Vol. 87 (1995) *ACTA PHYSICA POLONICA A* No. 2

Proceedings of the XXIII International School of Semiconducting Compounds, Jaszowiec 1994

DEFORMATION POTENTIALS IN IV–VI QUANTUM WELLS

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Theoretical studies of the deformation potentials in quantum wells and superlattices are presented. It is shown that a difference exists between the bulk deformation potentials and deformation potentials in the low dimensional structures made of narrow-gap semiconductors.

PACS numbers: 73.40.Lq, 71.50.+t

1. Introduction

To analyse the electronic properties of semiconductor superlattices (SLs) or quantum wells (QWs) it is necessary to know the basic parameters of the layers of which the structures are composed: the band gaps, effective masses parallel to the interfaces, etc. In turn, to determine those parameters properly, it is necessary to take into account the strains in the interfaces as well as in the bulk of the layers. The strain induced energy shifts are usually calculated from the corresponding deformation potentials (DPs). For SLs and QWs made of the IV–VI semiconducting materials, the strain induced shifts of energy levels are considered in Refs. [1–4]. It is commonly assumed that the DPs in QWs and SLs are the same as those in bulk crystals. For example, for the DPs of PbTe and SnTe SLs theoretical results of Refs. [5] and [6] are taken as a rule.

The purpose of the present contribution is to consider the difference between DPs in QWs and bulk material. We show that such difference does exist for the case of narrow-gap materials with the interband k–p interaction. This is because of pronounced effect of the size quantization on energy levels in QWs made of the narrow-gap materials.

2. Energy spectrum and deformation potentials

The energy spectrum near the L-point of the BZ in the IV–VI semiconductors is determined by the eigenstates of the Kohn–Luttinger matrix Hamiltonian [7]:

$$H_k = \begin{bmatrix} \epsilon_1 & 0 & -\mathrm{i}Z & -Y-\mathrm{i}X \\ 0 & \epsilon_1 & -Y+\mathrm{i}X & -\mathrm{i}Z \\ \mathrm{i}Z & -Y-\mathrm{i}X & \epsilon_2 & 0 \\ -Y+\mathrm{i}X & \mathrm{i}Z & 0 & \epsilon_2 \end{bmatrix} \tag{1}$$

where $\epsilon_{1,2} = E_{\mathrm{c,v}} \pm \frac{p^2}{2m^*}$, with $\frac{p^2}{2m^*} \equiv \frac{p_z^2}{2m_z^*} + \frac{p_\perp^2}{2m_\perp^*}$. $\widehat{m}^*$ are the far-band masses and $E_{\mathrm{c,v}}$ are the edges of the conduction and valence bands. $Z = v_z p_z$, $X, Y = v_\perp p_{x,y}$ and v is interband matrix element of velocity. The direction of z-axis is chosen to be parallel to the [111] crystallographic axis.

The effect of strain is to change the positions of the band edges

$$E_{\mathrm{c,v}} \to \tilde{E}_{\mathrm{c,v}} = E_{\mathrm{c,v}} + \Delta_{\mathrm{c,v}}, \tag{2}$$

where $\Delta_{\mathrm{c,v}}$ is the strain induced band shift. The latter can be expressed by the deformation potential of the band, $D_{\mathrm{c,v}}$ and the deformation ε:

$$\Delta_{\mathrm{c,v}} = \varepsilon D_{\mathrm{c,v}}. \tag{3}$$

In a simple case of dilation, the deformation is equal to the relative volume change: $\varepsilon = \Delta V/V$, and hence

$$D_{\mathrm{c,v}} = D_{\mathrm{d}}{}^{\mathrm{c,v}} + \frac{1}{3} D_{\mathrm{u}}^{\mathrm{c,v}}, \tag{4}$$

where D_{u} and D_{d} are the deformation potentials of the [111] valley [5, 6].

Solving the secular equation one obtains the energy spectrum

$$E_{1,2}(\boldsymbol{p}) = \frac{(\tilde{E}_{\mathrm{c}} + \tilde{E}_{\mathrm{v}})}{2} \pm \sqrt{\left(\frac{\tilde{E}_{\mathrm{g}}}{2} + \frac{p^2}{2\widehat{m}^*}\right)^2 + v_\perp^2 p_\perp^2 + v_z^2 p_z^2}, \tag{5}$$

where

$$\tilde{E}_{\mathrm{g}} = E_{\mathrm{g}} + \Delta_{\mathrm{c}} - \Delta_{\mathrm{v}}; \qquad E_{\mathrm{g}} = E_{\mathrm{c}} - E_{\mathrm{v}}. \tag{6}$$

For $\mathrm{Pb}_{1-x}\mathrm{Sn}_x\mathrm{Te}$ with $x > 0.4$, the gap parameter $\tilde{E}_{\mathrm{g}}$ is negative, and the band inversion starts at the point $\tilde{E}_{\mathrm{g}} = 0$.

