]. It has been demonstrated that the terahertz radiation can be generated from group-III acceptors in Ge in the absence [4] and presence [5–7] of stress. Therefore, research on the stress dependence of the oscillator strengths of optical transitions between group-III acceptor states in Ge is an important issue.

The oscillator strengths of optical transitions between group-III acceptor states in Ge have been studied experimentally and theoretically in the absence of external stress. Rotsaert *et al* [8, 9] first obtained the oscillator strengths by integrating the experimental absorption spectra. Clauws *et al* [10] then calculated the oscillator strengths of electric-dipole transitions in the effective mass approximation. The calculation considered various species of group-III acceptors by introduction of a semi-empirical impurity potential with a local form. However, they found their results are not in quantitative agreement with the experimental data [8, 9]. In addition, Buczko and Bassani [11] performed a similar calculation by using an impurity potential in a different form, and their results are in quantitative agreement with the theory of Clauws *et al* [10]. In the experimental aspect, Andreev *et al* [12, 13] determined not only the oscillator strengths but also the linewidth by very high-resolution (up to 0.01 cm^{-1}) absorption spectra. Their experimental results of oscillator strengths are in quantitative agreement with the theoretical

data [10, 11]. Rodriguez *et al* [14] have studied the relative intensities of electric-dipole transitions for acceptors in group-IV semiconductors under an infinitesimal stress by group-theoretical analysis. However, in the presence of finite stress, their results are no longer applicable due to the strain-induced couplings between acceptor states. To our knowledge, except for [15], no calculated result regarding the case of finite stress has been published.

In this paper, we calculate the oscillator strengths of electric-dipole transitions between group-III acceptor states in Ge under stress along the [001] crystallographic direction by the effective mass approximation, and take into account the cases of zero stress, infinitesimal stress, and finite stress in the low-stress (0.3 kbar), and the high-stress ($\gtrsim$3 kbar) regions. Our results are in excellent agreement with the experimental data [12, 13] at zero stress. In the presence of [001] infinitesimal stress, we calculate the intensity parameters, u and v [14] of $\Gamma_8 \rightarrow \Gamma_8$ transitions for various species of group-III acceptors in Ge. Our results are in excellent agreement with experimental data of Ga acceptors in Ge [16]. For the case of finite stress, we find the oscillator strengths of some transitions are susceptible to the stress. Therefore, the relative intensities in the low-stress region can deviate significantly from those predicted by the group-theoretical analysis at zero stress.

The organization of the rest of the paper is as follows. In section 2, we present the theoretical approaches. In section 3, we present and discuss the results for zero stress, infinitesimal stress, low stress, and high stress. We present the calculated absorption spectra for Ga acceptors in Ge under [001] stress for comparison with experimental spectra [17]. Finally, we draw conclusions in section 4.

2. Theory

To study the stress dependence of electric-dipole transitions between group-III acceptor states in Ge, we have calculated the electronic structure using the effective mass theory [18]. The wavefunctions of acceptor states are expressed as a sum of products of envelope functions and Bloch functions of the jth valence band $u_{J^j M^j}$. By taking into account the couplings of the heavy-hole ($u_{\frac{3}{2},\pm\frac{3}{2}}$), the light-hole ($u_{\frac{3}{2},\pm\frac{1}{2}}$), and the split-off-hole ($u_{\frac{1}{2},\pm\frac{1}{2}}$) bands, we express the wavefunctions of acceptor states as

$$\Psi = \sum_{j=1}^{6} \sum_{lm} g_{jlm}(r) Y_{lm}(\theta,\phi) u_{J^j M^j}, \tag{1}$$

where we have expanded the envelope functions in a sum of products of radial functions and spherical harmonics. The impurity potential we adopted is a sum of the Coulomb contribution V_{C} and the central-cell correction V_{cc}, and is expressed in a semi-empirical form:

$$V = V_{\mathrm{C}} + V_{\mathrm{cc}} \qquad V_{\mathrm{C}} = \frac{e^2}{\epsilon r}\left[1 + (\epsilon - 1)\exp\left(-\frac{\alpha r}{a_{\mathrm{B}}^*}\right)\right]$$
$$V_{\mathrm{cc}} = \frac{Ae^2}{2\epsilon r}\exp\left(-\frac{\beta r}{a_{\mathrm{B}}^*}\right), \tag{2}$$

where α, β, and A are dimensionless parameters; ϵ is the dielectric constant, e the elementary charge, and $a_{\mathrm{B}}^* = \epsilon\gamma_1\hbar^2/m_0e^2$ the effective Bohr radius in which γ_1 and m_0 are the first Luttinger parameter and the free-electron mass, respectively. In the absence of stress, the acceptor states transform like basis functions of the irreducible representations Γ_6, Γ_7, and Γ_8 of the $\mathrm{T_d'}$ group. In the presence of stress along the [001] direction, the Γ_8 state of the $\mathrm{T_d'}$ group split into one Γ_6 and one Γ_7 states of the $\mathrm{D_{2d}'}$ group, and the Γ_6 (Γ_7) state of the $\mathrm{T_d'}$ group becomes the Γ_6 (Γ_7) state of the $\mathrm{D_{2d}'}$ group. In this work, the acceptor states and their notations are the same as those in our previous work [18], except where otherwise noted.

