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Influence of quantum confinement on the carrier contribution to the elastic constants in quantum confined heavily doped non-linear optical and optoelectronic materials: simplified theory and the suggestion for experimental determination

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Abstract. In this paper we study the carrier contribution to elastic constants in quantum confined heavily doped non-linear optical compounds on the basis of a newly formulated electron dispersion law taking into account the anisotropies of the effective electron masses and spin orbit splitting constants together with the proper inclusion of the crystal field splitting in the Hamiltonian within the framework of k.p formalism. All the results of heavily doped three, and two models of Kane for heavily doped III-V materials form special cases of our generalized analysis. It has been found, taking different heavily doped quantum confined materials that, the carrier contribution to the elastic constants increases with increase in electron statistics and decrease in film thickness in ladder like manners for all types of quantum confinements with different numerical values which are totally dependent on the energy band constants. The said contribution is greatest in quantum dots and least in quantum wells together with the fact the heavy doping enhances the said contributions for all types of quantum confined materials. We have suggested an experimental method of determining the carrier contribution to the elastic constants in nanostructured materials having arbitrary band structures.

1. Introduction

In recent years with the advent of fine line lithography, organometallic chemical vapor deposition, molecular beam epitaxy and other experimental techniques low dimensional structures having quantum confinement in one, two and three dimensions such as quantum wells(QWs), quantum well wires(QWWs), and quantum dots(QDs) have in the last few years attracted much attention for not only their potential in uncovering new phenomena in nanoscience but also for their extremely exciting device applications in nanotechnology in general. Although extensive works have already been done, nevertheless it appears from the literature that the carrier contribution to elastic constants in heavily doped quantum confined non-linear optical and optoelectronic materials has yet to be studied in details.

In this context, we wish to note that the theory for determining the carrier contribution to the elastic constants in ultra thin films of p-type Si already exists [1]. It has been shown that the carrier contribution to the second and the third order elastic constants depends on the density-of-states function [2]. Sreedhar and Gupta [2] formulated the same for non-parabolic materials whose energy band structures are defined

by the two-band model of Kane. It has therefore different values in various materials and varies with the electron concentration, with the thickness of ultra thin films and with the temperature for semiconductors and their heterostructures having various carrier energy spectra. The nature of these variations has been investigated by Ghatak and co-workers [3-4] and a few others [5]. Some of the significant features, which have emerged from these studies, are:

(a) The carrier contribution of the elastic constants increases monotonically with electron concentrations in bulk materials having different band structures.
(b) The nature of the variations is significantly affected by the presence of the band non-parabolicity.
(c) The said contribution has relatively large values in ultra thin films.

The above characteristics are considered as theoretical predictions, and no experimental results are available to the knowledge of the authors in support of these predictions. Therefore, it would be of much interest to study the carrier contribution to the elastic constants for the present generalized systems and to suggest an experimental method of determining them in this context for quantum confined heavily doped materials having arbitrary band structures.

2. Theoretical background

The dispersion relation of the conduction electrons in bulk specimens of non-linear optical materials within the framework of **k.p** formalism can be expressed as [6]

$$\gamma(E) = f_1(E)k_x^2 + f_2(E)k_z^2 \tag{1}$$

where the notations are defined in the above reference.

The Gaussian distribution of $F(V)$ of the impurity potential is given by

$$F(V) = (\pi\eta^2)^{-1/2}\exp(-V^2/\eta^2) \tag{2}$$

where η is the impurity screening potential.

Combining equations (1) and (2), the dispersion relation of the conduction electrons in bulk specimens of heavily doped non-linear optical material can be written, after tedious mathematics, as

$$\frac{k_z^2}{Q_1(E,\eta)} + \frac{k_s^2}{Q_2(E,\eta)} = 1 \tag{3}$$

$$Q_1(E,\eta) = \frac{2m_{\parallel}^*}{\hbar^2}\left[X(E,\eta) + iY(E,\eta)\right],\ Q_2(E,\eta) = \frac{2m_{\perp}^*}{\hbar^2}\left[\frac{X(E,\eta) + iY(E,\eta)}{\left(\frac{b_{\parallel}}{b_{\perp}}\frac{c_{\parallel}}{c_{\perp}}\right) + V(E,\eta) + iW(E,\eta)}\right],$$

where the notations are defined in [6].

