ISSN 1330–0008
CODEN FIZAE4

ON A SIMPLE ANALYSIS OF THE BURSTEIN-MOSS SHIFT IN QUANTUM CONFINED STRUCTURES OF TERNARY AND QUATERNARY COMPOUNDS

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Received 17 October 1991
UDC 621.315

Original scientific paper

In this paper an attempt is made to study the Burstein-Moss shift in quantum wires and quantum dots of ternary and quaternary compounds on the basis of three-band Kane model, taking into account the influence of warped energy surface of the heavy hole band. It is found, taking n-$Hg_{1-x}Cd_xTe$ and $In_{1-x}Ga_xAs_yP_{1-y}$ lattice matched to InP as examples, that the Burstein-Moss shift exhibits oscillations of non-ideal Heaviside step functions for quantum wires and quantum dots with respect to doping and film thickness, respectively. Besides, the three-band Kane model enhances the Burstein-Moss shift and the numerical values of the shift are greatest in quantum dots for both compounds. In addition, the corresponding results for two-band Kane model and that of wide band-gap materials have also been obtained as special cases of our generalized analysis under certain limiting conditions.

1. Introduction

With the advent of fine line lithography[1)], molecular beam epitaxy[2)], metal-organic chemical vapour deposition[3)] and other experimental techniques, low-dimensional structures[4,5)] having quantum confinement in two and three dimensions such as quantum wires (QWs) and quantum dots (QDs) have in the last few years attracted much attention not only for their potential in uncovering new phenomena in solid state electronics but also for their interesting device applications. Heterostructures based on various materials are currently being studied because of the enhancement of carrier mobility[6]. These properties make such heterostructures suitable for applications in quantum-well lasers[7], optical modulators[8], heterojunction FETs[9] and other devices. In QWs, the motions of the electrons are quantized in the two perpendicular directions in wave-vector space and the carriers can only move in the single free direction[10]. In QDs, the dimensions of the quantum well increases from 1D to 3D, the freedom of motion of free carriers is not allowed and the density-of-states function is changed from Heaviside step function to Dirac's delta function[11,12].

For non-parabolic semiconductors the absorption edge lay at much shorter wavelength when it was very n-type than if it was intrinsic and the explanation of this effect is well-known[13]. Though, the Burstein-Moss shift (BMS) has been studied for various materials under different physical conditions, nevertheless it appears that the same shift in quantum confined structures has been relatively less studied. It appears from the literature that the BMS in QWs and QDs of non-parabolic semiconductors has yet to be studied by considering the various band models. It would, therefore, be of much interest to investigate the BMS in QWs and QDs of ternary and quaternary compounds, taking n-$Hg_{1-x}Cd_xTe$ and $In_{1-x}Ga_xAs_yP_{1-y}$, lattice matched to InP as examples, respectively.

The compound $Hg_{1-x}Cd_xTe$ is the classic narrow-gap semiconductor and is an important optoelectronic compound, because by varying the alloy composition, its band gap can be adjusted to cover the spectral range from 0.8 μm to 30 μm[15]. $Hg_{1-x}Cd_xTe$ finds extensive applications in infrared detector materials and photovoltaic detector arrays in $8-12$ μm wave bands[16]. The above uses have spurred a $Hg_{1-x}Cd_xTe$ technology for the production of high mobility crystal. The same material is ideally suited for studying the physics of narrow-gap compounds since the relevant material parameters are within easy experimental reach[17]. It may be noted in this context that the quaternary compounds have also received considerable attention as a widely used material for heterojunction lasers[19] and the avalanche photo diodes[20]. This material is being used extensively in PETs', transferred electron devices and detectors[21]. Thus it would be of interest to study the BMS in quantum confined structures of such ternary and quaternary compounds because of their importance in semiconductors device and technology as stated above.

In what follows, in Sect. 2.1 of theoretical background we shall derive the BMS in QWs of such materials on the basis of three-band Kane model[22] and taking into account the influence of the warped energy surface of the heavy hole band[23]. In Sect. 2.2 we shall derive the same in QDs. In Sect. 2.3 we shall obtain the corresponding results of two-band Kane model and that of wide gap materials as special cases of our generalized analysis. We shall study the doping and thickness dependences of the BMS in QWs and QDs of such compounds.

