

# **Influence of Quantum Confinement on the Carrier Contribution to the Elastic Constants in Nonlinear Optical and Optoelectronic Materials: Simplified Theory and Suggestion for Experimental Determination: Part - I**

K.P. GHATAK\*, S. BHATTACHARYA\*, S. SINGHA ROY\* AND L. J. SINGH\*\*

*\* Department of Electronic Science, University of Calcutta, 92,  
Acharya Prafulla Chandra Road, Kolkata – 700 009, India*

*\*\*Department of Electronics and Communication Engineering, Sikkim Manipal  
Institute of Technology, Majhitar, Rangpo, East Sikkim – 737132, India*

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An attempt is made in the first part of this paper to study the carrier contribution to elastic constants in quantum wells (QWs) and quantum well wires (QWWs) of nonlinear optical compounds on basis of a newly formulated electron energy spectrum taking into account the combined influences of the anisotropies in the effective electron mass, the spin-orbit splitting and the presence of crystal field splitting respectively. The corresponding results for quantum confined III-V, ternary and quaternary types of optoelectronic materials form a special case of our generalized analysis. The carrier contribution to the elastic constants has also been studied for QWs and QWWs of II-VI and IV-VI compounds. It has been found, taking QWs and QWWs of CdGeAs<sub>2</sub>, InAs, Hg<sub>1-x</sub>Cd<sub>x</sub>Te, In<sub>1-x</sub>Ga<sub>x</sub>As<sub>y</sub>P<sub>1-y</sub> lattice matched to InP, CdS and PbSe as examples for numerical computations that the second and third order elastic constants increase with increasing carrier degeneracy and decreasing film thickness respectively in various oscillatory manners emphasizing the influence of dimensional quantizations and the energy band constants in different cases. An experimental method of determining the said contribution in QWs and QWWs having arbitrary dispersion laws has also been suggested and the present simplified analysis is in agreement with the suggested relationship. The well-known results for wide-gap materials having nondegenerate electron concentration have also been obtained as special cases of our generalized theory under certain limiting conditions.

*Keywords:* Carrier contribution; Quantum Wells; Quantum Well Wires; second and third order elastic constants; nonlinear optical and optoelectronic materials; **k,p** theory.

## INTRODUCTION

With the advent of fine lithographical methods, molecular beam epitaxy, organometallic vapor phase epitaxy and other experimental techniques, low dimensional structures having quantum confinement in one, two and three dimensions such as QWs, QWWs and quantum dots have in the last few years attracted much attention not only for their potential in uncovering new phenomena in nonlinear optical science and technology but also for their interesting device applications [1]. In QWs, the restriction of the motion of the carriers in the direction normal to the film leading to the quantum size effect allowing two-dimensional (2D) carrier transport parallel to the surface of the film. Heterostructures based on various materials are being currently studied because of the enhancement of carrier mobility [2] and such 2D systems find extensive applications in quantum well lasers, field effect transistors, high-speed digital networks, optical modulators and also in other quantum-effect devices [3]. In QWWs, the carriers are quantized in two transverse directions, and only one-dimensional motion of the carriers is being allowed. The quantum devices like QWW waveguides [4] and QWW transistors [5] have also been fabricated. The optoelectronic transport in QWWs may be studied by utilizing the similarities with an optical and microwave wave-guides. Though considerable work has been done, nevertheless it appears from the literature that the carrier contribution to the elastic constants in QWs and QWWs of nonlinear optical, III-V, ternary, quaternary, II-VI and IV-VI materials have yet to be theoretically worked out by considering the various significant features of the respective energy band spectra within the framework of **k.p** formalism.

In this context, we wish to note that the theory for determining the carrier contribution to the elastic constants in ultrathin films of p-type Si already exists [6]. It has shown that the carrier contribution to the second and third order elastic constants depends on the density-of-states function [6]. Sreedhar and Gupta [7] formulated the same for small-gap optoelectronic 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 electron concentration, with doping, with the magnitude of reciprocal quantizing magnetic field, and with the superlattices period as in superlattices of small-gap materials having various carrier energy spectra. The nature of these variations has been investigated by Ghatak and co-workers [6, 8, 9] and few others [7, 10, 11]. Some of the significant features, which have emerged from these studies, are:

- a) The carrier contribution to the elastic constants increases monotonically with electron concentration in bulk materials.
- b) The nature of the variations is significantly affected by the band non-parabolicity.
- c) The said contribution has significantly different values in superlattices.

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 a much interest to study the carrier contribution to the elastic constants for the present generalized QWs and QWWs of nonlinear optical materials and III-V, ternary, quaternary, II-VI and IV-VI types of optoelectronic compounds since the density-of-states function for the aforementioned systems increase much more rapidly with carrier energy in various oscillatory manners than that of the monotonic variation for the bulk specimens of the constituent materials.

In this context, we wish to note that the nonlinear optical compounds are being increasing used in nonlinear optics and light emitting devices [12]. Rowe and Shay [13] have demonstrated that the quasi-cubic model can be used to explain the observed splitting and symmetry properties of the conduction and valence bands at the zone center in  $\mathbf{k}$ -space of such compounds. The s-like conduction band is singly degenerate and the p-like valence band is triply degenerate. Incorporating the anisotropic crystal potential to the Hamiltonian and the special features of the nonlinear optical compounds, Kildal [14] proposed the energy spectrum of the conduction electrons under the assumptions of the isotropic momentum matrix element and the isotropic spin-orbit splitting respectively although the anisotropies in the aforementioned band parameters are the significant physical features of the said materials [12]. In this paper, in Section A, we shall study the carrier contribution to the elastic constants in QWs and QWWs of nonlinear optical compounds by including the combined influence of the anisotropies of the said energy band constants together with the inclusion of the crystal field splitting respectively.

It is worth remarking that III-V compounds are being extensively used in integrated optoelectronics [15], photo refractive materials [16], distributed feedback lasers [17] and infrared photo detectors [18]. The three-band model of Kane [19] is valid for III-V, ternary and quaternary types of optoelectronic materials but must be used as such for studying the optoelectronic properties of n-InAs where the spin orbit splitting constant is of the order of band gap.

We shall study the carrier contribution to the elastic constants in QWs and QWWs of III-V compounds in Section B of this paper. We shall show that the results for III-V quantum confined systems form special cases of our generalized analysis, as presented in Section A, under certain limiting conditions. In section-B, we shall also consider the simplified cases of the two-band model of Kane and that of wide gap materials. It may be noted that the two-band model of Kane and the parabolic energy bands can be derived from the three-band model of Kane under certain limiting conditions. For the purpose of numerical computations, we shall take  $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$  and  $\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$  lattice matched to InP as examples of ternary and quaternary compounds. In this context, we wish to note that the ternary alloy  $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$  is a classic narrow-gap compound and is an important of optoelectronic material. Its band gap can be varied to cover the spectral range from  $0.8\mu\text{m}$  to over  $30\mu\text{m}$  by adjusting the alloy composition [20].  $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$  finds extensive use in infrared detector materials and photovoltaic detector arrays [21] in the  $8\text{-}12\mu\text{m}$  wave bands. The above uses have spurred an  $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$  technology for the production of high mobility single crystals with specially prepared surfaces and the same material is ideally suitable for narrow-subband physics because the relevant material constants are within the easy experimental reach [22]. Moreover, the quaternary alloy,  $\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$ , lattice matched to InP, also finds extensive applications in the fabrication of photodetectors [23], heterjunction lasers [24], light-emitting diodes [25], avalanche photodiodes [26], field effect transistors, detectors and other devices. In addition, new type of investigated optical devices such as switches, modulators, solar cells and filters are made from the quaternary systems [27].