Having obtained the acceptor states, we can then go on to calculate the electric-dipole transitions between these states. We consider that the transitions occur at liquid-helium temperature $T = 4.22$ K. At such a low temperature, we suppose that all the holes are in the ground state $1\Gamma_8^+$ in the absence of stress, and in the $1\Gamma_6^+$ and the $1\Gamma_7^+$ states, into which the $1\Gamma_8^+$ state split when a [001] stress is applied. The absorption coefficient of the electric-dipole transition for group-III acceptors in Ge can be written as

$$\alpha(\hbar\omega;\mathbf{e}) = \frac{2\pi^2\hbar e^2\gamma_1 N}{cm_0\sqrt{\epsilon}} \sum_{\mu\nu}\sum_{n=1}^{\infty} w(1\Gamma_\mu^+) f_{1\Gamma_\mu^+, n\Gamma_\nu^-}(\mathbf{e})$$
$$\times\, \delta(E(n\Gamma_\nu^-) - E(1\Gamma_\mu^+) - \hbar\omega), \tag{3}$$

where $E(n\Gamma_\nu^\pm)$ is the energy level of the $n\Gamma_\nu^\pm$ state, $\mathbf{e}$ the polarization unit vector of light, $w(1\Gamma_\mu^+)$ the probability that a hole is in the $1\Gamma_\mu^+$ state, N the acceptor concentration, and c the speed of light in vacuum. The indices μ and ν run over all the irreducible representations. The $f_{1\Gamma_\mu^+, n\Gamma_\nu^-}(\mathbf{e})$ is the oscillator strength for the electric-dipole transition from the $1\Gamma_\mu^+$ state to the $n\Gamma_\nu^-$ state [19],

$$f_{1\Gamma_\mu^+, n\Gamma_\nu^-}(\mathbf{e}) = \frac{2m_0}{\gamma_1\hbar^2}\frac{1}{g_\mu}(E(n\Gamma_\nu^-) - E(1\Gamma_\mu^+))$$
$$\times \sum_{qq'} |\langle 1\Gamma_{\mu(q)}^+ |\mathbf{e}\cdot\mathbf{r}| n\Gamma_{\nu(q')}^-\rangle|^2, \tag{4}$$

where g_μ is the degeneracy of the $1\Gamma_\mu^+$ state, and the q (q') runs over all the degenerate partners of the $1\Gamma_\mu^+$ ($n\Gamma_\nu^-$) state. For the case of the $\mathrm{D_{2d}'}$ group, all the acceptor states are doubly degenerate due to the time-reversal symmetry. Hence, there are four terms in the sum of equation (4). Two of them are zero if we choose an appropriate orthogonal set of the degenerate states. The remaining two terms have the same value because of the time-reversal symmetry. Therefore, equation (4) can be written as

$$f_{1\Gamma_\mu^+, n\Gamma_\nu^-}(\mathbf{e}) = \frac{4m_0}{\gamma_1\hbar^2}\frac{1}{g_\mu}(E(n\Gamma_\nu^-) - E(1\Gamma_\mu^+))|\langle 1\Gamma_\mu^+|\mathbf{e}\cdot\mathbf{r}|n\Gamma_\nu^-\rangle|^2. \tag{5}$$

Here, for simplicity, we drop the indices q and q', and the $\langle 1\Gamma_\mu^+|\mathbf{e}\cdot\mathbf{r}|n\Gamma_\nu^-\rangle$ is one of the non-zero matrix elements. Substituting equation (1) into the $\langle 1\Gamma_\mu^+|\mathbf{e}\cdot\mathbf{r}|n\Gamma_\nu^-\rangle$ and using the facts that the envelope functions are slowly varying outside the central-cell region and that the wavefunctions of odd parity states have almost vanished in the central-cell region, we can

further express the matrix element as

$$\langle 1\Gamma_\mu^+|\mathbf{e}\cdot\mathbf{r}|n\Gamma_\nu^-\rangle = \sum_{l}^{(\text{even})} \sum_{\substack{l'=l\pm1\\ l'\geqslant 1}} \sum_{mm'} \sum_{j=1}^{6} \int_0^\infty \mathrm{d}r\, r^3 g_{jlm}^{1\Gamma_\mu^+ *} g_{jl'm'}^{n\Gamma_\nu^-} \times \int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi} \mathrm{d}\Omega Y_{lm}^* Y_{l'm'} \cos\theta_r, \quad (6)$$

where $\mathrm{d}\Omega = \sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi$ and θ_r is the angle between **e** and **r**.

In this paper, we denote the light with the polarization vector parallel (perpendicular) to the stress direction [001] by $\mathbf{E}_\parallel$ ($\mathbf{E}_\perp$). For $\mathbf{E}_\parallel$, the $1\Gamma_6^+ \to n\Gamma_6^-$ and the $1\Gamma_7^+ \to n\Gamma_7^-$ transitions are forbidden, while for $\mathbf{E}_\perp$, all the transitions are allowed.

3. Results and discussion

In this section, we systematically study the electric-dipole transitions for group-III acceptors in Ge under [001] stress. We examine the cases of different stresses, including, from low to high, zero stress, infinitesimal stress, the low-stress region ($\leqslant$0.3 kbar), and the high-stress region ($\gtrsim$3 kbar). In the following discussion, we denote the irreducible representations, symmetry, and acceptor states of the T_d' group by $\bar{\Gamma}_\nu$, $\bar{\Gamma}_\nu^u$, and $n\bar{\Gamma}_\nu^u$ (i.e. the symbols with a bar), respectively, in order to avoid confusing the notations of the T_d' group with those of the D_{2d}' group.

