PHYSICAL REVIEW B VOLUME 21, NUMBER 12 15 JUNE 1980

Transverse electron effective mass in a semiconductor superlattice

D. Mukherji and B. R. Nag
Center of Advanced Study in Radio Physics and Electronics, 92 Acharya Prafulla Chandra Road, Calcutta-700009 India
(Received 24 August 1979)

An analytical expression involving the electron effective mass in the transverse direction has been obtained for a semiconductor superlattice. Numerical results presented indicate that the transverse mass depends on electron energy, and in most cases has a value close to the energy-dependent electron effective mass in the layer having the smaller band gap.

I. INTRODUCTION

The energy-wave-vector relationship for semiconductor superlattices has been worked out elsewhere by the authors,[1] taking into consideration all the complexities of the band structures of the constituent materials. The electron effective mass in the longitudinal direction may be readily worked out[2] from these expressions. The electron effective mass in the transverse direction has not, however, been worked out explicitly, and discussion on this is not available in the literature. It has so far been tacitly assumed that in these directions, the electron is always characterized by the isotropic mass corresponding to the material with the smaller band gap,[3] usually GaAs. The underlying idea has been that the electron occupies real states only in the GaAs layers, being characterized by imaginary wave vectors in the so-called barrier layers. This concept needs to be examined critically, to determine whether the presence of the alternate barrier layers affects the transverse mass at all. We derive in this note an analytical expression for the electron effective mass in the transverse direction. Numerical results are also given to indicate how far the values differ from the values corresponding to the layers with the lower energy band gap.

II. TRANSVERSE EFFECTIVE MASS IN A SUPERLATTICE

A superlattice is composed of alternate layers of two different materials. Let the material with the smaller band gap be characterized by a conduction-band edge E_{c1}, a band-edge effective mass m_1^*, and electron wave vectors k_1 and $k_\perp$ in the longitudinal and transverse directions. Then the total electron energy E, measured from E_{c1} is given by

$$E=\frac{\hbar^2k_1^2}{2m_1^*f_1(E)}+\frac{\hbar^2k_\perp^2}{2m_1^*f_1(E)}\,, \tag{1}$$

where the factor $f_1(E)=(1+\alpha_1E)$ is introduced to account for the nonparabolic relation between the energy and the wave vector; $\alpha_1={}^1/E_{G1}$, where E_{G1} is the direct band gap for the material.[4] Let the conduction band edge and band-edge effective mass in the second layer (the so-called barrier layer) be E_{c2} and m_2^*, and let k_2 be the electron wave vector in the longitudinal direction in this layer. Since the total energy E and the transverse wave vector $k_\perp$ are conserved when an electron moves across the layers, we have

$$E_{c1}+E=\frac{\hbar^2k_2^2}{2m_2^*f_2(E)}+\frac{\hbar^2k_\perp^2}{2m_2^*f_2(E)}+E_{c2}\,, \tag{2}$$

where $f_2(E)=1+\alpha_2(E_{c1}+E-E_{c2})$ is the factor due to nonparabolicity,[5,6] with $\alpha_2=1/E_{G2}$, where E_{G2} is the direct band gap in the second material.[7]

Rearranging (1) and (2), we get

$$k_1=[(2m_1^*/\hbar^2)E(1+\alpha_1E)-k_\perp^2]^{1/2}, \tag{3}$$

and

$$K_2=ik_2=\{(2m_2^*/\hbar^2)[1-\alpha_2(V-E)](V-E)+k_\perp^2\}^{1/2}, \tag{4}$$

where $V=(E_{c2}-E_{c1})$ is the potential barrier encountered by the electron.

The electron wave functions in layers 1 and 2 may be expressed as

$$\psi_1(z)=A\exp[ik_1(z-a)]+B\exp[-ik_1(z-a)]\,, \tag{5}$$

and

$$\psi_2(z)=C\exp[K_2(z-d)]+D\exp[-K_2(z-d)]\,, \tag{6}$$

where a and b denote the widths of layers 1 and 2 and $d=(a+b)$ is the superlattice periodicity. The superlattice wave vector k is introduced through the relation

$$\psi_3(z)=\psi_1(z-d)\exp(ikd)\,, \tag{7}$$

where ψ_3 is the electron wave function in the third layer (identical to the first layer, but separated from it by d).