The II-VI compounds are suitable for optoelectronic communication [28], advanced microwave devices [18], light emitting diodes [29] and infrared detectors [30,31]. The carriers of the II-VI materials are defined by the Hopfield model [32] where the splitting of the two-spin states by the spin-orbit coupling and the crystalline field has been taken into account to describe the carrier energy spectra of these materials. In Section C, we shall study the carrier contribution to the elastic constants in QWs and QWWs of II-VI type of optoelectronic compounds on basis of the Hopfield model by formulating the appropriate carrier statistics.

The IV-VI materials find extensive applications in infrared detectors, thermoelectric devices, superlattices and quantum confined systems [33]. The dispersion relation of the carriers of IV-VI materials has been formulated by Cohen [34] by including the band non-parabolicity and the anisotropies

of the effective-masses of the carriers respectively. In Section D, we shall study the carrier contribution to the elastic constants in QWs and QWWs in IV-VI compounds on the basis of the Cohen model. We shall show that under certain limiting conditions, all the results for all the models will be reduced to that of the relatively wide-gap materials under non degenerate electron concentration, which are well known in the literature [35]. The above statement will exhibit the indirect accuracy of our mathematical formulation. In Section E, we shall suggest an experimental method of determining the carrier contribution to the elastic constants in materials having arbitrary dispersion laws. The effects of carrier degeneracy and the nanothickness on the carrier contribution to the second and third order elastic constants in QWs and QWWs of nonlinear optical, III-V, ternary, quaternary, II-VI and IV-VI compounds have been studied respectively by taking n-CdGeAs<sub>2</sub>, InAs, Hg<sub>1-x</sub>Cd<sub>x</sub>Te, In<sub>1-x</sub>Ga<sub>x</sub>As<sub>y</sub>P<sub>1-y</sub> lattice matched to InP, CdS and PbSe as examples for numerical computations.

## THEORETICAL BACKGROUND

### A Formulations of the carrier contribution to the second and third order elastic constants in QWs and QWWs of nonlinear optical materials on basis of a newly formulated electron dispersion law

The form of the **k.p** matrix for the nonlinear optical compounds can be written as

$$H = \begin{bmatrix} H_1 & H_2 \\ H_2^+ & H_1 \end{bmatrix} \tag{1}$$

where

$$H_1 = \begin{bmatrix} E_g & P_{II}k_z & 0 & 0 \\ P_{II}k_z & -\left(\delta + \frac{1}{3}\Delta_{II}\right) & (2\Delta_{\perp}/3) & 0 \\ 0 & (2\Delta_{\perp}/3) & -\frac{2}{3}\Delta_{II} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad H_2 = \begin{bmatrix} 0 & 0 & f_{,-} & f_{,-} \\ 0 & 0 & 0 & 0 \\ -f_{,-} & 0 & 0 & 0 \\ f_{,-} & 0 & 0 & 0 \end{bmatrix}$$

in which  $E_g$  is the band gap,  $P_{\parallel}$  and  $P_{\perp}$  are the momentum matrix elements parallel and perpendicular to the direction of the  $\mathbf{c}$  axis, respectively,  $\delta$  is the crystal-field splitting constant,  $\Delta_{\parallel}$  and  $\Delta_{\perp}$  are the spin-orbit splitting parameters parallel and perpendicular to the direction of the  $\mathbf{c}$  axis, respectively,

$$\mathbf{f}_{\pm} \equiv \left( \mathbf{P}_{\perp} / \sqrt{2} \right) (\mathbf{k}_x \pm i\mathbf{k}_y) \quad \text{and } i = \sqrt{-1}.$$

Thus by diagonalizing the above matrix, the generalized electron energy spectrum in the bulk specimens of the nonlinear optical compounds can be expressed as

$$\gamma(E) = f_1(E)k_x^2 + f_2(E)k_z^2 \quad (2)$$

where

$$\gamma(E) \equiv \left\{ E(E + E_g) \left[ (E + E_g) \times (E + E_g + \Delta_{\parallel}) + \delta \left( E + E_g + \left( \frac{1}{3} \right) \Delta_{\parallel} \right) \right] + \left( \frac{2}{9} \right) \times \right.$$

$$\left. E \times (E + E_g) (\Delta_{\parallel}^2 - \Delta_{\perp}^2) \right\}, \quad k_x^2 \equiv k_x'^2 + k_x''^2$$

$$f_1(E) \equiv \left\{ \hbar^2 E_g (E_g + \Delta_{\perp}) \cdot \left[ 2m_{\perp}^* (E_g + \frac{2}{3} \Delta_{\perp}) \right]^{-1} \right\} \times \left[ \delta \left( E + E_g + \left( \frac{1}{3} \right) \Delta_{\parallel} \right) + \right.$$

$$\left. (E + E_g) \left( E + E_g + \left( \frac{2}{3} \right) \Delta_{\parallel} \right) + \left( \frac{2}{9} \right) (\Delta_{\parallel}^2 - \Delta_{\perp}^2) \right]$$

$$f_2(E) \equiv \left\{ \hbar^2 E_g (E_g + \Delta_{\parallel}) \cdot \left[ 2m_{\parallel}^* (E_g + \left( \frac{2}{3} \right) \Delta_{\parallel}) \right]^{-1} \right\} \times$$

$$\left[ (E + E_g) \left( E + E_g + \left( \frac{2}{3} \right) \Delta_{\parallel} \right) \right]$$

in which  $E$  is the electron energy as measured from the edge of the conduction band in the vertically upward direction,  $\hbar = h/2\pi$ ,  $h$  is the Planck constant, and  $m_{\parallel}^*$  and  $m_{\perp}^*$  are the effective masses of the electron at the edge of the conduction band parallel and perpendicular to the direction of the  $\mathbf{c}$  axis, respectively.

The dispersion relation of the conduction electrons in QWs and QWWs of nonlinear optical compounds can, respectively, be written as

$$\gamma(E)=f_1(E)k_s^2 + f_2(E). (\pi n_z/d_z)^2 \tag{3}$$

and

$$\gamma(E)=f_1(E)k_x^2 + f_1(E).( \pi.n_y/d_y)^2 + f_2(E).( \pi.n_z/d_z)^2 \tag{4}$$

where  $n_y (=1,2,3,\dots)$  and  $n_z (=1,2,3,\dots)$  are the size quantum numbers along y and z directions respectively and  $d_y$  and  $d_z$  are the corresponding nanothicknesses along y- and z- directions respectively. The carrier statistics, in QWs and QWWs can, respectively, be expressed as

$$n_0 = (2\pi)^{-1}C_1[L_1(E_F)+L_2(E_F)] \tag{5}$$

and

$$n_0 = (2/\pi)C_2[L_3(E_F)+L_4(E_F)] \tag{6}$$

where,  $C_1 \equiv \sum_{n_z=1}^{n_z \max}$ ,  $L_1(E_F) \equiv [[\gamma(E_F)-f_2(E_F).( \pi n_z/d_z)^2]/f_1(E_F)]$ ,

$$L_2(E_F) \equiv C_3 k_1, \quad C_3 \equiv \sum_{r=1}^s,$$

$$k_1 \equiv (k_B T)^{2r} (1 - 2^{1-2r}) \zeta(2r) \frac{\partial^{2r}}{\partial E_F^{2r}} [L_1(E_F)]$$