3.1. Zero stress

Figure 1 shows the oscillator strengths as functions of the parameter A for electric-dipole transitions of G ($1\bar{\Gamma}_8^+ \to 1\bar{\Gamma}_8^-$), D ($1\bar{\Gamma}_8^+ \to 2\bar{\Gamma}_8^-$), and C ($1\bar{\Gamma}_8^+ \to 1\bar{\Gamma}_7^-, 3\bar{\Gamma}_8^-$) lines. The parameter A can be regarded as the strength of the effective central-cell force exerted on the hole, and includes all the contributions of the impurity potential except for the Coulomb potential V_C. These contributions are (a) the difference in the screened potential induced by the positive point charge at the impurity site with the charge magnitude equal to that of the core electrons between the impurity and the host atoms, (b) the difference in the screened potentials induced by the core electrons between the impurity and the host atoms, (c) the difference in the effective repulsive potentials, which is the kinetic energy of the valence electrons in nature, localized in the central-cell region, and originates from the requirement that the wavefunctions of the valence electrons are orthogonal to those of the core electrons, (d) the lattice relaxation around the impurity site induced by the presence of the impurity [20, 21]. The sum of the contribution (a) and V_C is just the difference in the screened point charge potential induced by the nucleus. The sum of the potentials (a) and (b) is attractive for the valence electrons and localized in the central-cell region because they are induced by charges of the same magnitude but opposite sign. The effect (c) should be the primary contribution, and the effective potentials are positive for the valence electrons but negative from the standpoint of the valence holes. Therefore, the effective central-cell force exerted on the hole is small for the isocoric impurity Ga ($A = 1.00$), attractive for the heavier impurities In ($A = -13.71$) and Tl ($A = -26.29$),

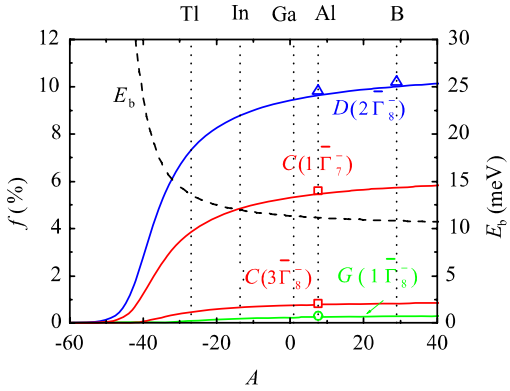

Figure 1. Oscillator strengths of electric-dipole transitions for G ($1\bar{\Gamma}_8^+ \to 1\bar{\Gamma}_8^-$), D ($1\bar{\Gamma}_8^+ \to 2\bar{\Gamma}_8^-$), and C ($1\bar{\Gamma}_8^+ \to 1\bar{\Gamma}_7^-, 3\bar{\Gamma}_8^-$) lines and the binding energy of the ground state as functions of the strength parameter A. The points are experimental data of [12] and [13].

and repulsive for the lighter impurities Al ($A = 7.52$) and B ($A = 28.96$) [18]. The oscillator strengths decrease with the attractive force, as shown in figure 1, because the probability of the hole in the central-cell region increases with the attractive force for the ground state and the integral in equation (6) over the central-cell region gives almost no contribution to the whole dipole matrix element. The oscillator strengths almost vanish when the attractive force is so large that the wavefunction of the ground state is totally localized in the central-cell region ($A < -50$). On the other hand, the oscillator strengths increase slowly with the repulsive force because the size of the central-cell region is much smaller than that of the ground-state wavefunction. As a result, the deviation of the oscillator strength of the D line transition from that of the pure point charge (with $A = 0$) for Tl is three times larger in magnitude than that for B, even though the magnitude of A for Tl is smaller than that for B. The dashed line in figure 1 is for the binding energy of the ground state. It decreases slowly with the repulsive force, but increases dramatically with the attractive force when the attractive force is so large ($A < -35$) that an appreciable part of the wavefunction of the ground state is localized in the central-cell region. When this happens, the effective mass theory is no longer applicable. The points in figure 1 are the oscillator strengths measured by Andreev *et al* for acceptors B and Al [12, 13]. As can be seen, there is an excellent agreement between the calculated and the experimental results.

3.2. Infinitesimal stress

Rodriguez *et al* found that the relative intensities of the infinitesimal-stress-induced components of the $\bar{\Gamma}_8 \to \bar{\Gamma}_7$ and the $\bar{\Gamma}_8 \to \bar{\Gamma}_6$ transitions can be determined by the group-theoretical analysis, and those of the $\bar{\Gamma}_8 \to \bar{\Gamma}_8$ transitions depend on two intensity parameters u and v [14]. For $\mathbf{E}_\parallel$, the relative intensities of the $\Gamma_6 \to \Gamma_7$ and the $\Gamma_7 \to \Gamma_6$ components are $1/2-v$ and $1/2+v$, respectively; for $\mathbf{E}_\perp$, those of the $\Gamma_6 \to \Gamma_6$, the $\Gamma_6 \to \Gamma_7$, the $\Gamma_7 \to \Gamma_6$, and the $\Gamma_7 \to \Gamma_7$ components are $3u/8$, $(1-3u/4+v)/2$, $(1-3u/4-v)/2$, and

Table 1. Intensity parameters for group-III acceptors in Ge.

