Effective-mass superlattice

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(Received 28 February 1984)

A new type of superlattice which is constructed with a periodic modulation of effective mass is proposed. Candidate materials for this superlattice are presented. The analysis shows that there exist continuously electronic subbands in real space.

I. INTRODUCTION

There has long been much interest in physics and electronics of synthesized semiconductors which consist of alternating ultrathin layers with its period less than the electron mean free path, i.e., semiconductor superlattices. Two types of superlattices were initially proposed and have both been investigated.[1-3] The compositional superlattices are constructed with a periodic modulation of composition, such as AlGaAs/GaAs, and the doping superlattice with a periodic modulation of space charge by ionized impurity such as *n-i-p-i* crystals. In either type of superlattice, the periodic variation of potential typically exists in both the conduction and valence bands. Thus, the electronic subbands appear periodically in real space.

This paper will propose a new type of superlattice where the electronic subbands appear continuously in real space. This superlattice is constructed with a periodic modulation of effective mass, but no modulation of the electron affinity and the work function. It can be called the effective-mass superlattice or mass-modulation superlattice. Candidate materials for this superlattice, as well as an analysis for the electronic subbands, are presented and discussed.

II. EFFECTIVE-MASS SUPERLATTICE

Although the lattice-constant match is not required for a strained-layer superlattice,[4,5] we take the matching condition into account to facilitate the fabrication of the effective-mass superlattice. The built-in potential does not appear in the conduction band when neither the electron affinity nor the work function changes from one layer to another.

It is difficult to select the proper semiconductor layers useful for the fabrication of effective-mass superlattices, since the values of some physical parameter of AlP are not readily available. Some material properties of III-V compound semiconductors are listed in Table I. The values of AlP were calculated by the extrapolation with respect to the band gaps of AlAs and AlSb. Referring to the band structure and lattice-constant chart of III-V semiconductors,[6] we can suggest the following pairs of semiconductor layers for the effective-mass superlattice:

TABLE I. Material properties of III-V compound semiconductors. Parenthetical values are of the estimation from the proportionality variation with respect to band gaps of Al-group compounds.

Semiconductor	χ (eV)	m_l/m_e[g]	Minimum valley	Band gap (eV)	Lattice constant (Å)
AlP	(3.44)	(0.56)	X	2.46	5.4625
AlAs	3.5[a]	0.5	X	2.16	5.6611
AlSb	3.6[b]	0.39	X,L	1.63	6.1355
GaP	4.0[c]	0.35	X	2.26	5.4495
GaAs	4.07[d]	0.07	Γ	1.43	5.653
GaSb	4.06[c]	0.049	Γ	0.721	6.094
InP	4.40[e]	0.073	Γ	1.34	5.868
InAs	4.55[f]	0.027	Γ	0.359	6.058
InSb	4.59[c]	0.0135	Γ	0.175	6.478

[a]A. G. Milnes and D. L. Feucht, *Heterojunctions and Metal-Semiconductor Junctions* (Academic, New York, 1972), p. 9.
[b]T. E. Fischer, Phys. Rev. **139**, A1228 (1965).
[c]A. M. Cowley and S. M. Sze, J. Appl. Phys. **36**, 3212 (1965).
[d]G. W. Gobeli and F. G. Allen, Phys. Rev. **137**, A245 (1965).
[e]T. E. Fischer, Phys. Rev. **142**, 519 (1966).
[f]T. E. Fischer, F. G. Allen, and G. W. Gobeli, Phys. Rev. **163**, 703 (1967).
[g]M. Neuberger, *III-V Semiconducting Compounds* (Plenum, New York, 1971).

TABLE II. Examples of semiconductor layers for the effective-mass superlattice.

