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LETTER TO THE EDITOR

Optical properties of strained GaAs layers

Zhi-Zhong Xu

Chinese Centre of Advanced Science and Technology (World Laboratory) and Department of Physics, Fudan University, Shanghai 200433, People's Republic of China

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Abstract. Optical properties, including oscillator strengths for interband transitions and optical third-order non-linear susceptibilities, are calculated in the tight-binding frame for strained GaAs layers grown on $\text{Ge}_x\text{Si}_{1-x}(001)$ substrates. The dependences of the optical properties on the substrate alloy composition, x , as well as the strains in the GaAs layers are discussed.

GaAs is an important material for fabricating optoelectronic devices and many of its optical properties are superior to those of Si. However, Si is the most mature semiconductor technology including its substrates. The growth of GaAs on Si is therefore of interest for optical applications, with potential for integrated optoelectronics. A GaAs layer grown on an Si substrate is strained because the GaAs layer cannot lattice-match with the Si substrate. The strains change the band structures as well as the physical properties of the GaAs layers: one of the most effective methods in band engineering is to grow a strained layer on a substrate (Bean 1992, O'Reilly 1989). By choosing a substrate material with proper lattice constants in order to control the strain in the epitaxial layer, it is possible to obtain excellent characteristics for the strained layer. Considering that the lattice constant of Ge is equal to that of GaAs, the $\text{Ge}_x\text{Si}_{1-x}$ alloy (in which the lattice constant can be modified by changing the alloy composition x) may be chosen as the substrate for the GaAs epitaxial layer. Due to the serious lattice mismatch between GaAs and Si (about 4%), the critical thickness is small for GaAs layers grown on $\text{Ge}_x\text{Si}_{1-x}$ substrates with small x . However, it is expected that a high-quality GaAs layer thick enough for fabricating devices will be achieved before long, though many technological problems remain unsolved. In this letter, the optical properties, including the oscillator strengths for the optical transitions, and the optical third-order non-linear susceptibilities are calculated in the tight-binding frame for the strained GaAs layers grown on $\text{Ge}_x\text{Si}_{1-x}(001)$ substrates, and their dependences on the substrate alloy composition x are discussed. Compared with work on strained quantum wells, the confined-size effect has been neglected. Therefore, it is supposed in our calculation that the strained GaAs layers have a large thickness.

The tight-binding parameters used by Priester *et al* (1988) are adopted in this work. Since only the nearest-neighbouring interactions are considered in Priester *et al's* parameters, the calculated results for the conduction band energy level at the L point cannot agree very well with experiment though those at the Γ point and the X point coincide with the experiments in general. Based on Priester *et al's* parameters, two next-neighbouring interaction parameters $\epsilon(\text{spa})$ and $\epsilon(\text{spc})$, which represent the interactions between s state and p state for two anions and for two cations, are introduced with values of -0.07 and

-0.1 separately. They are determined by fitting the experimental values of the conduction band energy level at the L point for the GaAs. Table 1 shows the results calculated with our parameters and Priester *et al*'s parameters for the energy gaps at the Γ , X and L points and the spin-orbit splitting Δ_0 at the valence band top of GaAs. The experimental values (Madelung 1982) are also listed in the table.

Table 1. The calculated and experimental values of the energy gaps at the Γ , X and L points and the spin-orbit splitting Δ_0 at the valence band top for bulk GaAs given in eV.

	$E_g(\Gamma)$	$E_g(X)$	$E_g(L)$	Δ_0
This work	1.55	2.03	1.82	0.35
Priester <i>et al</i>	1.55	2.03	1.69	0.35
Experiment	1.52	1.98	1.81	0.35

