Alloy-disorder-scattering-limited mobility of electrons in a superlattice

Partha Ray and P. K. Basu
Institute of Radio Physics and Electronics, University of Calcutta, 92 Acharya Prafulla Chandra Road, Calcutta 700 009, India
(Received 25 March 1991; revised manuscript received 12 December 1991)

This paper examines the effect of the alloy-disorder scattering on the electron transport in a superlattice along the growth direction. The relaxation time is calculated by using Fermi's golden rule and the wave functions obtained from both the tight-binding and the Kronig-Penney models. The mobility is calculated using the Boltzmann transport equation. Numerical values for a GaAs/$Al_xGa_{1-x}As$ superlattice indicate that these two wave functions yield almost the same values of the mobility, which are substantially higher than the values obtained by other workers for polar-optic-phonon and interface-roughness scattering.

I. INTRODUCTION

Electronic properties of multilayered semiconductor structures such as multiple quantum wells (MQW's) and superlattices (SL's) have been investigated by many workers over the past few decades.[1] Previously, the emphasis was mainly on the study of electron transport along the layer planes. In recent years, more attention has been directed toward investigation of the transport properties along the direction of growth of the layers.[2–7] Recent studies indicate that transport takes place mainly due to the miniband conduction and not by hopping, as had been conjectured earlier.[8,9] Attempts have been made to explain the experimental results on electron mobility by considering scattering due to deformation-potential acoustic phonons,[2] longitudinal polar-optic (LO) phonons (both bulklike and confined[7]), and interface roughness (IFR).[6] The last mechanism is thought to be the most important in reducing the difference between the experimental and the theoretical values.

The SL structures are made of alternate layers of a binary- and a ternary-alloy semiconductor, and the electrons are therefore subject to alloy-disorder scattering.[10] This mechanism has been studied in the bulk[10] and in the heterojunctions,[11–14] and has been found to play an important role under certain situations. However, the effect of this scattering mechanism on the miniband conduction in a SL has not been studied to date. In the present work we report the results of such an investigation for a GaAs/$Al_xGa_{1-x}As$ SL. The expressions for the relaxation times due to alloy-disorder scattering are derived by using the analytic wave functions obtained from both the tight-binding (TB) and the Kronig-Penney (KP) models.[15–17] The expressions are given in Sec. II and the method of calculation of the mobility is also outlined there. The numerical values for a GaAs/$Al_xGa_{1-x}As$ SL are presented in Sec. III and are compared with the values for other scattering mechanisms.

II. THEORY

A. Wave functions

The SL potential is assumed to be of the simple KP type,[15–17] as shown in Fig. 1. The dispersion relation for the miniband is expressed by the following transcendental equation considering the effective-mass mismatch between the well and the barrier layers:[16,17]

$$\cosh(2k_2b)\cos(2k_1a) + K^{-}\sinh(2k_2b)\sin(2k_1a)=\cos(k_zL)\ , \quad (1)$$

where

$$k_2=\frac{[2m_B(V_0-E)]^{1/2}}{\hbar}\ , \quad k_1=\frac{(2m_WE)^{1/2}}{\hbar}\ ,$$

$$K^{\pm}=\frac{(\lambda k_2/k_1\pm k_1/\lambda k_2)}{2}\ , \quad \lambda=\frac{m_W}{m_B}\ .$$

In the above $2a$ is the well width, $2b$ is the barrier width, L is the SL period, $m_{W(B)}$ is the effective mass of the electrons in the well (barrier) layer, k_z is the z component of the electron wave vector, V_0 is the barrier height at the heterointerface, and E is the electron energy.

We have expressed the miniband dispersion relation in the following phenomenological form:[7]

$$E(k)=\hbar^2k_{\parallel}^2/2m_{\parallel}+\Delta[1-\cos(k_zL)]\ , \quad (2)$$

where $m_{\parallel}$ is the electron mass along the layer planes, 2Δ is the miniband width obtained from Eq. (1), and $k_{\parallel}$ is the in-plane component of the electron wave vector.