The use of equation (3) leads to the expressions of the carrier statistics in QWs, QWWs and QDs of heavily doped non-linear optical materials respectively as

$$n_0 = (2\pi)^{-1}C_1\left[T_1(E_F,\eta) + T_2(E_F,\eta)\right] \tag{4}$$

$$n_0 = \frac{2}{\pi}C_2\left[T_3(E_F,\eta) + T_4(E_F,\eta)\right] \tag{5}$$

and

$$n_0 = \left(\frac{2}{d_x d_y d_z}\right)C_3\left[F_{-1}(\eta_n)\right] \tag{6}$$

where $C_3 = \sum_{n_x=1}^{n_{x\max}} \sum_{n_y=1}^{n_{y\max}} \sum_{n_z=1}^{n_{z\max}}$, $\eta_n = \left[E_F - \omega\right]/k_B T$, ω can be derived from the equation $\frac{\left(n_z\pi/d_z\right)^2}{Q_1\left(\omega,\eta\right)} + \frac{\left(n_x\pi/d_x\right)^2 + \left(n_y\pi/d_y\right)^2}{Q_2\left(\omega,\eta\right)} = 1$, $F_j\left(\eta\right)$ is the one parameter Fermi-Dirac integral of order j and the other notations have already been defined in [6].

The carrier contribution to the second and third order elastic constants can in general be written as [2]

$$\Delta C_{44} = \frac{G_0^2}{9}\frac{\partial n_0}{\partial E_F} \tag{7}$$

and

$$\Delta C_{456} = -\frac{G_0^3}{27}\frac{\partial^2 n_0}{\partial E_F^2} \tag{8}$$

where G_0 is the deformation potential constant.

Thus using the appropriate equations, we can determine the carrier contributions to the elastic constants for heavily doped quantum confined nonlinear optical and optoelectronic materials.

Under the conditions $\Delta_{\square} = \Delta_{\perp} = \Delta$ (the isotropic spin orbiting constant), $\delta = 0$, $m_{\square}^* = m_{\perp}^* = m^*$ (the isotropic effective electron mass at the edge of the conduction band), the equation (1) assumes the form

$$\frac{\hbar^2 k^2}{2m^*} = \gamma(E), \quad \gamma(E) \equiv \frac{E\left(E+E_g\right)\left(E+E_g+\Delta\right)\left(E_g+\frac{1}{3}\Delta\right)}{E_g\left(E_g+\Delta\right)\left(E+E_g+\frac{2}{3}\Delta\right)} \tag{9}$$

The equation (9) describes the dispersion relation of the conduction electrons in III-V, ternary, and quaternary materials and is well known in the literature as the three-band model of Kane, which should in turn be used as such for studying the electronic properties of such compounds where the spin orbit splitting constant is of the order of band gap.

2.1 Suggestion for the experimental determination of the carrier contribution to the elastic constants in quantum confined materials having arbitrary band structures

It is well known that in the presence of a classically large magnetic field, the thermoelectric power is independent of scattering mechanisms. The magnitude of the thermoelectric power $\left(T_0\right)$ in the present case can be written as [7]

$$T_0 = \left(\frac{1}{eTn_0}\right)\int_{-\infty}^{\infty}(E-E_F)R(E)\left[-\frac{\partial f}{\partial E}\right]dE \tag{10}$$

where $R(E)$ is the total number of states and f is the distribution function. The equation (10) can be written as

$$T_0 = \left(\pi^2 k_B^2 T/3en_0\right)\left(\frac{\partial n_0}{\partial E_F}\right) \tag{11}$$

Using Equations (7), (8) and (11), we get

$$\Delta C_{44} = -\left(G_0^2 e T_0 n_0/3\pi^2 k_B^2 T^2\right) \tag{12}$$

$$\Delta C_{456} = \left(n_0 e G_0^3 T_0^2/3\pi^4 k_B^3 T\right)\left(1+\frac{n_0}{T_0}\frac{\partial T_0}{\partial n_0}\right) \tag{13}$$

Therefore, we can determine ΔC_{44} and ΔC_{456} by knowing the experimental values of T_0.

Thus, we can summarize the whole mathematical background in the following way. From the expression of carrier statistics in quantum confined heavily doped nonlinear optical materials by incorporating all the system parameters, we have formulated the generalized expressions for ΔC_{44} and ΔC_{456} respectively. The expressions of ΔC_{44} and ΔC_{456} for quantum confined heavily doped optoelectronic materials form a special case of our analysis. From our generalized formulation, the well-known expressions of n_0, ΔC_{44} and ΔC_{456} in bulk specimens of wide gap materials can easily be derived which is an indirect mathematical test of our present analysis. In addition, we have suggested an experimental method for determining the ΔC_{44} and ΔC_{456} for quantum confined materials having arbitrary dispersion laws.

3. Results and discussion

Using the appropriate equations together with the parameters as given in [6] we have plotted the normalized ΔC_{44} and normalized ΔC_{456}, as functions of inverse film thickness for QWs, QWWs and QDs of n-$CdGeAs_2$ as shown by curves e and f, d and c and b and a respectively in Figure 1. In Figure 2, we have plotted all the cases of Figure 1 for quantum confined $Hg_{1-x}Cd_xTe$.

It appears from the figures that the normalized ΔC_{44} and ΔC_{456} for quantum confined materials are oscillatory functions of $1/d_x$. The oscillatory dependence is due to the crossing over of the Fermi level by the size quantized levels. For each coincidence of a size quantized level with the Fermi level, there would be a discontinuity in the DOS function resulting in a peak of oscillations in different manners, which are totally band structure dependent. The normalized ΔC_{44} and ΔC_{456} in QDs are larger than that of the corresponding QWs, which is the direct signature of the special physical characteristics of the quantum confined systems in general.