2. Theoretical background

2.1. Formulation of BMS in QWs of ternary and quaternary compounds

The energy spectrum of the conduction electrons in bulk specimens of ternary and quaternary compounds can be expressed, in accordance with three-band Kane model, as[22)]

$$\frac{\hbar^2 k^2}{2m^*} = \gamma(E), \qquad \gamma(E) = \frac{E(E+E_g)(E+E_g+\Delta)(E_g+(2/3)\Delta)}{E_g(E_g+\Delta)(E+E_g+(2/3)\Delta)}\,, \tag{1a}$$

where $\hbar = h/2\pi$, h is the Planck's constant, $\vec{k}$ is the wave-vector, m^* is the effective electron mass at the edge of the conduction band, E is the total electron energy as measured from the edge of the conduction band in the vertically upward direction in the absence of any quantization, E_g is the band-gap and Δ is the spin-orbit splitting of the valence band. The modified electron dispersion law in QWs can be written following Eq. (1a) as

$$\gamma(E) = \frac{\hbar^2\pi^2}{2m^*}\left[\left(\frac{n_x}{d_x}\right)^2 + \left(\frac{n_y}{d_y}\right)^2\right] + \frac{\hbar^2 k_z^2}{2m^*}\,, \tag{1b}$$

where n_x and n_y are the size quantum numbers along x and y directions, respectively, and d_x and d_y are the widths of the QWs along the respective directions. The use of Eq. (1b) leads to the expression of the density-of-states function as

$$N_{1D}(E) = (\sqrt{2m*}/\hbar)\sum_{n_x=1}^{n_{x\,max}}\sum_{n_y=1}^{n_{y\,max}}\left[\Theta_1(E)/\Psi_1(E,n_x,n_y)\right]H(E-E_1)\,, \tag{2}$$

where

$$\Theta_1(E) = \gamma(E)\left[E^{-1} + (E+E_g)^{-1} + (E+E_g+\Delta)^{-1} - \left(E+E_g+\frac{2}{3}\right)^{-1}\right],$$

$$\psi_1(E,n_x,n_y) = \left[\gamma(E) - \frac{\hbar^2\pi^2}{2m^*}\left(\left(\frac{n_x}{d_x}\right)^2 + \left(\frac{n_y}{d_y}\right)^2\right)\right].$$

H is the Heaviside step function and E_1 can be obtained from Eq. (1b) by putting $E = E_1$ and $k_z = 0$.

Combining Eq. (2) with the Fermi-Dirac occupation probability factor, the electron concentration per unit length in QWs of ternary and quaternary materials can be written in accordance with three-band Kane model as

$$n_{1D} = \frac{\sqrt{2m^*}}{\pi\hbar} \sum_{n_x=1}^{n_{x\,max}} \sum_{n_y=1}^{n_{y\,max}} [\psi_1(E_F, n_x, n_y) + \psi_2(E_F, n_x, n_y)], \tag{3}$$

where

$$\psi_2(E_F, n_x, n_y) = \sum_{r=1}^{S} 2(k_B T)^{2r}(1 - 2^{1-2r})\zeta(2r)\frac{\mathrm{d}^{2r}}{\mathrm{d}E_F^{2r}}\,.$$

r is the set of real positive integers, k_B is the Boltzmann constant, T is the temperature, $\zeta(2r)$ is the zeta function of order $2r$[14] and E_r is the Fermi energy in the QWs.

The heavy hole spectrum can be written in accordance with the warped energy band model as[23]

$$E_h = \frac{\hbar^2 k^2}{2m_0}\gamma_1 - \frac{\hbar^2}{m_0}\left[\gamma_2^2 k^4 - 3(\gamma_3^2 - \gamma_2^2)(k_x^2 k_y^2 + k_y^2 k_z^2 + k_z^2 k_x^2)\right]^{1/2}, \tag{4}$$

where m_0 is the free electron mass and γ_1, γ_1 and γ_3 are the well-known Luttinger constants[23].

