Electronic Contribution to the Elastic Constants in Strained Layer Quantum Dot Superlattices of Non-Parabolic Semiconductors with Graded Interfaces

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Most papers in the area of semiconductor superlattices (SLs) are based on the assumption that the interface between the layers are sharply defined with the zero thickness so as to be devoid of any interface effects. The advanced experimental techniques may produce SL with physical interface between the two materials crystallographically abrupt, but the bonding environment of the atoms adjoining these interface will change at least on an atomic scale as the potential form changes from a well (barrier) to a barrier (well), an intermediate potential region exists for the charge carriers. Thus, the influence of the finite thickness of the interface on the carrier dispersion law becomes very important. In this paper we study the electronic contribution to the elastic constants in strained layer quantum dot superlattices of non-parabolic semiconductors with graded structures and compare the same with that of the constituent materials, by formulating the appropriate dispersion laws. It is found, taking InSb/GaSb quantum dot strained superlattices of non-parabolic semiconductors as an example, that the carrier contribution to the second- and third-order elastic constants oscillates with the electronic concentration together with the fact that the nature of oscillations are totally dispersion relation dependent. We have also suggested an experimental method for determining the electronic contribution to the elastic constants in quantum-confined materials having arbitrary carrier energy spectra. In addition, the well-known results for bulk specimens of wide-gap stress free materials have been obtained as special cases from our generalized formulation under certain limiting conditions.

Keywords: Elastic Constants, Strained Layer Quantum Dot Superlattices, Graded Interfaces, Dispersion Relation, Suggestion for the Experimental Determination of the Elastic Constants.

1. INTRODUCTION

With the advent of molecular beam epitaxy, organometallic chemical vapor phase epitaxy, fine line lithography and other experimental techniques, it has become possible to fabricate Superlattices (SLs) of non-parabolic semiconductors composed of alternate layers of two different materials with controlled thickness, many of which are currently under study due to their new physical properties.¹,² The SL, as originally proposed by Esaki and Tsu,³ has found wide applications in many device structures, such as photo detectors,⁴ avalanche photo diodes,⁵ transistors,⁶ tunneling devices,⁷ light emitters,⁸ etc.

The most extensively studied SL is consisting of alternate layers of GaAs and Ga₁₋ₓAlₓAs. In addition to the SLs with usual structure, the SLs with more complex structures such as PbTe/SnTe,⁹ II-VI,¹⁰ strained layer,¹¹ and HgTe/CdTe,¹² etc have also been proposed. These complex
structures have provided additional degrees of freedom through band gap engineering, so that the more parameters could be available for obtaining of the desired electronic and optical properties. It is worth remarking that the most papers in this vital area of modern nanostructured electronics are based on the assumption that the interface between the layers is sharply defined with the zero thickness so as to be devoid of any interface effects: the SL potential distribution may be considered as a one dimensional array of rectangular potential wells. The advanced experimental techniques may produce SL with physical interface between the two materials crystallographically abrupt, but the bonding environment of the atoms adjoining these interface will change at least on an atomic scale as the potential form changes from a well (barrier) to a barrier (well), an intermediate potential region exists for the charge carriers. Thus, the influence of the finite thickness of the interface on the carrier energy spectra becomes very important since the dispersion relation of the carriers of the interface will change at least on an atomic scale so as to be devoid of any interface effects: the SL between the layers is sharply defined with the zero thickness of ultra thin films and with the temperature for the present system. The corresponding results for bulk specimens of stress free wide-gap materials have also been obtained from our generalized formulation for the purpose of assessing the influence of strain and interface width respectively. As already remarked we have also suggested the experimental methods for determining such contribution for materials having arbitrary dispersion laws. We shall study the doping dependence of $\Delta C_{44}$ and $\Delta C_{456}$ taking strained quantum dot InAs/GaSb SL as an example for the purpose of numerical computations.