$k_B$  is the Boltzmann constant, T is the temperature,  $\zeta(2r)$  is the Zeta function of order 2r,  $L_3(E_F) \equiv [[\gamma(E_F)-f_1(E_F).( \pi.n_y/d_y)^2$

$$-f_2(E_F).( \pi.n_z/d_z)^2] \{f_1(E_F)\}^{-1}]^{1/2}, L_4(E_F) \equiv C_3 k_3$$

$$C_2 \equiv \sum_{n_y=1}^{n_y \max} \sum_{n_z=1}^{n_z \max}$$

and  $E_F$  is the corresponding Fermi energy. The carrier contribution to the second and the third order elastic constants can, in general, be written as [6-7]

$$\Delta C_{44} = \left( -G_o^2 / 9 d_y^{g_1} d_z^{g_2} \right) \left( \partial n_o / \partial E_F \right) \tag{7}$$

and

$$\Delta C_{456} = \left( -G_o / 9 \right) \frac{\partial}{\partial E_F} (\Delta C_{44}) \tag{8}$$

where  $G_o$  is the deformation potential constant,  $g_1 = 0$  and  $g_2 = 1$  for QWs and  $g_1 = g_2 = 1$  for QWWs respectively. We can now combine the Equations (5), (6), (7) and (8) to get the respective expressions of  $\Delta C_{44}$  and  $\Delta C_{456}$  in QWs and QWWs of nonlinear optical compounds as

$$\Delta C_{44} = \left(-G_o^2/9d_y^{g_1} d_z^{g_2}\right)(2\pi)^{-1} C_1 \left[L_1'(E_F) + L_2'(E_F)\right] \quad (9)$$

$$\Delta C_{456} = \left(G_o^3/27d_y^{g_1} d_z^{g_2}\right)(2\pi)^{-1} C_1 \left[L_1''(E_F) + L_2''(E_F)\right] \quad (10)$$

and

$$\Delta C_{44} = \left(-G_o^2/9d_y^{g_1} d_z^{g_2}\right)(2/\pi) C_2 \left(L_3'(E_F) + L_4'(E_F)\right) \quad (11)$$

$$\Delta C_{456} = \left(G_o^3/27d_y^{g_1} d_z^{g_2}\right)(2/\pi) C_2 \left(L_3''(E_F) + L_4''(E_F)\right) \quad (12)$$

respectively in which the single and double primes denote the first order and the second order differentiations of the respective differentiable functions with respect to  $E_F$  respectively

## B Formulations of $\Delta C_{44}$ and $\Delta C_{456}$ in QWs and QWWs of III-V materials as special cases of Section A.

(i) Under the conditions  $\Delta_{\parallel} = \Delta_{\perp} = \Delta$  (the isotropic spin-orbit splitting constant),  $\delta = 0$  and  $m_{\parallel}^* = m_{\perp}^* = m^*$  (the isotropic effective electron mass at the edge of the conduction band), the Equation (2) assumes the form

$$\frac{\hbar^2 k^2}{2m^*} = \frac{E(E + E_g)(E + E_g + \Delta)(E_g + (2/3)\Delta)}{E_g(E_g + \Delta)(E + E_g + (2/3)\Delta)} \quad (13)$$

The above equation is the well-known three-band model of Kane [19], which is a valid model for studying the optoelectronic properties of III-V, ternary and quaternary materials. Thus the expressions of  $n_0$ ,  $\Delta C_{44}$  and  $\Delta C_{456}$

for QWs and QWWs of III-V materials can, respectively, be written from the Equations (5), (9) and (10) and the Equations (6), (11) and (12) as

$$n_0 = (m^*/\pi\hbar^2)C_1[L_5(E_F)+L_6(E_F)] \quad (14)$$

$$\Delta C_{44} = \left(-G_o^2/9d_y^{g_1}d_z^{g_2}\right)(m^*/\pi\hbar^2)C_1(L_5'(E_F)+L_6'(E_F)) \quad (15)$$

$$\Delta C_{156} = \left(G_o^3/27d_y^{g_1}d_z^{g_2}\right)(m^*/\pi\hbar^2)C_1(L_5''(E_F)+L_6''(E_F)) \quad (16)$$

and

$$n_0 = \left(4\sqrt{2m^*}/h\right)C_2[L_7(E_F)+L_8(E_F)] \quad (17)$$

$$\Delta C_{44} = \left(-G_o^2/9d_y^{g_1}d_z^{g_2}\right)\left(4\sqrt{2m^*}/h\right)C_2[L_7'(E_F)+L_8'(E_F)] \quad (18)$$

$$\Delta C_{156} = \left(G_o^3/27d_y^{g_1}d_z^{g_2}\right)\left(4\sqrt{2m^*}/h\right)C_2[L_7''(E_F)+L_8''(E_F)] \quad (19)$$

where

$$L_5(E_F) \equiv \left[ \frac{E_F(E_F+E_g)(E_F+E_g+\Delta)(E_g+2/3\Delta)}{E_g(E_g+\Delta)(E_F+E_g+2/3\Delta)} - \left( \frac{\hbar^2\pi^2}{2m^*} \right) \left( \frac{n_z}{d_z} \right)^2 \right], L_6(E_F) \equiv C_3k_5,$$

$$L_7(E_F) \equiv \left[ L_5(E_F) - \left( \frac{\hbar^2\pi^2}{2m^*} \right) \left( \frac{n_y}{d_y} \right)^2 \right]^{1/2} \quad \text{and} \quad L_8(E_F) \equiv C_3k_7$$

(ii) Under the conditions  $\Delta \gg E_g$  or  $\Delta \ll E_g$ , the Equation (13) gets simplified as

$$E(1 + \alpha E) = \hbar^2 k^2 / 2m^*, \quad \alpha \equiv 1/E_g \quad (20)$$

which is known as the simplified two-band model of Kane and it is often used to study the optoelectronic properties of III-V materials excluding n-InAs [19]. Thus, under these inequalities, the Equations (14) to (19) get simplified as

$$n_0 = (m^*/\pi \cdot \hbar^2) C_1 [L_9(E_F) + L_{10}(E_F)] \quad (21)$$

$$\Delta C'_{41} = \left( -G_o^2 / 9 d_y^{g_1} d_z^{g_2} \right) \left( m^* / \pi \cdot \hbar^2 \right) C_1' \left( L'_{10}(E_F) + L'_{10}(E_F) \right) \quad (22)$$

$$\Delta C_{456} = \left( G_o^3 / 27 d_y^{g_1} d_z^{g_2} \right) \left( m^* / \pi \cdot \hbar^2 \right) C_1 \left( L_9''(E_F) + L_{10}''(E_F) \right) \quad (23)$$

$$n_0 = \left( 4\sqrt{2m^*} / h \right) \cdot C_2 [L_{11}(E_F) + L_{12}(E_F)] \quad (24)$$

$$\Delta C_{44} = \left( -G_o^2 / 9 d_y^{g_1} d_z^{g_2} \right) \left( 4\sqrt{2m^*} / h \right) C_2 [L'_{11}(E_F) + L'_{12}(E_F)] \quad (25)$$

and

$$\Delta C'_{450} = \left( G_o^3 / 27 d_y^{g_1} d_z^{g_2} \right) \left( 4\sqrt{2m^*} / h \right) C_2 [L''_{11}(E_F) + L''_{12}(E_F)] \quad (26)$$