To consider the effect of strain on energy spectrum in QWs, we introduce the definition of deformation potential in a general form

$$\tilde{D}_{\mathrm{c,v}} = \left.\frac{\partial E_{1,2}}{\partial \varepsilon}\right|_{\varepsilon=0 p=0}. \tag{7}$$

It follows from Eq. (5) that for bulk material, $\tilde{D}_{\mathrm{c,v}} = D_{\mathrm{c,v}}$, i.e. the calculated DPs are the same as those inserted in the Hamiltonian.

3. Deformation potentials in QWs

Consider now the effect of one-dimensional confinement in a IV–VI QW grown in the [111] direction. We assume that QW is a rectangular one and deep in the sense that the following condition is fulfilled

$$\xi \equiv \frac{m_{\perp}^{*} W L^2}{\hbar^2} \gg 1, \tag{8}$$

where $m_{\perp}^{*}$ is the in-plane effective mass of the confined particles, L is the well thickness and W is the band offset (the energy difference between the band edges in the well and the barrier). We assume $W = 40$ meV [8], $L = 10$–40 nm and $m_{\perp}^{*} = 0.2m$. For these parameters the condition (8) is well fulfilled.

The size quantization effect can approximately be taken into account by the following substitution in Eq. (5):

$$p_z \to p_n = \frac{\hbar n \pi}{L}\left(1 - \sqrt{\frac{2}{\xi}}\right), \qquad n = 1, 2, 3 \ldots \tag{9}$$

Since the energy depends now on quantum number n, and $p_z \neq 0$ the DP definition of Eq. (7) takes the form

$$\tilde{D}_{\mathrm{c,v}}^{n} = \left.\frac{\partial E_{1,2}^{n}}{\partial \varepsilon}\right|_{\varepsilon = 0, p_{\perp} = 0} \tag{10}$$

and hence for the DPs we obtain

$$\tilde{D}_{\mathrm{c,v}}^{n} = \frac{D_{\mathrm{c}} + D_{\mathrm{v}}}{2} \pm \frac{D_{\mathrm{c}} - D_{\mathrm{v}}}{2\sqrt{1 + \eta^2}}, \tag{11}$$

where

$$\eta = \frac{2 v_z p_n}{E_{\mathrm{g}}\left[1 + \left(\frac{p_n}{p_0}\right)^2\right]}, \qquad p_0^2 = \hat{m}_z^{*} E_{\mathrm{g}}. \tag{12}$$

The plus and minus on the right side of Eq. (11) correspond respectively to the c and v on the left side of that equation. From Eq. (11) one can conclude that for $v_z \to 0$ or $p_n \to 0$ ($L \to \infty$), $\tilde{D}_{\mathrm{c,v}}^{n} = D_{\mathrm{c,v}}$, as it should be. On the other hand, the non-parabolicity of the spectrum ($v_z \neq 0$) makes the DPs in QWs different from their values in the bulk material and mixes up the bulk conduction and valence band DPs. The QW DPs depend both on the energy spectrum of the bulk materials, of which the QW is built up, and parameters of the QW.

The parameter η is proportional to p_n for $p_n \ll p_0$, has a maximum at $p_n = p_0$, and decreases as $2 v_z \hat{m}_z^{*}/p_n$ for $p_n \gg p_0$. To estimate η we can use typical of IV–VI QWs parameters: $v_z \approx 7 \times 10^5$ m/s, $E_{\mathrm{g}} \approx 0.2$ eV, $L = 10$ nm. For this set of parameters and the ground state $n = 1$ one obtains $\eta \approx 0.4$. Parameter η increases with the increase in n. Thus, for excited states the difference between the bulk and the QW DPs further increases. This may be of great importance in the interpretation of optical experiments in strained QWs and SLs. As it follows from Eq. (11) the non-parabolicity influences DPs even more in QWs made of a material with a band inversion, i.e., with $E_{\mathrm{g}} < 0$, as it is in the case of SnTe. The non-parabolicity influence is also more pronounced in thinner QWs.

In conclusion, we predict that in a very narrow QW made for example of SnTe sandwiched between barriers of PbTe, the energy levels of the holes in SnTe will be quite different from that calculated on the basis of the bulk DPs. This is owing to the inapplicability of the bulk DPs to that case. We suggest that the derived QW DPs are relevant to that case.

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