2. THEORETICAL BACKGROUND

The dispersion relation of the conduction electrons in bulk specimens of stressed non-parabolic semiconductors can be expressed, in the absence of any quantization, as

$$[k_x/a_i^*(E)]^2 + [k_y/b_i^*(E)]^2 + [k_z/f_i^*(E)]^2 = 1 \quad (1)$$

where

$$[a_i^*(E)]^2 = L_i^*(E)[A_i^*(E) + (1/2)D_i^*(E)]^{-1},$$

$$i = 1, 2, L_i^*(E) = [3E^2 + Eq_i - R_i],$$

$$q_i = [(3E_{gi}/2e_i^2) - (3e_i^2/c_i)]$$

where $E_{gi}$ is the band gap, $e_i$ are the momentum matrix elements, $c_i$ is the conduction band deformation potential constant, $e_i$ is the trace of the strain tensor $\tilde{e}_i$, which is given by

$$\tilde{e}_i = \begin{bmatrix} e_{xxi} & e_{xyi} & 0 \\ e_{xyi} & e_{yyi} & 0 \\ 0 & 0 & e_{zzi} \end{bmatrix} \quad (2)$$

$e_{xxi}$, $e_{xyi}$, $e_{yyi}$, and $e_{zzi}$ are the various elements of $\tilde{e}_i$.

$$R_i = [e_i^{-2}(g_i)^2(e_{yyi})^2 + (3/2)e_i^{-2}c_i e_i(E_{gi} - c_i e_i)]$$

$g_i$ is a constant describing the strain interaction between the conduction and valence bands,

$$A_i^*(E) = (E + G_i^*)/(E + H_i)^{-1},$$

$$G_i^* = [E_{gi} - c_i^2 e_i + 3\tilde{b}_0 e_{xxi} - \tilde{b}_0 e_i(a_{0i} + c_i^2 e_i)]$$

$$a_{0i} = -(x_i + 2y_i)/3, \quad \tilde{b}_0 = (x_i - y_i)/3, \quad \tilde{b}_0 = 2Z_i/\sqrt{3}, x_i, y_i$$
and $Z_i$ are the matrix elements of the strain projection operator,

$$H_i = [E_i + c_i^r e_i], \quad D_i^*(E) = \rho_i (E + H_i)^{-1},$$

$$\rho_i = [d_i \epsilon_{c y}(3)^{1/2}]$$

$$[b_i^*(E)]^2 = L_i^*(E) [A_i^*(E) - (1/2)D_i^*(E)]^{-1},$$

$$[f_i^*(E)]^2 = L_i^*(E)/C_i^*(E), \quad C_i^*(E) = (E + G_i^*) (E + H_i)^{-1},$$

and

$$G_i^* = [E_{g z} - c_i^r e_i - (a_0 + c_i^r)e_i + \bar{b}_0 \epsilon_{c y} - \bar{b}_0 e_i]$$

Therefore the dispersion law of the electrons in strained layer SLs of non-parabolic semiconductors with graded interfaces can be written as, by extending the method as given in Ref. [19], as

$$\cos(L_0 k) = \phi(E)/2$$

where $L_0 = L_1 + L_2$ is the period length, $L_1$ and $L_2$ are the widths of the barrier and well respectively,

$$\phi(E) = \left\{ 2 \cosh[\beta(E) \cos[\gamma(E)]
+ T(E) \sinh[\beta(E) \sin[\gamma(E)]
+ \Delta_0 \left\{ \frac{K_0^2(E)}{K'(E)} - 3K'(E) \right\} \cosh[\beta(E)] \sin[\gamma(E)]
+ \left( 3K_0^2(E) \frac{K'(E)}{K_0^2(E)} - \frac{K'(E)}{K_0^2(E)} \right) \sinh[\beta(E)] \cos[\gamma(E)] \right\}
+ \Delta_0 \left\{ \left( 2[K_0^2(E)]^2 - 2[K'(E)]^2 \right) \cosh[\beta(E)] \cos[\gamma(E)]
+ \frac{1}{12} \left( 5K_0^2(E) - \frac{K'(E)^3}{K_0^2(E)} - 34K'(E)K_0^2(E) \right) \sinh[\beta(E)] \sin[\gamma(E)] \right\}\right\},$$

$$T(E) = \left( \frac{K_0^2(E)}{K'(E)} - \frac{K'(E)}{K_0^2(E)} \right), \quad \beta(E) = K_0(E)(L_1 - \Delta_0)$$