Since the lattice constant of GaAs cannot match with that of $\text{Ge}_x\text{Si}_{1-x}$ alloys, there are strains in the GaAs layer grown on the $\text{Ge}_x\text{Si}_{1-x}(001)$ substrate. The strains change both the bond lengths and bond angles in the GaAs layer. The change of the bond angles modifies not only the geometrical structure factor but also the tight-binding parameters for the off-diagonal interaction through varying the direction cosine of the bond angles (Xu 1993). The change of the bond lengths modifies the off-diagonal tight-binding parameters according to the empirical scaling rule (Harrison 1980)

$$V_{\alpha\beta} = V_{\alpha\beta}^0 (d/d_0)^{-n(\alpha\beta)}$$

where $V_{\alpha\beta}^0$ and $V_{\alpha\beta}$ are the unstrained and strained tight-binding parameters for the interactions between the α state and β state respectively. d and d_0 are the unstrained and strained bond lengths; $n(\alpha\beta)$ is the scale index. In order to consider the influence of the strain on the electronic band structures correctly, the scale index $n(\alpha\beta)$ is determined by fitting the experimental values of the hydrostatic deformation potentials for the Γ direct energy gap, $a(\Gamma)$, and for the X and L indirect energy gaps $E_1(X)$ and $E_1(L)$ (Xu 1993). Though the correct values of the hydrostatic deformation potentials can be obtained by adjusting the scale index $n(\alpha\beta)$, the shear deformation potentials are independent of the scale index $n(\alpha\beta)$. The incorrect shear deformation potentials may result in a wrong order of the energies for the splitting levels X_x (X_y) and X_z which come from the X conduction band valley under the uniaxial strain along the [001] direction. In order to count the variations of the energy band structures by the uniaxial strains correctly, a new scale index, F , is used according to the method proposed by Munoz and Armelles (1993). In this method the tight-binding parameters of interactions between s^* and p (p_x , p_y , p_z) states, which determine the shear deformation potentials of the X indirect energy gap $E_2(X)$, are given as a function of strain components $e_x = e_y$ and e_z in the following way

$$V_{s^*a,pxc} = V_{s^*a,pyc} = (d/d_0)^{n(s^*a,pc)+1} V_{s^*a,pc}^0 [(1 - e_x) - F(e_z - e_x)]$$

$$V_{s^*a,pzc} = (d/d_0)^{n(s^*a,pc)+1} V_{s^*a,pc}^0 [(1 - e_z) + 2F(e_z - e_x)].$$

The new scale index, F , is determined by fitting the experimental values of shear deformation potentials $E_2(X)$ for the bulk GaAs. Table 2 lists the scale indices $n(\alpha\beta)$ and F obtained in this work. Table 3 gives the hydrostatic and shear deformation potentials calculated with these scale indices listed in table 2 and their experimental values (Madelung 1982). Here, b represents the shear deformation potential of the valence band top which concerns the splitting of the heavy- and light-hole levels.

Table 2. The scale indices $n(\alpha\beta)$ and F .

α, β	s, s	sa, pc	s*a, pc	pa, sc	pa, s*c	pp σ	pp π	F
$n(\alpha\beta)$	3.7	2.1	3.0	3.8	2.0	2.0	2.0	-1.06

Table 3. The deformation potentials of GaAs in eV.

	$a(\Gamma)$	$E_1(X)$	$E_1(L)$	$E_2(X)$	b
Calculated	-8.37	1.34	-4.05	6.47	-2.81
Experiment	-6.7 to -9.77	1.35	-4.10	6.5	-2.0

The oscillator strengths are calculated with the formula given by Lew Yan Voon and Ram-Mohan (1993).

$$f_{nm}^i(k) = (2m_0/\hbar^2) |\langle mk | \partial H / \partial k_i | nk \rangle|^2 / [E_m(k) - E_n(k)]$$

where i represents the polarization direction for the incident light, m and n are the band indices for states which have eigenenergies $E_m(k)$ and $E_n(k)$ and m_0 is the free-electron mass. $\partial H / \partial k_i$ is the partial differential of the tight-binding Hamiltonian matrix with respect to the i th component of the wavevector k . Here, the eigenenergies $E_m(k)$, $E_n(k)$ and the wavefunctions $|mk\rangle$, $|nk\rangle$ are obtained by diagonalizing the Hamiltonian matrix and all calculations are carried out in the tight-binding representation with a local basis set.

