Complemental Theory for Vertical Transport in Semiconductor Superlattices

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In a superlattice, it is known that localized electronic states are formed due to an electric field applied along the growth axis. Therefore, an electron changes its nature from a wave to a particle. Such change of electronic nature imposes on us to apply different frameworks of transport theory depending of strength of electric field. In this paper, we show such complemental nature of electrons can be described in a unified way by considering electronic acceleration during a scattering event. Based on the unified picture and by means of the Monte Carlo simulation, we calculate drift velocities of electrons in a superlattice. Crossover between band-transport in low fields and hopping-transport in high fields is studied and discussed.

1. Introduction

Vertical transport in a superlattice is a phenomenon where complementarity of an electron plays an important roll. Without applied electric fields, an electron acts like a wave; an electronic eigenstate is a Bloch function specified with a momentum (or a wave vector). The Bloch states are extending over the entire crystal, and their positions are undefined. As far as an applied electric field is small compared with the band width, this 'band picture' remains valid. Therefore, electronic transport in a low electric field is regarded as propagation of wave, described in the momentum-space. On the other hand, when a high electric field is applied, localized Stark-ladder states are formed.[1,2] Contrary to the Bloch states, Stark-ladder states have no momentum and their positions are unambiguously defined. In this case, an electron acts like a particle, and electronic transport as hopping motion in the real-space takes place.[3] Such change of electronic nature due to electric fields has imposed on us to apply different theoretical frameworks depending on applied electric field to study transport phenomena in superlattices. Although a number of theoretical studies have been carried out to investigate vertical transport properties in superlattice, as far as we know these studies are concerning only one of two limiting cases.[4-7]

In this paper, we show that these two limiting cases of electronic transport can be unified by taking electronic acceleration during a scattering into account. Instead of a Bloch function in low electric fields or a Stark-ladder state in high electric fields, we consider a wave-packet whose extension length depends on duration time of a scattering as an initial- and a final-state of a scattering. Such a wave-packet has a momentum as well as potential energy due to electric field, and thus can exhibit both band-transport and hopping-transport. Following motion of wave-packets by the Monte Carlo method, we investigate vertical transport properties of superlattice independent on strength of applied electric field.

2. Complemental Theory of Scattering

We consider a superlattice with period L. When no electric field is applied, an electronic state, a Bloch state, is specified with a wave vector $\boldsymbol{k}$. When an electric field F is applied along the growth axis of a superlattice, an electronic state is accelerated along the electric field as

$$\hbar \frac{\partial k_z}{\partial t} = -eF. \tag{1}$$

If there is no scattering, an electron keeps monotonic motion in the Brillouin zone. As a result of this motion called Bloch oscillation, localized Stark-ladder states are formed. Within a single band approximation, we can express a Stark-ladder state localizing in a nth quantum well, $\chi_{\boldsymbol{k}_\perp n}(\boldsymbol{r})$, as a superposition of Bloch functions on the path of Bloch oscillation as [8]

$$\chi_{\boldsymbol{k}_\perp n}(\boldsymbol{r}) = \frac{\sqrt{\Omega L}}{2\pi} \int_{-\pi/L}^{\pi/L} e^{\mathrm{i}k'_z nL} \phi_{\boldsymbol{k}'}(\boldsymbol{r}, t) dk'_z, \tag{2}$$

where Ω is the crystal dimension along the growth axis, and

$$\phi_{\boldsymbol{k}}(\boldsymbol{r}, t) = \exp\left[-\frac{\mathrm{i}}{\hbar}\int_0^t \varepsilon_{\boldsymbol{k}(t')} dt'\right] \phi_{\boldsymbol{k}}(\boldsymbol{r}), \tag{3}$$

is a Bloch function with time-dependent phase factor. Since value of $\boldsymbol{k}$ changes with time, time dependent phase

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factor of Bloch functions, $\exp(-i\varepsilon_{\boldsymbol{k}}/\hbar)$, also changes with time. Thus, we have to take into account phase change of Bloch functions in making the superposition. Since k_z is related to time by eq. (1), we can also regard $\chi_{\boldsymbol{k}_\perp n}(\boldsymbol{r})$ as a *time average* of Bloch functions over a period of Bloch oscillation.

The fact that a Stark-ladder state is a time average of Bloch functions indicates that, if scattering potential acts just in an instant, we can regard a scattering as transition between Bloch states. However, this is incorrect. It has been pointed out that a scattering takes a finite time to happen and that electron is still accelerated during a scattering. This effect is known as intra-collisional field effect (ICFE), and scattering rates can change due to the ICFE.[9,10] In principle, the ICFE exists not only in superlattices but also in bulk materials. However, the ICFE will be much more important in superlattices than in bulk materials because change of momentum during a scattering event can be as large as width of the Brillouin zone.

