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Transfer-matrix approach to the anisotropy of effective masses in [100] and [111] directions of diatomic crystals*

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Abstract. Recent applications of one-dimensional models with δ-function potentials to the theory of quasicrystals and certain mesoscopic phenomena is a suggestion for other applications of such models. In the present paper effective masses of carriers in diatomic crystals in [111] and [100] crystallographic directions are calculated on the basis of rigorously solvable one-dimensional models of zincblende structures and by using an appropriate transfer-matrix approach. The numerical analysis performed by using the analytically derived expressions leads to particular details rich enough to confirm a new semiempirical rule for the effective masses of both electrons and holes in given families of zincblende semiconductors.

1. Introduction

Effective masses belong the most peculiar characteristics of semiconducting materials; and the anisotropy of the effective masses of heavy holes in $A^{III}B^{V}$ crystals remains still a hot spot in modern experimental research [1, 2], compare also [3]. The corresponding theoretical treatments approach the problem in the framework of more or less sophisticated approximations like e.g. eight-band $\vec{k} \cdot \vec{p}$ calculations (see [1, 4] and references therein) and are in good agreement with the experimental findings, especially as regards (Ga, Al)As structures.

At the same time it is commonly recognised that rigorously solvable one-dimensional models are the basis for understanding the common physics behind various particular results valid for concrete structures [5]. Nowadays, "There are a few happy cases ... in which one can find solvable models rich enough to contain essential features ... and to serve as starting point for gaining control of general situations by suitable approximations" [5].

As regards the one-dimensional models in the effective mass theory, the most general results considering diatomic models of crystals with point interactions were obtained recently in our papers [6, 7] by using the transfer-matrix approach. As a matter of fact, these models correspond to the situation in the [100] crystallographic

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direction in the so-called zincblende structure. It is of certain interest (and this is our aim in the present paper) to perform analogous calculations for the effective masses in [111] direction, which could enable us to evaluate from a most general point of view the anisotropy in the effective masses in the most important directions in such crystals, i.e. the [100] and [111] directions. The starting point for the model under consideration can be traced back to the classical works by Seraphin [8] and Phariseau [9].

2. General considerations

Consider the model of a diatomic crystal with attractive δ-function potentials and lattice constant $2a$. The potential energy of an electron in such a crystal field is given by

$$E_p(x) = -\eta_1 \sum_{n=-\infty}^{\infty} \delta(x-2na) - \eta_2 \sum_{n=-\infty}^{\infty} \delta(x-2na-b) \tag{1}$$

where

$$\eta_i = \frac{a\hbar^2}{m} u_i(2a, p_i), \quad u_i(2a, p_i) = \frac{m}{\hbar^2}\frac{qp_i}{a} > 0, \qquad i = 1, 2 \tag{2}$$

Here η_i is a measure for the strength of the corresponding δ-function potential and, in fact

$$\eta_i = qp_i, \qquad i = 1, 2. \tag{2'}$$

The quantity $u_1 + u_2$ is proportional to the mean electron potential energy averaged over one unit cell, and p_i is measured by the "δ-potential well area" of the i-th atom in a unit cell.

The representative character of one-dimensional models is best seen when working in the framework of the transfer-matrix approach we are using here. The conceptional basis of this is the fact that the leading idea of a transfer matrix is a simple one, namely: "the system is divided into subunits, individual atoms for a 1D system, planes of atoms for a 3D system" [10]. Hence, the one-dimensional "lattice constant" $2a$ is in fact the distance between the two planes of the same kind of atoms in given direction, and b is the distance between two planes, respectively occupied by atoms of different kind (taken into the sense $\eta_1 \to \eta_2$). Thus, the [100] direction in zincblende structure corresponds to the case when $b = a$ (i.e. equidistant diatomic lattice), and the [111] direction is obtained when $b = a/2$ (compare [9]). Of course the one-dimensional lattice constant corresponding to models of different crystallographic orientation will have different value. This is a point we shall turn back in the next section.