In this work, the oscillator strengths for the interband transitions from three levels of valence band top, including heavy-, light- and split-off hole states, to the bottom level of the conduction band are calculated. The calculated results are shown in figure 1, where the solid lines denote the oscillator strengths for the polarization in the layer plane and the dot-dash lines denote those perpendicular to the layer plane. HC, LC and SC represent the transitions from the heavy-, light- and split-off hole states to the bottom state of the conduction band separately. It can be seen from figure 1 that for the transition from the heavy-hole state to the conduction band state, only the oscillator strength with polarization in the layer plane, $f_{HC}^{[100]}$, is not equal to zero and decreases with the substrate alloy composition, x . The oscillator strength with polarization perpendicular to the layer plane $f_{HC}^{[001]}$ is equal to zero for all the compositions of the substrate alloy x and is not shown in the figure. For the transition from the light-hole state to the conduction band state, with the decrease of x , the $f_{LC}^{[100]}$ grows and the $f_{LC}^{[001]}$ drops. For the transition from the split-off hole state to the conduction band state, $f_{SC}^{[100]} = f_{SC}^{[001]}$ at $x = 1$ and when x decreases, $f_{SC}^{[100]}$ drops and $f_{SC}^{[001]}$ grows. When $x = 1$, at which there is no strain in the GaAs layer, the levels of the light- and heavy-hole states are degenerate and the total oscillator strengths for the [100] polarization should be equal to $f_{HC}^{[100]} + f_{LC}^{[100]} = f_{LC}^{[100]}$ because $f_{HC}^{[100]} = 0$. Similarly, the total oscillator strengths for the [001] polarization should be equal to $f_{LC}^{[001]} + f_{SC}^{[001]}$ as $x = 1$. The calculated results show that at $x = 1$, $f_{HC}^{[001]} + f_{LC}^{[001]} = f_{LC}^{[001]} = 13.12$, implying that the isotropic symmetry of the bulk GaAs and the value of 13.12 is also approximately in agreement with the calculated results of 16.06–17.97, produced by Gorczyca *et al* (1991).

When the light frequencies ω_1 , ω_2 and ω_3 are much smaller than the E_g/h , where E_g is the energy gap of the material, the third-order non-linear optical susceptibility $\chi_{\alpha\alpha\alpha\alpha}^{(3)}(\omega_1\omega_2\omega_3)$ can be approximately written as (Jha and Blemborgen 1968, Wynne 1969)

$$\chi_{\alpha\alpha\alpha\alpha}^{(3)} = e^4 U_\alpha / 24h^4 \omega_1 \omega_2 \omega_3 (\omega_1 + \omega_2 + \omega_3)$$

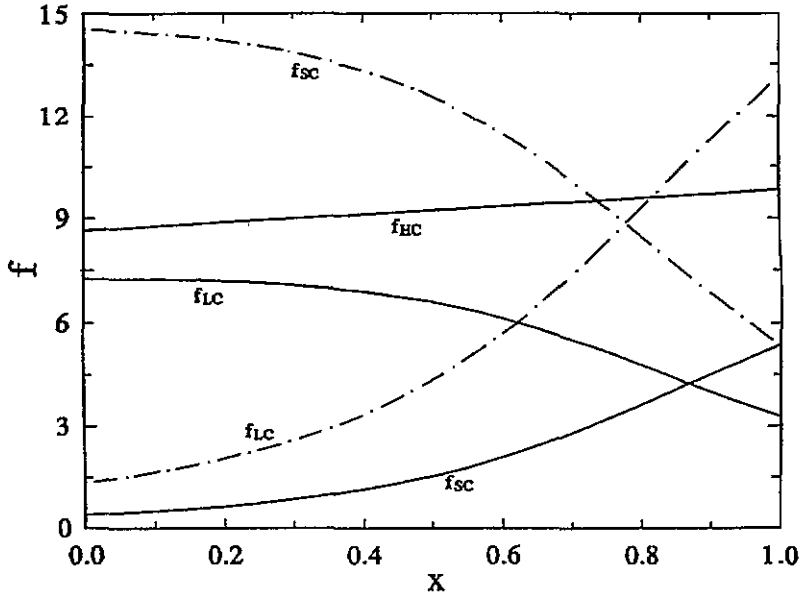


Figure 1. The oscillator strengths for interband transitions from three hole states to the conduction band bottom state for the strained GaAs/Ge_xSi_{1-x}(001) as a function of the substrate alloy composition x .