 © 1980 The American Physical Society

The disperation relation for the superlattice is obtained by matching the wave functions and their derivatives at the layer boundaries, and takes the form

$$\frac{K_2^2-k_1^2}{2k_1K_2}\sinh(K_2b)\sin(k_1a)+\cosh(K_2b)\cos(k_1a)=\cos(kd)\,. \quad (8)$$

It should be pointed out that (8) is identical in form to the expression obtained earlier,[1] but here it becomes the complete dispersion relation for the superlattice, since (3) and (4) involve the total energy E including that arising from the transverse wave vector.

The electron effective mass in the transverse direction is, by definition, given as

$$m_\perp^*=\left[\frac{1}{\hbar^2k_\perp}\frac{\partial E}{\partial k_\perp}\right]^{-1}\,. \quad (9)$$

Equation (8) may, therefore, be differentiated to yield

$$\frac{K_2^2+k_1^2}{2k_1K_2}\left[\frac{K_2}{k_1}\left(\frac{m_1^*\delta_1}{m_\perp^*}-1\right)+\frac{k_1}{K_2}\left(\frac{m_2^*\delta_2}{m_\perp^*}-1\right)\right]\sinh(K_2b)\sin(k_1a)$$
$$+\frac{K_2^2-k_1^2}{2k_1K_2}\left[\left(\frac{m_2^*\delta_2}{m_\perp^*}-1\right)k_1b\cosh(K_2b)\sin(k_1a)-\left(\frac{m_1^*\delta_1}{m_\perp^*}-1\right)K_2a\sinh(K_2b)\cos(k_1a)\right]$$
$$+\left[\left(\frac{m_2^*\delta_2}{m_\perp^*}-1\right)k_1b\sinh(K_2b)\cos(k_1a)+\left(\frac{m_1^*\delta_1}{m_\perp^*}-1\right)K_2a\cosh(K_2b)\sin(k_1a)\right]=0\,, \quad (10)$$

where $\delta_1=(1+2\alpha_1E)$ and $\delta_2=[1-2\alpha_2(V-E)]$. It is clear that (10) can only be solved numerically, and this has been done for a typical superlattice structure in the next section.

III. ESTIMATION OF TRANSVERSE MASS

A direct consequence of Eq. (8) is that the conduction band above E_{c1} is split up into a number of minibands. It can also be shown that in all cases of practical importance (with regard to electron concentration and temperature) only the lowermost miniband is likely to be occupied. We therefore present results for the first miniband only in a superlattice structure consisting of 50-Å-wide GaAs layers alternating with 10-Å-wide AlAs layers. The effective masses and bandgaps for these layers are $0.067m_0$, $0.15m_0$, 1500 meV, and 2860 meV, respectively. The transverse mass is worked out as a function of electron energy in two cases, viz., $V=500$ (Fig. 1) and 1100 meV (Fig. 2).[8] The curves (a) in the two figures denote $m_\perp^*$ when the effective masses in the individual layers are considered to be independent of energy, i.e., $\alpha_1=\alpha_2=0$. It is seen that (i) $m_\perp^*$ is different from m_1^* and the maximum difference of about 7 % occurs for the lower barrier at the lower miniband edge. The difference between $m_\perp^*$ and m_1^* also decreases with increasing barrier height. (ii) $m_\perp^*$ decreases with increasing electron energy.

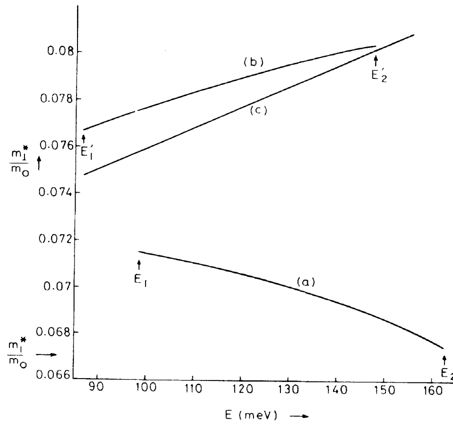

FIG. 1. $m_\perp^*$ as a function of E, with $V=500$ meV: (a) effective masses in layers assumed energy independent, (b) effective masses in layers assumed energy dependent, (c) $m_\perp^*(1+2\alpha_1E)$. E_1, E_2, E_1', and E_2' are the miniband edges for parabolic and nonparabolic cases.