As we have shown in [6], the general expression for the effective masses in terms of the corresponding transfer matrix $M(E)$ is given by

$$m^*_{k=0,\frac{\pi}{2a}} = \mp \frac{\hbar^2}{4a^2}\frac{d}{dE}\left[\frac{1}{2} TrM(E)\right] \tag{3}$$

Taking into account the general dispersion relation, derived by Phariseau [9], it is easy to obtain for the [111] crystallographic direction we are here interested in

$$\frac{1}{2} TrM(E) = \cos 2X - \frac{A_1 + A_2}{2X} \sin 2X + \frac{A_1 A_2}{2X^2} \sin \frac{X}{2} \sin \frac{3X}{2} \tag{4}$$

where we have introduced the dimensionless variable

$$X = \frac{a\sqrt{2mE}}{\hbar} \tag{5}$$

and the dimensionless parameters

$$A_i = a^2 u_i(a) = \frac{m}{2\hbar^2} a\eta_i, \qquad i = 1, 2. \tag{6}$$

Here we have taken into account eqs. (2) and (2′) together with (see [6])

$$u_i(2a) = \frac{1}{2} u_i(a), \qquad i = 1, 2.$$

It is not out of place to outline the physical meaning of the above introduced parameters A_i. Obviously, it is desirable to characterise the material by two types of physical quantities: one for the chemical nature of the constituent atoms and another one for the empty lattice of the crystal. For our simplest model the different atoms are represented by different strengths η_i of the δ-function potentials. Thus, A_i count for both the different constituent atoms comprising the crystal and the lattice constant. As it is seen from eq. (4) the energy band structure depends on both parameters A_1 and A_2 in the same manner. Now, from (3) and (4) follows

$$\left(\frac{m^*}{m}\right)_{k=0,\frac{\pi}{2a}} = \pm\left\{\frac{\sin 2X}{2X}\left[1 + \frac{A_1 + A_2}{4X}\left(2 \operatorname{cotg} 2X - \frac{1}{X}\right)\right] + \right.$$

$$\left. + \frac{A_1 A_2}{16X^3} \sin \frac{X}{2} \sin \frac{3X}{2}\left[\frac{4}{X} - \operatorname{cotg} \frac{X}{2} - 3 \operatorname{cotg} \frac{3X}{2}\right]\right\}. \tag{7}$$

For the [100] direction we have (compare [6])

$$\frac{1}{2} TrM(E) = 2 \prod_{i=1}^{2} \left(\cos X - \frac{A_i}{2X} \sin X\right) - 1 \tag{8}$$

and, consequently

$$\left(\frac{m^*}{m}\right)_{k=0,\frac{\pi}{2a}} = \pm \frac{\sin 2X}{2X}\left(1 - \frac{A_1 + A_2 + A_1 A_2}{4X^2} + \right.$$

$$\left. + \frac{A_1 + A_2}{2X} \operatorname{cotg} 2X + \frac{A_1 A_2}{4X^3} \operatorname{tg} X\right) \tag{9}$$

Now we are in a position to evaluate the anisotropy of effective masses comparing the corresponding values in the most important crystallographic directions, namely [100] and [111]. Since the above derived expressions (7) and (9) are

Table 1. Experimental data for the electrons in some zincblende compounds

Compound	ΔE [eV]	$(m_e^*/m)_{[100]}$
after [11]		
InSb	0.265	0.013
In As	0.46	0.022
InP	1.48	0.0812
after [4]		
GaAs	1.430	0.0670
$(Ga_{0.75}Al_{0.25})As$	1.823	0.0942

too cumbersome for an immediate physical interpretation, the next section is devoted to relevant numerical calculations.

It is easy also to observe some interesting empirical relations between the widths of the energy gaps and the effective masses. Consider e.g. a family of zincblende compounds, in which the one element is fixed (say GaAs, (GaAl)As, AlAs). It is easy to observe that the ratio of the energy gaps and the ratio of the effective masses of the heavy holes are relatively close, despite some differences in the different experimental data (compare e.g. [1–4] and references therein). This is a suggestion for the existence of an empirical rule and in the next section we present our numerical calculations which strongly support the validity of such a rule.

Another empirical rule considers the relation between the energy gaps and the effective masses of the electrons in analogous families of zincblende compounds. As it is seen from Table 1, the ratio of the energy gaps approximately equals the ratio of the electron effective masses for certain pairs of zincblende compounds. Our numerical calculations, which confirm this empirical rule and are based on eqs. (8) and (9), are also presented in the next section.

3. Numerical analysis and discussion

The experimental data confirm the presence of anisotropy in the effective masses of (heavy) holes in [100] and [111] directions [1–4], thus in what follows we shall concentrate our attention on the anisotropy in this case.