By considering the ICFE, a scattered state will be expressed as a superposition of various Bloch functions changing during a scattering, and such a state will be somewhat localizing one. Based on this idea and on the analogy of eq. (2), we write an initial- and a final-state of scattering as a superposition of various time-dependent Bloch functions as [11,12]

$$\tilde{\chi}_{\boldsymbol{k}n}(\boldsymbol{r}) = \sqrt{\frac{\Omega}{2\pi\Delta}} \int_{k_z-\Delta/2}^{k_z+\Delta/2} e^{ik'_z nL} \phi_{\boldsymbol{k}'}(\boldsymbol{r},t) dk'_z. \quad (4)$$

In eq. (4), Δ is a change of wave vector during a scattering. In this study, we regard interval of two successive scattering as duration of a scattering. In the real-space, $\tilde{\chi}_{\boldsymbol{k}n}(\boldsymbol{r})$ is a wave-packet distributing around the nth quantum well. When electrons are frequently scattered before they are accelerated up to the edge of the Brillouin zone, $\Delta \ll 2\pi/L$ is satisfied and $\tilde{\chi}_{\boldsymbol{k}n}(\boldsymbol{r})$ becomes just a Bloch function with a wave vector $\boldsymbol{k}$. On the other hand, when electrons exhibit Bloch oscillation before they are scattered, that is $\Delta > 2\pi/L$ is satisfied, we can regard that $\tilde{\chi}_{\boldsymbol{k}n}(\boldsymbol{r})$ is just a Stark-ladder state localizing in the nth quantum well. Therefore, we may expect that $\tilde{\chi}_{\boldsymbol{k}n}(\boldsymbol{r})$ interpolates between an extending Bloch function and a localized Stark-ladder state.

Energy of $\tilde{\chi}_{\boldsymbol{k}n}(\boldsymbol{r})$ is given by

$$\tilde{E}_{\boldsymbol{k}n} = \langle \varepsilon_{\boldsymbol{k}} \rangle_\Delta + eFn, \quad (5)$$

where the first term is kinetic energy as an average of kinetic energies of Bloch functions give by

$$\langle \varepsilon_{\boldsymbol{k}} \rangle_\Delta = \frac{1}{\Delta} \int_{k_z-\Delta/2}^{k_z+\Delta/2} \varepsilon_{\boldsymbol{k}'} dk'_z. \quad (6)$$

The second term in eq. (5) is potential energy due to applied electric field. Group velocity of $\tilde{\chi}_{\boldsymbol{k}n}(\boldsymbol{r})$ along the electric field is also given by an average of group velocities of constituent Bloch functions as

$$\langle v_g \rangle_\Delta(k_z) = \frac{1}{\Delta} \int_{k_z-\Delta/2}^{k_z+\Delta/2} \frac{1}{\hbar} \frac{\partial \varepsilon_{\boldsymbol{k}'}}{\partial k'_z} dk'_z. \quad (7)$$

This equation indicates that $\langle v_g \rangle_\Delta(k_z)$ approaches to zero with increasing Δ, reflecting the fact that a Stark-ladder state has no momentum in the direction of electric field.

In this study, we consider the electron-LO phonon emission and ionized impurity as scattering potential. Considering the case where the system is at low temperatures, we have neglected phonon absorption processes. For the LO-phonon emission process, matrix element of scattering Hamiltonian $\mathcal{H}'$ between a state $|\boldsymbol{k}\,0\rangle$ and a state $|\boldsymbol{k}+\boldsymbol{q}\,n\rangle$ is given by

$$\begin{aligned} &M_{\boldsymbol{k}0;\boldsymbol{k}+\boldsymbol{q}n}(\Delta) \\ &\quad \equiv \langle \tilde{\chi}_{\boldsymbol{k}0}(\boldsymbol{r}) | \mathcal{H}' | \tilde{\chi}_{\boldsymbol{k}+\boldsymbol{q}n}(\boldsymbol{r}) \rangle \\ &\quad = \frac{2\pi}{\Delta} \int_{k_z-\Delta/2}^{k_z+\Delta/2} \exp\left[-\frac{i}{\hbar} \int_0^t (\varepsilon_{\boldsymbol{k}'} - \varepsilon_{\boldsymbol{k}'+\boldsymbol{q}}) dt' \right. \\ &\qquad \left. + i(k_z+q_z)nL \right] dk'_z \langle \phi_{\boldsymbol{k}} | \mathcal{H}' | \phi_{\boldsymbol{k}+\boldsymbol{q}} \rangle. \end{aligned} \quad (8)$$

