A New Method For Calculating The Sublevels Of Multi-Quantum Well Structures

Xing-Kui Cheng[1*] , Jun-Ming Zhou[2] ,and Qi Huang[2]

[1]Institute of Physics , Shandong University, Jinan 250100, China

[2] Institute of Physics, Chinese Academy of Sciences, Beijing 100080,China

Abstract: The sublevels of multi-quantum well structures (MQW) are calculated by the electron interference model and Kronig-Penney model, respectively. Comparing the values calculated theoretically with results measured in experiment, we can see that the values calculated theoretically by the electron interference model are all in excellent agreement with the results measured in experiments. Whereas, most of results calculated by Kronig-Penney model are out of accord with ones measured in experiments and the reason why the theoretical calculation is inconsistent with the experimental result is discussed. Calculating the sublevels of MQW by the electron interference is still easier and more convenient than that by Kronig-Penney model.

Keywords: Kronig-Penney model, Electron interference model, Multi- quantum well structures

1. Introduction

It is important to design an optimum multi-quantum well structure (MQW) for fabricating QW infrared detectors. So far, there are some of methods in calculation of sublevels of MQW, such as Kronig-Penney model [1], transfer matrix method [2] etc, therein, Kronig-Penney model is a basic and important method in calculating sublevels of MQW. But in studying of photocurrent spectrum of GaAs/$Al_xGa_{1-x}As$ MQW structures, we found that positions of peaks of photocurrent measured in experiment are out of accord with the ones calculated theoretically based on K.P. model. Thus it is imperative to find a way for solution of the problem. Then we proposed a new method based on electronic reflection and interference at interface of well/barrier in MQW [3,4] and referred to it as the electron interference model. In this paper, we calculate the sublevels of GaAs/$Al_xGa_{1-x}As$ MQW structures using electron interference model and Kronig-Penney model, respectively, and make the results theoretically calculated by two different models compare with ones measured in experiment.

2. Sample preparation and measurement results

A GaAs layer doped with Si to 4×10^{18} cm^{-3} with a thickness of 1 μm (bottom contact layer) is firstly grown on semi-insulating GaAs substrate by Metalorganic Chemical Vapor Deposition (MOCVD) technique. Then a GaAs/$Al_{0.22}Ga_{0.78}As$ MQW structure with 50 periods is grown on the doped GaAs layer. Each period of MQW structure consists of a 4nm well of GaAs (Si-doped n = 2×10^{18} cm^{-3}) and a 30 nm barrier of $Al_{0.22}Ga_{0.78}As$. Finally, a Si-doped GaAs layer (n = 4×10^{18} cm^{-3}) with 0.5μm thickness (top contact layer) is grown on the top of the MQW structure.

The MOCVD grown multi-layer structure sample is processed into rectangular test structure

*xkcheng@sdu.edu.cn

whose opposite polished facets is parallel to each other and form a 45^0 angle with respect to the substrate surface. When measuring infrared absorption of the multi-quantum wells structure, incident light is perpendicular to the polished facets[5]. The infrared absorption spectrum measured at room temperature is shown in Fig. 1. It can be seen that there are several peaks which locate at ν=706, 770, 986, 1046, 1168, 1282 and 1653 cm^{-1}, respectively. The measured sample is labeled as sample 1.

To further demonstrate validity of the electronic interference model for calculation of sublevels of MQW structures, we prepared another sample of $GaAs/Al_{0.3}Ga_{0.7}As$ MQW grown by molecular beam epitaxy (MBE).

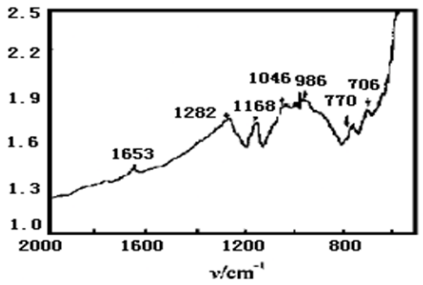

Fig.1. the infrared absorption spectrum measured at room temperature for GaAs/ $Al_{0.22}Ga_{0.78}As$ MQW structure

The $GaAs/Al_{0.3}Ga_{0.7}As$ MQW structure with 25 periods consists of a 5 nm well of GaAs (Si-doped $n = 7\times10^{17}$ cm^{-3}) and a 50 nm barrier of $Al_{0.3}Ga_{0.7}As$. The MQW structure (labeled as sample 2) photocurrent spectrum measured at T = 77 K by a Fourier transform infrared spectrometer (MAGNA-IR 760) is shown in Fig. 2. It can be seen that there are several peaks which are situated at ν_p=1312, 1439, 1477 and 1581 cm^{-1}, respectively.

