Monte Carlo Studies of Miniband Conduction in Extreme Type-II Superlattices

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Miniband charge transport was investigated by Monte Carlo simulations of electronic motion in short period superlattices of type-II energy band alignment (InAs/GaSb composition). The strong decrease of the miniband energy width when the electronic in-plane energy increases, characteristic of type-II superlattices, leads to a conductivity that is very sensitive to a magnetic field applied parallel to the axis of the superlattice. For structures with a miniband energy width greater than the optic phonon energy, the differential conductance can be changed from positive to negative by the magnetic field, due to the suppression of optic phonon emission.

1 Introduction

Miniband conduction in a superlattice is characterized by a negative differential resistance when the intensity of the electric field exceeds a critical value, F_c, which is required for electrons to reach high enough crystal momentum values (about one third of the mini-Brillouin width), to manifest Bragg reflections by the superlattice [1]. The Esaki-Tsu model [2] is the simplest one to describe miniband transport. It assumes catastrophic scattering and leads to an analytical electronic drift velocity. A more complete description, however, requires the inclusion of multiple scattering processes, with a complicated dependence of the scattering amplitude on sample parameters and external fields. In such a case, Monte Carlo simulations have been used to model the conductivity for various type-I band alignment systems [3, 4], which produces a semiclassical description in which Wannier-Stark quantization [5] is not included.

An InAs/GaSb heterojunction forms an extreme type-II band alignment, where the conduction band of InAs lies below the top of the valence band of GaSb. In short period InAs/GaSb superlattices, quantum confinement leads to a positive difference between the energy of conduction band and valence band states, and a semiconducting energy gap is recovered. However, in opposition to the behavior seen in type-I systems, the carrier tunneling probability between adjacent wells, and hence the miniband width, decreases very rapidly when the in-plane energy of the carriers increases, in sharp contrast to type-I superlattices.

In this work, we studied theoretically the miniband transport in InAs/GaSb superlattices in a quantizing magnetic field applied along the axis of the superlattice, using Monte Carlo simulations. The magnetic field causes the electronic miniband to develop into a series of Landau level minibands (LLMB). The characteristic parameters of the LLMB's were obtained from 8-band $\mathbf{k}\cdot\mathbf{p}$ calculations, and they were used as input in the Monte Carlo simulations. The Monte Carlo simulations showed that at low magnetic fields, electrons gain kinetic energy from the external electrical field, climb the ladder of Landau levels through quasi-elastic scattering, and relax their energy through optical phonon emission; in this range of magnetic fields, electrons may have on average a high crystal momentum, and conductivity can be high. As the magnetic field rises, the energy separation between adjacent LLMB's increases, and ultimately a complete transition into a quantum box superlattice transport regime is reached. The transition into the quantum box superlattice regime occurs when the fundamental LLMB width becomes less than the cyclotron energy. For high enough magnetic fields, the miniband energy width will also become less than the optical phonon energy; in this range of magnetic fields, optical phonon scattering is completely suppressed, and electron scattering becomes limited to quasi-elastic transitions between states of opposite k_z, leading to a low average electronic crystal momentum, and hence a low vertical conductivity. These effects are specific to the extreme type-II structures, in which the miniband width decreases with applied magnetic field.

2 Model

When a magnetic field is applied parallel to the axis of the superlattice, the continuous in-plane kinetic energy spectrum of electrons, $\frac{\hbar^2 k^2}{2m*}$, is broken into a ladder of discrete Landau levels of energy $\hbar\omega_c(N+\frac{1}{2})$, where $\omega_c = eB/m^*$ is the in-plane cyclotron frequency for electrons. In the tight-binding approximation, the total energy spectrum of electrons will be given by a set of LLMB's

$$E(N,k_z) = \hbar\omega_c\left(N+\frac{1}{2}\right) - \frac{\Delta}{2}\cos k_z d, \qquad (1)$$