$\Delta_0$ is the interface width,

$$\gamma(E) = K'(E)(L_2 - \Delta_0),$$

$$K'(E) = \left\{ (E + G_i^*)^{-1} (E + H_i) (3E_i^2 + EQ_1 - R_1) - (E + G_i^*)^{-1} (E + G_i^* + \frac{1}{2} \rho_i) k_i^2
- (E + G_i^*)^{-1} (E + G_i^* - \frac{1}{2} \rho_i) k_i^2 \right\}^{1/2},$$

$$K_0(E) = \left\{ (V_0 - E - H_2)(E_1 + G_i^*)^{-1} (3E_i^2 + EQ_1 - R_2) + (E_1 + G_i^*)^{-1} \left( E + G_i^* + \frac{1}{2} \rho_i \right) k_i^2
+ (E_1 + G_i^*)^{-1} \left( E + G_i^* - \frac{1}{2} \rho_i \right) k_i^2 \right\}^{1/2}$$

$$E_i = E - V_{0}, \quad \text{and} \quad V_0 = (E_{g z} - E_\text{g z})$$

Therefore the electron energy spectrum in strained layer quantum dot SLs of non-parabolic semiconductors with graded interfaces can be written as

$$(n_z \pi/d_z)^2 = \left[ -\theta_0^2 + (\delta(E')/L_0^2) \right]$$

where $n_z = 1, 2, 3, \ldots$ is the size quantum number along $z$-direction, $d_z$ is the width along $z$ direction, $\theta_0 = \left( n_z \pi / d_z \right)^2 + \left( n_z \pi / d_y \right)^2$, $n_x$ and $n_y$ are size quantum numbers along $x$ and $y$ directions, $d_x$ and $d_y$ are the widths along $x$ and $y$ directions, $\delta(E') = \cos^{-1} \left( 1/2 \psi(E') \right)^2$

$$\psi(E') = \left\{ 2 \cosh[\beta(E') \cos[\gamma(E')]$$
$$+ T(E') \sinh[\beta(E') \sin[\gamma(E')]$$
$$+ \Delta_0 \left\{ \frac{K_0^2(E)}{K'(E)} - 3K'(E) \right\} \cosh[\beta(E')] \sin[\gamma(E')]$$
$$+ \left( 3K_0^2(E) - \frac{K'(E)^3}{K_0^2(E)} \right) \sinh[\beta(E')] \cos[\gamma(E')] \right\}
+ \Delta_0 \left\{ \left( 2[K_0^2(E)]^2 - 2[K'(E)]^2 \right) \cosh[\beta(E')] \cos[\gamma(E')]
+ \frac{1}{12} \left( 5K_0^2(E) - \frac{K'(E)^3}{K_0^2(E)} - 34K'(E)K_0^2(E) \right) \sinh[\beta(E')] \sin[\gamma(E')] \right\}\right\},$$

$$\beta(E') = K_0(E')(d_z - \Delta_0),$$

$$K_0(E') = \left\{ (V_0 - E - H_2)(E_1 + G_i^*)^{-1} (3E_i^2 + EQ_1 - R_2) + (E_1 + G_i^*)^{-1} \left( E + G_i^* + \frac{1}{2} \rho_i \right) k_i^2
+ (E_1 + G_i^*)^{-1} \left( E + G_i^* - \frac{1}{2} \rho_i \right) k_i^2 \right\}^{1/2}$$

$E_i = E - V_0$ and $V_0 = (E_{g z} - E_\text{g z})$ is the potential barrier encountered by the electron.