3. Analysis and Discussion

3.1. Calculation of sublevels of MQW by electron interference model

Supposing that Z direction is parallel to MQW structure growth axis, periodic potential in $GaAs/Al_xGa_{1-x}As$ MQW structure can be expressed by $U_0(z) = U_0(z + nd)$, where $d = L_w + L_b$, n = ±1,±2,±3,… . Here L_w is well width, and L_b and U_0 is barrier width and height, respectively, as shown in Fig. 3. When an electron wave propagates from interface $A_1(A_2,A_3,\ldots)$ to interface $B_1(B_2, B_3, \ldots)$ in MQW in z direction, its phase shift can be given by

$$\theta = 2\pi\frac{L_b}{\lambda_b}$$

where λ_b is wavelength of electrons propagating in barrier layers in the direction parallel to MQW structure growth axis. Part of the electron wave arriving at the interface $B_1(B_2, B_3,\ldots)$ is transmitted, while the rest of the waves is reflected. The reflected part of the wave travels back to the interface $A_1(A_2, A_{3,\ldots})$, and then it is reflected again to the interface $B_1(B_2, B_3,\ldots)$ and

transmit through it .The phase difference of the two parts of electron wave transmitting through interface $B_1(B_2, B_3, \ldots)$ is given by

$$\phi = 2\theta = 2\pi \frac{2L_b}{\lambda_b}$$

According to wave theory, if the phase difference is even times of π, i.e. ,

$$\phi = 2\theta = 2\pi \frac{2L_b}{\lambda_b} = 2n\pi, \quad n = 1,2,3 \ldots$$

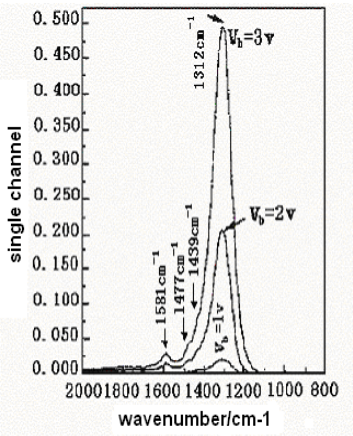

Fig.2. photocurrent spectrum measured at T=77K for sample 2

The two parts of the electron waves will have constructive interference. This means that the transmissivity of electron wave through the potential barrier reaches its maximum value. The energy of the electron with a maximum of transmissivity through the potential barrier can be written as[3, 4]

$$E = E^n = U_0 + \frac{\hbar^2}{2m_b}\left(\frac{\pi}{L_b}\right)^2 n^2 , \qquad (1)$$

$$n = 1,2,3 \ldots$$

where $\hbar$ is Planck constant divided by 2π and $m_b=(0.067+0.083x)m_0$[6], here m_0 is free electron mass. Taking x=0.22 and L_b=30nm for sample 1, we obtain from equation (1) that

$$E^n - U_0 = 4.9n^2 \quad \text{meV}, \quad n=1, 2, 3, \ldots \qquad (2)$$

Energy E_0 of an electron on ground state in quantum well can be calculated by[3]

$$E = \frac{\hbar^2}{2m_w}\left(\frac{\pi}{L_w}\right)^2\left(n+\frac{1}{2}\right)^2, n = 0,1,2\ldots$$

Letting n=0, $$E_0 = \frac{\hbar^2}{8m_w}\left(\frac{\pi}{L_w}\right)^2 \quad . \qquad (3)$$