where

$$L_9(E_F) \equiv \left[ E_F (1 + \alpha \cdot E_F) - \left( \hbar^2 \pi^2 / 2m^* \right) \left( \frac{n_z}{d_z} \right)^2 \right],$$

$$L_{10}(E_F) \equiv C_3 k_0 \cdot L_{11}(E_F) \equiv \left[ L_0(E_F) - \left( \hbar^2 \pi^2 / 2m^* \right) \left( \frac{n_y}{d_y} \right)^2 \right]^{1/2}$$

$$\text{and } L_{12}(E_F) \equiv C_3 k_{11}$$

(iii) For relatively wide-gap compounds  $E_g \rightarrow \infty$  and the expressions of  $n_0$ ,  $\Delta C_{44}$  and  $\Delta C_{456}$  for QWs and QWWs of wide-gap materials assume the forms as

$$n_0 = \left( \frac{m^* k_B T}{\pi \hbar^2} \right) \times C_1 [F_0(\eta_1)] \tag{27}$$

$$\Delta C_{44} = \left( -G_o^2 / 9 d_y^{g_1} d_z^{g_2} \right) \times \left( \frac{m^*}{\pi \hbar^2} \right) C_1 [F_{-1}(\eta_1)] \tag{28}$$

$$\Delta C_{456} = \left( G_o^3 / 27 d_y^{g_1} d_z^{g_2} \right) \times \left( \frac{m^*}{\pi \hbar^2 k_B T} \right) C_1 [F_{-2}(\eta_1)] \tag{29}$$

and

$$n_0 = \frac{2}{h} \sqrt{2\pi m^* k_B T} \cdot C_2 [F_{-1/2}(\eta_2)] \tag{30}$$

$$\Delta C_{44} = \left( -G_o^2 / 9 d_y^{g_1} d_z^{g_2} \right) \frac{2}{h} \sqrt{2\pi m^* / k_B T} \cdot C_2 [F_{-3/2}(\eta_2)] \tag{31}$$

$$\Delta C_{456} = \left( G_o^3 / 27 d_y^{g_1} d_z^{g_2} k_B T \right) \frac{2}{h} \sqrt{2\pi m^* / k_B T} \cdot C_2 [F_{-5/2}(\eta_2)] \tag{32}$$

where

$$\eta_1 \equiv \left[ E_F - \left( \frac{\hbar^2}{2m^*} \right) (\pi n_z / d_z)^2 \right] / k_B T, \quad \eta_2 \equiv \left[ \eta_1 - \left( \frac{\hbar^2 \pi^2}{2m^* k_B T} \right) (n_y / d_y)^2 \right]$$

and  $F_t(\eta)$  is the one parameter Fermi-Dirac integral of order  $t$  [35] which can be defined as

$$F_1(\eta) = (\Gamma(t+1))^{-1} \int_0^{\infty} x^t [1 + \exp(x - \eta)]^{-1} dx \quad \text{for } t > -1 \quad (33)$$

or for all  $t$ , analytically continued as a complex contour integral around the negative  $x$  axis as

$$F_1(\eta) = (\Gamma(-t)/2\pi\sqrt{-1}) \int_{\infty}^0 x^t [1 + \exp(-x - \eta)]^{-1} dx \quad (34)$$

(iv) For bulk specimens of wide-gap materials, the expressions of the carrier concentration,  $\Delta C_{44}$  and  $\Delta C_{456}$  can, respectively be written, from Equations (27) to (32) after converting the respective summation to the respective integration, as

$$n_o = N_c F_{1/2}(\eta_o) \quad (35)$$

$$\Delta C'_{44} = (-G_o^2 N_c / 9k_B T) (F'_{1/2}(\eta_o)) \quad (36)$$

and

$$\Delta C'_{456} = (G_o^3 N_c / 27(k_B T)^2) (F'_{3/2}(\eta_o)) \quad (37)$$

where  $N_c \equiv 2(2\pi m^* k_B T / h^2)^{3/2}$ ,  $\eta_o \equiv E_{F_o} / k_B T$ , and  $E_{F_o}$  is the Fermi-energy as measured from the edge of the conduction band in the vertically upward direction in the absence of any quantization.

(v) Under the condition of carrier nondegeneracy,  $\eta_o < 0$  and the Equations (35) to (37) get simplified to the well-known forms as [6]

$$n_o = N_c \exp(\eta_o) \quad (38)$$

$$\Delta C'_{44} = \frac{-G_o^2 n_o}{9k_B T} \quad (39)$$

and

$$\Delta C_{456} = \frac{G_o^3 n_o}{27(k_B T)^2} \quad (40)$$

### C Formulations of $\Delta C_{44}$ and $\Delta C_{456}$ in QWs and QWWs of II - VI materials

The energy spectra of both the carriers of II-VI compounds can be expressed as [32]

$$E = Ak_s^2 + Bk_z^2 + Ck_s \quad (41)$$

where  $A \equiv \hbar^2 / 2m_{\perp}^*$ ,  $B \equiv \hbar^2 / 2m_{\parallel}^*$  and C represents the splitting of the two spin states by the spin-orbit coupling and the crystalline field respectively. The expressions of  $n_o$ ,  $\Delta C_{44}$  and  $\Delta C_{456}$  in QWs and QWWs of II-VI compounds can, respectively, be written as

$$n_o = (16.\pi.A^2)^{-1} [C_1 [L_{13}(E_F) + L_{14}(E_F)]] \quad (42)$$

$$\Delta C_{44} = \left(-G_o^2 / 9d_y^{g_1} d_z^{g_2}\right) (16.\pi.A^2)^{-1} \left(C_1 \left(L'_{13}(E_F) + L'_{14}(E_F)\right)\right) \quad (43)$$

$$\Delta C'_{456} = \left(G_o^3 / 27d_y^{g_1} d_z^{g_2}\right) (16.\pi.A^2)^{-1} \left(C_1 \left(L''_{13}(E_F) + L''_{14}(E_F)\right)\right) \quad (44)$$

and

$$n_o = (\pi)^{-1} [C_2 [L_{15}(E_F) + L_{16}(E_F)]] \quad (45)$$

$$\Delta C_{44} = \left(-G_o^2 / 9d_y^{g_1} d_z^{g_2}\right) (\pi)^{-1} \left(C_2 \left(L'_{15}(E_F) + L'_{16}(E_F)\right)\right) \quad (46)$$

$$\Delta C_{456} = \left( G_o^3 / 27 d_y^{g_1} d_z^{g_2} \right) (\pi)^{-1} \left( C_2 \left( L_{15}''(E_F) + L_{16}''(E_F) \right) \right) \quad (47)$$

where

$$L_{13}(E_F) = [2C^2 - 4.A.B.(\pi.n_z / d_z)^2 + 4AE_F \pm 2C\{C^2 - 4AB(\pi.n_z / d_z)^2 + 4AE_F\}^{1/2}], L_{14}(E_F) = C_3 k_{13},$$

$$L_{15}(E_F) = [(4A^2)^{-1}L_{13}(E_F) - (\pi.n_y / d_y)^2]^{1/2}, \text{ and } L_{16}(E_F) = C_3 k_{15}$$

Under the conditions  $A = B = \hbar^2/2m^*$  and  $C \rightarrow 0$ , the Equations (42) to (47) get simplified to the Equations (27) to (32) respectively.