Therefore the BMS in QWs can be expressed as

$$\delta_{1d} = E_F + E_g + E_2\,, \tag{5}$$

where

$$E_2 = \frac{\hbar^2\gamma_1}{2m_0}\left[A + B(E_F)\right] - \frac{\hbar^2}{m_0}\Big[\gamma_2^2\left[A + B(E_F)\right]^2$$

$$+3(\gamma_3^2 - \gamma_2^2)(\pi^2/d_x d_y) + 3(\gamma_3^2 - \gamma_2^2)AB(E_F)\Big]^{1/2},$$

$$A = \pi^2(d_x^{-2} + d_y^{-2}) \quad \text{and} \quad B(E_F) = 2m^*\hbar^{-2}\gamma(E_F) - A\,.$$

2.2. Formulation of BMS in QDs of ternary and quaternary compounds

From Eq. (1b) the electron energy spectrum in QDs of the materials considered can be written as

$$\gamma(E') = (\hbar^2\pi^2/2m^*)\left[(n_x/d_x)^2 + n_y/d_y)^2 + n_z/d_z)^2\right], \tag{6}$$

where E' is the 3D quantized energy in the present case, d_z and n_z are the film thickness and the size quantum number along th z-direction, respectively. The use of Eq. (6) leads to the expression of the density-of-states function as

$$N_{3D} = (2/d_x d_y d_z) \sum_{n_x=1}^{n_{x\,max}} \sum_{n_y=1}^{n_{y\,max}} \sum_{n_z=1}^{n_{z\,max}} \delta'(E - E'), \tag{7}$$

where δ' is the Dirac's delta function. Thus combining Eq. (7) with the Fermi-Dirac occupation probability factor, the electron concentration per unit volume in QDs of ternary and quaternary materials can be expressed as

$$n_{3D} = (2/d_x d_y d_z) \sum_{n_x=1}^{n_{x\,max}} \sum_{n_y=1}^{n_{y\,max}} \sum_{n_z=1}^{n_{z\,max}} F_{-1}(\eta), \tag{8}$$

where $\eta = (k_B T)^{-1}(\varepsilon_F - E')$, ε_F is the Fermi energy in QDs and $F_j(\eta)$ is the Fermi-Dirac integral of order j which can be written following Ref. 25 as

$$F_j(\eta) = \frac{1}{\sqrt{j+1}} \int_0^\infty y^j [1 + \exp(y - \eta)]^{-1} \mathrm{d}y, \tag{9}$$

for $y > -1$, or for all y analytically continued as a complex contour integral around the negative axis,

$$F_j(\eta) = C_j \int_{(-\infty)}^{(0+1)} y^j [1 + \exp(y - \eta)]^{-1} \mathrm{d}y, \tag{10}$$

where $\sqrt{j+1}$ is the complete gamma function and $C_j = \sqrt{-j}/2\pi\sqrt{-1}$. Therefore the BMS in QDs of nonparabolic materials is given by

$$\delta_{3D} = \varepsilon_F + E_g + E_3, \tag{11}$$

where

$$E_3 = \frac{\hbar^2 \gamma_1 D_1}{2m_0} - \frac{\hbar^2}{m_0} \Big[\gamma_2^2 D_1^2 + 3(\gamma_3^2 - \gamma_2^2) e_1 \Big]^{1/2},$$

$$D_1 = \pi^2 (d_x^{-2} + d_y^{-2} + d_z^{-2}) \quad \text{and} \quad e_1 = \pi^4 (d_x^{-2} d_y^{-2} + d_y^{-2} d_z^{-2} + d_z^{-2} d_x^{-2}).$$