	B		Al		Ga		In		Tl	
Final state	u	v	u	v	u	v	u	v	u	v
$1\Gamma_8^-$	0.98	−0.13	0.99	−0.11	0.99	−0.10	1.00	−0.07	1.00	0.04
$2\Gamma_8^-$	0.12	0.33	0.12	0.33	0.12	0.33	0.13	0.33	0.13	0.33
$3\Gamma_8^-$	0.79	−0.41	0.79	−0.41	0.79	−0.41	0.79	−0.41	0.79	−0.40
$4\Gamma_8^-$	0.08	0.27	0.08	0.28	0.09	0.28	0.09	0.29	0.10	0.30

$3u/8$, respectively. The values of u and v of the $1\bar{\Gamma}_8^+ \rightarrow n\bar{\Gamma}_8^-$ transitions for various species of group-III acceptors in Ge are listed in table 1. As table 1 shows, the intensity parameters (and hence the relative intensities) do not correlate significantly with the species of group-III acceptors except for the $1\bar{\Gamma}_8^+ \rightarrow 1\bar{\Gamma}_8^-$ transition. Martin *et al* obtained the values of the parameters, $u = 0.95 \pm 0.05$ and $v = -0.1 \pm 0.05$, for Ge:Ga by the piezospectroscopic measurement [16]. Our result, $u = 0.99$ and $v = -0.10$, shows a better agreement with the experiment than that of [22], $u = 0.91$ and $v = -0.29$.

3.3. Low-stress region

Even though the group-theoretical analysis of [14] provides information about the relative intensities at infinitesimal stress, it is not applicable to the case of finite stress due to the strain-induced couplings between acceptor states of the same symmetry. In this section, we study the stress dependence of the oscillator strengths of the stress-induced components of the G, D, C, and B line transitions in the low-stress region ($\leqslant$0.3 kbar). In such a low-stress region, the energy levels of the initial and the final states of the G, D, and C line components do not either cross or anticross. Here, we consider the acceptor Ga for the G, D, and C line transitions. For the cases of the other species of group-III acceptors, the results are similar to the case of the Ga acceptor. As to the B line transition, we consider the acceptor In for comparison with experiment.

3.3.1. G line. In the presence of [001] stress, the G line splits into four components, G_1 ($1\Gamma_6^+ \rightarrow 1\Gamma_6^-$), G_2 ($1\Gamma_6^+ \rightarrow 1\Gamma_7^-$), G_3 ($1\Gamma_7^+ \rightarrow 1\Gamma_6^-$), and G_4 ($1\Gamma_7^+ \rightarrow 1\Gamma_7^-$) [18]. Figure 2 shows the stress dependence of the oscillator strengths of the G line components for (a) $\mathbf{E}_\parallel$ and (b) $\mathbf{E}_\perp$. As can be seen, the oscillator strengths are susceptible to the stress in the low-stress region. In addition, with the increase of stress, the oscillator strengths of G_1 for $\mathbf{E}_\perp$ and G_2 for $\mathbf{E}_\parallel$ first decrease to zero and then increase.

We further inspect the compositions of acceptor states to gain more insight into the stress dependence of oscillator strengths. In the absence of stress, the initial states of the G line components, $1\Gamma_6^+$ and $1\Gamma_7^+$, have an s ($l = 0$) composition of 71% and a d ($l = 2$) composition of 28%. The final states, $1\Gamma_6^-$ and $1\Gamma_7^-$, have a p ($l = 1$) composition of 90% and an f ($l = 3$) composition of 9%. In the stress region from 0 to 0.3 kbar, the compositions are not susceptible to the stress because the couplings of the $1\Gamma_6^+$, $1\Gamma_7^+$, $1\Gamma_6^-$, and $1\Gamma_7^-$ states with other acceptor states of the same symmetry are weak. As a result, the dipole matrix elements of equation (6)

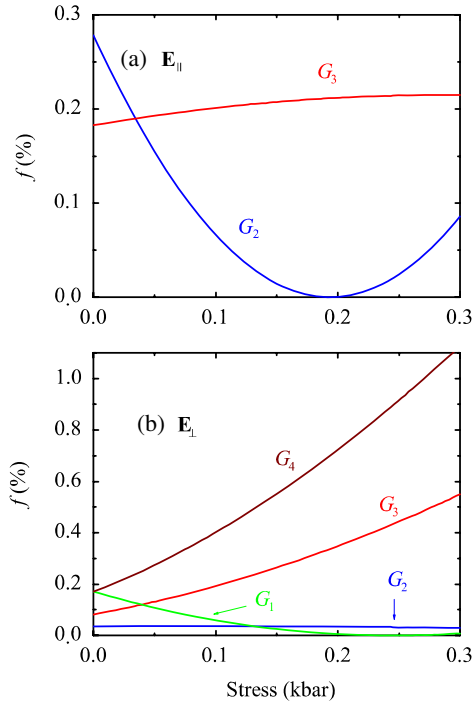

Figure 2. Oscillator strengths of G line components for Ge:Ga as functions of uniaxial stress along the [001] direction for (a) $\mathbf{E}_\parallel$ and (b) $\mathbf{E}_\perp$.

contain significant s $\rightarrow$ p and d $\rightarrow$ p components (denoted by M_{sp} and M_{dp}, respectively), a small d $\rightarrow$ f component M_{df}, and negligible higher-order components. Furthermore, the components M_{sp} and M_{dp} have comparable magnitudes but opposite signs so that the sum of M_{sp} and M_{dp} is small in magnitude and comparable with M_{df}. This is the reason why the oscillator strength of the G line transition, as figure 1 shows, is much smaller than those of the C and D line transitions, even though the final state of the G line transition has a greater overlap with the ground state than those of C and D line transitions. Because of the significant overlap between the wavefunctions of the initial and the final states, and the almost complete cancellation between the M_{sp} and the M_{dp} components, the weak strain-induced couplings between the acceptor states still have a considerable influence on the stress dependence of oscillator strengths as figure 2 shows.