$N = 0, 1, \ldots$, where Δ is the miniband width, and d is the superlattice period. For a type-I superlattice, Δ is usually taken to be independent of N and B, however, for a type-II superlattice, Δ will be dependent on the in-plane energy. For an InAs/GaSb superlattice, we performed 8-band $\mathbf{k}\cdot\mathbf{p}$ calculations, and found that the energy width of the electronic miniband, $\Delta(N,B)$, on magnetic field intensity, B, can be fitted for all Landau levels, N, with a single parameter α, such that

$$\Delta(N,B) = \Delta_0 \mathrm{e}^{-\alpha\left(N+\frac{1}{2}\right)\hbar\omega_c} \tag{2}$$

where Δ_0 and α are parameters, obtained by fitting the theoretical result of the $\mathbf{k}\cdot\mathbf{p}$ calculations with Eq. (2).

Table 1 summarizes the miniband parameters obtained from the 8-band $\mathbf{k}\cdot\mathbf{p}$ calculations for three InAs superlattices: all three structures had the same thickness in the InAs layers (50 Å), but differed in the width of the GaSb layers (60 Å for structure #1, 70 Å for structure #2, and 80 Å for structure #3).

Table I. Structure parameters extracted from $\mathbf{k}\cdot\mathbf{p}$ calculations and used as input in the Monte Carlo simulations.

Structure	period d (Å)	Δ_0 (meV)	α (eV^{-1})
#1	110	34.5	18.1
#2	120	24.2	21.8
#3	130	17.5	25.6

Monte Carlo calculations were done for all three structures. The electric field was applied parallel to the superlattice axis. The natural basis states for electrons are the LLMB states $|N,X,k_z>$: the integer for the Landau level (N), the guiding center coordinate (X), and the wavevector along the superlattice direction (k_z). The effect of the electric field is taken into account using the acceleration theorem. We followed the usual Monte Carlo scheme, described in Ref.[3], which consists of modeling the motion of an electron as a sequence of free flights interrupted by collisions. The duration of each flight, the scattering mechanism operating at the end of the flight, and the quantum state of the electron after the instantaneous scattering process, were chosen stochastically using a random number generator. At the end of the flight electrons were scattered by acoustic or optic phonons, including Umklapp processes. The average crystal momentum was computed after 500 thousand flights. All calculations were done assuming a level broadening of $\gamma = 0.5$ meV. Figure 1 shows the average electron drift velocity as a function of applied electric field, obtained from the Monte Carlo calculations for the structures described in Table 1, when $B = 0$. The conductance increases when the width of the miniband increases; this is because for very short period structures, the miniband width is larger than the LO optical phonon energy ($\hbar\omega_{\mathrm{LO}}$ =30 meV). As a result, electrons have a very efficient route to relax their energy, i.e. by optic phonon emission, and the electrons may acquire a large average crystal momentum. In contrast, if the miniband width is less than the optical phonon energy, electrons can relax energy only through quasi-elastic acoustic phonon emission. This process is much less efficient, and for the same electric field the electron's average momentum is much smaller, due to an increased probability of Bloch transport. Further, for a structure with a miniband width greater than $\hbar\omega_{\mathrm{LO}}$, (structure #1) electrons have a small probability of acquiring crystal momentum beyond $\sim \pi/3d$, and the negative differential conductivity regime is almost absent.

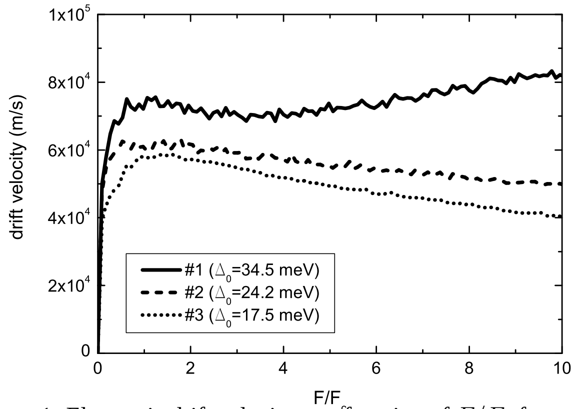

Figure 1. Electronic drift velocity as a function of F/F_c for structures described in Table 1.