2.3. *Special cases*

(a) Under the conditions $\Delta \gg E_g$ (e.g. n-InSb) or $\Delta \ll E_g$ (e.g. n-GaAs), Eq. (1a) assumes the form

$$\hbar^2 k^2 / 2m^* = E(1 + \alpha E), \qquad \alpha = 1/E_g, \tag{12}$$

which is the well-known two-band Kane model[26]. The basic forms of all aforementioned equations will be unchanged for two-band Kane model where

$$\gamma(E) = E(1 + \alpha E) \qquad \text{and} \qquad \Theta_1(E) = 1 + 2\alpha E. \tag{13}$$

(b) For relatively wide band-gap materials $\alpha \to 0$. In this case, all equations considered will also be unaltered where

$$\gamma(E) = E \qquad \text{and} \qquad \Theta_1(E) = 1. \tag{14}$$

3. Results and discussion

Using Eqs. (3) and (5) and taking the values of the energy band parameters[23,27,28] for $Hg_{1-x}Cd_xTe$ and $In_{1-x}Ga_xAs_yP_{1-y}$ lattice matched to InP as given in Table 1, we have plotted the normalized BMS as functions of electron concentration per unit length and film thickness as shown in Figs. 1 and 2, respectively, in accordance with both the three- and two-band Kane models for QWs of both compounds, respectively. Using Eqs. (8) and (11) and taking the parameters as used in obtaining Figs. 1 and 2, we have further plotted the normalized BMS as functions of electron concentration per unit volume and film thickness as shown in Figs. 3 and 4, respectively, in accordance with the aforementioned band models for QDs of both compounds. From the figures and the above discussion, the following features follow.

TABLE 1.

Parameters	InP	GaP	$In_{1-x}Ga_xAs_yP_{1-y}$
γ_1	4.95	4.05	$Q(x, y)$
γ_2	1.65	0.49	$Q(x, y)$
γ_3	2.35	1.25	$Q(x, y)$
m^*/m_0			$0.080 - 0.0393y$
Δ			$(0.114 + 0.26y - 0.22y^2)$ eV
E_g			$(1.337 - 0.73y + 0.13y^2)$ eV

$Q(x, y) = (1 - x)yB_{AC} + (1 - x)(1 - y)B_{AD} + xyB_{BC} + x(1 - y)B_{BD}$
for the material $A_{1-x}B_xC_yD_{1-y}$, $x = 0.1844y[0.4184 - 0.013y]^{-1}$

Energy band parameters of $In_{1-x}Ga_xAs_yP_{1-y}$ lattice matched to InP and $Hg_{1-x}Cd_xTe$, respectively.

a) Parameters for $In_{1-x}Ga_xAs_yP_{1-y}$, lattice matched to InP[27].

$E_g = [-0.302 + 1.93x + 5.35x\,10^{-4}\,T(1 - 2x) - 0.810x^2 + 0.832x^3]$ eV,
$m^* = 3\hbar^2 E_g(x)/4P^2(x)$, $P^2(x) = (\hbar^2/2m_0)(18+3x)$, $\Delta = 0.63+0.24x-0.27x^2]$ eV,
$\gamma_1 = 8.3$, $\gamma_2 = 7.4$, $\gamma_3 = 7.5$,

b) Parameters for n-$Hg_{1-x}Cd_xTe$[23,28].

1. It appears from Figs. 1 and 2 that the BMS in QWs increases with increasing electron concentration and decreasing film thickness, respectively, for both compounds. The BMS oscillates both with n_{1D} and d_x in a step-like manner which reflects the dependence of the density-of-states function with energy in QWs. The influence of 1D motion is immediately apparent from Fig. 2 since the BMS has become strongly dependent on the thickness of the QWs in contrast with bulk specimens of the corresponding compounds. The step functional oscillations of BMS is non ideal due to the presence of finite temperature. The influence of spin-orbit splitting of the valence band in the dispersion relation of the conduction electrons in accordance with three-band Kane model enhances the values of the BMS for the whole range of the variables considered. The numerical values of the BMS for quaternary compounds are greater than those of ternary materials.