As to the G_1 line for $\mathbf{E}_\perp$ and the G_2 line for $\mathbf{E}_\parallel$, M_{sp} has a larger magnitude than M_{dp} and has the same sign as M_{df} at zero stress. With the increase of stress, M_{sp} (M_{dp}) decreases (increases) markedly in magnitude, but M_{df} changes slowly. Therefore, the oscillator strength decreases with stress until it reduces to zero. If the stress goes on increasing, the M_{dp}

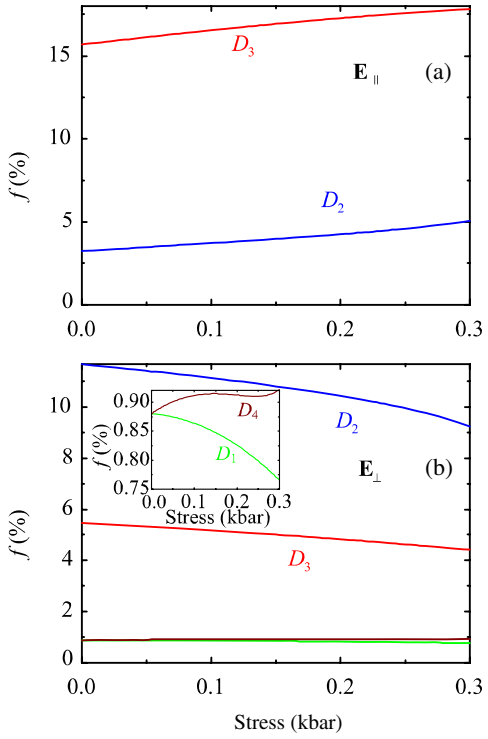

Figure 3. Oscillator strengths of D line components for Ge:Ga as functions of uniaxial stress along the [001] direction for (a) $\mathbf{E}_{\parallel}$ and (b) $\mathbf{E}_{\perp}$.

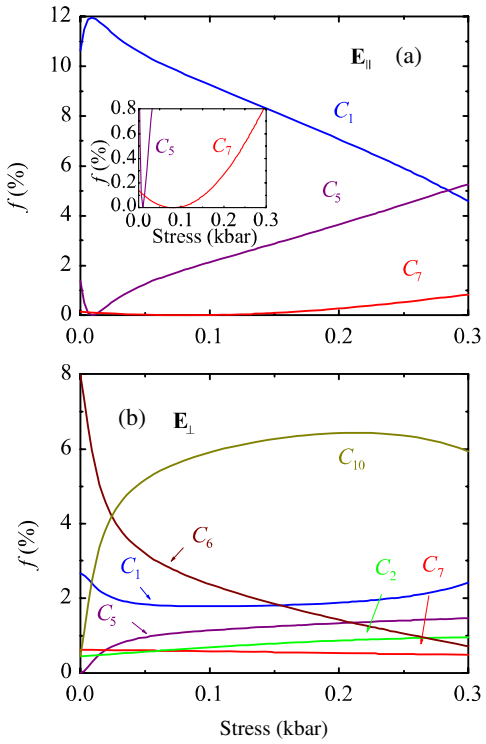

Figure 4. Oscillator strengths of C line components for Ge:Ga as functions of uniaxial stress along the [001] direction for (a) $\mathbf{E}_{\parallel}$ and (b) $\mathbf{E}_{\perp}$.

becomes larger in magnitude than the sum of $M_{\rm sp}$ and $M_{\rm df}$, leading to the increase in the oscillator strength with stress.

3.3.2. D line. In the presence of [001] stress, the D line splits into four components, D_1 ($1\Gamma_6^+ \rightarrow 2\Gamma_6^-$), D_2 ($1\Gamma_6^+ \rightarrow 2\Gamma_7^-$), D_3 ($1\Gamma_7^+ \rightarrow 2\Gamma_6^-$), and D_4 ($1\Gamma_7^+ \rightarrow 2\Gamma_7^-$) [18]. The final states of the D line components, $2\Gamma_6^-$ and $2\Gamma_7^-$, have a 55% p and a 43% f composition at zero stress. In general, the sum of $M_{\rm sp}$, $M_{\rm dp}$, and $M_{\rm df}$ is not small in magnitude for the D line components. Therefore, the D line transition is one of the most prominent transitions. With the increase of stress, the couplings between acceptor states do not cause large changes in the oscillator strengths, as figure 3 shows.

3.3.3. C line. At zero stress, the C line is associated with the $1\bar{\Gamma}_8^+ \rightarrow 1\bar{\Gamma}_7^-$ and the $1\bar{\Gamma}_8^+ \rightarrow 3\bar{\Gamma}_8^-$ transitions [18]. In the presence of [001] stress, the $1\bar{\Gamma}_7^-$ state becomes the $3\Gamma_7^-$ state, and the $3\bar{\Gamma}_8^-$ state splits into the $3\Gamma_6^-$ and the $4\Gamma_7^-$ states. As a result, the C line splits into six components, C_1 ($1\Gamma_6^+ \rightarrow 3\Gamma_7^-$), C_2 ($1\Gamma_6^+ \rightarrow 3\Gamma_6^-$), C_5 ($1\Gamma_6^+ \rightarrow 4\Gamma_7^-$), C_6 ($1\Gamma_7^+ \rightarrow 3\Gamma_7^-$), C_7 ($1\Gamma_7^+ \rightarrow 3\Gamma_6^-$), and C_{10} ($1\Gamma_7^+ \rightarrow 4\Gamma_7^-$) [18]. Here, the notation of the C line components is the same as that of [17]. It is known that the main transition of the C line at zero stress is $1\bar{\Gamma}_8^+ \rightarrow 1\bar{\Gamma}_7^-$ [10, 11, 23]. This can also be seen in figure 1. Therefore, the main C line components should be those whose final state is $3\Gamma_7^-$ at [001] infinitesimal stress. They are C_1 (for $\mathbf{E}_{\parallel}$) and C_6 (for $\mathbf{E}_{\perp}$) as can be seen in figure 4. However, since a small stress can cause a strong coupling between the $3\Gamma_7^-$ and the $4\Gamma_7^-$ states, the oscillator strengths of the C line components whose final states are the $3\Gamma_7^-$ and the $4\Gamma_7^-$ states change rapidly with stress when the stress is close to zero. The main C line component for $\mathbf{E}_{\parallel}$ ($\mathbf{E}_{\perp}$) becomes C_5 (C_{10}) when the stress is larger than 0.28 (0.02) kbar. In addition, in comparison with the coupling between the $3\Gamma_7^-$ and the $4\Gamma_7^-$ states, the couplings of the $3\Gamma_7^-$ ($4\Gamma_7^-$) state with other acceptor states should be insignificant so that the sum of the oscillator strengths of the C_1 and the C_5 components and the sum of the C_6 and the C_{10} components are not susceptible to the stress.