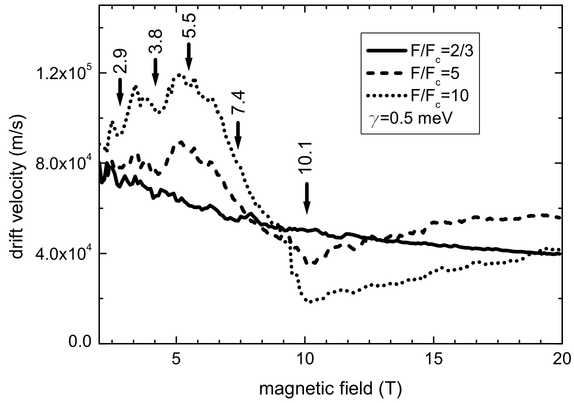

Figure 2. Electronic drift velocity as a function of B for structure #1 (Table 1).

Next we examine the effect of a magnetic field applied perpendicular to the layers. Figure 2 shows the calculated drift velocity, v_d, for structure #1 described in Table 1, for a range of electric fields, $F/F_c = 2/3$, $F/F_c = 5$, and $F/F_c = 10$. For this structure, the zero-field miniband width is larger than the LO phonon energy. In the low electric field regime, $F < F_c$, electrons remain most of the time around the Γ-point of the mini-Brillouin zone, and no miniband effects are seen. When a magnetic field is applied, the average drift velocity simply decreases monotonously, due to the slow dependence of the scattering rates on the magnetic field intensity. At high electric fields, $F >> F_c$, however, electrons acquire a large crystal momentum, and the miniband transport is in full operation. Under these conditions the magnetic field has a dramatic effect on the average drift velocity. A notable feature in Fig. 2 is the pronounced decrease in v_d centered at 7.4 T. At this magnetic field intensity, the miniband energy width becomes smaller than the LO phonon energy, thus optic phonon emission is greatly suppressed, and the superlattice changes from a regime of positive to one of negative differential resistance. This feature is unique to type-II superlattice systems, whereby the miniband energy width depends on the in-plane kinetic energy. The Monte Carlo study also shows conductivity steps at the magnetic field values where an excited Landau level is shifted out of energy resonance with the fundamental one (10.1T, 5.5T, 3.8T 2.9T,...) . At these fields, elastic inter Landau level scattering is reduced and the probability of electrons climbing the ladder of Landau levels to states with enough energy to emit an optical phonon decreases, leading to a decrease in conductivity (Fig.1). These steps, however, are not equally spaced in reciprocal field, as expected for type-I systems, due to the strong dependence of the miniband energy width on the magnetic field.

3 Conclusion

The $\mathbf{k} \cdot \mathbf{p}$ calculation showed that in extreme type-II superlattices of InAs/GaSb composition the width of the LLMB's decrease with applied magnetic field, and the dependence of the width on magnetic field can be approximated by an exponential function quite well. The Monte Carlo calculations showed that a magnetic field applied parallel to the superlattice axis could strongly suppress conductivity, due to the increasing isolation of the LLMB's from one another. For structures with a zero-field miniband energy width greater than the optic phonon energy, the differential conductance can be changed from positive to negative by an applied magnetic field, due to the suppression of optic phonon emission.

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References

[1] *Semiconductor Superlattices*, edited by H.T.Grahn, World Scientific, Singapore (1995).

[2] L.Esaki and R. Tsu, IBM Journal of Research and Development **14**, 61 (1970).

[3] A. Sibille, J.F.Palmier, M.Hadjazi, H.Wang, G.Etemadi, E.Dutisseuil, and F.Mollot, Superlatt. Micr. **13**, 247 (1993).

[4] N. Mori, C.Hamaguchi, L.Eaves, and P.C.Main, VLSI Des. **13**, 45 (2001).

[5] A. Wacker, Physics Reports **357**, 1 (2002).