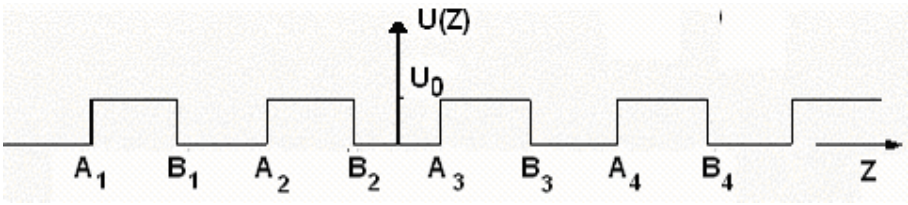

Fig.3. Potential distribution in GaAs/$Al_{0.22}Ga_{0.78}$As MQW

Taking $m_w=0.067m_0$ and L_w=4nm, from equation (3) we obtain E_0 = 87.7mev. Due to the fact that if the concentration of electrons being high enough, exchange interaction among electrons increases, the energy E_0 of an electron on the ground state in quantum well will decreases by about 20meV at room temperature [7] . Therefore, the energy E_0 on ground state in well locates at 67.7 (meV) above the well bottom.

Fermi energy of an electron in a quantum well is given by

$$E_F = \frac{\hbar^2 K_F^2}{2m_w} \quad , \qquad (4)$$

where $K_F=\sqrt{2\pi\sigma}$, $\sigma = n_0L_w$ is electron sheet density, n_0 is bulk electron density. Taking $n_0 = 2 \times 10^{18}$ cm^{-3} , L_w = 4 nm, and $m_w=0.067m_0$, E_F can be calculated to be 28 meV, namely, E_F is at 28 meV above ground state E_0 or at 95.7 mev above well bottom.

Difference of energy band gap for GaAs/Al_xGa_{1-x}As MQW can be given by $\Delta E_g = 1.247x(eV)$[8] , and the well depth or barrier height can be given by [9]

$U_0=\Delta Ec=0.65\Delta Eg$.

Letting x=0.22 , We have $U_0=\Delta Ec$=178mev, then $U_0 - E_F$=178-95.7=82.3mev. From equation (2) we have

$$E^n - E_F=(E^n - U_0)+(U_0 - E_F)=4.9n^2+82.3 \quad (meV), \quad n=1, 2, 3\ldots, \quad (5)$$

We consider that each of the levels between the ground state E_0 and Fermi level E_F is occupied by electrons at room temperature, in the case of light excitation , the electrons occupying Fermi level E_F can be excited to the energy states E^n (called conduction states , n=1,2,3…) above the barriers, forming a series of absorption peaks. Positions of the absorption peaks should be determined by the values of (E^n - E_F) which are defined as electron transition energy. The transition energies between Fermi level E_F and sublevels E^n above barriers, which are calculated by electron interference model, for sample 1 are listed in Table 1.

In measurement of infrared absorption, optical transition energy of an electron is obtained by formula $E_T = \hbar\omega = \hbar\tilde{\upsilon} = \hbar c\nu_p$, where E_T is optical transition energy , $\hbar$ is Planck constant, c the speed of light in vacuum, and ν_p light wave-numbers at absorption peak. Therefore, the optical transition energy corresponding to the infrared absorption peaks shown in Fig.1 are given to be 87.5meV, 95.5meV, 129.7meV, 159meV, and 205meV, respectively, and they are also listed in table 1. The transitions of electrons from Fermi level E_F in well to the sublevels E^n (n=1,2,…) above barriers for MQW are shown schematically in Fig.4.

Likewise, we can calculate from equation (3) the energy of ground state in quantum well for an MQW labeled as sample 2, obtaining

E_0 =87.5meV.

Taking exchange interaction of electrons into consideration, the ground state energy E_0 in quantum well decreases by about 20meV [7], therefore ,the level E_0 should be at 67.5 (meV) above well bottom.

Fermi level can be calculated from equation (4) to be 12.5meV, i.e., it locates at 12.5meV above E_0 or at 80 meV above well bottom.

Taking L_b=50nm, m_b =(0.067+0.083x)m_0 [6] ,and x=0.3 , we obtain from equation (1)

$$E^n - U_0 = 1.6n^2(\text{meV}) \quad , n=1,2,3\ldots . \qquad (6)$$

Using $\Delta E_g = 1.247x$[8] (eV) and $\Delta Ec = U_0 = 0.65\Delta Eg$[9] , and letting x=0.3, we obtain

U_0 =243 meV , then U_0 -E_F =163mev. Hence,

$$E^n - E_F = (E^n - U_0) + (U_0 - E_F) = 1.6n^2 + 163(\text{meV}), \quad n=1, 2, 3\ldots . \qquad (7)$$

For sample 2 the values of transition energy (E^n-E_F) calculated by equation (7) are listed in table 2.

