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ON THE BRUSTEIN-MOSS SHIFT IN 3D QUANTUM DOTS OF Te

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An attempt is made to study the Brustein-Moss shift in 3D quantum dots of Te in accordance with Ba and K models as given elsewhere. It is found, that the same shift in 3D quantum dots of Te increases with electron concentration and decreases with increasing film width in an oscillatory manner, respectively. Besides the model Ba enhances the numerical value of the shift than that of model K.

1. Introduction

With the advent of fine line lithographical methods[1], molecular-beam epitaxy[2], organometallic vapour-phase epitaxy[3] and other experimental techniques, low-dimensional structures[4-5], having quantum confinement in 1, 2 and 3 dimensions such as quantum wells, quantum wires and quantum dots 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 devices applications. Heterostructures based on various materials are currently being studied because of the enhancement of carrier mobility[6]. These properties make heterostructures suitable for applications in quantum well laser[7], heterojunction FET's[8], high-speed digital networks[9], optical modulators[10] and the other devices. As the dimensionality of the quantum well increases from 1D to 3D, the

degree of freedom of the free carrier motion decreases drastically and the density-of-states function is changed from 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 was well-known in the literature[13-13]. The Brustein-Moss shift (hereafter referred to as BMS) has been studied for various materials having different dispersion relations under various physical conditions[15,16]. It appears from the literature that the BMS in quantum dots (QDs) of Te has yet to be investigated by considering the various band models. This is very important since Te has intensively been investigated for its various peculiar electronic properties[17]. In what follows, we shall study the doping and thickness dependences of 3D dots of Te in accordance with various band models.

2. *Theoretical background*

The dispersion relation of the conduction electrons in bulk specimens of Te in accordance with K model can be written[17] as

$$E_{c61/62} = ak_{\perp}^2 + bk_z^2 + E_g \pm [M^2k_{\perp}^2 + N^2k_z^2]^{1/2}, \tag{1}$$

where the notations are defined in the above reference. Thus the modified electron energy spectrum in QDs of Te is given by

$$\varepsilon' = \pi^2 a\,[(n_{xc}/L_x)^2 + (n_{yc}/L_y)^2] + b\pi^2\,(n_{zc}/L_z)^2 + E_g \pm$$
$$\pm\,[M^2\pi^2\,\{(n_{xc}/L_x)^2 + (n_{yc}/L_y)^2\} + N^2\pi^2\,(n_{zc}/L_z)^2)^{1/2}, \tag{2}$$

where ε' is the 3D quantized total energy of the electrons in the present case, n_{xc}, n_{yc} and n_{zc} are the size quantum numbers of the conduction electrons along x,y and z-directions, respectively, and L_x, L_y and L_z are the widths of the QDs of Te along x, y and z-directions, respectively. The total electron concentration is given by

$$n_0 = C_0 \sum_{n_{xc}n_{yc}n_{zc}} [F_{-1}(\eta_0)], \tag{3}$$

where

$$C_0 \equiv [8\pi^3 L_x L_y L_z], \quad \eta_0 \equiv (k_B T)^{-1}\,[E_F - \varepsilon'],$$

E_F is the Fermi energy in the present case, k_B is Boltzmann constant, T is temperature and $F_j(\eta_0)$ is the one parameter Fermi-Dirac integral of order j as defined by Blakemore[18]. The dispersion relation of the topmost valence band in accordance with K model is given by

$$E_{v4} = Ak_{\perp}^2 + Bk_z^2 + \beta k_{\perp}^4 + \beta' k_{\perp}^2 k_z^2 - 2\,|\Delta_1| + [(2|\Delta_1| +$$
$$+\,\eta k_{\perp}^2 + \zeta k_{\perp}^4 + \zeta' k_{\perp}^2 k_z^2)^2 + S^2 k_z^2]^{1/2}, \tag{4}$$

where the notations are given in Ref. 17.

