The density of states and dielectric constant of monolayer superlattice $Ga_{0.47}In_{0.53}As/InP(110)$

1989 J. Phys.: Condens. Matter 1 3551

(http://iopscience.iop.org/0953-8984/1/22/013)

J. Phys.: Condens. Matter 1 (1989) 3551–3554. Printed in the UK

LETTER TO THE EDITOR

The density of states and dielectric constant of monolayer superlattice $Ga_{0.47}In_{0.53}As/InP(110)$

Zhizhong Xu
Department of Physics, Fudan University, Shanghai, People's Republic of China

Received 17 January 1989

Abstract. The DOS, JDOS and $\varepsilon_2(\Omega)$ of monolayer superlattice $Ga_{0.47}In_{0.53}As/InP(110)$ have been calculated using the tight-binding approach and compared with those of alloy $Ga_{0.235}In_{0.765}P_{0.5}As_{0.5}$, which has the same stoichiometric composition as the monolayer superlattice. The effects of the superlattice periodicity on the electronic structure and optical properties of materials are discussed. The roles played by momentum matrix elements in the superlattices and alloys are pointed out.

A considerable amount of research has been done on the electronic structures and optical properties of superlattices (Chang and Schulman 1985, Ninno *et al* 1986, Gell *et al* 1987, Sander and Chang 1987, Sander and Baja 1987). Most of them have concentrated on the structure near the band edges. We have calculated the density of state (DOS) and the imaginary part of dielectric constant $\varepsilon_2(\Omega)$ of the monolayer superlattice $Ga_{0.47}In_{0.53}As/InP(110)$ in the whole Brillouin zone and compared these results with those of the alloy $Ga_{0.235}In_{0.765}P_{0.5}As_{0.5}$, which has the same stoichiometric composition as the monolayer superlattice, in order to show the influence of the superlattice periodicity on the electronic structures and optical properties of superlattices. Chang and Schulman (1985) have shown that the momentum matrix elements play important roles in determining the optical constants of superlattices. We have also calculated the joint density of state (JDOS) for these two materials and point out the different effects of the momentum matrix elements.

The imaginary part of dielectric constant can be given by the expression (Ehrenreich and Philips 1962)

$$\varepsilon_2(\Omega) = (4\pi^2e^2)(m\Omega)^{-2}\left(\sum_{jn}\int_{BZ}[2/(2\pi)^3]\,d\boldsymbol{k}|\langle j\boldsymbol{k}|\boldsymbol{e}\cdot\boldsymbol{p}|n\boldsymbol{k}\rangle|^2\right)$$
$$\times\,\delta(E_j(\boldsymbol{k}) - E_n(\boldsymbol{k}) - \hbar\Omega). \tag{1}$$

Here m and e are the mass and charge of electrons. The summation is taken over all occupied states n and unoccupied states j, and the integral is confined in the Brillouin

0953-8984/89/223551 + 04 $02.50

zone. $\boldsymbol{e}$ gives the direction of polarisation. If the momentum matrix elements $\langle j\boldsymbol{k}|\boldsymbol{e}\cdot\boldsymbol{p}|n\boldsymbol{k}\rangle$ are taken as constants, $\varepsilon_2(\Omega)$ can be approximated by the expression

$$\varepsilon_2(\Omega) = (A/\Omega^2)J(\Omega) \tag{2}$$

where

$$J(\Omega) = \left(\sum_{jn}\int_{\mathrm{BZ}} [2/(2\pi)^3]\,\mathrm{d}\boldsymbol{k}\right)\delta(E_j(\boldsymbol{k}) - E_n(\boldsymbol{k}) - \hbar\Omega) \tag{3}$$

is the joint density of state, and A is a constant including the momentum matrix elements.

The slab model with supercell is applied to the monolayer superlattice. All calculations are carried out using the tight-binding method proposed by Vogl *et al* (1983). For alloys, we have used the virtual crystal approximation, and a non-linear correction (Mbaye and Verle 1984) is made. The integrals in (1) are evaluated with the method suggested by Gilat and Raubenheimer (1965), and by taking 408 sampling points within the irreducible $\frac{1}{48}$ Brillouin zone for alloys and 245 points within $\frac{1}{8}$ Brillouin zone for superlattices. The summations are taken over three valence bands and five conduction bands.