The transition energy measured on the basis of photocurrent spectrum for sample 2 are given by formula $E_T = hc\nu_p$,where ν_p is light wave-numbers at photocurrent peaks, to be 163meV,178meV,183meV,and 196meV, respectively ,as shown in table 2.

3.2 Calculation of sublevels of MQW by Kronig-Penney model

According to Kronig-Penney(K.P.) model, the minimum energy of every odd-index band in well for a MQW structure can be calculated by[1]

$$\tan\left[\frac{L_w}{2\hbar}\left(2m_w E_{min}\right)^{\frac{1}{2}}\right] - \left[\frac{m_w}{m_b}\left(\frac{U_0}{E_{min}} - 1\right)\right]^{\frac{1}{2}} \tanh\left\{\frac{L_b}{2\hbar}\left[2m_b(U_0 - E_{min})\right]^{\frac{1}{2}}\right\} = 0 \ , \qquad (8)$$

for $E < U_0$,

where $\hbar$ is Planck constant divided by 2π. Substituting L_w=4nm, L_b=30nm, m_w=0.067m_0, m_b = (0.067+0.083x)m_0[6] (here x=0.22 and m_0 being free electronic mass) , and U_0=0.178eV given above for sample 1 into equation (8), we obtain by graphing

E_{1min} = 0.137e V.

The maximum energy of every odd-index band in well for the GaAs/$Al_{0.22}Ga_{0.78}$As MQW structure can be calculated by[1]

$$\tan\left[\frac{L_w}{2\hbar}\left(2m_w E_{max}\right)^{\frac{1}{2}}\right] - \left[\frac{m_w}{m_b}\left(\frac{U_0}{E_{max}} - 1\right)\right]^{\frac{1}{2}} \coth\left\{\frac{L_b}{2\hbar}\left[2m_b(U_0 - E_{max})\right]^{\frac{1}{2}}\right\} = 0 \ , \qquad (9)$$

for $E < U_0$.

From equation (9) we can obtain by same method that E_{1max}=0.141eV. Letting

$E_1 = \frac{1}{2}(E_{1min} + E_{1max})$, we have E_1=0.139eV.

Due to the electron exchange interactions, it leads the lowering of level E_1 in well by about 20meV[7], hence the level E_1(called ground state) lies at 0.119eV above the well bottom.

According to the criterion that if $2m_w U_0 L_w^2/\hbar^2 < \pi^2$, there is only one confined level in the quantum well[10], we can judge that there is only one confined level in the wells for sample 1.

The minimum energy of every odd-index band above barriers for GaAs /$Al_{0.22}Ga_{0.78}$As MQW can be calculated by[1]

$$\tan\left[\frac{L_w}{2\hbar}\left(2m_w E_{min}\right)^{\frac{1}{2}}\right] + \left[\frac{m_w}{m_b}\left(1 - \frac{U_0}{E_{min}}\right)\right]^{\frac{1}{2}} \tan\left\{\frac{L_b}{2\hbar}\left[2m_b(E_{min} - U_0)\right]^{\frac{1}{2}}\right\} = 0 \ , \qquad (10)$$

for $E > U_0$.

Likewise, from equation (10) we obtain

E_{3min}=0.205V, E_{5min}=0.302eV

Table.1. Theoretically calculated transition energies between ground state in well and sublevels above barrier comparing with results measured in experiment for an MQW structure labeled as sample 1

Theoretically Calculated transition energy				Measured results	
K.P. model (meV)		Interference model (meV)		Positions of absorption peaks (cm^{-1})	Transition energy (meV)
E_F	147	E_F	95.7		
E_1	119	E_0	67.7		
ΔE_2	62	ΔE^1	**87.2**	706	**87.5**
ΔE_{2-1}	**90**				
ΔE_3	80	ΔE^2	**101.9**	770	**95.5**
ΔE_{3-1}	**108**				
ΔE_4	145	ΔE^3	**126.4**	1046	**129.7**
ΔE_{4-1}	173				
ΔE_5	184	ΔE^4	**160.7**	1282	**159**
ΔE_{5-1}	212				
ΔE_6	249	ΔE^5	**204.8**	1653	**205**
ΔE_{6-1}	277				