The SL envelope function is obtained in several ways. Dharssi and Butcher[6,7] have used the TB approximation

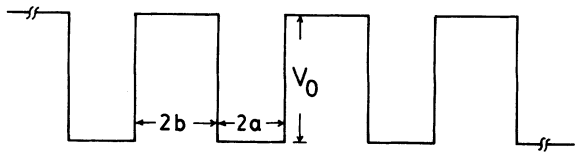

FIG. 1. The potential profile in a superlattice. The well and the barrier are made of GaAs and $Al_xGa_{1-x}As$, respectively.

to write the envelope function as

$$\psi_{\mathbf{k}}=(L/V)^{1/2}\exp(ik_{\parallel}\cdot\rho)\times\sum_{n=-N/2}^{N/2}\phi(z-nL)\exp(ik_z nL)\ , \tag{3}$$

the normalization constant being determined from

$$\phi(z-nL)\phi(z-mL)=\delta_{n,m}\phi^2(z-nL)\ , \tag{4}$$

where $\phi(z)$ is the normalized eigenfunction for an isolated QW. We have employed in our calculation this TB wave function as well as the following analytical envelope function obtained by Aitelhabti, Vasilopoulos, and Currie[15] from the KP model:

$$\phi_W(z)=N^{-1/2}\exp(-ik_1L/2)\exp(ink_zL)\times[b_2\exp(iX)+\beta\exp(-iX)]\ ,$$
$$\text{for } (n-1)L+a<z<nL-a \tag{5}$$

and

$$\phi_B(z)=N^{-1/2}\exp(-ik_1L/z)\exp(ink_zL)\times[p\cosh(Y)+q\sinh(Y)]\ ,$$
$$\text{for } nL-a<z<nL+a \tag{6}$$

with

$$b_2=\tfrac{1}{2}(\lambda k_2/k_1+k_1/\lambda k_2)\sinh(2k_2b)\ ,$$
$$X=k_1[z-(n-\tfrac{1}{2})L]\ ,$$
$$Y=k_2(z-nL+a)\ ,$$
$$\beta=a_1\sin(k_1L)-b_1\cos(k_1L)-\sin(k_zL)\ ,$$
$$a_1+ib_1=[\cosh(2k_2b)+i\tfrac{1}{2}(\lambda k_2/k_1-k_1/\lambda k_2)\times\sinh(2k_2b)]\exp(2ik_1b)\ ,$$
$$p=b_2\exp(ik_1a)+\beta\exp(-ik_1a)\ ,$$
$$q=[b_2\exp(ik_1a)-\beta\exp(-ik_1a)](ik_1/\lambda k_2)\ .$$

The normalization constant N, obtained by normalizing the wave function in the interval

$$(n-1)L+a<z<nL+a\ ,$$

may be expressed as

$$N=A\sin^2(k_zL)-(2A\beta_0+B)\sin(k_zL)+C\ , \tag{7}$$

where $A=L-P^+D$,

$$B=2b_2((2b-P^-D)\cos(2k_1a)+\{1/k_1-(k_1/\lambda k_2)[\cos(4k_2b)-1]/2k_2\}\times\sin(2k_1a))\ ,$$

and

$$\dot{C}=A(\beta_0^2+b_2^2)+B\beta_0\ ,$$

with

$$P^{\pm}=1\pm(k_1/\lambda k_2)^2\ ,$$
$$\beta_0=a_1\sin(k_1L)-b_1\cos(k_1L)\ .$$

B. Scattering probability

The theory of electronic scattering in a QW due to random alloy-disorder potential has been reported in a number of papers.[11–14] The scattering potential in a ternary alloy $A_xB_{1-x}C$ under virtual-crystal approximation is $(1-x)\Delta E$ and $x\,\Delta E$, respectively, at sites A and B. We assume that the scattering potential $V_i(r_i,z_i)$ at a site (r_i,z_i) is a spherically symmetric square well of height ΔE and radius r_0. The method of calculating the scattering probability for such a potential has been discussed earlier. The potential is expanded in the following two-dimensional (2D) Fourier series as[11,12]