where

$$U_{\alpha} = (2/8\pi^3) \int_{BZ} f_0(E) \partial^4 E(\mathbf{k}) / \partial k_{\alpha}^4 d\tau_{\mathbf{k}}.$$

Here, the polarizations of all three optical fields are supposed to be the same and denoted by α , and only the polarization component of the induced field in the same direction is considered. $E(\mathbf{k})$ represents the eigenenergy, which is the conduction band energy for n type GaAs/Ge_xSi_{1-x}(001) and the valence band energy for p type GaAs/Ge_xSi_{1-x}(001). k_{α} is the α th component of the wavevector and $f_0(E)$ is the Fermi distribution function. For simplification, it is supposed that the absolute temperature $T = 0$ and so,

$$f_0(E) = \begin{cases} 0 & \text{if } E > E_F \\ 1 & \text{if } E < E_F \end{cases}$$

where E_F is the Fermi level. $d\tau_{\mathbf{k}}$ is the space element in \mathbf{k} space and the integral is performed in the whole Brillouin zone. In order to compare the values of the $\chi_{\alpha\alpha\alpha\alpha}^{(3)}$ for various alloy composition, x , clearly, $\hbar\omega_1$ and $\hbar\omega_2$ are taken to be 0.117 eV ($\lambda_1 = \lambda_2 = 10.16 \mu\text{m}$) and $\hbar\omega_3$ is taken to be -0.135 eV ($\lambda_3 = 9.2 \mu\text{m}$) according to the experimental arrangement described by Wynne (1969).

The third-order non-linear optical susceptibilities $\chi^{(3)}$ for the n type and p type GaAs/Ge_xSi_{1-x}(001) with $x = 0, 0.5, 1$ as a function of the electronic concentration, n , and hole concentration, p , are shown in figure 2 and figure 3 respectively. For most concentrations of electrons or holes, the $\chi^{(3)}$ of the n type GaAs/Ge_xSi_{1-x}(001) is always positive and the $\chi^{(3)}$ of the p type GaAs/Ge_xSi_{1-x}(001) is negative. So, the absolute values of $\chi^{(3)}$ are given in figure 3. In figure 2, the short-dash line and long-dash line denote the third-order susceptibility with [100] polarization $\chi_{xxxx}^{(3)}$ and with [001] polarization $\chi_{zzzz}^{(3)}$ at $x = 0$ respectively, the dot-dash line and double-dots-dash line denote the $\chi_{xxxx}^{(3)}$ and $\chi_{zzzz}^{(3)}$

at $x = 0.5$ and the solid line denotes the $\chi_{xxxx}^{(3)} = \chi_{zzzz}^{(3)}$ at $x = 1$. (When $x = 1$, there is no strain in the GaAs layers and it is the same as the bulk GaAs.) It can be seen from figure 2 that when $x = 1$, the electronic $\chi_{xxxx}^{(3)}$ ($= \chi_{zzzz}^{(3)}$) almost varies with the electronic concentration n linearly in the logarithmic coordinates and can be approximately written as

$$\chi_{xxxx}^{(3)} = \chi_{zzzz}^{(3)} = 2.64 \times 10^{-25} n^{0.912} (\text{esu}).$$