#### D Formulations of $\Delta C_{44}$ and $\Delta C_{456}$ in QWs and QWWs of IV - VI materials

The electron dispersion law in IV-VI compounds can be written in accordance with Cohen [33] as

$$E(1 + \alpha.E) = p_x^2/2m_1 + p_y^2/2m_2 + p_z^2/2m_3 + \frac{\alpha.E.p_y^2}{2} \left( \frac{1}{m_2} - \frac{1}{m_2'} \right) - \frac{\alpha.p_y^4}{4m_2.m_2'} \quad (48)$$

where  $m_1$  and  $m_3$  are the band-edge effective electron masses in the transverse directions,  $m_2$  is the band-edge effective electron mass in the longitudinal direction and  $m_2'$  is the longitudinal band-edge effective mass of the holes. The carrier statistics in QWs and QWWs of IV-VI materials can, respectively, be expressed as

$$n_o = \left( g_v \sqrt{m_1 m_3} / \pi \hbar^2 \right) \sum_{n_y=1}^{n_y^{\max}} [L_{17}(E_F) + L_{18}(E_F)] \quad (49)$$

and

$$n_o = \left( 2g_v \sqrt{2m_1} / \pi \hbar \right) C_2 [L_{19}(E_F) + L_{20}(E_F)] \quad (50)$$

where

$$L_{17}(E_F) \equiv [E_F(1+\alpha.E_F) - (\hbar^2 / 2m_2).(\pi.n_y / d_y)^2 - (\alpha.E_F \hbar^2 \pi^2 / 2) (n_y / d_y)^2 \\ [(m_2)^{-1} - (m'_2)^{-1}] - (\alpha.\hbar^4 \pi^4 / 4m_2 m'_2) (n_y / d_y)^4],$$

$$L_{18}(E_F) = C_3 k_{17}, L_{19}(E_F) \equiv [L_{17}(E_F) - (\hbar^2 \pi^2 / 2m_3)(n_z / d_z)^2]^{1/2},$$

and  $L_{20}(E_F) \equiv C_3 k_{19}$

Thus using the Equations (7), (8), (49) and (50), the expressions of  $\Delta C_{44}$  and  $\Delta C_{456}$  in QWs and QWWs of IV-VI compounds can, respectively, be expressed as

$$\Delta C_{44} = \left(-G_o^2 / 9d_y^{g_1} d_z^{g_2}\right) \left(g_v \sqrt{m_1 m_3} / \pi \hbar^2\right) \sum_{n_y=1}^{n_{max}} [L'_{17}(E_F) + L'_{18}(E_F)] \tag{51}$$

$$\Delta C'_{456} = \left(G_o^3 / 27d_y^{g_1} d_z^{g_2}\right) \left(g_v \sqrt{m_1 m_3} / \pi \hbar^2\right) \sum_{n_y=1}^{n_{max}} [L''_{17}(E_F) + L''_{18}(E_F)] \tag{52}$$

and

$$\Delta C'_{44} = \left(-G_o^2 / 9d_y^{g_1} d_z^{g_2}\right) \left(2g_v \sqrt{2m_1} / \pi \hbar\right) C_2 [L'_{19}(E_F) + L'_{20}(E_F)] \tag{53}$$

$$\Delta C_{456} = \left(G_o^3 / 27d_y^{g_1} d_z^{g_2}\right) \left(2g_v \sqrt{2m_1} / \pi \hbar\right) C_2 [L''_{19}(E_F) + L''_{20}(E_F)] \tag{54}$$

Under the conditions,  $\alpha \rightarrow 0$  and  $m_1 = m_2 = m_3 = m^*$ , the Equations (49) to (54) get simplified to the Equations (27) and (32) respectively.

**E Suggestion for the experimental determination of  $\Delta C_{44}$  and  $\Delta C_{456}$  for materials having arbitrary dispersion laws**

It is well known that in the presence of a large magnetic field, the thermoelectric power is determined only by the dispersion laws [36]. The magnitude of the thermoelectric power for the present system can be written as [36]

$$L_o = \left( \frac{1}{eTn_o} \right) \int_{\epsilon_o}^{\epsilon_o} (E - E_f) R(E) \left[ - \frac{\partial f_o}{\partial E} \right] dE \quad (55)$$

where  $R(E)$  is the total number of states and  $f_o$  is the Fermi-Dirac distribution function. Following Tsidilkovski [37], the Equation (55) can be expressed as

$$L_o = \left( \pi^2 k_B T / 3en_o \right) \left( \frac{\partial n_o}{\partial E_f} \right) \quad (56)$$

Using the Equations (7), (8) and (55), we get

$$\Delta C_{44} = -G_o^2 en_o L_o / 3\pi^2 k_B T d_y^{g_1} d_z^{g_2} \quad (57)$$

$$\Delta C_{456} = \left( G_o^3 n_o / 3d_y^{g_1} d_z^{g_2} \right) \left( eL_o / \pi^2 k_B T \right)^2 \left[ 1 + \frac{n_o}{L_o} \frac{\partial L_o}{\partial n_o} \right] \quad (58)$$

Therefore, we can, experimentally, determine  $\Delta C_{44}$  and  $\Delta C_{456}$  for any degenerate material having arbitrary dispersion law by knowing the experimental  $n_o$  versus  $L_o$  curve.

Thus, we can summarize the whole theoretical background in the following way. We have formulated the expressions for the carrier statistics in QWs and QWWs of nonlinear optical compounds (on the basis of a new dispersion law), III-V, ternary, quaternary, II-VI and IV-VI types of optoelectronic materials without any approximations of the energy band constants, from which we have obtained the corresponding  $\Delta C_{44}$  and  $\Delta C_{456}$  respectively. The results of the three and the two band models of Kane have formed the special cases of our generalized analysis. Besides, under certain limiting conditions, all the models reduce to the well-known results of the  $\Delta C_{44}$  and  $\Delta C_{456}$  for bulk specimens of wide-gap materials under the condition of carrier nondegeneracy. The above statement is the indirect test of our mathematical analysis. In addition, we have suggested an experimental method of determining  $\Delta C_{44}$  and  $\Delta C_{456}$  in materials having arbitrary dispersions laws.

**RESULTS AND DISCUSSION**

Using the Equations (5), (9) and (10) together with the parameters [24]  $\Delta_{11}=0.30\text{eV}$ ,  $\Delta_{\perp}=0.36\text{eV}$ ,  $m^*_{11}=0.035m_0$ ,  $m^*_{\perp}=0.039m_0$ ,  $\delta=-0.21\text{eV}$ ,  $E_g=0.57\text{eV}$ ,  $G_o = 15\text{eV}$ ,  $d_z=20\text{nm}$  and  $T=4.2\text{K}$ , we have plotted in Figure 1 the normalized  $\Delta C_{44}$  ( $\Delta C_{44}/T_1$ ,  $T_1 = -G_o^3 n_o / 9k_B T$ ) and the normalized  $\Delta C_{456}$  ( $\Delta C_{456}/T_2$ ,  $T_2 = G_o^3 n_o / 27(k_B T)^2$ ) in QWs of CdGeAs<sub>2</sub> versus film thickness as shown by curves a and a' respectively in which the curves b and b' exhibit the same dependences for n-InAs (by using the Equations (14), (15) and (16)) in accordance with the three-band model of Kane and by taking the values of the band constants as  $\Delta=0.43\text{eV}$ ,  $m^*=0.026m_0$ ,  $G_o = 13\text{eV}$  and  $E_g=0.36\text{eV}$  at 4.2K [19]. The curves c and c' are valid for n-CdS (by using the Equations (42) to (44)) where we have used  $m^*_{11}=0.7m_0$ ,  $m^*_{\perp}=1.5m_0$ ,  $G_o = 10\text{eV}$  and  $C = \pm 1.4 \times 10^{-10}\text{eVm}$  as the experimental values of the energy band parameters of n-CdS [39]. By using the Equations (49), (51) and (52) together with the parameters  $g_v = 4$ ,  $G_o = 15\text{eV}$ ,  $m_1 = m_3 = 0.040m_0$ ,  $m_2 = 0.07m_0$ ,  $m_2' = 0.068m_0$  and  $E_g = 0.15\text{eV}$  [19], we have plotted in Figure 1, the normalized  $\Delta C_{44}$  and  $\Delta C_{456}$  as functions of film thickness in QWs of n-PbSe as shown by the curves d and d' respectively. The circular plots in Figure 1 have been obtained by using the Equations (57) and (58) together with the experimental curves of  $L_o$  versus  $n_o$  and  $d_z$  respectively for QWs of CdS [38].