In the table $\Delta E_n=E_n-E_F$, n=2,3,4,5,6, $\Delta E^n=E^n-E_F$, n=1,2,3,4,5 and $\Delta E_{n-1}=E_n-E_1$,n=2,3,4,5,6

The minimum energy of every even -index band above barriers for GaAs /$Al_{0.22}Ga_{0.78}As$ MQW can be calculated by[1]

$$\cot\left[\frac{L_w}{2\hbar}\left(2m_w E_{min}\right)^{\frac{1}{2}}\right]-\left[\frac{m_w}{m_b}\left(1-\frac{U_0}{E_{min}}\right)\right]^{\frac{1}{2}}\tan\left\{\frac{L_b}{2\hbar}\left[2m_b(E_{min}-U_0)\right]^{\frac{1}{2}}\right\}=0\,, \qquad (11)$$

for $E > U_0$.

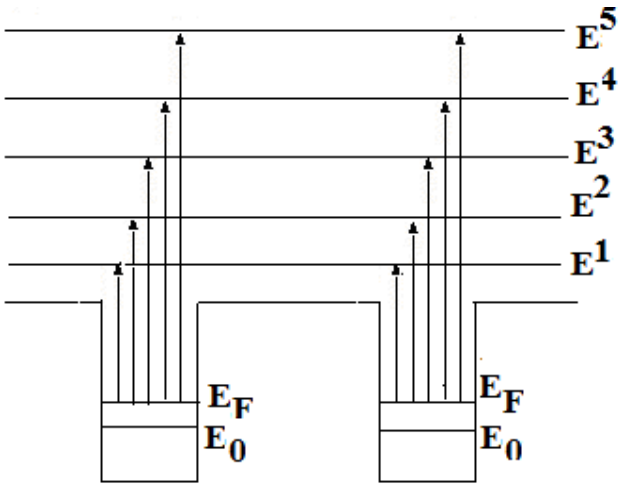

Fig.4. Optical transitions of electrons from E_F in well to E^n (n=1,2,3…) above barriers for MQW structure. (according to electron interference model)

From equation (11) we obtain

E_{2min}=0.192eV , E_{4min}=0.268eV , and E_{6min}=0.370eV

The maximum energy of every odd-index band above barriers for GaAs /$Al_{0.22}Ga_{0.78}As$ MQW can be calculated by [1]

$$\tan\left[\frac{L_w}{2\hbar}\left(2m_w E_{max}\right)^{\frac{1}{2}}\right]-\left[\frac{m_w}{m_b}\left(1-\frac{U_0}{E_{max}}\right)\right]^{\frac{1}{2}}\cot\left\{\frac{L_b}{2\hbar}\left[2m_b(E_{max}-U_0)\right]^{\frac{1}{2}}\right\}=0, \qquad (12)$$

for $E>U_0$.

From equation (12) we have E_{3max}=0.248eV ,and E_{5max}=0.357eV.

The maximum energy of every even-index band above barriers for GaAs /$Al_{0.22}Ga_{0.78}As$ MQW can be calculated by [1]

$$\cot\left[\frac{L_w}{2\hbar}\left(2m_w E_{max}\right)^{\frac{1}{2}}\right]+\left[\frac{m_w}{m_b}\left(1-\frac{U_0}{E_{max}}\right)\right]^{\frac{1}{2}}\cot\left\{\frac{L_b}{2\hbar}\left[2m_b(E_{max}-U_0)\right]^{\frac{1}{2}}\right\}=0, \qquad (13)$$

for $E>U_0$.

From equation (13), we have E_{2max}=0.226eV, E_{4max}=0.315eV, and E_{6max}=0.421eV.

Letting $E_n=\frac{1}{2}(E_{nmin}+E_{nmax})$, we have

E_2=0.209eV, E_3=0.227eV, E_4=0.292eV, E_5=0.331eV, and E_6=0.396eV.