Scattering rate of a state $|\boldsymbol{k}\ n\rangle$ is obtained from the Fermi's golden rule and by taking summation with final states as

$$\begin{aligned} &W_{\boldsymbol{k}n}(\Delta) \\ &\quad = \frac{2\pi}{\hbar} \sum_{\boldsymbol{k}'n'} |M_{\boldsymbol{k}n,\boldsymbol{k}'n'}(\Delta)|^2 \\ &\quad \times \delta[\langle \varepsilon_{\boldsymbol{k}} \rangle_\Delta - \langle \varepsilon_{\boldsymbol{k}'} \rangle_\Delta + eFL(n-n') \pm \hbar\omega_{LO}], \end{aligned} \quad (9)$$

where $\hbar\omega_{LO}$ is the LO phonon energy. The summation of final-states in eq. (9) is taken for states which satisfy $\langle \varepsilon_{\boldsymbol{k}'} \rangle_\Delta > 0$. The wave-packet has an extension length which is roughly evaluated by $1/\Delta$. The uncertainty principle between position and wave number of a states shows us that position change smaller than the extension length of the state may be meaningless. Therefore we limit the n' for the summation in eq. (9) only when $|L(n-n')| > 1/\Delta$ is satisfied. This limitation of hopping length assures that no hopping takes place when $\Delta \simeq 0$ and thus an electronic state behaves as a wave.

In order to investigate transport properties, we carried out Monte Carlo simulation as follows:
(i) Electronic states is accelerated by the applied electric field as given by eq. (1) (free flight).
(ii) We determine duration of free flight, τ, with a random number c distributing between 0 and 1 as

$$\int_0^\tau W_{\boldsymbol{k}n}(\Delta) dt' = \ln(c), \quad (10)$$

is satisfied. Since $\Delta = eF\tau$ scattering rate $W_{\boldsymbol{k}n}(\Delta)$ depends on the duration of free flight.

(iii) Final state is chosen with a random number and transition probability given by eq. (9).
These procedures are repeated until we obtain stable transport properties. After simulation for time T, we evaluate drift velocity of electrons as

$$v_d = \frac{1}{T}\left[\int_0^T \langle v_g \rangle_\Delta (k_z) dt + L\sum_l \Delta n_l\right], \qquad (11)$$

where $L\Delta n_l$ is hopping length of the wave-packet at the lth scattering. The first term in eq. (11) derives from electronic motion as a wave, and the second term comes from hopping motion of a wave-packet in the real-space.

3. Results and Discussion

We carried out single electron Mote Carlo simulation for a GaAs(40Å)/AlAs(20Å) superlattice to evaluate drift velocities. This superlattice structure is of interest because miniband width t is slightly larger than the LO phonon energy. If t is much larger than $\hbar\omega_{LO}$, electrons are most likely to be scattered by LO phonons before they reach the edge of Brillouin zone, and thus Stark-ladder states can not be formed. In such a case, electronic transport will be always governed by wave-like behavior of electrons. In the present structure, however, Stark-ladders are formed when impurity scattering rate is small, whereas band-transport is realized when impurity scattering is sufficiently high. Therefore, we can treat impurity density as a parameter which determines degree of localization of electrons.

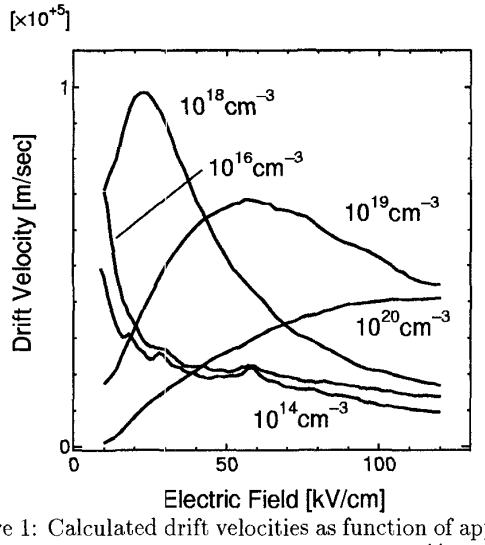

Figure 1: Calculated drift velocities as function of applied electric field with impurity densities from 10^{14}cm^{-3} to 10^{20}cm^{-3}.

Figure 1 shows drift velocities calculated from Monte Carlo simulation for 2 nsec time with various impurity densities. For lower impurity densities (10^{14} cm^{-3} and 10^{16} cm^{-3}), drift velocity curves show distinct negative differential conductance (NDC) in all region of the electric fields. Increase of impurity density brings about enhancement of drift velocity. For 10^{18}cm^{-3} impurities, we see that drift velocity is largely enhanced, especially in the electric fields $F = 20 \sim 50$ kV/cm. On the other hand, the increase of impurity scattering also brings about decrease of drift velocity in low electric field region as disappearance of NDC. Further increase of impurity density causes in turn decrease of drift velocity with disappearance of the NDC. For 10^{20}cm^{-3} impurities, NDC does not appear. Such behavior of drift velocity in a superlattice has already been studied by L. Esaki and R. Tsu within the path integration method.[13] However, the simple method without ICFE can not describe the appearance of resonant LO phonon scattering as described below.