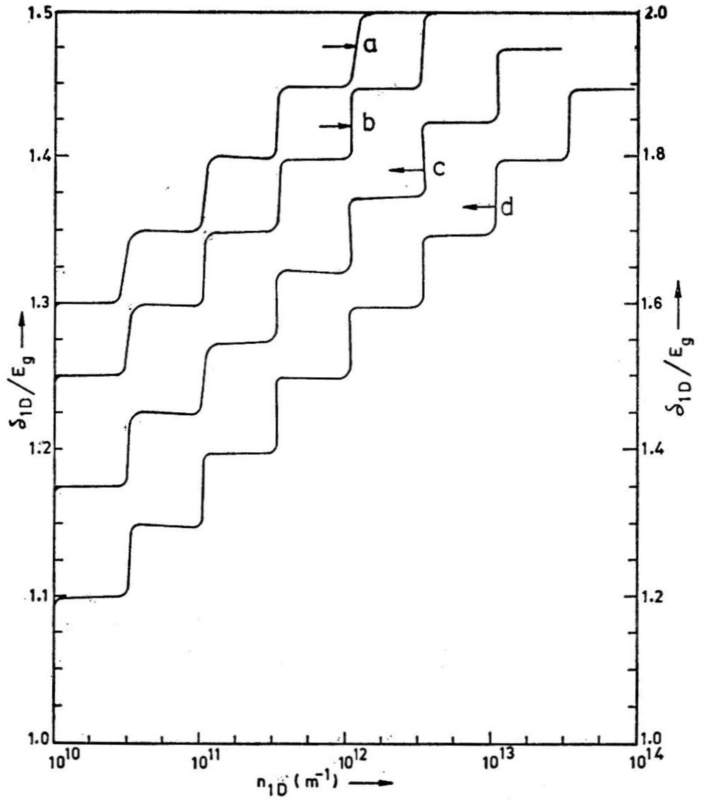

Fig. 1. Plot of the normalized BMS versus n_{1D} in QWs in accordance with (a) three-band Kane model for $In_{1-x}Ga_xAs_yP_{1-y}$, lattice matched to InP; (b) two-band Kane model for $In_{1-x}Ga_xAs_yP_{1-y}$, lattice matched to InP; (c) three-band Kane model for $Hg_{1-x}Cd_xTe$ and (d) two-band Kane model for $Hg_{1-x}Cd_xTe$ ($x = y = 0.5$, $T = 4.2$ K, $d_x = d_y = 40$ nm).