In the case of excitation of light, the electrons on level E_1 in well can transit to the states E_n above the barriers, forming a series of absorption peaks. The positions of the absorption peaks

should be determined by values of (E_n - E_1), n=2,3… . For sample 1 the values of (E_n-E_1) calculated by K.P model are listed in table1. The transitions of the electrons from E_1 in well to E_n above barriers are shown schematically in Fig.5.

Likewise, the sublevels of MQW for GaAs/$Al_{0.3}Ga_{0.7}As$ (sample 2) are calculated by K.P model to be E_1=0.162eV, E_2=0.257eV, E_3=0.261eV,E_4=0.298eV,E_5=0.313eV,and E_6=0.352eV. Due to the exchange interaction of electrons, it leads the level E_1 in well lowering by about 20meV[7], hence level E_1 lies at 0.142eV above the well bottom. The transition energy (E_n-E_1), calculated by K.P model, between E_1 in well and E_n above barriers are listed in table 2.

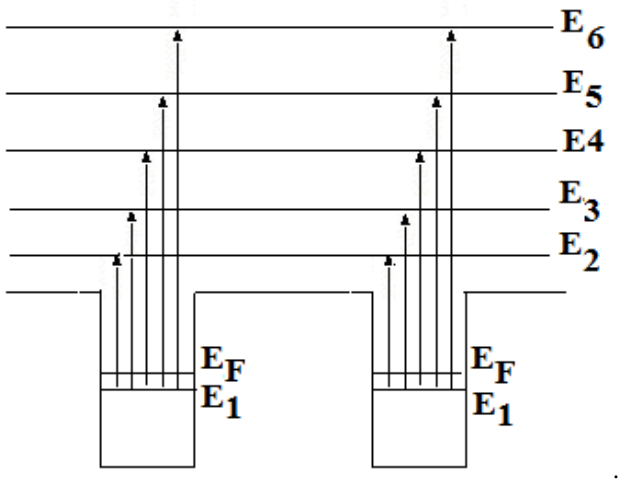

Fig.5. Optical transitions of electrons from E_1 in well to E_n (n=2,3…) above barriers for MQW structure (according to K.P. model).

3.3. Comparison

Based On the electron interference model, we calculate sublevels of a GaAs/$Al_{0.22}Ga_{0.78}As$ MQW structure (labeled as sample 1) grown by MOCVD and of a GaAs/$Al_{0.3}Ga_{0.7}As$ MQW structure (labeled as sample 2) grown by MBE, respectively. Thereby, we obtain the transition energies between the ground state E_0 (strictly speaking Fermi level E_F) in well and the sublevels E^n (n=1,2,3…) above barriers for the two samples. Comparing them one by one with the transition energies measured in experiments, shown in table 1 and table 2, we can see that no matter whether they are calculated from sample 1 or from sample 2, the transition energies calculated theoretically by the electron interference model are all in excellent agreement with ones measured in experiments.

Table 2. Theoretically calculated transition energies between ground state in well and sublevels above barrier comparing with results measured in experiment for an MQW structure labeled as sample 2

Theoretically Calculated values				Measured results	
K.P. model (meV)		interference model (meV)		positions of photocurrent peaks (cm^{-1})	transition energies (meV)
E_F	154.5	E_F	80		
E_1	142	E_o	67.5		
ΔE_2	102	ΔE^1	**164.**	1312	**163**
ΔE_{2-1}	115				
ΔE_3	106.5	ΔE^2	**169.**		
ΔE_{3-1}	119				
ΔE_4	143.5	ΔE^3	**177.**	1439	**178**
ΔE_{4-1}	156				
ΔE_5	158.5	ΔE^4	**188.**	1477	**183**
ΔE_{5-1}	171				
ΔE_6	197.5	ΔE^5	**203**	1581	**196**
ΔE_{6-1}	210				

In the table $\Delta E_n=E_n-E_F$, n=2,3,4,5,6, $\Delta E^n=E^n-E_F$, n=1,2,3,4,5 and $\Delta E_{n-1}=E_n-E_1$,n=2,3,4,5,6

Note that the absorption peak at $\nu = 986\ cm^{-1}$, shown in Fig.1, is determined by width and depth of quantum well, and it is not related to electronic interference . The peak at $\nu=1168\ cm^{-1}$ may be caused by vibrations of Si - C bond in the material.