Semiconductors	a (Å)	χ (eV)	ϵ_g (eV)	$m_{2,1}/m_e$	m_2/m_1	Figure
$Al_{0.23}Ga_{0.3}In_{0.47}P$	5.653	(4.07)	(2.13)	m_2/m_e (0.13) (0.4)	1.9 5.7	1(a)
$Ga_{0.86}In_{0.14}P_{0.78}Sb_{0.22}$	5.653	(4.07)	(1.89)	m_2/m_e (0.4)	5.7	1(b)
GaAs	5.653	4.07	1.43	m_1/m_e 0.07		1(a) 1(b)
$Al_{0.5}In_{0.5}As_{0.49}Sb_{0.51}$	6.094	(4.06)	(1.3)	m_2/m_e (0.067)	1.4	1(c)
GaSb	6.094	4.06	0.721	m_1/m_e 0.049		1(c)
$Al_{0.12}Ga_{0.61}In_{0.27}P$	5.572	(4.04)	(2.2)	m_2/m_e (0.4)	4.2	5
$GaAs_{0.6}P_{0.4}$	5.572	(4.04)	(1.9)	m_1/m_e (0.095)		5

(i) $Al_{0.23}Ga_{0.3}In_{0.47}P/GaAs$,

(ii) $Ga_{0.86}In_{0.14}P_{0.78}Sb_{0.22}/GaAs$,

and

(iii) $Al_{0.5}In_{0.5}As_{0.49}Sb_{0.51}/GaSb$,

where the lattice constant and electron affinity are matched for each pair. Other estimated values are summarized in Table II. In Fig. 1 each cross point of the lattice-constant line (single-dot—dashed line) with the electron-affinity line (double-dot—dashed line) indicates candidate material for effective-mass by combination with GaAs in (a) and (b), and with GaSb in (c).

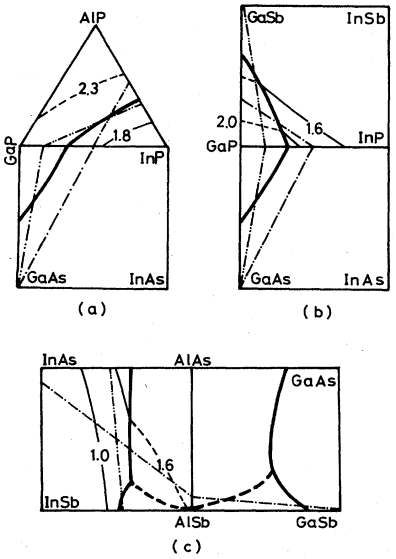

FIG. 1. Material examples for the effective-mass superlattice. Bold-solid line: border of Γ and X (or L) valleys; Bold-dashed line: border of X and L valleys; Solid line: equal band gap of Γ valley; Dashed line: equal band gap of X valley; Single-dot—dashed line: equal lattice-constant line; Double-dot—dashed line: equal electron-affinity line. (a), $Al_{0.23}Ga_{0.3}In_{0.47}P/GaAs$; (b), $Ga_{0.86}In_{0.14}P_{0.78}Sb_{0.22}/GaAs$; (c), $Al_{0.5}In_{0.5}As_{0.49}Sb_{0.51}/GaSb$.

Since the values of effective masses in L and X valleys of AlP and GaSb are not known, we assume that the effective mass of an indirect-band-gap semiconductor is $0.4m_e$, where m_e is the rest mass of a free electron. The band structure, with a direct- or indirect-band gap of $Al_{0.23}Ga_{0.3}In_{0.47}P$ is known with certainty in the present material values, and thus effective masses of both cases are listed. As cited in Table II for the candidate materials for the effective-mass superlattice, we could expect to achieve a mass ratio in the range $m_2/m_1=1.4$—5.7.

III. ELECTRONIC SUBBANDS

To derive electronic subbands in the effective-mass superlattice, we use the Kronig-Penny model.[7] A schematic figure for the effective-mass superlattice is shown in Fig. 2, where the layer thicknesses for the effective mass m_1 and m_2 ($\neq m_1$) are a and b, respectively. These two layers are assumed in the analysis to be infinitely repeated.