Our experimental suggestions for the determination of ΔC_{44} and ΔC_{456} are valid for materials having arbitrary dispersion relations. Since the experimental curves of n_0 versus T_0 are not available in the literature to the best our knowledge for the present generalized systems, we cannot compare our theoretical formulation with the proposed experiment although the generalized analysis as presented in this context can be checked when the experimental investigations of T_0 would appear in the literature for our generalized systems.

We wish to note that in view of large changes of the elastic constants with d_x, detailed experimental work on second- and third- order elastic constants as functions of d_x would be interesting for the present systems. It may be suggested that the experiments on the velocity of sound involving the shear mode as function of film thickness 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 experimental determinations of ΔC_{44} and ΔC_{456}, beside the suggested methods of determining them as given by equation (7) and (8) respectively. It may be noted that our study covers different materials having various electronic dispersion laws and the formulations of ΔC_{44} and ΔC_{456} are based on the dispersion relations in such compounds would be useful and the equation (7) and (8) are important in probing the band structures of different materials. It is worth noting that the influence of energy band models on ΔC_{44} and ΔC_{456} in various types of materials can also be assessed from our present work.

We have not considered other types of compounds or external physical variables for numerical computations in order to keep the presentation brief. With different sets of energy band parameters, we shall get different numerical values of ΔC_{44} and ΔC_{456} although the nature of variation of the said elastic constants with respect to d_x as shown here would be similar for the other types of materials.

We must note that the study of transport phenomena and the formulation of the electronic properties of quantum confined compounds are based on the dispersion relations in such materials. The theoretical results of our paper can be used to determine the ΔC_{44} and ΔC_{456} for the constituent bulk semiconductors in the absence of size effects. Finally, it may be also noted that the objective of the present work is not solely to investigate ΔC_{44} and ΔC_{456} but also to suggest their experimental determination for the materials having arbitrary band structures which, in turn, is again dimension independent.

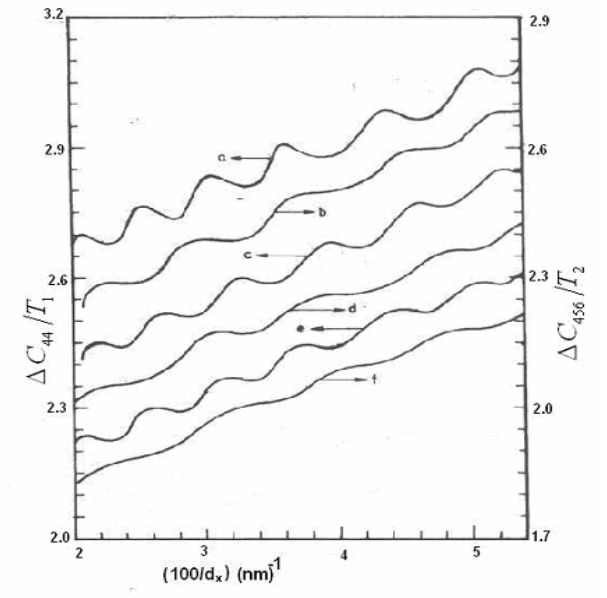

Figure 1. The curves e and f, d and c and b and a exhibit the plots of the normalized ΔC_{44} and ΔC_{456} as functions of inverse d_x for QWs, QWWs and QDs of $CdGeAs_2$ respectively.

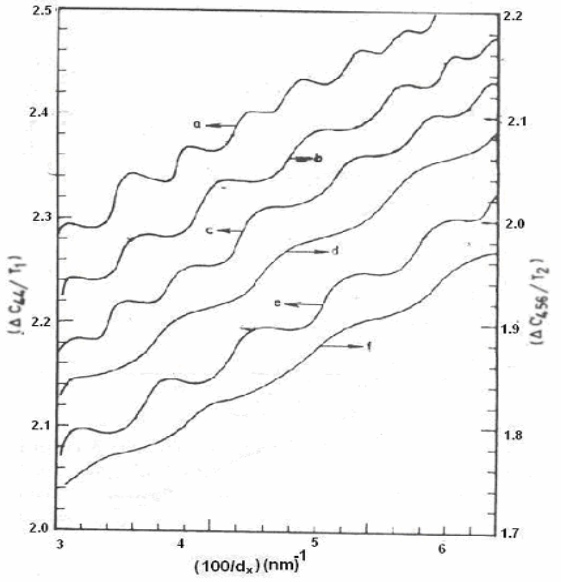

Figure 2. The plots of the normalized ΔC_{44} and ΔC_{456} for $Hg_{1-x}Cd_xTe$ as function of $1/d_x$ for all cases of Fig.1

4. References

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