It should be pointed that according to the electronic interference model, the photocurrent produced by the transitions of electrons from E_F to E^1 overlaps with one from E_F to E^2, so that only a strongest peak of photocurrent at 1312cm-^{1} is observed in the photocurrent spectrum measured, shown in Fig.2.

Meanwhile, using K.P. model, we calculate sublevels of the GaAs/$Al_{0.22}Ga_{0.78}$As MQW structure and of the GaAs/$Al_{0.3}Ga_{0.7}$As MQW structure, respectively. Thereby, we obtain the transition energies between ground state E_1(or Fermi level E_F) in well and sublevels E_n (n=2,3…)

above barriers for sample 1 and sample 2. Comparing them one by one with ones measured in experiments ,shown in table 1 and table 2, we can see that for sample 1 only two of transition energies calculated by K.P. model, i.e. the value of (E_2- E_1) or/and of (E_3- E_1), are approximately in accord with experimental results. The rest of values calculated theoretically are out of accord with the results measured in infrared absorption experiment, while for sample 2 theoretically calculated values of transition energies are all out of accord with the results measured in photocurrent.

In addition, for GaAs/Al_xGa_{1-x}As MQW with other structure parameters, using electron interference model , the theoretically calculated transition energy between ground state E_0 (strictly speaking, Fermi level E_F) in well and the sublevels E^n (n=1,2,3…) above barriers are all in excellent agreement with measured ones[11].

Microscopic particles (e.g. electrons) have wave-particle duality, which has the characteristics of both wave and particle. In K.P. model, it is assumed that the wave function and its first derivative at the interface between well and barrier layer are continuous .i.e. the electron probability current density (like particle current density) through interface is continuous. This means that the behavior of electrons through interface is considered as like–particles. In electron interference model, we take only electron reflection and interference at interface between well and barrier layer into account, no matter whether electron wave-function and its first derivative at interface is continuous or not. This means that the behavior of electrons through interface is considered as like-wave. In fact, the behavior of the electrons, which propagate along the direction of growth of multiple quantum wells structure, through interface is like-wave and not like-particle. Therefore, the results calculated theoretically for GaAs/Al_xGa_{1-x}As MQW structure based on the electron interference model are all in excellent agreement with ones measured in experiment. Whereas the results calculated theoretically based on K.P. model are basically out of accord with ones measured in experiment

The electron interference model can be applied to the design of quantum well infrared detector. For fabricating a quantum well infrared detector with a specific response peak wavelength and bandwidth, we can design the structure parameters of MQW, such as depth and

width of the well, barrier width and doping density in well, and calculate the difference of energy between the conduction states E^n (n=1,2,3…) above barriers and the ground state E_0 in well, then adjust the difference of the energy between energy states by varying the structure parameters of MQW. Finally we can fabricate desirable quantum well infrared detector with special wavelength of responsive peak and bandwidth [12,13].

4. Conclusions

Based on the above analysis, we can conclude as follows:

1. The sublevels of MQW structures for GaAs/$Al_xGa_{1-x}As$ can be calculated by the electron interference model, and the theoretically calculated results are all in excellent agreement with ones measured in experiments. But calculating the sublevels of MQW structures by K.P. model, most of the results calculated are out of accord with the results measured in experiment.

2. Behavior of the electrons, which propagate along the direction of growth of multiple quantum wells structure, through interface is like-wave and not like-particle, therefore, the results calculated theoretically for GaAs/$Al_xGa_{1-x}As$ MQW structures based on electron interference model are all in excellent agreement with ones measured in experiment. Whereas the results calculated theoretically based on K.P. model are basically out of accord with ones measured in experiment

3. Comparing the electron interference model with Kronig--Penney model, we can see that the formulas used in calculation of sublevels of MQW structures by the electron interference model are simpler. Therefore, calculating sublevels of GaAs/$Al_xGa_{1-x}As$ MQW structure by the electronic interference model is still easier and more convenient than that by K.P. model.

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