The wave functions for an electron are given by

$$\psi_1(x)=K_1e^{i\alpha x}+K_2e^{-i\alpha x} \quad \text{for } 0<x<a \ , \tag{1a}$$

where

$$\alpha\equiv\frac{(2m_1\epsilon)^{1/2}}{\hbar} \tag{1b}$$

and

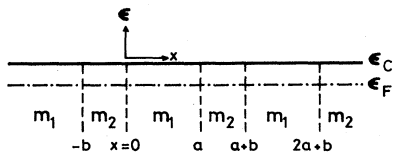

FIG. 2. Schematic figure of the effective-mass superlattice where the effective masses m_1 and m_2 are not equal, $m_1\neq m_2$.

$$\psi_2(x)=K_3e^{i\beta x}+K_4e^{-i\beta x} \text{ for } -b<x<0 , \tag{2a}$$

where

$$\beta=\frac{(2m_2\epsilon)^{1/2}}{\hbar} . \tag{2b}$$

Here, K_1, K_2, K_3, and K_4 are determined by the boundary conditions[8,9]

$$\psi_1(0)=\psi_2(0) \text{ and } \frac{1}{m_1}\frac{d\psi_1}{dx}\bigg|_0=\frac{1}{m_2}\frac{d\psi_2}{dx}\bigg|_0 , \tag{3a}$$

$$\psi_1(a)=\psi_2(-b)e^{ik(a+b)}$$

and (3b)

$$\frac{1}{m_1}\frac{d\psi_1}{dx}\bigg|_a=\frac{1}{m_2}\frac{d\psi_2}{dx}\bigg|_{-b}e^{ik(a+b)} ,$$

where k denotes the wave number along the x direction.

From Eqs. (1), (2), and (3) we can derive the equation for the energy ϵ versus the momentum $\hbar k$:

$$A\cos(\alpha a+\beta b)-B\cos(\alpha a-\beta b)=\cos[k(a+b)] , \tag{4a}$$

where

$$A\equiv\frac{[(m_2/m_1)^{1/2}+1]^2}{4(m_2/m_1)^{1/2}} , \tag{4b}$$

$$B\equiv\frac{[(m_2/m_1)^{1/2}-1]^2}{4(m_2/m_1)^{1/2}} . \tag{4c}$$

The effective mass of a transit electron perpendicular to the multilayer surface, i.e., the x direction is given by

$$\frac{m^*}{(m_1m_2)^{1/2}}=\frac{1}{\alpha\beta(a+b)^2}\frac{g^3(\epsilon)}{f(\epsilon)g^2(\epsilon)+[1-f^2(\epsilon)]g(\epsilon)-[1-f^2(\epsilon)]h(\epsilon)} , \tag{5a}$$

where

$$f(\epsilon)=A\cos(\alpha a+\beta b)-B\cos(\alpha a-\beta b) , \tag{5b}$$

$$g(\epsilon)=A(\alpha a+\beta b)\sin(\alpha a+\beta b)-B(\alpha a-\beta b)\sin(\alpha a-\beta b) , \tag{5c}$$

$$h(\epsilon)=A(\alpha a+\beta b)^2\cos(\alpha a+\beta b)-B(\alpha a-\beta b)^2\cos(\alpha a-\beta b) . \tag{5d}$$

Here, the energy available is restricted in the range satisfying Eq. (4).

To see the electronic subbands in the effective-mass superlattice, we calculate them for the case

$$\frac{a}{b}=\left[\frac{m_2}{m_1}\right]^{1/2} \text{ or } \alpha a=\beta b , \tag{6}$$

that is, the layer-thickness ratio equals the square root of the effective-mass ratio. Equation (4a) becomes

$$A\cos(2\alpha a)-B=\cos\left\{ka\left[1+\left[\frac{m_2}{m_1}\right]^{1/2}\right]\right\} . \tag{7}$$

The results are shown in Figs. 3 and 4. The band gap between the ground state and the first excited state becomes wider with the increase in the effective-mass ratio. As shown in Fig. 4, the effective mass near the bottom of the first excited state becomes smaller than either of m_1 and m_2.

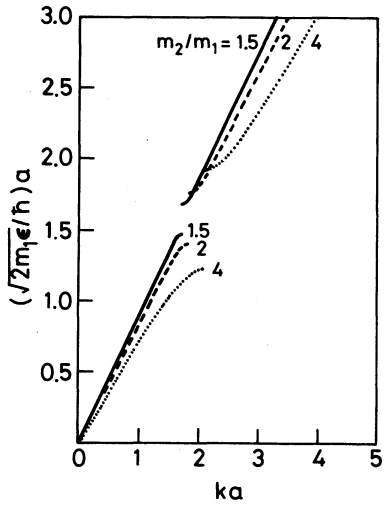

FIG. 3. Electronic subbands of effective-mass superlattice where the layer-thickness ratio equals the square root of the effective-mass ratio, $a/b=(m_2/m_1)^{1/2}$. The greater mass ratio produces the wider band gap.