In the tight-binding method, the wavefunction $\psi_{n\boldsymbol{k}}(\boldsymbol{r})$ is written as

$$\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = \sum_{\beta\mu} C_{\beta\mu}(n,\boldsymbol{k})\varphi_{\beta\mu}(\boldsymbol{k},\boldsymbol{r}) \tag{4}$$

where

$$\varphi_{\beta\mu}(\boldsymbol{k},\boldsymbol{r}) = (N)^{1/2}\sum_{m}\exp[\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}_m - \boldsymbol{t}_\beta)]a_{\beta\mu}(\boldsymbol{r} - \boldsymbol{R}_m - \boldsymbol{t}_\beta) \tag{5}$$

is the Bloch sum. Here $a_{\beta\mu}(\boldsymbol{r} - \boldsymbol{R}_m - \boldsymbol{t}_\beta)$ is the wavefunction of the electron in the μ state of β atom which is situated in the mth cell. If the momentum matrix elements between two different atoms $\langle a_{\beta\mu}(\boldsymbol{r})|\boldsymbol{p}|a_{\beta'\mu'}(\boldsymbol{r} - \boldsymbol{R}_m - \boldsymbol{t}_{\beta'})\rangle$ are neglected in tight-binding approximation, we can obtain the expression

$$\langle n\boldsymbol{k}|\boldsymbol{p}|n'\boldsymbol{k}'\rangle = \sum_{\beta}\sum_{\mu\mu'} C_{\beta\mu}(n,\boldsymbol{k})^* C_{\beta\mu'}(n\boldsymbol{k}')\boldsymbol{P}^{\beta}_{\mu\mu'} \tag{6}$$

with

$$P^{\beta}_{\mu\mu'} = \int a_{\beta\mu}(\boldsymbol{r})^*\boldsymbol{p}a_{\beta\mu'}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}. \tag{7}$$

The Wigner–Eckart theorem (Tinkham 1964) is applied to (7) and we obtain the expressions from (6)

$$\begin{aligned}\langle n\boldsymbol{k}|p_x|n'\boldsymbol{k}'\rangle = \sum_{\beta}\,[&(C_{\beta s}(n,\boldsymbol{k})^* C_{\beta p_x}(n'\boldsymbol{k}') + C_{\beta p_x}(n,\boldsymbol{k})^* C_{\beta s}(n',\boldsymbol{k}'))T^{\beta}_{10}\\ &+ \mathrm{i}(C_{\beta p_z}(n,\boldsymbol{k})^* C_{\beta p_y}(n',\boldsymbol{k}') - C_{\beta p_y}(n,\boldsymbol{k})^* C_{\beta p_z}(n',\boldsymbol{k}'))T^{\beta}_{11}\\ &+ (C_{\beta s^*}(n,\boldsymbol{k})^* C_{\beta p_x}(n',\boldsymbol{k}') + C_{\beta p_x}(n,\boldsymbol{k})^* C_{\beta s^*}(n',\boldsymbol{k}'))^* T^{\beta}_{10}]\end{aligned} \tag{8}$$

and other similar expressions for p_y and p_z. Here, $T^{\beta}_{ll'}(T^{\beta}_{10}, T^{\beta}_{11}, {}^*T^{\beta}_{10})$ are the reduced matrix elements that are independent of the magnetic quantum numbers but only dependent on the azimuthal quantum numbers l, l'. Considering that the momentum $\boldsymbol{p}$ is a polar vector, the momentum matrix elements between two atomic states with the

Table 1. The values of adjustable parameters $T^{\beta}_{ll'}$.

	T^{a}_{10}	$^{*}T^{a}_{10}$	T^{c}_{10}	$^{*}T^{c}_{10}$
GaAs	9.98	11.09	11.09	4.43
InP	23.66	13.26	1.02	5.10
InAs	24.19	7.44	0.93	7.44

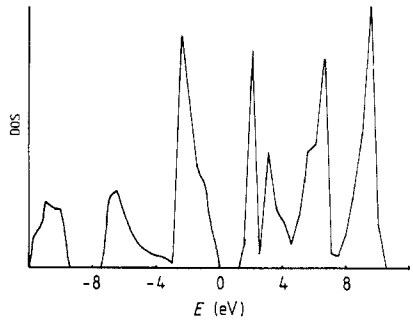

Figure 1. The DOS of monolayer superlattice $Ga_{0.47}In_{0.53}As/InP(110)$.

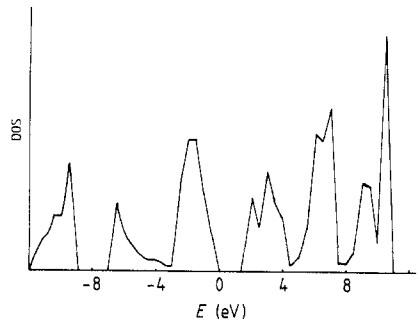

Figure 2. The DOS of alloy $Ga_{0.235}In_{0.765}P_{0.5}As_{0.5}$.

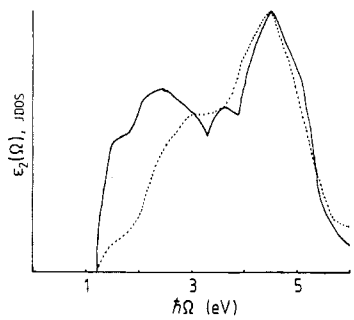

Figure 3. The $\varepsilon_2(\Omega)$ and JDOS of monolayer superlattice $Ga_{0.47}In_{0.53}As/InP(110)$. The full curve shows $\varepsilon_2(\Omega)$ and the broken curve shows JDOS.