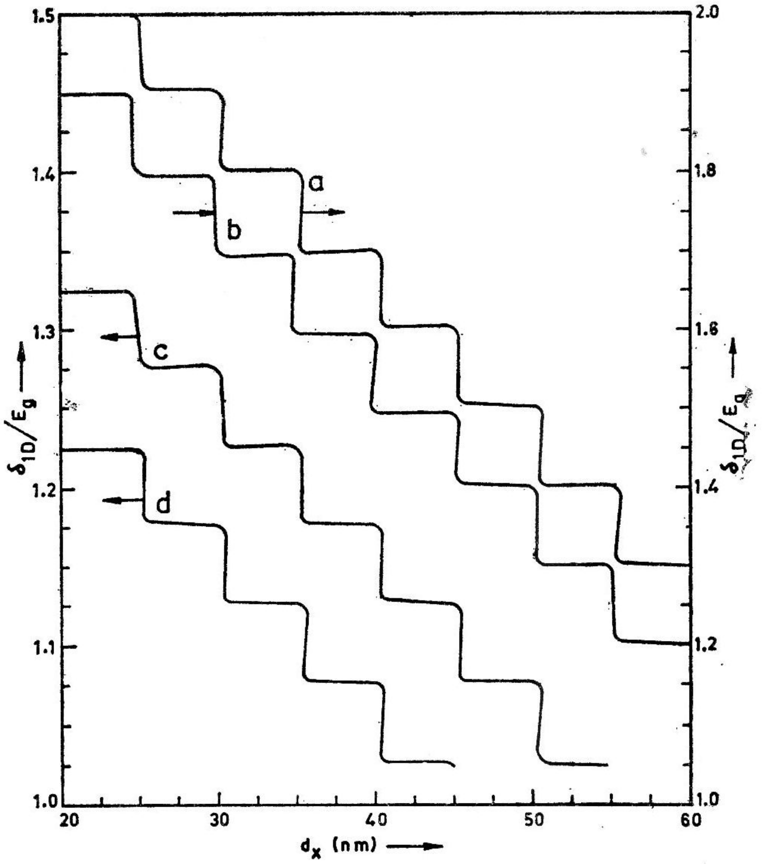

Fig. 2. Plots of the normalized BMS versus d_x in QWs for all the cases of Fig. 1 $(x = y = 0.5$, $T = 4.2$ K, $d_y = 40$, $n_{1D} = 10^{11}$ m^{-1}.

2. It appears from Figs. 3 and 4 that the BMS increases with increasing electron concentration and decreasing film thickness very sharply in nonideal steps on QDs of ternary and quaternary materials. It may be noted that the 3D quantization in QDs leads to the discrete energy levels which produces very large changes. Under such quantization, there remains no free electron states and consequently the crossing of the Fermi levels by the size quantized subbands under 3D quantization would have much more greater impact on the redistribution of the electrons as compared to found for ID quantization. It is basically this impact which results in the increased sharpness of the oscillatory variations of the BMS in QDs as compared to QWs.

In this paper we have first formulated the simple expressions of the electron statistics and the BMS for ternary and quaternary compounds by using the generalized three-band Kane model and the warping of the heavy hole band without any approximations among the energy band constants. The three-band Kane model is also valid for III-V compound semiconductors, in general, but must be used as such

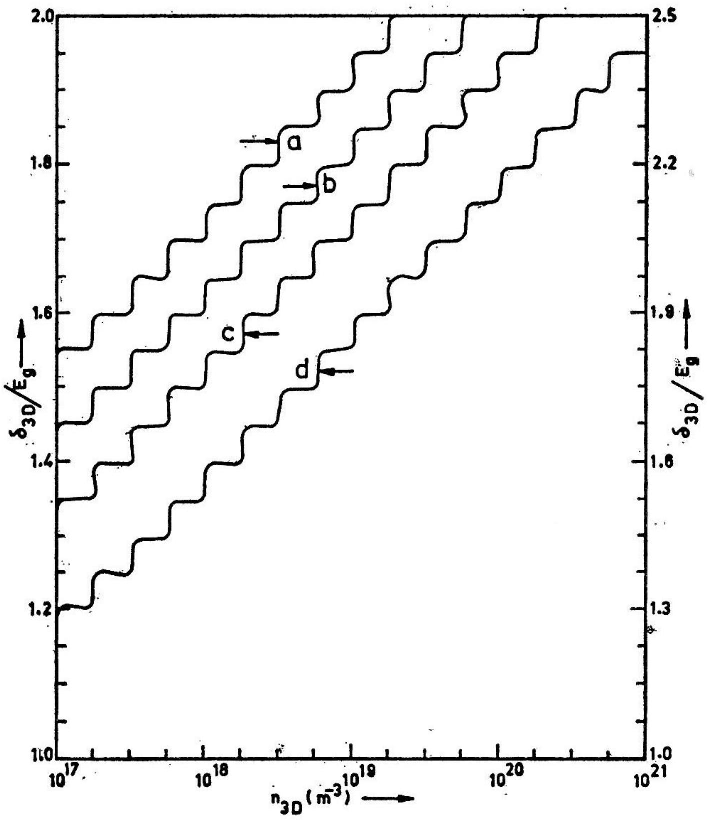

Fig. 3. Plots of the normalized BMS versus n_{3D} in QDs for all cases of Fig. 1 ($x = y = 0.5$, $d_x = d_y = d_z = 40$ nm, $T = 4.2$ K).