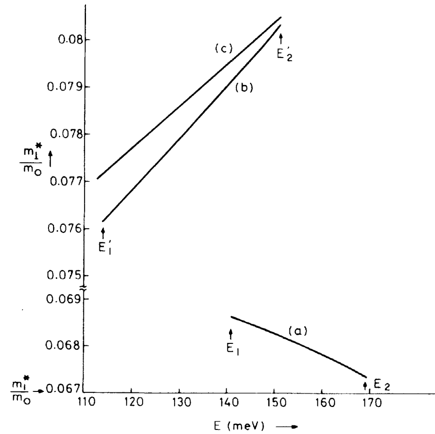

FIG. 2. $m_\perp^*$ as a function of E, with $V=1100$ meV; (a) effective masses in layers assumed energy independent, (b) effective masses in layers assumed energy dependent, (c) $m_\perp^*(1+2\alpha_1E)$. E_1, E_2, E_1', and E_2' are the miniband edges for parabolic and nonparabolic cases.

The energy dependence of the isotropic effective masses in the individual layers is important in superlattice structures because the electron energies encountered in the minibands are usually quite far from E_{c1} and E_{c2}. The values of $m_\perp^*$ when this dependence is taken into account are shown by the curves (b). For comparison with the corresponding energy dependent effective mass in the first layer, the quantity $m_1^*(1+2\alpha_1 E)$ is also shown alongside [curves (c)]. It is seen that $m_\perp^*$ differs from the effective mass in the first layer by about $\pm.002 m_0$ for the system considered. The difference is also found to increase with decrease in the barrier height.

It is interesting to note that whereas $m_\perp^*$ is greater then the energy-dependent effective mass in the first layer for a low barrier, the situation is reversed for a high barrier. This happens because the energy dependence of the effective mass in the barrier layer always causes it to be smaller than m_2^* for the energies considered ($E < V$). As the barrier height increases, the effective mass in the second layer gets further reduced for the same energy, until for large barriers this mass actually becomes less than the effective mass in the first layer. In this situation, the contribution of the second layer is to reduce $m_\perp^*$ to a value smaller than the effective mass in the first layer.

IV. CONCLUSION

We have obtained an analytical expression for the effective mass in the transverse direction in a semiconductor superlattice, beginning with the dispersion relation for the superlattice. Numerical solution of the expression indicates that the transverse mass represents a complex average over the effective masses in the individual superlattice layers. The mechanism of this averaging process involves the electron energy, probably as a consequence of the fact that the nature of the transit of the electron through the barrier layer depends on its energy. The value of the transverse mass is, in general fairly close to the effective mass in the layer with the smaller band gap.

---

[1] D. Mukherji and B. R. Nag, Phys. Rev. B 12, 4338 (1975).

[2] D. Mukherji and B. R. Nag, Phys. Status Solidi B 75, K35 (1976).

[3] A. Ya. Shik, Sov. Phys. Semicond. 8, 1195 (1975).

[4] E. O. Kane, J. Phys. Chem. Solids 1, 249 (1957).

[5] W. P. Dumke, Phys. Rev. B 2, 987 (1970).

[6] G. Lewicki and C. A. Mead, J. Phys. Chem. Solids 29, 1255 (1968).

[7] Although the Γ-point minimum is not the lowest in materials like AlAs, used as the barrier layer in superlattice structures, it has been shown by the authors with the help of a tunneling formalism that only the electron states corresponding to the Γ-point minimum in such cases are responsible for the formation of minibands. D. Mukherji and B. R. Nag, Solid-State Electron. 21, 555 (1978).

[8] The proper choice for the barrier height in GaAs and AlAs structures has been dealt with in Ref. 7.