Using the Equations (6), (11) and (12) together with the parameters as given above we have plotted in Figure 2 the normalized  $\Delta C_{44}$  and  $\Delta C_{456}$  in QWws of CdGeAs<sub>2</sub> versus film thickness as shown by curves a and a' respectively in which the curves b and b' exhibit the same dependences for QWws of n-InAs (by using the Equations (17), (18) and (19)) in accordance with the three-band model of Kane. The curves c and c' are valid for QWws of n-CdS where we have used the Equations (45) to (47) for plotting the normalized  $\Delta C_{44}$  and  $\Delta C_{456}$  respectively. By using the Equations (50), (53) and (54), we have plotted in Figure 2, the normalized  $\Delta C_{44}$  and  $\Delta C_{456}$  as functions of film thickness in QWws of n-PbSe as shown by the curves d and d' respectively.

Using the appropriate Equations together with the material constants [40]  $\Delta = (0.63 + 0.24x + 0.27x^2) \text{ eV}$ ,  $G_o = 15\text{eV}$ ,  $E_g = (-0.302 + 1.93x + 5.25 \times 10^{-4} T(1-2x) - 0.810x^2 + 0.832x^3)\text{eV}$ ,  $m^* = 3\hbar^2 / 4P^2$ ,  $P^2 = (\hbar^2 / 2m_o)(18 + 3x)$  and  $T = 4.2 \text{ K}$  for n-Hg<sub>1-x</sub>Cd<sub>x</sub>Te and  $E_g = (1.337 - 0.73y + 0.13y^2) \text{ eV}$ ,  $m^* = (0.080 - 0.0396y)m_o$ ,  $\Delta = (0.114 + 0.26y - 0.22y^2)\text{eV}$ ,  $G_o = 14\text{eV}$  and  $y = (0.1896 - 0.4052x)(0.1896 + 0.0123x)^{-1}$  for the energy band con-

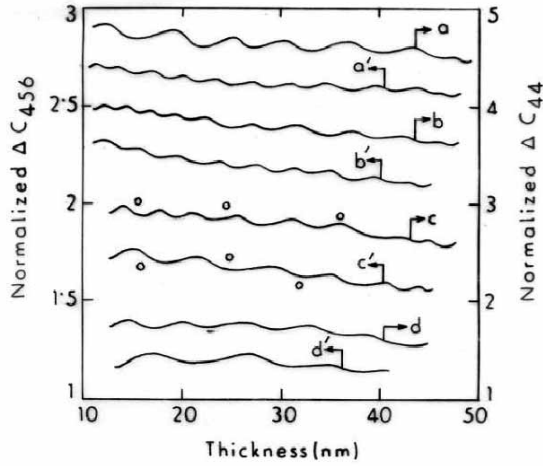


FIGURE 1

Plot of the normalized  $\Delta C_{44}$  at 4.2K as functions of film thickness in QWs of (a) CdGeAs<sub>2</sub>; (b) InAs; (c) CdS; and (d) PbSe ( $n_0 = 10^{14} \text{m}^{-2}$ ). The plots  $a'$ ,  $b'$ ,  $c'$ , and  $d'$  are valid for the normalized  $\Delta C_{456}$  of the aforementioned materials. The circular plots have been obtained by using the Equations (57) and (58) together with the experimental curves of  $L_0$  versus  $n_0$  and  $d_z$  respectively for QWs of CdS [38].

stants of  $\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$  lattice matched to InP, we have plotted in Figure 3 the normalized  $\Delta C_{44}$  and  $\Delta C_{456}$  respectively as functions of film thickness in QWs of the said ternary and quaternary materials in accordance with the three band model of Kane for  $x = 0.3$  and  $0.4$  respectively. The circular plots have been obtained by using Equations (57) and (58) together with the experimental curves of  $L_0$  versus  $n_0$  and  $d_z$  respectively for QWs of  $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$  for  $x = 0.4$  [38]. In Figure 4, all the cases of Figure 3 have been drawn for QWs of  $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$  and  $\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$  lattice matched to InP for  $x = 0.3$  and  $0.4$  respectively.

In Figure 5, we have drawn the normalized  $\Delta C_{44}$  and  $\Delta C_{456}$  in QWs of CdGeAs<sub>2</sub> as functions of surface electron concentration as shown by curves a and a' respectively. The curves b and b' exhibits the same dependence for QWs of  $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ . Besides the plots c and c' are valid for QWs of PbSe.

The influence of quantum confinement is immediately apparent from Figures 1 to 4 since the  $\Delta C_{44}$  and  $\Delta C_{456}$  depend strongly on the thickness of the quantum confined systems in direct contrast with the bulk specimens of the said compounds. The  $\Delta C_{44}$  and  $\Delta C_{456}$  exhibit strong oscillatory dependence on the thickness. The appearance of the humps in Figures 1 to 4 is due to the redistribution of the electrons amongst the quantized energy levels

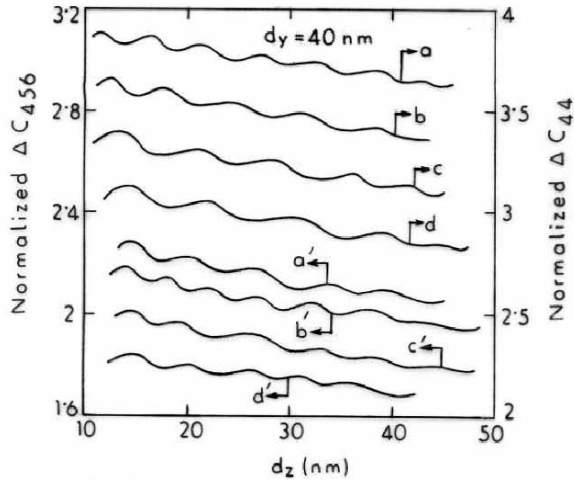


FIGURE 2  
Plots of the normalized  $\Delta C_{44}$  at 4.2K as functions of film thickness in QWs of (a) CdGeAs<sub>2</sub>; (b) InAs; (c) CdS; and (d) PbSe ( $n_0 = 10^{10} \text{m}^{-1}$ ). The plots a', b', c', and d' are valid for the  $\Delta C_{456}$  of the aforementioned materials.