for n-InAs where the spin-orbit splitting constant is of the order of band gap. For many important semiconductors $\Delta \gg E_g$ (e.g. n-InSb) or $\Delta \ll E_g$ (e.g. GaAs), where the two-band Kane model is applicable. Thus our simple analysis is valid for various materials under different quantum confined conditions. Besides, the influence of the energy band models on the BMS in QWs of ternary and quaternary materials can also be assessed from our work. The BMS could have been plotted with other physical variables. We have numerically plotted a few cases for the purpose of condensed presentation. Since the experimental results are not available in the literature to the best of our knowledge, we can not compare our theoretical analysis with experimental data. The general qualitative features of the BMS as shown here would be valid for most n-type semiconducting materials. Finally it may be noted that the basic purpose of the present work is not only to investigate the BMS but also to formulate the appropriate density-of-states function since the different electronic properties and transport coefficients are based on this function in quantum confined structures.

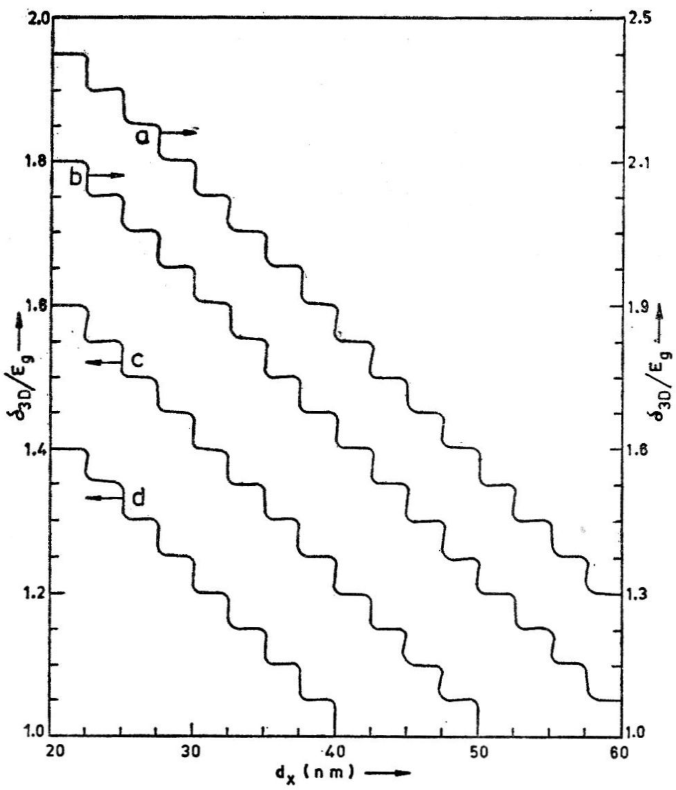

Fig. 4. Plot of the normalized BMS versus d_x in QDs for all cases of Fig. 1 ($x = y = 0.5$, $d_y = d_x = 40$ nm, $n_{3D} = 10^{19}$ m^{-3}, $T = 4.2$ K).

Acknowledgements

One of the authors (KPG) is grateful to Indian National Science Academy for a Visiting Fellowship at IIT, Kharagpur (award letter number BS/VF/3/930 dated 14th May, 1991). The authors are grateful to Professor D. N. Bose for critically reading the manuscript.

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O JEDNOSTAVNOJ ANALIZI BURSTEIN-MOSSOVOG POMAKA U KVANTNIM OGRANIČENIM STRUKTURAMA TERNARNIH I KVATERNARNIH SPOJEVA

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UDK 621.315

Originalni znanstveni rad

Koristeći Kaneov model s tri vrpce proučavan je Burstein-Mossov pomak u kvantnim točkama i kvantnim žicama ternarnih i kvaternarnih spojeva. U obzir je uzeta iskrivljenost energetske plohe teških šupljina. Uzevši n-$Hg_{1-x}Cd_xTe$ i $In_{1-x}Ga_xAs_yP_{1-y}$ kao primjere, nađeno je da Burstein-Mossov pomak pokazuje neidealne oscilacije Heavisideove step funkcije u odnosu na dopiranje i debljinu sloja. Burstein-Mossov pomak najveći je u kvantnim točkama za oba spoja. Odgovarajući rezultati za Kaneov model s dvije vrpce i velik energetski procijep dobiveni su uz određene granične uvjete.