$$\gamma(E') = K'(E')(d_z - \Delta_0),$$

$\psi(E') = \left\{ 2 \cosh[\beta(E') \cos[\gamma(E')]$$
$$+ T(E') \sinh[\beta(E') \sin[\gamma(E')]$$
$$+ \Delta_0 \left\{ \frac{K_0^2(E)}{K'(E)} - 3K'(E) \right\} \cosh[\beta(E')] \sin[\gamma(E')]$$
$$+ \left( 3K_0^2(E) - \frac{K'(E)^3}{K_0^2(E)} \right) \sinh[\beta(E')] \cos[\gamma(E')] \right\}
+ \Delta_0 \left\{ \left( 2[K_0^2(E)]^2 - 2[K'(E)]^2 \right) \cosh[\beta(E')] \cos[\gamma(E')]
+ \frac{1}{12} \left( 5K_0^2(E) - \frac{K'(E)^3}{K_0^2(E)} - 34K'(E)K_0^2(E) \right) \sinh[\beta(E')] \sin[\gamma(E')] \right\}\right\},$$

$$\beta(E') = K_0(E')(d_z - \Delta_0),$$

$$K_0(E') = \left\{ (V_0 - E - H_2)(E_1 + G_i^*)^{-1} (3E_i^2 + EQ_1 - R_2) + (E_1 + G_i^*)^{-1} \left( E + G_i^* + \frac{1}{2} \rho_i \right) k_i^2
+ (E_1 + G_i^*)^{-1} \left( E + G_i^* - \frac{1}{2} \rho_i \right) k_i^2 \right\}^{1/2}$$

$E_i = E - V_0$ and $V_0 = (E_{g z} - E_\text{g z})$ is the potential barrier encountered by the electron.

$$\gamma(E') = K'(E')(d_z - \Delta_0),$$
Elastic Constants in Strained Layer Quantum Dot Superlattices of Non-Parabolic Semiconductors

Singh et al.

The Eq. (8) and (9) represent the expressions for \( \Delta C_{44} \) and \( \Delta C_{456} \) for the present system. The expression for \( n_0 \) for the constituent non-parabolic materials will be given by Eq. (5) where \( E' \) has to be determined from

\[
\begin{align*}
[&n_i, \pi/(d_i \alpha_i(E'))^2]\quad+\quad[n_i, \pi/(d_i \beta_i(E'))^2] \\
&+\quad[n_i, \pi/(d_i \gamma_i(E'))^2] = 1
\end{align*}
\]

In the absence of stress and under the substitution \( \varepsilon_i^2 = 3h^2 E_{	ext{g}}/4m^* \), where \( m^* \) is the effective electron mass at the edge of the conduction band, the Eq. (1) assumes the form

\[
E(1 + \alpha \cdot E) = \frac{h^2 k^2}{2m^*}
\]

where \( \alpha = 1/E_{\text{g}} \) and \( h \) is Dirac’s constant.

The Eq. (11) is known in the literature as the two band model of Kane.20 Besides, this particular equation is being extensively used to study the electronic properties of nanostructured III-V compounds, ternary and quaternary alloys, and is a special case of Eq. (1). The expressions of \( n_0, \Delta C_{44} \), and \( \Delta C_{456} \) can, respectively, be written as

\[
\begin{align*}
n_0 &= N_c [F_{1/2} (\eta) + (15 \alpha \cdot k_B T/4) F_{3/2} (\eta)] \\
\Delta C_{44} &= -(G_0^2/9) \frac{\partial n_0}{\partial E_F} \\
\Delta C_{456} &= (G_0^3/27) \frac{\partial^2 n_0}{\partial E_F^2}
\end{align*}
\]

where \( G_0 \) is the deformation potential.