Of course, one could expect different values of the effective masses in the two directions as an immediate result of the fact that in the [100] direction we have equal spacing between any two adjacent atomic planes, and in the [111] direction this equidistant model has to be replaced with another one, in which the ratio of the two spacings is 1/3. Strictly speaking, there is an additional essential argument which has also to be taken into account, namely: if $2a$ is the lattice constant in the equidistant model, then the lattice constant in the one-dimensional model corresponding to the [111] crystallographic direction is $2a\sqrt{3}$. What is more, on account of eqs. (6) and (2), it is evident that the A_i $(i = 1, 2)$ has to be also replaced by

Table 2. Anisotropy in the effective masses of holes for models with first energy gap

A_1	A_2	$(m_h^*/m)_{[100]}$	$(m_h^*/m)_{[111]}$	$\frac{(m_h^*)_{[111]}}{(m_h^*)_{[100]}}$
0.2	0.1	0.01056	0.04169	3.95
0.4	0.2	0.02205	0.08887	4.03
0.6	0.1	0.05765	0.13298	2.31
0.6	0.3	0.03459	0.14263	4.12
0.6	0.5	0.01153	0.16612	5.73
0.8	0.1	0.08457	0.19270	2.28
0.8	0.3	0.06040	0.19760	3.27
0.8	0.5	0.03624	0.21401	5.90
1.0	0.1	0.11414	0.26421	2.31
1.0	0.3	0.08877	0.26500	2.98

$A_i\sqrt{3}$. Hence, the replacement $2a \to 2a\sqrt{3}$ implies the replacement $A_i \to A_i\sqrt{3}$, a fact we have taken into account by the numerical calculations for the [111] direction.

In Table 2 we present the anisotropy of the effective masses of holes in [100] and [111] crystallographic directions making use of our above derived formulae [9] and (7), respectively. By the calculations we have chosen $2a = 5$ Å.

From Table 2 it is clearly seen that the so calculated effective masses in [111] direction are always greater than those in [100] direction, the ratio being in the interval $2.28 \div 5.90$. Some experimental values for the effective masses of heavy holes in certain zincblende compounds give for this ratio values in the interval $2.05 \div 2.60$ (see e.g. [1–4] and references therein). Hence, there is a surprisingly good qualitiative agreement, especially taking into account the highly simplified models used in our calculations.

It is worth noting that the so calculated effective masses have reasonable values and the best agreement with the experimental data for the anisotropic effect may be obtained when $A_1/A_2 > 5 \Rightarrow \eta_1/\eta_2 > 5$, i.e. when there exists a strong difference between the two constituent atoms.

Table 3. Effective masses of holes in [111] direction for models with first energy gap

$A_1/\sqrt{3}$	$A_2/\sqrt{3}$	$\Delta E_{[111]}$	$(m_h^*/m)_{[111]}$ (theory)	$(m_h^*/m)_{[111]}$ (empirical rule)
0.6	0.1	0.23524	0.13298	
0.6	0.3	0.25071	0.14263	0.14172
0.6	0.5	0.28658	0.16612	0.16200
1.0	0.1	0.41916	0.26421	
1.0	0.3	0.42142	0.26500	0.26563
0.8	0.1	0.32378	0.19270	
0.8	0.3	0.33154	0.19760	0.19732
0.8	0.5	0.35504	0.21401	0.21130

Table 4. Effective masses of holes in [111] direction for models with second energy gap

$A_1/\sqrt{3}$	$A_2/\sqrt{3}$	$\Delta E_{[111]}$	$(m_h^*/m)_{[111]}$ (theory)	$(m_h^*/m)_{[111]}$ (empirical rule)
0.6	0.1	0.18014	0.02318	
0.6	0.3	0.11042	0.01410	0.01421
0.6	0.5	0.04843	0.00616	0.00623
0.8	0.1	0.25277	0.03308	
0.8	0.3	0.18354	0.02384	0.02402
0.8	0.5	0.11783	0.01523	0.01542
1.0	0.1	0.32497	0.04341	
1.0	0.3	0.25649	0.03400	0.03426
1.0	0.5	0.19076	0.02514	0.02548
1.0	0.9	0.10782	0.01423	0.01440
1.7	0.5	0.44027	0.06400	
1.7	1.0	0.32163	0.04645	0.04675
1.7	1.5	0.31916	0.04730	0.04639

The very fact that the ratio of the energy gaps of two zincblende compounds (from one family) approximately equals the ratio of their (heavy) hole effective masses in one and the same crystallographic direction enables us to compute the effective mass in the one compound when the effective mass in the other is known, provided the ratio of the energy gaps is also known.