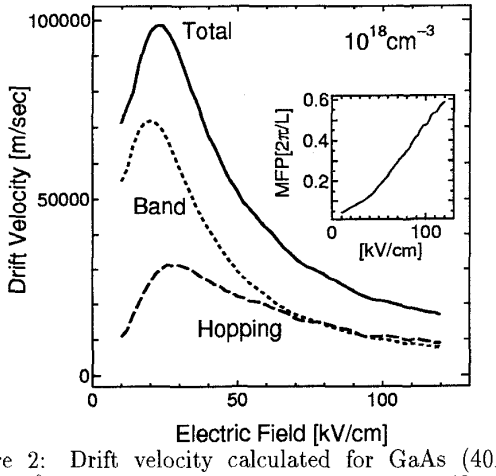

Figure 2: Drift velocity calculated for GaAs (40Å)/ AlAs(20Å) superlattice with impurity density 10^{18}cm^{-3}. The dotted- and dashed-curves denote contribution of band-transport and hopping motion, respectively. Inset: Mean free path in the momentum-space along the electric field as a function of electric field.

The curve for 10^{14} cm^{-3} impurities have some peaks. These peaks are attributed to the resonant LO phonon scattering; When energy difference of Stark-ladder states between neighboring wells is close to the LO phonon energy, that is, $eFnL \simeq \hbar\omega_{LO}$ is satisfied, LO phonon scattering rate increases resonantly, and as a result, enhancement of drift velocity occurs. The peaks at $F \simeq 20$, 30 and 60 kV/cm are assigned to resonance with indices $n =$ 3, 2 and 1, respectively. Such resonance occurs only when localized states are formed. Therefore, we cannot expect resonance with index $n > 4$. We note that gross feature of this curve is similar to theoretical results obtained by V. V.Bryksin and P. Kleinert [4] where hopping between Stark-ladder states in high electric fields is studied. Increase of impurity scattering make such resonance unclear. In the curve for 10^{16}cm^{-3} impurities, such peaks are quite blurry except one with the index $n = 1$ (which is located at $F \simeq 60$kV/cm). There are no such peaks in the

curve for 10^{18}cm^{-3} impurities, although NDC appears.

Figure 2 shows calculated drift velocity with impurity density 10^{18}cm^{-3}. Components of band-transport and hopping-transport are also shown by dotted- and dashed curves, respectively. We see that the component of band-transport plays an important roll especially in lower electric fields. Importance of hopping motion increases with increasing electric field. For $F > 60$ kV/cm, both of those two transport modes have nearly the same significance. Inset is electronic mean free path (MFP) in the momentum-space as a function of applied electric field. We see that MFP $\simeq 0.2 \times 2\pi/L$ at $F \simeq 60$ kV/cm where hopping-transport becomes as large as band-transport.

With 10^{20}cm^{-3} impurities, band-transport dominates transport properties as shown in Fig. 3, though the component of hopping motion increases with increasing electric field. In this case, the mean free path in the momentum-space is less than $0.06\pi/L$, and the NDC completely disappears .

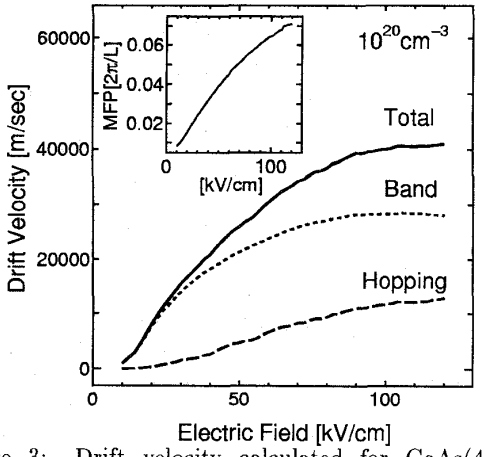

Figure 3: Drift velocity calculated for GaAs(40Å)/AlAs(20Å) superlattice with impurity density 10^{20}cm^{-3}.

We have to note that the theory shown in this study is based on the single band approximation and thus effect of higher bands is neglected. Electrons at the Brillouin zone edge can go up to higher band, instead of doing Bragg reflection. This is known as the Zener tunneling. In real-space picture, the Zener tunneling is described as transition to higher states in the neighboring quantum well. When two localized states in neighboring wells are close in energy, this effect can be very large resonantly. In the present structure, GaAs(40Å)/AlAs(20Å), the second miniband lies in quite higher energy, and such resonance occurs in very high electric field. In the present study, therefore, we have neglected the effect of higher bands.

Acknowledgments

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