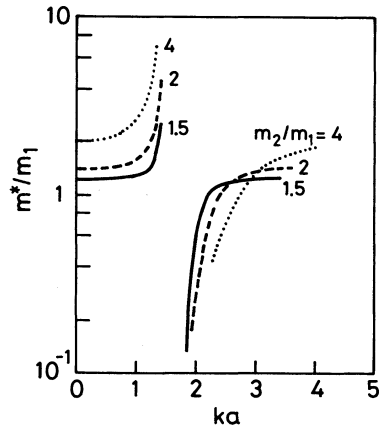

FIG. 4. The effective mass m^* of the effective-mass superlattice for $a/b=(m_2/m_1)^{1/2}$. At the bottom of a ground state, $m^*=(m_1m_2)^{1/2}$. Near the bottom of a first excited state, m^* becomes less than m_1 ($<m_2$).

IV. DISCUSSION

The band gap between the ground state and the first excited state is calculated with respect to the layer thickness a for the effective mass $m_1 = 0.07m_e$ of GaAs. As can be seen in Fig. 5, the gap larger than 6.4 meV ($T = 77$ K) can be expected. The layer thickness a becomes larger for the given energy gap, as the effective-mass ratio becomes greater. However, the layer thickness b for the effective mass m_2 is less dependent on the effective-mass ratio from 4 to 1.5, i.e., $b \sim 65$ Å at 6.4 meV.

As can be confirmed in Eq. (4a), we can obtain the maximum energy gap with the condition $\alpha a = \beta b$ for the sum $(\alpha a + \beta b)$ constant. The A and B in Eq. (7) are independent of the energy as can be seen in Eqs. (4b) and (4c). The variation of energy against the momentum $\hbar k$ is repeated for every 2π of $2\alpha a$. Thus, all energy gaps are equal for the constant effective-mass ratio. This could be an interesting characteristic for device applications.

To have a high effective-mass ratio, it is favorable to combine a direct-band-gap semiconductor layer with an indirect-band-gap semiconductor layer. The use of $GaAs_{0.6}P_{0.4}$, which is generally used for a light-emitting diode, must be combined with $Al_{0.12}Ga_{0.61}In_{0.27}P$, which definitely has an indirect-band gap as shown in Fig. 6. Their properties are given in Table II. In the layer system of $Al_{0.5}In_{0.5}As_{0.49}Sb_{0.51}/GaSb$, the use of $Al_{0.22}Ga_{0.78}Sb$ in place of GaSb decreases the electron affinity. It would be possible to combine an indirect-band-gap AlInAsSb layer with a direct-band-gap $Al_xGa_{1-x}Sb$ ($x \lesssim 0.23$) layer for the superlattice. However, the different locations of the conduction minima in a momentum space, Γ—X or Γ—L, has not been taken into account in the analytical process. It was points out in a theoretical study of electron transport that the electron coupling probability from Γ (X) states to $X(\Gamma)$ states is poor when compared with Γ-Γ state coupling.[4,10,11] Thus, the effective-mass superlattice of the direct-indirect combination would be less useful in a practical application involving the applied field perpendicular to the heterointerface, but parallel to it there would be some applications resulting from the real-space transfer.[12]

To provide more definite statements about the layer combinations for the effective-mass superlattice, we need more detailed physical parameter values of the candidate materials. This effective-mass superlattice can be produced for holes in the valence band by using the semiconductors with an equal sum of the electron affinity and the band gap and with equal work function. However, the effective-mass ratio of holes would be less than that of electrons. For further study, the effective-mass superlattice must be analyzed by taking into account the effect of the difference in the density of states for electron distribution which would shift the Fermi level.

V. CONCLUSIONS

It was proposed in this paper that a new superlattice can be constructed by varying effective masses periodically rather than the potentials. In this superlattice, which can be called the effective-mass superlattice, electronic subbands exist continuously in real space, in contrast to previous superlattices in which the subbands exist periodically.