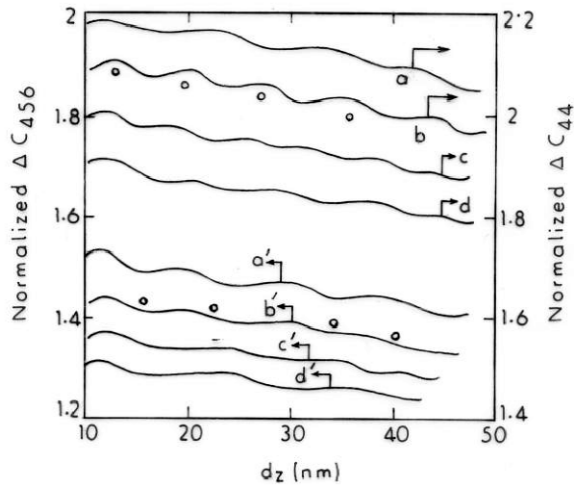


FIGURE 3  
The plots a and b exhibit the thickness dependence of the normalized  $\Delta C_{44}$  in QWs of Hg<sub>1-x</sub>Cd<sub>x</sub>Te in accordance with the three band model of Kane (by using the Equations (14) and (15)) for  $x = 0.3$  and  $0.4$  respectively. The plots c and d exhibit the same dependence for QWs of In<sub>1-x</sub>Ga<sub>x</sub>As<sub>y</sub>P<sub>1-y</sub> lattice matched to InP for  $x = 0.3$  and  $0.4$  respectively. The curves a' and b' show the dependence of the normalized  $\Delta C_{456}$  (by using Equations (14) and (16)) for QWs of Hg<sub>1-x</sub>Cd<sub>x</sub>Te and the curves c' and d' exhibit the same dependences for QWs of In<sub>1-x</sub>Ga<sub>x</sub>As<sub>y</sub>P<sub>1-y</sub> lattice matched to InP for  $x = 0.3$  and  $0.4$  respectively. The circular plots have been obtained by using Equations (57) and (58) together with the experimental curves of  $L_{00}$  versus  $n_0$  and  $d_z$  respectively for QWs of Hg<sub>1-x</sub>Cd<sub>x</sub>Te for  $x = 0.4$  [38].

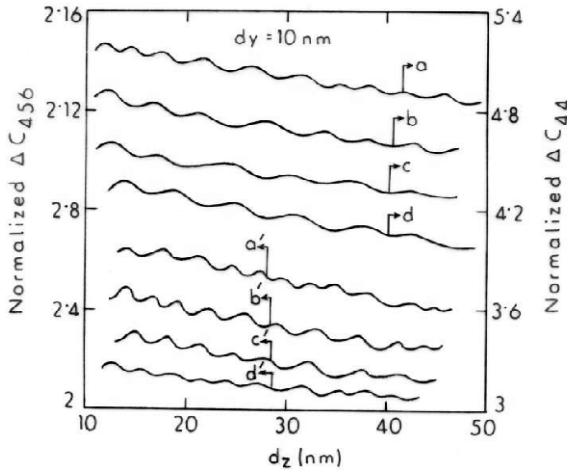


FIGURE 4

The plots a and b exhibit the thickness dependence of the normalized  $\Delta C_{44}$  in QWs of  $Hg_{1-x}Cd_xTe$  in accordance with the three band model of Kane (by using the Equations (17) and (18)) for  $x = 0.3$  and  $0.4$  respectively. The plots c and d exhibit the same dependence for QWs of  $In_{1-x}Ga_xAs_yP_{1-y}$  lattice matched to InP for  $x = 0.3$  and  $0.4$  respectively. The plots  $a'$  and  $b'$  show the dependences of the normalized  $\Delta C_{456}$  (by using Equations (17) and (19)) for QWs of  $Hg_{1-x}Cd_xTe$  and the curves  $c'$  and  $d'$  exhibit the same dependences for QWs of  $In_{1-x}Ga_xAs_yP_{1-y}$  lattice matched to InP for  $x = 0.3$  and  $0.4$  respectively.

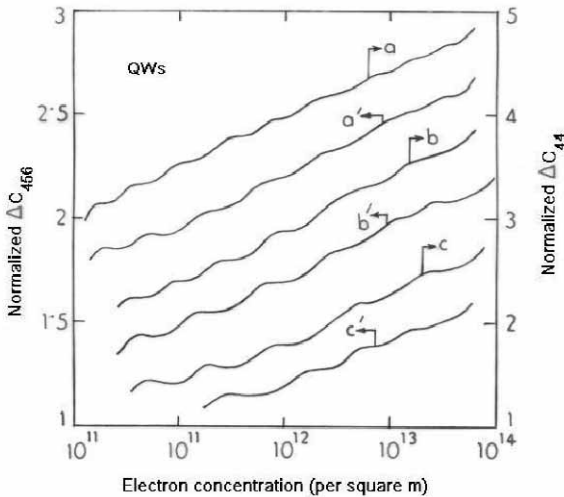


FIGURE 5

The plots  $a$  and  $a'$  exhibit the variations of the normalized  $\Delta C_{44}$  and  $\Delta C_{456}$  with respect to surface electron concentration in QWs of  $CdGeAs_2$ . The plots  $b$  and  $b'$ , and  $c$  and  $c'$  show the same variations in QWs of  $Hg_{1-x}Cd_xTe$  and  $PbSe$  respectively ( $d_z = 70$  nm).

when the size quantum number corresponding to the highest occupied level changes from one fixed value to the other. The  $\Delta C_{44}$  and  $\Delta C_{456}$  in quantum confined materials can become several orders of magnitude larger than that in the bulk specimens of the same materials which is also a direct consequence of system asymmetry through dimensional reduction. By comparing among the Figures 1 to 4, we can easily assess the influence of energy band constants on the  $\Delta C_{44}$  and  $\Delta C_{456}$  for QWs and QWWs of CdGeAs<sub>2</sub>, InAs, Hg<sub>1-x</sub>Cd<sub>x</sub>Te, In<sub>1-x</sub>Ga<sub>x</sub>As<sub>y</sub>P<sub>1-y</sub> lattice matched to InP, CdS and PbSe respectively with respect to the film thickness.

From Figure 5, we observe that the  $\Delta C_{44}$  and  $\Delta C_{456}$  oscillate with  $n_0$  in different manners which are the characteristic features of the dimension reduction. The oscillatory dependence is influenced by the crossing of the Fermi level by the size-quantized levels in steps. Since the Fermi-energy in quantum confined materials is an oscillatory function of  $n_0$  and film thickness and also since the  $\Delta C_{44}$  and  $\Delta C_{456}$  are functions of  $E_F$ , therefore the  $\Delta C_{44}$  and  $\Delta C_{456}$  oscillate with  $n_0$  and film thickness respectively. From the plots of the Figures 1 and 2, it appears that the presence of crystal field splitting constant enhances the numerical value of the  $\Delta C_{44}$  and  $\Delta C_{456}$  in QWs of CdGeAs<sub>2</sub>. Besides the numerical values of the  $\Delta C_{44}$  and  $\Delta C_{456}$  are greatest for CdGeAs<sub>2</sub> for all types quantum confined materials as considered here together with the fact that the values of the  $\Delta C_{44}$  and  $\Delta C_{456}$  in the QWWs are larger than that of the same for the QWs. The said fact is the consequence of the dispersion relations of the materials and the appropriate dimension reduction.