$$V_i(r_i,z_i)=\sum_{\mathbf{q}_{\parallel}}2\pi\,\Delta E\frac{r_zJ_1(r_zq_{\parallel})}{q_{\parallel}}\exp[i\mathbf{q}_{\parallel}\cdot(\mathbf{r}-\mathbf{r}_i)]\ ,$$
$$r_z^2=r_0^2-(z-z_i)^2 \tag{8}$$

where J_1 is the Bessel function of the first kind and of order 1.[18] For this form of potential the matrix element for transition from a state $\mathbf{k}$ to another state $\mathbf{k}'$ becomes

$$\langle\mathbf{k}'|V_i|\mathbf{k}\rangle=\int d^2r\int_{z_i-r_0}^{z_i+r_0}dz\,\psi^*_{\mathbf{k}'}\psi_{\mathbf{k}}2\pi\,\Delta E\frac{r_zJ_1(r_zq_{\parallel})}{q_{\parallel}}\times\exp[i\mathbf{q}_{\parallel}\cdot(\mathbf{r}-\mathbf{r}_i)]\ . \tag{9}$$

Since $r_zq_{\parallel}\ll1$, $J_1(x)\simeq x/2$ is valid.[18] In the integration over z, the wave function is assumed to be constant over the small interval and is taken outside the integral. Considering all the alloy sites to be randomly distributed in the ratio $x:(1-x)$, one gets for the squared matrix element

$$|M(\mathbf{k},\mathbf{k}')|^2=(\tfrac{4}{3}\pi r_0^3\,\Delta E)^2(L/V)N_0x(1-x)\times\delta_{\mathbf{k}'_{\parallel},\mathbf{k}_{\parallel}+\mathbf{q}_{\parallel}}\int|\phi(z)|^4dz\ , \tag{10}$$

where N_0 is the number of alloy sites per unit volume, δ_{ij} is the Kronecker δ, and V is the volume of the crystal. The relaxation time is given by the expression

$$\tau^{-1}(\mathbf{k})=\frac{2\pi}{\hbar}\sum_{\mathbf{k}'}|M(\mathbf{k},\mathbf{k}')|^2(1-\cos\vartheta_{\mathbf{k}})\delta(E_{\mathbf{k}'}-E_{\mathbf{k}})\ , \tag{11}$$

where $\vartheta_{\mathbf{k}}$ is the angle between $\mathbf{k}$ and $\mathbf{k}'$, and $\delta(x)$ is Dirac's δ function. The summation over $\mathbf{k}'$ may be transformed into an integral by the following expression:

$$\sum_{\mathbf{k}'}\longrightarrow\frac{V}{8\pi^3}\int_0^{\infty}dk'_{\parallel}\,k'_{\parallel}\int_0^{2\pi}d\vartheta_{\mathbf{k}}\int_{-\pi/L}^{\pi/L}dk'_z\ . \tag{12}$$

Following Palmier and Ballini[2] we only consider the non-Umklapp process, and finally get

$$\tau^{-1}(\mathbf{k})=(\tfrac{4}{3}\pi r_0^3\,\Delta E)^2N_0x(1-x)(m_{\parallel}/\hbar^3)\int|\phi(z)|^4dz\ . \tag{13}$$

There is a difficulty inherent in the KP model in that it

provides no information about the transport in the layer planes. The effective mass in the layer planes, $m_{\parallel}$, is, therefore, not easy to calculate. To circumvent this difficulty we use, following Palmier and Chomette,[3] a mean effective mass $m_{\parallel}^{*}$ defined as

$$m_{\parallel}^{*}(am_1+bm_2)/(a+b) . \tag{14}$$

This approximation is quite reasonable in this case, where the effective masses of the well and the barrier layers are not too different from each other.