The modified hole energy E_v' in the QDs of Te can be written using equation (4) as

$$E_v' = A\pi^2 [(n_{xv}/L_x)^2 + (n_{yv}/L_y)^2] + B\pi^2 (n_{zv}/L_z)^2 + \beta\pi^4 [(n_{xv}/L_x)^2 + (n_{yv}/L_y)^2]^2 + \beta'\pi^4 (n_{zv}/L_z)^2 [(n_{xv}/L_x)^2 + (n_{yv}/L_y)^2] - 2|\Delta_1| + \left[2|\Delta_1| + \eta\pi^2 \{(n_{xv}/L_x)^2 + (n_{yv}/L_y)^2\} + \zeta\pi^4 \{(n_{xv}/L_x)^2 + (n_{yv}/L_y)^2\}^2 + \zeta'\pi^4 (n_{zv}/L_z)^2 \{(n_{xv}/L_x)^2 + (n_{yv}/L_y)^2\} + \zeta'\pi^4 \left(\frac{n_{zv}}{L_z}\right)^2 \left\{\left(\frac{n_{xv}}{L_x}\right)^2 + \left(\frac{n_{yv}}{L_y}\right)^2\right\}\right]^2 + S^2\pi^2 \left(\frac{n_{zv}}{L_z}\right)^2\Bigg]^{1/2} \quad (5)$$

Thus the BMS in accordance with K model can be written as

$$\delta_k = E_F + E_v'. \quad (6)$$

We shall now compare δ_k with that which will be found in accordance with Ba model. The dispersion relation of the conduction electrons in Te in accordance with Ba model can be expressed[17] as

$$E_{c61/62} = \frac{1}{2}[E_g + \varepsilon_\pm + (C_c - A_c) k_\perp^2 + (D_c - B_c) k_z^2] + \left[\frac{1}{4}[E_g - \varepsilon_\pm + (C_c + A_c) k_\perp^2 + (B_c + D_c) k_z^2]^2 + Q_c^2 k_\perp^2\right]^{1/2}, \quad (7)$$

where

$$\varepsilon_\pm \equiv -2|\Delta_1| \pm \sqrt{4\Delta_1^2 + S_c^2 k_z^2},$$

and the other notations are defined in the above reference.

The basic form of n_0 as given by equation (3) for K model will also be unchanged for Ba model in 3D QDs of Te where

$$\varepsilon' = \frac{1}{2}[E_g - 2|\Delta_1| \pm \sqrt{4\Delta_1^2 + S_c^2\pi^2 (n_{zc}/L_z)^2} + (C_c - A_c)\pi^2 \{(n_{xc}/L_x)^2 + (n_{yc}/L_y)^2\} + (D_c - B_c)(n_{zc}/L_z)^2 \pi^2] + \left[\frac{1}{4}[E_g + 2|\Delta_1| \pm \pm \sqrt{4\Delta_1^2 + S_c^2\pi^2 (n_{zc}/L_z)^2} + (C_c + A_c)\pi^2 \left\{(n_{xc}/L_x)^2 + \left(\frac{n_{yc}}{L_y}\right)^2\right\} + (B_c + D_c)\pi^2 (n_{zc}/L_z)^2]^2 + Q_c^2\pi^2 \{(n_{xc}/L_x)^2 + (n_{yc}/L_y)^2\}\right]^{1/2}.$$

In this case the BMS is given by

$$\delta_{Ba} = E_F + E_v' \tag{8}$$

where

$$E_v' = \frac{1}{2}\left[E_g - 2|\Delta_1| \pm \sqrt{4\Delta_1^2 + S_v^2\pi^2(n_{zv}/L_z)^2} + (C_v - A_v)\pi^2\{(n_{xv}/L_x)^2 + (n_{yv}/L_y)^2\} + (D_v - B_v)(n_{zv}/L_z)^2\pi^2\right] - \left[\frac{1}{4}\left[E_g + 2|\Delta_1| \pm \pm \sqrt{4\Delta_1^2 + S_v^2\pi^2(n_{zv}/L_z)^2} + (C_v + A_v)\pi^2\left\{(n_{xv}/L_x)^2 + \left(\frac{n_{yv}}{L_y}\right)^2\right\} + (B_v + D_v)\pi^2(n_{zv}/L_z)^2\right]^2 + Q_v^2\pi^2\{(n_{xv}/L_x)^2 + (n_{yv}/L_y)^2\}\right]^{1/2}$$