In Wynne's experiment (1969), the $\chi_{xxxx}^{(3)}$ ($= \chi_{zzzz}^{(3)}$) of the bulk GaAs is supposed to be changing linearly with the electronic concentration, n , and the measured value of the $\chi_{xxxx}^{(3)}/n$ is about $(4.4 \pm 2.2) \times 10^{-27}$ esu cm^{-3} . It can be seen from figure 4 in the paper of Wynne (1969) that the experimental points with larger concentration, n , deviate obviously from the line. However, if we also suppose that the change is linear, an average value of the $\chi_{xxxx}^{(3)}/n$ can be obtained to be 7.2×10^{-27} esu cm^{-3} , which is agreement with Wynne's experimental value roughly. As x departs from unity, the GaAs layer becomes strained. The strain reduces both the $\chi_{xxxx}^{(3)}$ and $\chi_{zzzz}^{(3)}$ and so they decrease with x . For larger concentration n ($n > 3 \times 10^{17}$ cm^{-3} at $x = 0.5$ and $n > 5 \times 10^{17}$ cm^{-3} at $x = 0$), the $\chi_{zzzz}^{(3)}$ is smaller than the $\chi_{xxxx}^{(3)}$. When $n < 1.6 \times 10^{17}$ cm^{-3} , the $\chi_{xxxx}^{(3)}$ oscillates around zero and the amplitude is about 1×10^{-10} esu. For $x = 0.5$, as $n < 2 \times 10^{16}$ cm^{-3} , the $\chi_{zzzz}^{(3)}$ also turns out to be negative. None of the negative values of the $\chi_{xxxx}^{(3)}$ and $\chi_{zzzz}^{(3)}$ are shown in figure 2.

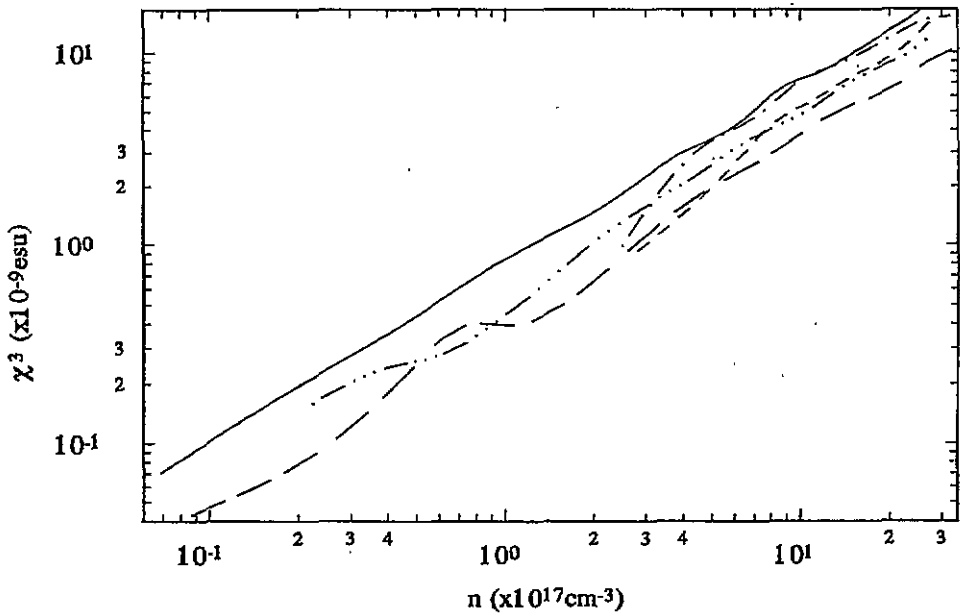


Figure 2. The third-order non-linear susceptibilities of n type strained GaAs/Ge $_x$ Si $_{1-x}$ (001) as a function of electronic concentration n . The short-dash line and long-dash line denote the susceptibilities with [100] polarization and [001] polarization for the substrate alloy composition $x = 0$. The dot-dash line and triple-dots-dash line denote the susceptibilities with [100] polarization and [001] polarization for the substrate alloy composition $x = 0.5$. The solid line denotes the susceptibilities for the substrate alloy composition $x = 1$.