C. Calculation of the mobility

In the presence of the electric field ξ_z, the perturbation g added to the equilibrium distribution function f_0 may be written in terms of the relaxation time as

$$g(\mathbf{k})=\frac{e\xi_z}{\hbar}\frac{\partial f_0}{\partial k_z}\tau(\mathbf{k}) . \tag{15}$$

The current density is

$$j_z=-\frac{e}{4\pi^3}\int d^3k g(\mathbf{k})v_z(\mathbf{k}) \tag{16}$$

and the mobility is

$$\mu_z=j_z/en\xi_z , \tag{17}$$

where the e and n are, respectively, the charge and the number density of electrons, and v_z is the drift velocity defined as

$$v_z=\frac{1}{\hbar}\frac{\partial E}{\partial k_z} . \tag{18}$$

III. RESULTS AND DISCUSSIONS

We have used the formulas derived earlier to calculate the mobility of electrons limited by alloy-disorder scattering in a $GaAs/Al_{0.3}Ga_{0.7}As$ superlattice. The following values of parameters are chosen for the calculation:[19]

$m^{*}(GaAs)=0.067m_0$;

$m^{*}(Al_xGa_{1-x}As)=(0.067+0.0735x)m_0$;

$E_g(x)=(1.501+1.239x+0.37x^2)$ eV ;

$a_0(x)=(0.5645+0.000\,78x)$ nm ; $r_0=0.44a_0$;

$\Delta E_c/\Delta E_v=57/43$; $\Delta E=0.6$ eV ; $V_0=231$ meV .

a_0 is the lattice constant.

The variation of the absolute magnitude of the wave function in the nth well and in the nth barrier is shown in Fig. 2 for equal well and barrier widths of 5 nm each. As may be seen from the figure, the KP model gives an almost sinusoidal variation of the wave function with a nonzero mean indicating a strong interwell coupling. The nature of the wave function in the barrier, calculated under the TB approximation, is, as usual, of decaying nature. It should be noted, however, that there is an equal amount of contribution to the wave function in the nth barrier from the $(n+1)$th well, as shown in Fig. 2. When

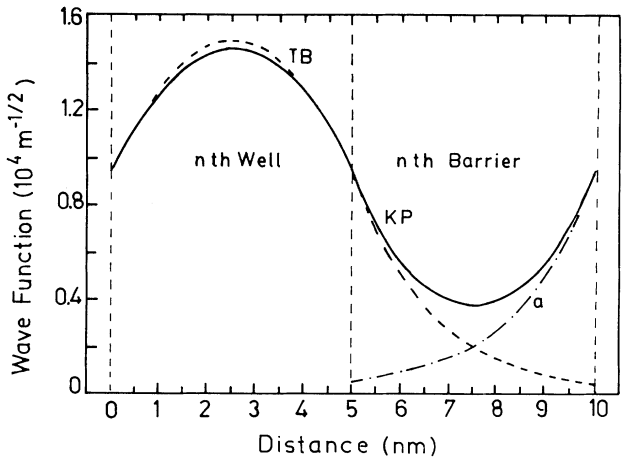

FIG. 2. The variation of envelope function in a superlattice, calculated with TB and KP models for a superlattice period of 10 nm. Curve a is the envelope function penetrating out of the $(n+1)$th well into the nth barrier.

the contributions from the nth and the $(n+1)$th wells are taken together, the TB wave function in the nth barrier appears to be almost identical with the corresponding KP wave function.

The values of the mobility limited by alloy-disorder scattering are presented in Fig. 3 as a function of the SL period for equal well and barrier widths. As explained above, the TB and KP wave functions are not much different; the values of the mobility obtained by using these two different wave functions are, therefore, almost identical.

The mobility values using both the TB and KP wave functions are found to increase slightly with the SL period, then attain a peak, and finally decrease. This is due to two mutually opposing factors. As the SL period or the well width increases, the wave function becomes