3. Results and discussion

Using Eqs. (6) and (3) and taking the parameters[17] $A = -2.57 \times 10^{-19}$ eV · m², $B = -4.09 \times 10^{-19}$ eV · m², $\beta = 1.1 \times 10^{-37}$ eV · m⁴, $\beta' = 0$ eV · · m², $2|\Delta_1| = 6.315 \times 10^{-2}$ eV, $\eta = -1.18 \times 10^{-19}$ eV · m², $\zeta = 4 \times 10^{-31}$ eV · m, $\zeta' = 0$ eV · m⁴, $|S| = 2.62 \times 10^{-9}$ eV · m, $a = 3.65 \times 10^{-19}$ eV · m², $b = 5.47 \times 10^{-16}$ eV · m, $|M| = 2.25 \times 10^{-10}$ eV · m, $|N| = 7.12 \times 10^{-10}$ eV · · m, $E_g = 0.337$ eV, $L_x = 40$ nm, $L_y = 50$ nm, $L_z = 60$ nm and $T = 4.2$ K which are valid of K model we have plotted the normalized BMS in QDs of Te as shown in Fig. 1 as a function of electron concentration in which the same dependence has also been plotted in accordance with Ba model and taking the parameters[17] $A_c = -0.65 \times 10^{-19}$ eV · m², $A_v = -1.21 \times 10^{-19}$ eV · m², $B_{c,v} = 3.77 \times 10^{-19}$ eV · m², $C_{cv} = 2.67 \times 10^{-19}$ eV · m², $D_{c,v} = 7.6 \times 10^{-19}$ eV · m², $2|\Delta_1| = 6.315 \times 10^{-2}$ eV, $E_g = 0.335$ eV, $|S|_{c,v} = 2.44 \times 10^{-19}$ eV · m, $|Q|_c = 3.8 \times \times 10^{-9}$ eV · m and $|Q|_v = 4 \times 10^{-9}$ eV · m. Using the above parameters as used in obtaining Fig. 1, we have shown in Fig. 2 the normalized dependence of BMS on the film thickness (taking cubic QD of Te) for both the models corresponding to an electron concentration of 10^{23} m^{-3}.

It appears from Fig. 1 that, the BMS increases with increasing electron concentration in an oscillatory manner and the Ba model enhances the numerical values of the BMS in the whole range of the concentrations considered. From Fig. 2 it can be stated that the BMS decreases with increasing film thickness. The main difference between the models lies in their $k_\perp$ dependence for energies and is caused by the various consideration of the non-parabolicity as noted the carrier energy spectra. It appears that a combination of model K and Ba taking into account a strong coupling between VH4, VH5 and CH61, CH62 and a weak one between VH4, VH5 and VH61, VH62 including $\vec{k}$-linear terms and trigonal warping terms for both the bands, would be the best description of the dispersion relations. It may be noted that 3D quantization leads to discrete energy levels somewhat like atomic energy levels which produces very sharp changes. Under such