Thus, combining Eqs. (5), (6), and (7), we get

\[
\begin{align*}
\Delta C_{44} &= \left(\frac{G_0^2}{9d_x d_y d_z k_B T}\right) \sum_{n_{\text{max}}} \sum_{n_{\text{max}}}
\quad\times\left[A(1 - A^2 + 3A \cos \lambda + 3A^2 \cos^2 \lambda)\right] \\
\Delta C_{456} &= \left(\frac{G_0^3}{27d_x d_y d_z k_B T}\right)
\quad\times\sum_{n_{\text{max}}} \sum_{n_{\text{max}}}
\quad\times\left[A(1 - A^2 + 2A \cos \lambda)^{-2}
\quad\times\left(1 - A^2 + 3A \cos \lambda + 3A^2 \cos^2 \lambda\right)
\quad-\quad4A(1 + A^2 - 2A \cos \lambda)\right] \\
&\quad\times\left(-2A + 3 \cos \lambda + 6A \cos^2 \lambda)\right]
\end{align*}
\]
scattering mechanisms. The magnitude of the thermoelectric power \( T_0 \) in the present case can be written as

\[
T_0 = \left( \frac{1}{eE_{T_0}} \right) \int_{-\infty}^{\infty} (E - E_f)R(E) \left[ -\frac{\partial f}{\partial E} \right] dE \tag{20}
\]

where \( R(E) \) is the total number of states and \( f \) is the distribution function. Following Tsidilkovski, Eq. (20) can be written as

\[
T_0 = (\pi^2 K_B^2 T/3e n_0) \frac{\partial n_0}{\partial E_f} \tag{21}
\]

Using Eqs. (6), (7), and (20), we get

\[
\Delta C_{44} = - \left( G_0^2 e T_0 n_0 / 3\pi^2 K_B^2 T^2 \right) \tag{22}
\]

\[
\Delta C_{456} = \left( n_0 e G_0^2 T_0 / 3\pi^2 K_B^2 T \right) \left( 1 + \frac{n_0}{T_0} \frac{\partial T_0}{\partial n_0} \right) \tag{23}
\]

Thus, we can summarize the whole mathematical background in the following way. From the expression of carrier statistics in strained layer quantum dot superlattices of non-parabolic semiconductors with graded structure by incorporating all the system parameters, we have formulated the generalized expressions for \( \Delta C_{44} \) and \( \Delta C_{456} \) respectively. The expressions of \( \Delta C_{44} \) and \( \Delta C_{456} \) for quantum dots of the constituent materials form a special case of our analysis where \( E' \) is the only dispersion relation dependent quantity. From our generalized formulation, we have obtained the well-known expressions of \( n_0, \Delta C_{44} \), and \( \Delta C_{456} \) in bulk specimens of wide gap stress free degenerate materials. This fact is the indirect mathematical test of our generalized analysis. In addition, we have suggested an experimental method for determining the \( \Delta C_{44} \) and \( \Delta C_{456} \) for materials having arbitrary dispersion laws.

3. RESULTS AND DISCUSSION

Using the Eqs. (5), (8), and (9) for the strained layer InAs/GaSb quantum dot SL together with the parameters\(^{18}\)

\[
m_0^* = 0.023 m_0, \quad E_{g1} = 0.41 \text{ eV}, \quad \epsilon_1 = 10 \times 10^{-11} \text{ eV m},
\]

\[
g_1 = 2 \text{ eV}, \quad c_1 = 20 \text{ eV}, \quad (S_{44})_1 = 0.3 \times 10^{-3} \text{ KBar}^{-1},
\]

\[
d_{01} = -4.4 \text{ eV}, \quad (a_{01} + c_1) = 8 \text{ eV}, \quad b_{01} = -1.8 \text{ eV},
\]

\[
(S_{11})_1 = 0.09 \times 10^{-3} \text{ KBar}^{-1},
\]

\[
(S_{12})_1 = 0.48 \times 10^{-3} \text{ KBar}^{-1}, \quad \sigma = 4 \text{ KBar}
\]

for InAs and

\[
m_0^* = 0.048 m_0, \quad E_{g2} = 0.81 \text{ eV}, \quad \epsilon_2 = 14 \times 10^{-11} \text{ eV m},
\]

\[
g_2 = 4 \text{ eV}, \quad c_2 = 30 \text{ eV}, \quad d_{02} = -6 \text{ eV},
\]