3.3.4. B line. In the presence of [001] stress, the B line transition $1\bar{\Gamma}_8^+ \rightarrow 4\bar{\Gamma}_8^-$ splits into four components. Dickey and Dimmock [24] measured the transition energies of two of the four B line components for Ge:In as functions of stress. We assigned the two components to the $1\Gamma_6^+ \rightarrow 5\Gamma_7^-$ (denoted by B_2) and the $1\Gamma_7^+ \rightarrow 4\Gamma_6^-$ (denoted by B_3) transitions in our previous work [18]. Figure 5 shows the stress dependence of the oscillator strengths of the B line components for Ge:In. As can be seen, the B_1 ($1\Gamma_6^+ \rightarrow 4\Gamma_6^-$) and the B_4 ($1\Gamma_7^+ \rightarrow 5\Gamma_7^-$) components are forbidden for $\mathbf{E}_{\parallel}$, and their oscillator strengths for $\mathbf{E}_{\perp}$ are smaller than those of the B_2 and the B_3 components in the low-stress region (<0.14 kbar). Therefore, only the B_2 and the B_3 components were observed in the experiment of [24]. At the stress close to 0.14 kbar, the oscillator strength of the B_2 component changes dramatically with stress due to the anticrossing between the $5\Gamma_7^-$ and the $6\Gamma_7^-$ states. Therefore, the B_2 component should be assigned to the $1\Gamma_6^+ \rightarrow 6\Gamma_7^-$ transition when the stress is higher than 0.14 kbar.

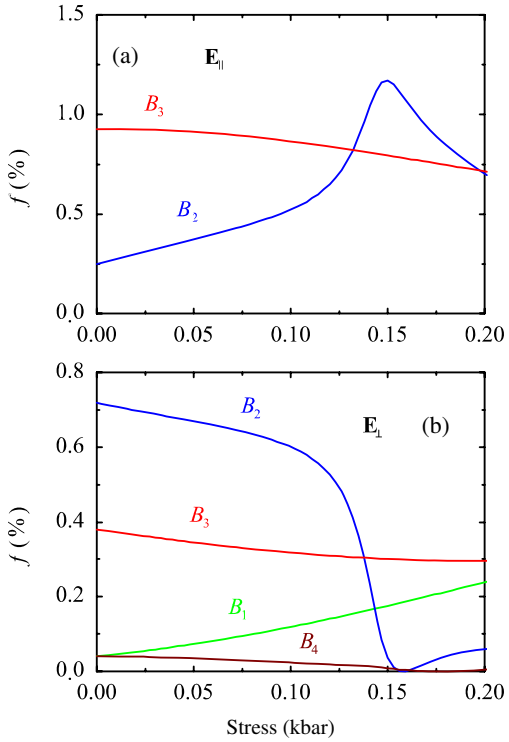

Figure 5. Oscillator strengths of B line components for Ge:In as functions of uniaxial stress along the [001] direction for (a) $\mathbf{E}_\parallel$ and (b) $\mathbf{E}_\perp$.

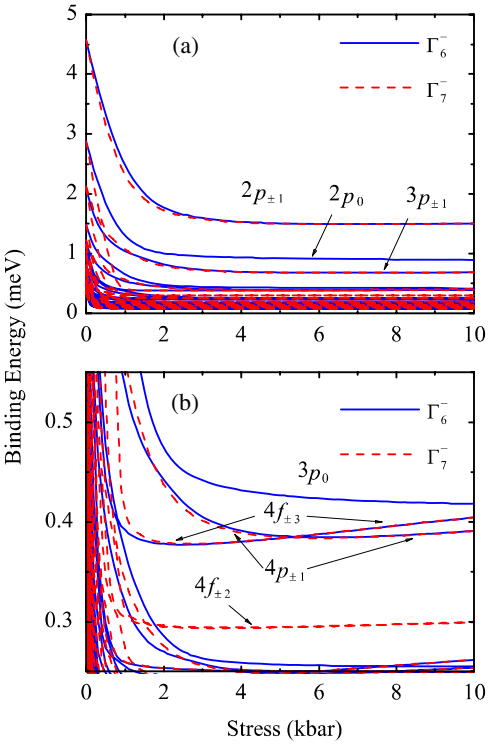

Figure 6. Binding energies of odd parity states as functions of uniaxial stress along the [001] direction for Ge:Ga. Panel (b) is a zoom-in of panel (a). The notation of acceptor states is explained in the text.