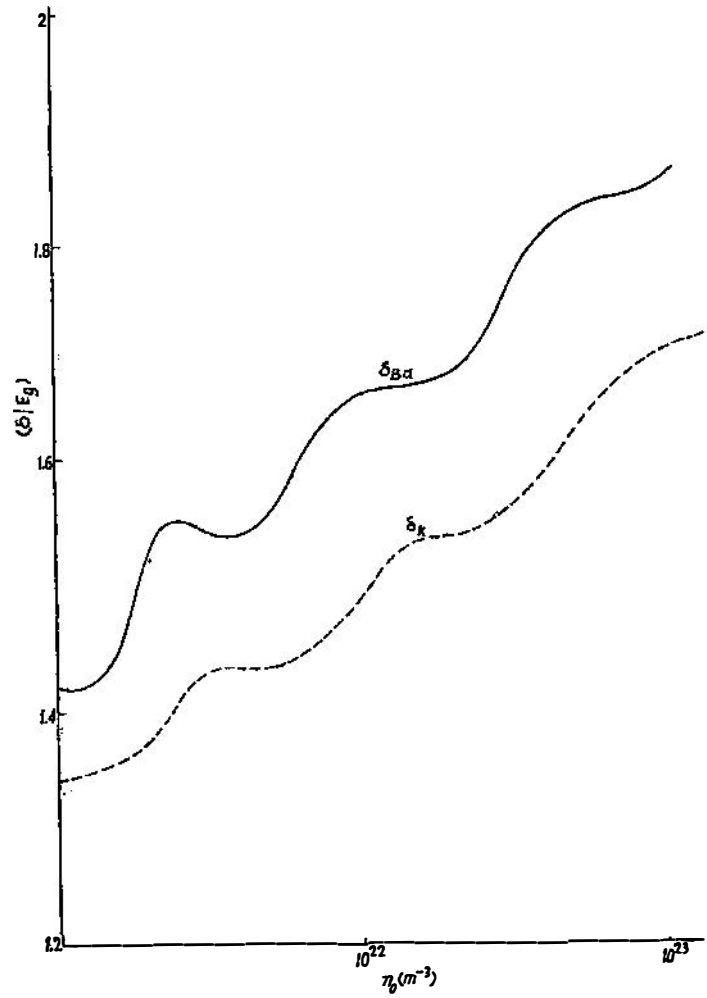

Fig. 1. Plot of the normalised BMS as a function of n_0 in accordance with Ba model in 3D QDs of Te. The dashed plot corresponds to K model.

quantization, there remains no free electron states and consequently the crossing of the Fermi level 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 1D quantization. It is basically this impact which results in the increasing sharpness of the oscillatory variations for both types of band models. The basic form of n_0 and as given by equation (3) will be unaltered for both types of band models. Only ε' and E_v' are band structure dependent quantities. This fact is again only true for 3D quantization of $\vec{k}$ space. The general features of the BMS in 3D QDs of Te as discussed here would be valid for most of the non-para-

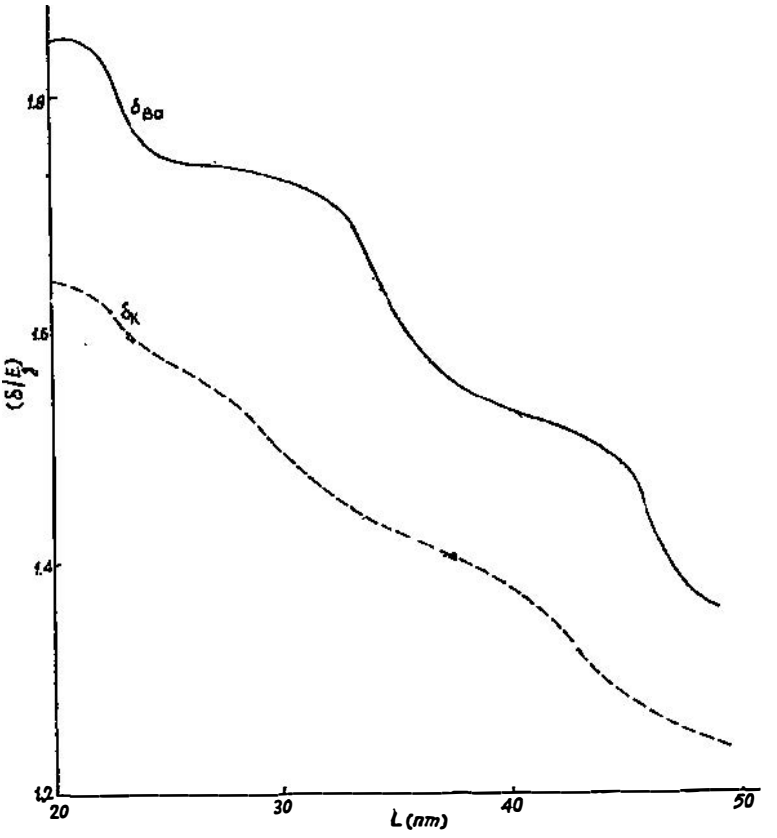

Fig. 2. Plot of the normalised BMS as a function of film thickness in accordance with Ba model in 3D QDs of Te. The dashed plot corresponds to K model.

bolic semiconductors. Finally it may be noted that the basic purpose of the present work is not solely to investigate the BMS in 3D QDs of Te but also to formulate the appropriate electron concentration since the different electronic properties of semiconductor microstructures are based the electron statistics in such materials.

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O BRUSTEIN-MOSSOVOM POMAKU U 3D KVANTNIM TOČKAMA TELURA

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Koristeći Ba i K model razmatrani su Brustein-Mossovi pomaci u 3D kvantnim točkama telura. Nađeno je da pomak oscilatorno raste s koncentracijom elektrona a pada s debljinom filma.