In Table 3 we present the above mentioned effective masses for a set of model diatomic compounds with first energy gap, calculated both explicitly after our above derived formulae and on the basis of the here introduced empirical rule. The analogous results for models with second energy gap are given in Table 4.

Holes and electrons are treated on the same footing in the simplest one-dimensional models. Thus, it is natural to complete our above considerations with analogical calculations for the effective masses of electrons. Of course, as it is well known, there is no anisotropy in the effective masses of electrons, hence we shall restrict our attention to the effective masses of electrons in [100] direction. As it is evident from Tables 5 and 6, there is a surprisingly good agreement between the exact theoretical values of these effective masses and their relevant counterparts, calculated from the corresponding empirical rule.

Of course, the more sophisticated version of the $\vec{k} \cdot \vec{p}$-theory developed in [4] is more powerful by the description of peculiarities characterising a particular material. But as we have shown, the basic facts may be obtained even by using an appropriate Kronig–Penney model. As regards the above empirical rule, it is in good agreement with the simplest $\vec{k} \cdot \vec{p}$-estimate [12] for the electron effective masses

$$\frac{m}{m^*} \simeq 1 + 2\frac{(\hbar^2/md^2)}{\Delta E},$$

(d is the lattice constant).

Table 5. Effective masses of electrons calculated in [100] direction for models with first energy gap

A_1	A_2	$\Delta E_{[100]}$	$(m_e^*/m)_{[100]}$ (theory)	$(m_e^*/m)_{[100]}$ (empirical rule)
0.6	0.1	0.32737	0.05171	
0.6	0.3	0.20040	0.03236	0.03165
0.6	0.5	0.06817	0.01127	0.01076
1.0	0.3	0.48737	0.07551	
1.0	0.5	0.35513	0.05636	0.05502
1.0	0.8	0.14123	0.02165	0.02188
1.0	0.9	0.07395	0.01237	0.01145
1.7	0.5	0.91702	0.13526	
1.7	1.0	0.56189	0.08877	0.08287
1.7	1.5	0.16875	0.02888	0.02489
1.9	0.1	1.35193	0.18615	
1.9	1.0	0.73858	0.11414	0.10155
1.9	1.8	0.08873	0.01571	0.01222

A more detailed comparison with the particular experimental data seems to be out of place first of all due to the discrepancies between the results obtained by different experimental methods, and secondly because it is rather over the top to expect detailed predictions from a simplest model approach. Nevertheless, a semi-quantitative discussion is possible, e.g. comparing the experimental data from Table 1 with the relevant computed values shown in Table 5. Thus, we arrive at the conclusion that our approach is instructive enough to describe the data for the electron effective masses in InP, InAs and InSb when we attach $A_1 = 1.0$ to the In-atom, the values of A_2 for P-, As- and Sb-atoms being 0.3, 0.8 and 0.9, respectively.

Table 6. Effective masses of electrons calculated in [100] direction for models with second energy gap

A_1	A_2	$\Delta E_{[100]}$	$(m_e^*/m)_{[100]}$ (theory)	$(m_e^*/m)_{[100]}$ (empirical rule)
0.6	0.1	0.43360	0.01773	
0.6	0.3	0.56095	0.02280	0.02293
0.6	0.5	0.68951	0.02786	0.02819
1.0	0.3	0.81614	0.03293	
1.0	0.5	0.94815	0.03780	0.03825
1.0	0.9	1.21573	0.04813	0.04905
1.7	0.5	1.40181	0.05573	
1.7	1.0	1.75621	0.06839	0.06982
1.7	1.5	2.11722	0.08106	0.08417
1.9	0.1	1.25010	0.05066	
1.9	1.0	1.89034	0.07346	0.07660
1.9	1.8	2.48096	0.09372	0.10054

At the end let us point to the fact that it seems really exciting that such details can be discussed at least from a conceptional point of view on the basis of one-dimensional models.

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