3.4. High-stress region

Figure 6 shows the binding energies of odd parity states as functions of stress up to 10 kbar for Ge:Ga. As can be seen, some of the states, which are not degenerate in the low-stress region, become nearly degenerate in the high-stress region ($\gtrsim$3 kbar). Such an extra degeneracy has been discussed in detail in our previous work [18]. In the high-stress region, the acceptor states can be regarded as belonging to a single valence band, and the effective mass Hamiltonian has a nearly azimuthal symmetry. Therefore, the wavefunctions of the acceptor states can be expressed as

$$\Psi_{JM}^{m} = \sum_{l\geqslant|m|} g_{JMlm}(r)Y_{lm}(\theta,\phi)u_{JM} \qquad (7)$$

with J, M, and m as good quantum numbers. Furthermore, for the ground state and the odd parity states, we found by the calculation of l compositions as functions of stress that only the acceptor states close to the anticrossing point can have different non-negligible l compositions, even though l is not a good quantum number. Therefore, l can approximately be regarded as a good quantum number in the high-stress region. In figure 6, we use nX_m to denote the acceptor states in the high-stress region. Here, X denotes a lower-case letter for the angular momentum l (s, p, d, f, ... for $l = 0, 1, 2, 3, \ldots$, respectively), and n is a positive integer for sorting of the acceptor states with the same l and m according to their energy levels. As can be seen, the nX_m and the nX_{-m} states are degenerate in the high-stress region.

Figure 7 shows the stress dependence of oscillator strengths of electric-dipole transitions from the ground state $1\Gamma_7^+$ to the odd parity states $n\Gamma_\nu^-$ ($\nu = 6, 7$; $n = 1, 2, \ldots, 6$). The results agree with the selection rules of the electric-dipole transitions: $\Delta l = \pm1$, $\Delta m = 0$, for $\mathbf{E}_\parallel$ and $\Delta l = \pm1$, $\Delta m = \pm1$, for $\mathbf{E}_\perp$. In the high-stress region, the ground state is s-like. Therefore, for $\mathbf{E}_\parallel$ ($\mathbf{E}_\perp$), only the transitions whose final states are np_0 ($np_{\pm1}$) can have non-negligible oscillator strengths. In addition, as mentioned previously, the G line components are weak in the low-stress region because of the appreciable d composition of the $1\Gamma_6^+$ and the $1\Gamma_7^+$ states. However, with the increase of stress, the d (s) composition of $1\Gamma_7^+$ decreases (increases) so that for $\mathbf{E}_\perp$, the oscillator strengths of the G_3 and G_4 components, which correspond to the $1\Gamma_7^+ \rightarrow 2p_{\pm1}$ transitions in the high-stress region, increase with stress, and hence the $1\Gamma_7^+ \rightarrow 2p_{\pm1}$ transitions become the main transitions in the high-stress region.

3.5. Absorption spectra

We have calculated the electric-dipole transitions between acceptor states of opposite parity. Jones and Fisher [25] measured the absorption spectrum for various species of group-III acceptors in Ge in the absence of stress, and observed the absorption from the ground $1\bar{\Gamma}_8^+$ to the $2\bar{\Gamma}_8^+$ states. In addition, Vickers *et al* [17] measured the absorption spectra of Ge:Ga in the low-stress region, and observed the stress-induced components of the $1\bar{\Gamma}_8^+ \rightarrow 3\bar{\Gamma}_8^+$ transition. It is worth mentioning that although the envelope functions of an acceptor state have a common parity, the total wavefunction

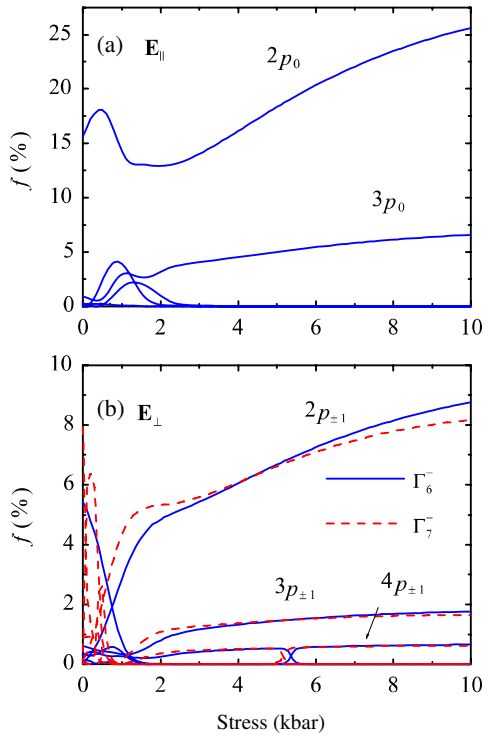

Figure 7. Oscillator strengths of electric-dipole transitions from the ground state $1\Gamma_7^+$ to the odd parity states $n\Gamma_\nu^-$ ($\nu = 6, 7$; $n = 1, 2, \ldots, 6$) for Ge:Ga as functions of uniaxial stress along the [001] direction for (a) $\mathbf{E}_\parallel$ and (b) $\mathbf{E}_\perp$. The transitions which have non-negligible oscillator strengths in the high-stress region are denoted by the final states with the same notation as in figure 6.