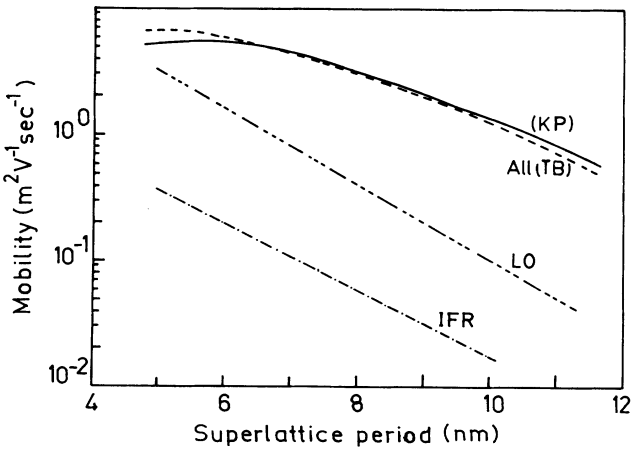

FIG. 3. Mobility of electrons in a $GaAs/Al_xGa_{1-x}As$ superlattice vs the superlattice period for equal well and barrier widths. The curves labeled "All" show the alloy-disorder-scattering-limited mobility obtained in the present work using TB and KP wave functions. Curves labeled IFR and LO are due to Dharssi and Butcher (Refs. 6 and 7), using the TB wave function.

more confined within the wells, thereby reducing the probability of scattering in the alloy regions and increasing the mobility. On the other hand, as the SL period or the barrier width increases, there is less coupling between the wells, and the miniband width becomes less. There is a consequent increase in the effective mass and a decrease in the mobility.

It is also useful to compare the present theoretical values with the values obtained for IFR and LO-phonon scatterings. We have included in Fig. 3 the results obtained by Dharssi and Butcher[6,7] using a TB envelope function for both of these scattering processes. It is found that the values of the alloy-disorder-scattering-limited mobility obtained by us are almost an order of magnitude larger than the values limited by LO-phonon scattering when the SL period exceeds 8 nm. The mobilities limited by IFR scattering are still lower. It may, therefore, be concluded that alloy-disorder scattering makes an insignificant contribution to the miniband conduction in a $GaAs/Al_xGa_{1-x}As$ SL.

ACKNOWLEDGMENT

One of us (P.R.) was supported in part by the Council for Scientific and Industrial Research, India.

[1]See, e.g., papers in the spacial issue on quantum-well heterostructures and superlattices, published in the IEEE J. Quantum Electron. **QE-24**, 1579 (1988).
[2]J. F. Palmier and Y. Ballini, J. Phys. (Paris) **41**, L539 (1980).
[3]J. F. Palmier and A. Chomette, J. Phys. (Paris) **43**, 381 (1982).
[4]A. Sibille, J. F. Palmier, C. Minot, J. Harmand, and C. Dubon-Chevallier, Superlatt. Microstruct. **3**, 553 (1987).
[5]B. Deveaud, J. Shah, T. C. Damen, B. Lambert, and A. Regreny, Phys. Rev. Lett. **58**, 2582 (1987).
[6]I. Dharssi and P. N. Butcher, J. Phys. Condens. Matter **2**, 4629 (1990).
[7]I. Dharssi and P. N. Butcher, J. Phys. Condens. Matter **2**, 119 (1990).
[8]R. Tsu and G. Dohler, Phys. Rev. B **12**, 680 (1975).
[9]B. Deveaud, J. Shah, T. C. Damen, B. Lambert, A. Chomette, and A. Regreny, IEEE J. Quantum Electron. **QE-24**, 1641 (1988).
[10]J. W. Harrison and J. R. Hauser, Phys. Rev. B **13**, 5347 (1976).
[11]P. K. Basu and B. R. Nag, Surf. Sci. **142**, 256 (1984).
[12]P. K. Basu and D. Roychoudhuri, J. Appl. Phys. **68**, 3442 (1990).
[13]S. B. Ogale and A. Madhukar, J. Appl. Phys. **56**, 368 (1984).
[14]Y. Takeda and A. Sasaki, Jpn. J. Appl. Phys. **24**, 1307 (1985).
[15]D. Aitelhabti, P. Vasilopoulos, and J. F. Currie, Can. J. Phys. **68**, 268 (1990).
[16]E. Merzbacher, *Quantum Mechanics*, 2nd ed. (Wiley, New York, 1970).
[17]D. Mukherji and B. R. Nag, Phys. Rev. B **12**, 4338 (1975).
[18]*Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1970), Chap. 9.
[19]H. Hillmer, A. Forchel, S. Hansmann, M. Morohashi, E. Lopez, H. P. Meier, and K. Ploog, Phys. Rev. B **39**, 10 901 (1989).