It may be noted that our experimental suggestion for the determination of  $\Delta C_{44}$  and  $\Delta C_{456}$  for materials having arbitrary dispersion laws is based on the Equations (57) and (58). Only the experimental values of  $L_0$  for any material as function of electron concentration will generate the experimental values of  $\Delta C_{44}$  and  $\Delta C_{456}$  for that range of  $n_0$  for that material. Since the experimental values of  $L_0$  in the present case are not available in the literature excluding CdS and Hg<sub>1-x</sub>Cd<sub>x</sub>Te to the best of our knowledge, we cannot compare our theoretical formulation with the experiment for all the other materials we have considered in this paper, although the theoretical results as given in this context would be useful. The Equations (57) and (58) provide not only the experimental check of  $\Delta C_{44}$  and  $\Delta C_{456}$  but also a technique for probing the band structures of quantum confined materials. We wish to note that we have not considered the hot electron and the many body effects in this simplified theoretical formalism due to the absence of the proper analytical techniques in the literature for including them for the present gener-

alized systems as considered in this paper. Our simplified approach will be useful for the purpose of relative comparison when the methods for tackling the formidable problem of inclusion of the many body and the hot electron effects for present generalized systems will appear. It is worth remarking in this context that our simplified theoretical results for  $\Delta C_{44}$  and  $\Delta C_{456}$  in QWs and QWWs of n-CdS and  $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$  are in quantitative agreement with the suggested experimental method of determining  $\Delta C_{44}$  and  $\Delta C_{456}$ , for materials having arbitrary band structures, even in the absence of the consideration of the many body and the hot electron effects respectively. The inclusion of these effects would certainly increase the accuracy of the results although our suggestion for the experimental determination of  $\Delta C_{44}$  and  $\Delta C_{456}$  is independent of the inclusion of the said effects together with the fact that the basic qualitative features of  $\Delta C_{44}$  and  $\Delta C_{456}$  as discussed in this paper would not change in the presence of the aforementioned effects.

It may be noted that by neglecting the contribution of the remote bands, we have ignored the direct coupling between the heavy and light holes which can be described by Luttinger Hamiltonian formalism. The direct coupling between the heavy and light holes influences the hole dispersion laws, but in turn, does not contribute with respect to the electron energy spectrum. In this paper, we have considered n-type nonlinear optical and optoelectronic materials because of their availability [41] and consequently we have formulated  $\Delta C_{44}$  and  $\Delta C_{456}$  for electrons only. Thus, we have neglected the contribution of the remote band. For n-type materials, the  $\mathbf{k}\cdot\mathbf{p}$  formulation is valid [19]. Since we have considered n-type materials, we have not considered the Luttinger formulation. In this context, it may be stated that the coulomb interaction is of special importance in determining optical nonlinearities at low excitations. Since the optical nonlinearities at low excitations do not influence the  $\Delta C_{44}$  and the  $\Delta C_{456}$  in n-type nonlinear optical and optoelectronic materials, we have not considered the coulomb interaction in this paper.

In this paper, we have studied in section-A,  $\Delta C_{44}$  and  $\Delta C_{456}$  in QWs and QWWs of nonlinear optical materials using n-CdGeAs<sub>2</sub> as an example. In formulating the expressions of  $\Delta C_{44}$  and  $\Delta C_{456}$  in such quantum confined materials, we have considered the crystal field splitting, the anisotropies of the effective electron masses and spin-orbit splitting parameters since these are the significant physical features of such nonlinear optical compounds [24]. In the absence of crystal field splitting, together with the assumptions of isotropic effective electron mass and spin-orbit splitting, the expressions of the quantum confined  $\Delta C_{44}$  and  $\Delta C_{456}$  as given by the Equation (9), (10),

(11) and (12) convert into the corresponding Equations (15), (16), (18) and (19) as given in section-B. The Equations (15), (16), (18) and (19) are valid for QWs and QWWs of III-V, ternary and quaternary compounds whose energy band structures are defined by the three-band model of Kane. For many important optoelectronic materials  $\Delta \gg E_g$  or  $\Delta \ll E_g$ . Under these inequalities, the Equations (15), (16), (18) and (19) should, respectively, be replaced by the Equations (22), (23), (25) and (26). For wide band gap materials, the Equations (22), (23), (25) and (26) get transformed into the Equations (28), (29), (31) and (32) respectively. Besides, in absence of any quantum confinement, the Equations (28), (29), (31) and (32) converge to the Equations (36) and (37) respectively. In addition, under non-degenerate electron concentration the Equations (36) and (37) reduce to the well-known results as given by the Equations (39) and (40) respectively. Thus our generalized formulation covers various materials under different conditions of quantum confinements.

In Section C, we have studied the  $\Delta C_{44}$  and the  $\Delta C_{456}$  in QWs and QWWs of II-VI materials in accordance with the Hopfield model where the splitting of the two spin states by the spin-orbit coupling and crystalline field has been taken into account to describe the carrier energy spectrum in II-VI compounds. In Section D, we have investigated the  $\Delta C_{44}$  and the  $\Delta C_{456}$  for IV-VI quantum confined compounds on the basis of the Cohen model. It may be noted that the Cohen model is also used to study the optoelectronic properties of Bismuth. The importance of Bismuth with respect to the experimental and theoretical realization of quantum confinement is already well known in the literature [41]. Thus, our study is also valid for QWs and QWWs of Bismuth with the proper changes in the energy band constants. In Section E, we have suggested the experimental determination of  $\Delta C_{44}$  and  $\Delta C_{456}$  for materials having arbitrary dispersion laws.

It is worth remarking that the influence of energy band models on  $\Delta C_{44}$  and  $\Delta C_{456}$  in quantum confined nonlinear optical and optoelectronic materials can be assessed from the present work and this simplified analysis also covers various dimensionally reduced compounds in quantum regime having different electron energy spectra. We have not considered other types of quantum-confined materials or other physical variables in order to keep the presentation brief. With the different sets of energy band parameters, we shall get different numerical values of the  $\Delta C_{44}$  and  $\Delta C_{456}$  though the nature of variation of  $\Delta C_{44}$  and  $\Delta C_{456}$  with respect to  $d_z$  and  $n_0$  as shown here would be similar for the other types of the aforementioned compounds and this simplified analysis exhibits the basic qualitative features of the quantum

confined  $\Delta C_{44}$  and  $\Delta C_{456}$  for such materials. The variations of  $\Delta C_{44}$  and  $\Delta C_{456}$  are totally band structure dependent. We wish to note that in view of larger changes of the elastic constants for the present quantum confined systems, detailed experimental work on  $\Delta C_{44}$  and  $\Delta C_{456}$  as functions of  $n_0$  would be interesting for quantum confined materials having arbitrary dispersion laws. It may be suggested that the experiments of the velocity of sound involving the shear mode as function of carrier degeneracy may exhibit the carrier contribution to the elastic constants for the present system. It is worth noting that the above statement is another suggestion for the experimental determination of  $\Delta C_{44}$  and  $\Delta C_{456}$  besides the suggested experimental method of determining them as given by the Equations (57) and (58) respectively. It may also be remarked that our study covers quantum confined nonlinear optical and optoelectronic materials having different electron dispersion laws. We must note that the formulations of  $\Delta C_{44}$  and  $\Delta C_{456}$  for any type of material are based on the specific dispersion relation in such compound. Finally it may be noted that the basic aim of this present work is not solely to investigate the  $\Delta C_{44}$  and the  $\Delta C_{456}$  in the presence of quantum confinement together with the suggestion for their experimental determination but also to formulate the expression for determining the Fermi-energy since the investigation of the different properties of n-type nonlinear optical and optoelectronic compounds are based on the temperature dependent electron statistics in such materials having various energy band structures.

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