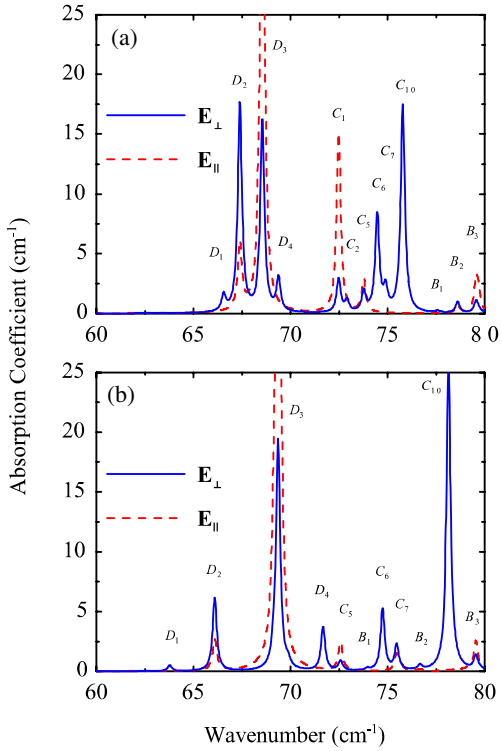

Figure 8. Absorption spectra for Ge:Ga under [001] stress of (a) 0.078 kbar and (b) 0.22 kbar at liquid-helium temperature ($T = 4.22$ K). The acceptor concentration is 6×10^{13} cm^{-3}. Each peak of the spectra is broadened by a Lorentzian line-shape function with a FWHM of 0.25 cm^{-1}.

does not have a definite parity because of the lack of inversion symmetry in the p-Ge system. Therefore, this could allow the electric-dipole transitions between acceptor states of the same parity. For the transitions between even parity states, the matrix element integral over all space is nearly equal to that over the central-cell region since the envelope functions are slowly varying outside the central-cell region. Therefore, the simple empirical form of the central-cell correction V_{cc} of equation (2) should not be applicable. On the contrary, for the electric-dipole transitions between acceptor states of opposite parity, the calculated results are not correlated closely with the detailed form of the V_{cc} since the wavefunctions of odd parity states almost vanish in the central-cell region. Adopting the central-cell correction V_{cc} in the form of equation (2) with an adjustable effective force parameter A, we obtain the transition energies [18] and the oscillator strengths for various species of group-III acceptors in Ge. The results show an excellent agreement with experiments.

For further comparison with the experimental absorption spectra of [17], we calculated the absorption spectra for Ge:Ga. The results are shown in figure 8. In the calculation, the acceptor concentration is taken to be 6×10^{13} cm^{-3}, and the stress for figures 8(a) and (b) is taken to be 0.078 and 0.22 kbar, respectively, with the same parameters as in [17]. We also replace the delta function in equation (3) with a Lorentzian line-shape function whose full width at half-maximum (FWHM) is taken to be 0.25 cm^{-1}. Here, the B_2 component is assigned to the $1\Gamma_6^+ \rightarrow 5\Gamma_7^-$ transition in panel (a) and to the $1\Gamma_6^+ \rightarrow 6\Gamma_7^-$ transition in panel (b) due to the anticrossing between the $5\Gamma_7^-$ and the $6\Gamma_7^-$ states, as mentioned previously. As can be seen, except for the presence of the transitions between even parity states, the calculated spectra are in good agreement with the experimental results, and successfully predict that the C_7 component for $\mathbf{E}_\parallel$ vanishes at 0.078 kbar but appears at 0.22 kbar. This can also be understood in terms of the stress dependence of the C_7 oscillator strength for $\mathbf{E}_\parallel$ in figure 4(a).

In panel (b), the transition energies of D_3 (69.4 cm^{-1}), C_1 (69.2 cm^{-1}), and C_2 (69.9 cm^{-1}) components are very close to each other, and the C_1 and C_2 components are much weaker than the D_3 component so that the D_3, C_1, and C_2 components are not resolved by experiment. In addition to the C_7, C_{10}, B_2, and B_3 components, there are 14 transition lines with transition energies between 75 and 80 cm^{-1}. These transitions, whose initial state is $1\Gamma_6^+$, are not labelled in panel (b) because they are too weak to be observed.

4. Conclusions

We have systematically studied the electric-dipole transitions between group-III acceptor states in Ge at zero, infinitesimal, low, and high stress along the [001] direction. At zero stress, our results are in excellent agreement with the experimental data. The binding energy of the ground state and the oscillator

strengths of electric-dipole transitions from the ground state to the odd parity states are more susceptible to the attractive central-cell force (e.g. for acceptor Tl) than to the repulsive one (e.g. for acceptor B). For the case of infinitesimal stress, we have calculated the intensity parameters, u and v, of transitions $1\bar{\Gamma}_8^+ \rightarrow n\bar{\Gamma}_8^-$ for various species of group-III acceptors in Ge. Except for the G line transition, the intensity parameters are not significantly correlated with the species of acceptor atoms. Our results for Ge:Ga agree well with the experimental data. At finite stress, the intensity parameters are no longer applicable due to the strain-induced couplings between acceptor states of the same symmetry. In fact, the oscillator strengths of certain transitions change appreciably even though only a small stress (<0.3 kbar) is applied. In the high-stress region, the nX_m and the nX_{-m} states are nearly degenerate. Because the ground state becomes s-like, only the transitions to the np_0 ($np_{\pm1}$) states for $\mathbf{E}_\parallel$ ($\mathbf{E}_\perp$) can have non-negligible oscillator strengths. For the same reason, the G_3 and G_4 components, which are weak in the low-stress region, become the main transitions for $\mathbf{E}_\perp$ in the high-stress region. We have calculated the absorption spectra at stresses of 0.078 and 0.22 kbar. Our results are in good agreement with the measured spectra [17], except for the presence of the transitions between even parity states, and successfully explain the disappearance of the C_7 component for $\mathbf{E}_\parallel$ at 0.078 kbar.

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