Some material examples for the superlattice have been presented as listed in Table II. The analysis has proven (i) the existence of subbands, (ii) the energy gap larger than the energy of either 77 K or room temperature can be

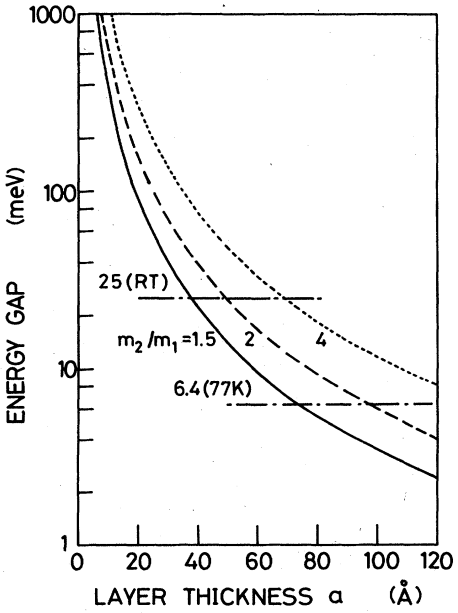

FIG. 5. Energy gap in electronic subbands of the effective-mass superlattice for the case of $a/b = (m_2/m_1)^{1/2}$ and $m_1 = 0.07m_e$ of GaAs.

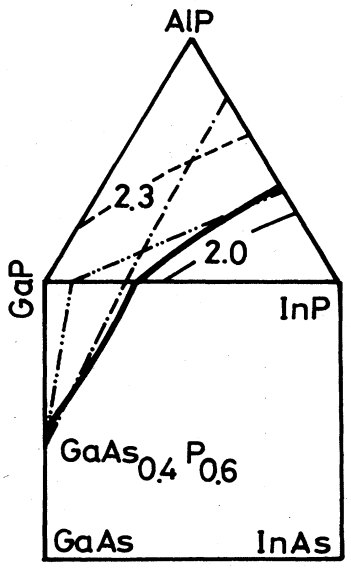

FIG. 6. Effective-mass superlattice by $Al_{0.12}Ga_{0.61}In_{0.27}P$ (indirect) and $GaAs_{0.6}P_{0.4}$ (direct). See Fig. 1 for description of lines.

created between electronic subbands, and (iii) energy variation is repeated for every 2π of $2\alpha a$ for the case $\alpha a = \beta b$, so that a constant effective-mass ratio leads to equal subband energy gaps. These equal gaps could be interesting in electronic applications.

ACKNOWLEDGMENTS

The author wishes to express his deep appreciation to Dr. Shigeo Fujita and Dr. Yoshikazu Takeda for stimulating discussions.

[1]L. Esaki and R. Tsu, IBM J. Res. Dev. **14**, 61 (1970).
[2]G. H. Döhler, Phys. Status Solidi B **52**, 79 (1972).
[3]See L. L. Chang, in *Proceedings of the 4th Molecular Beam Epitaxy Workshop,* edited by H. Morkoç [J. Vac. Sci. Technol. B **1**, 120 (1983)], as a recent review paper.
[4]G. C. Osbourn, J. Appl. Phys. **53**, 1586 (1982).
[5]G. C. Osbourn, R. M. Biefeld, and P. L. Gourley, Appl. Phys. Lett. **41**, 172 (1982).
[6]A. Sasaki, M. Nishiuma, and Y. Takeda, Jpn. J. Appl. Phys. **19**, 1695 (1980).
[7]R. de L. Kronig and W. J. Penny, Proc. R. Soc. London Ser. A **130**, 499 (1930).
[8]W. A. Harrison, Phys. Rev. **123**, 85 (1961).
[9]D. J. BenDaniel and C. B. Duke, Phys. Rev. **152**, 683 (1966).
[10]G. C. Osbourn, J. Appl. Phys. **53**, 1586 (1982).
[11]G. C. Osbourn and D. L. Smith, Phys. Rev. B **19**, 2124 (1979).
[12]K. Hess, H. Morkoc, H. Schichijo, and B. G. Streetman, Appl. Phys. Lett. **35**, 469 (1979).