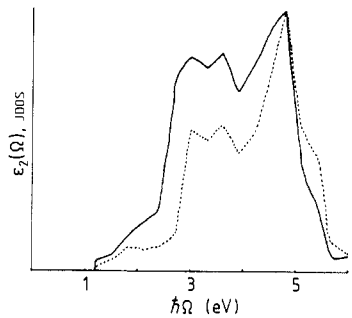

Figure 4. The $\varepsilon_2(\Omega)$ and JDOS of alloy $Ga_{0.235}In_{0.765}P_{0.5}As_{0.5}$. The full curve shows $\varepsilon_2(\Omega)$ and the broken curve shows JDOS.

same azimuthal quantum number l must be zero, i.e. $T^{\beta}_{11} = 0$. Then, for the III–V compound semiconductors, there remain four reduced matrix elements in (8): T^{a}_{10}, $^{*}T^{a}_{10}$, T^{c}_{10}, $^{*}T^{c}_{10}$, where a, c denote the anion and cation in a primitive cell respectively. These four reduced matrix elements are considered as four adjustable parameters and their values are determined by fitting the calculated values of $\varepsilon_2(\Omega)$ from (1) and (8) with experimental values for InP, GaAs and InAs. Table 1 shows the values of these four parameters, which are obtained by fitting with the experimental values given by Aspnes and Studna (1983). For the alloys $Ga_xIn_{1-x}P_yAs_{1-y}$, which are lattice-matched with InP, a linear approximative expression is assumed:

$$T^{\beta}_{ll'}(Ga_xIn_{1-x}P_yAs_{1-y}) = xT^{\beta}_{ll'}(GaAs) + yT^{\beta}_{ll'}(InP) + (1-x-y)T^{\beta}_{ll'}(InAs).$$

Figures 1 and 2 show the densities of state for monolayer superlattice $Ga_{0.47}In_{0.53}As/$

InP(110) and alloy $Ga_{0.235}In_{0.765}P_{0.5}As_{0.5}$ respectively. The superlattice periodicity can considerably modify the electronic structure near the high-symmetry points in the Brillouin zone (Chang and Schulman 1985), where the degenerate energy levels will be split and some sub-bands may hybridise each other. If the folding of the Brillouin zone leads two sub-bands to cross at some points, there may be some considerable changes near these points. However, it can be seen from figures 1 and 2 that they have roughly similar shapes.

The joint densities of state and the imaginary parts of dielectric constants are shown in figures 3 and 4 for $Ga_{0.47}In_{0.53}As/InP(100)$ and $Ga_{0.235}In_{0.765}P_{0.5}As_{0.5}$, respectively. The broken curves denote the JDOS and the full curves denote the $\varepsilon_2(\Omega)$. For the superlattice, which is anisotropic, the $\varepsilon_2(\Omega)$ shown in figure 3 is an average value for three different directions: one corresponds to the polarisation of light perpendicular to the layer surface and the other two correspond to polarisations of light parallel to the layer surface. The folding the of Brillouin zone will increase the number of levels at every point in $\boldsymbol{k}$-space and as a result many more direct transitions are allowed to occur, which are inhibited before the folding. As a result, the JDOS of superlattice turns round and many peaks disappear compared with the JDOS of the alloy shown in figure 4. However, by including the effects of momentum matrix elements, some peaks appear again in the figure of $\varepsilon_2(\Omega)$ for the superlattice.

From figures 3 and 4, we can conclude that the effects of momentum matrix elements are different for superlattices and alloys. For alloys, it can change only the amplitudes of peaks and cannot change the positions of peaks. Just because of this, the JDOS is a close approximation to $\varepsilon_2(\Omega)$ for some semiconductors and their alloys. However, for the superlattices, the momentum matrix elements can cause in the JDOS many more changes. So, when we calculate the $\varepsilon_2(\Omega)$ of superlattices, the momentum matrix elements must be considered.

This work was supported by the Chinese Natural Science Foundation.

References

Aspnes D E and Studna A A 1983 *Phys. Rev.* B **27** 985
Chang Yia-Chung and Schulman J N 1985 *Phys. Rev.* B **31** 2069
Ehrenreich H and Philips H R 1962 *Phys. Rev.* **128** 1622
Gell M A, Ninno D, Jaros M, Wolford D J, Keuch T F and Bradley J A 1987 *Phys. Rev.* B **35** 1196
Gilat G and Raubenheimer L J 1965 *Phys. Rev.* **144** 390
Mbave A A and Verle C 1984 *Phys. Rev.* B **29** 3756
Ninno D, Gell M A and Jaros M 1986 *J. Phys. C: Solid State Phys.* **19** 3845
Sander G D and Bajaj K K 1987 *Phys. Rev.* B **35** 2038
Sander G D and Chang Yia-Chung 1987 *Phys. Rev.* B **35** 1300
Tinkham M 1964 *Group Theory and Quantum Mechanics* (New York: McGraw–Hill)
Vogl P, Hjalmarson H P and Dow J D 1983 *J. Phys. Chem. Solids* **44** 365