Figure 3 shows the dependence of the $\chi_{xxxx}^{(3)}$ and $\chi_{zzzz}^{(3)}$ for the p type GaAs/Ge $_x$ Si $_{1-x}$ (001) on the concentration of holes, p , where the solid lines denote the $\chi_{xxxx}^{(3)}$ and the dot-dash lines denote $\chi_{zzzz}^{(3)}$. Comparing figure 3 with figure 2, figure 3 shows that when $x < 1$ the $\chi_{xxxx}^{(3)}$ grows and the $\chi_{zzzz}^{(3)}$ drops. The $\chi_{xxxx}^{(3)}$ at $x = 0.5$ is larger than that at $x = 0$ and the

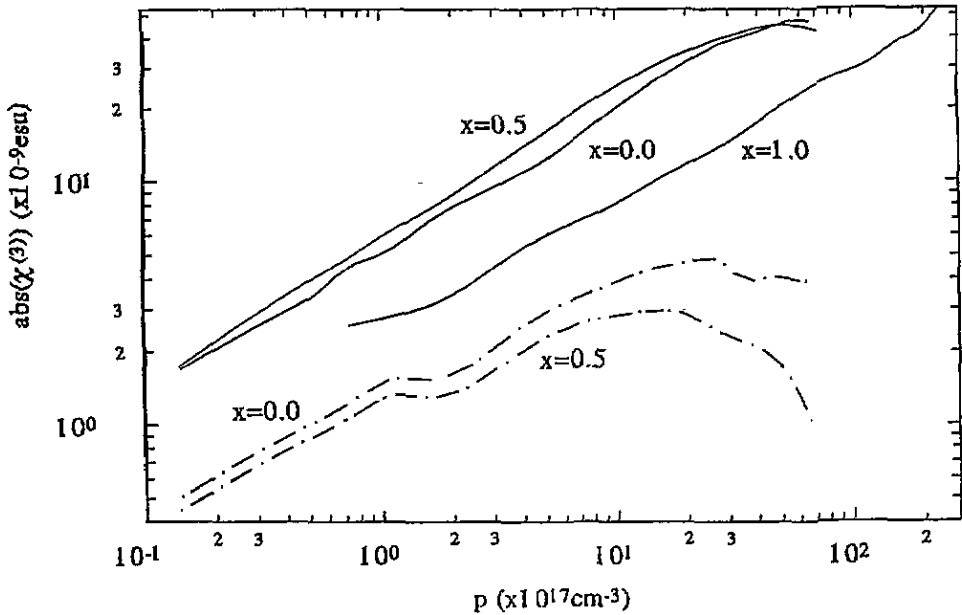


Figure 3. The third-order non-linear susceptibilities of the p type strained GaAs/Ge_xSi_{1-x}(001) as a function of the hole concentration p . The solid lines denote the susceptibilities with [100] polarization and the dot-dash lines denote those with [001] polarization.

$\chi_{zzzz}^{(3)}$ at $x = 0.5$ is smaller than that at $x = 0$. When $x > 0.5$ (for example, $x = 0.8$ or 0.9) the $\chi_{xxxx}^{(3)}$ may grow further for some concentrations p , but out of these concentrations $\chi_{xxxx}^{(3)}$ drops quickly. From the longitudinal coordinates of figure 2 and figure 3 it can be seen that most $\chi^{(3)}$ values of holes are larger than those of electrons. For example, as $x = 1$ and $n = 2.5 \times 10^{18} \text{ cm}^{-3}$, the electronic $\chi_{xxxx}^{(3)} = 1.6 \times 10^{-8} \text{ esu}$, but for the same x and the same concentration the hole $\chi_{xxxx}^{(3)} = 4.0 \times 10^{-8} \text{ esu}$.

Finally, it may be pointed out that the values of the $\chi^{(3)}$ given above are not very accurate because the used formula is approximate but it is useful to display what are the effects of the strain on the $\chi^{(3)}$ qualitatively. The calculated results show that the strain in the GaAs/Ge_xSi_{1-x}(001) reduces the $\chi^{(3)}$ of electrons and enhances the $\chi_{xxxx}^{(3)}$ of holes. So, it is favourable to use p type GaAs/Ge_xSi_{1-x}(001) for fabricating non-linear optical devices.

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What Gorczyca *et al* give in this article is the value of the interband matrix elements $E_{p0} = P^2/m_0$, where P is the quantum matrix elements between valence band top states and conduction band bottom states. The value shown in the text is calculated from the value of E_{p0} with the equation $f = E_{p0}/E_g$, where $E_g = 1.55 \text{ eV}$.

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