\[
(S_{44})_2 = 0.6 \times 10^{-3} \text{ KBar}^{-1}, \quad (a_{02} + c_2) = 10 \text{ eV},
\]

\[
b_{02} = -4 \text{ eV}, \quad (S_{11})_2 = 0.71 \times 10^{-3} \text{ KBar}^{-1},
\]

\[
(S_{12})_2 = 0.46 \times 10^{-3} \text{ KBar}^{-1}
\]

for GaSb

\[
\Delta_0 = 5 \text{ Å}, \quad L_0 = 120 \text{ Å}, \quad L_1 = 60 \text{ Å}, \quad T_B = 9.4 \text{ K},
\]

\[
d_s = d_t = 60 \text{ Å} \quad \text{and} \quad T = 4.2 \text{ K}
\]

we have plotted in Figure 1 the normalized \( \Delta C_{44} \) and \( \Delta C_{456} \) versus \( n_0 \) in stressed quantum dot InAs/GaSb SL with \( \Delta \neq 0 \) as shown by curves a and b. The curves c and d of Figure 1 exhibit the same dependence in absence of stress. The curves e, f, g, and h exhibit the dependence of \( \Delta C_{44} \) and \( \Delta C_{456} \) on \( n_0 \) for quantum dots of InAs/GaSb respectively.

![Fig. 1](image)

**Fig. 1.** Plots of the normalized \( \Delta C_{44} \) and \( \Delta C_{456} \) versus \( n_0 \) in stressed quantum dot InAs/GaSb SL with \( \Delta \neq 0 \) as shown by curves a and b. The curves c and d of Figure 1 exhibit the same dependence in absence of stress. The curves e, f, g, and h show the dependences of \( \Delta C_{44} \) and \( \Delta C_{456} \) on \( n_0 \) for quantum dots of InAs and GaSb respectively. It appears from Figure 1 that both \( \Delta C_{44} \) and \( \Delta C_{456} \) increase with increasing \( n_0 \) in different oscillatory manners for all types of materials as considered here. The natures of oscillations are totally determined by the respective dispersion relation. The combined influences of the strain and the finite width of the interface enhance the numerical values of both \( \Delta C_{44} \) and \( \Delta C_{456} \) respectively. The numerical values of \( \Delta C_{44} \) and \( \Delta C_{456} \) are greatest for the present system and the least for the quantum dot of GaSb respectively.

It may be noted that our experimental suggestions for the determination of \( \Delta C_{44} \) and \( \Delta C_{456} \) are valid for materials having arbitrary dispersion relations. Since the experimental curve of \( n_0 \) versus \( T_0 \) is not available in the literature to the best our knowledge for the present system, we cannot compare our theoretical formulation with the proposed experiment although the generalized analysis as presented in this context would be useful and the Eqs. (22) and (23) are important in probing the band structures of different materials.

We wish to note in view of large changes of the elastic constants with \( n_0 \), detailed experimental work on second- and third-order elastic constants as functions of \( n_0 \) would be
interesting for the present class of quantum confined materials. It may be suggested that the experiments on the velocity of sound involving the shear mode as function of \( n_0 \) may exhibit the carrier contribution to the elastic constants for materials having arbitrary carrier energy spectra. It is worth noting that the above statement again suggests the elasticity of sound involving the shear mode as function of energy spectral density quantity as already stated. Finally, it may be noted that the experiments on the velocity of sound in the aforementioned systems. The inclusion of these effects would increase the accuracy of the results although our suggestion for the experimental determination of \( \Delta C_{44} \) and \( \Delta C_{456} \) is independent of incorporating the said effects and the qualitative features of \( \Delta C_{44} \) and \( \Delta C_{456} \) would not change in the presence of the aforementioned effects. The formulation as presented in this paper is general and \( E' \) is the only band structure dependent quantity as already stated. Finally, it may be noted that the basic aim of the present paper is not solely to investigate that \( \Delta C_{44} \) and \( \Delta C_{456} \) but also to suggest the experimental determination of them for materials having arbitrary dispersion laws which, in turn, is again in dimension independent.

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References and Notes