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General Expressions for Ellipsoidal-Valley Quantum Transport in Arbitrary Growth Direction: Non-Equilibrium Green's Function

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A theoretical method for the calculation of quantum transport in an ellipsoidal valley is presented. This method is developed using a non-equilibrium Green's function framework. Importantly, it is instructive that k_z is separated into two parts so that the wrong figure shape of the transmission coefficients does not exist. The L-electron effect on AlAs–GaAs–AlAs double barrier structures oriented in the [001], [111], and [110] growth directions is explored using the proposed method. © 2011 The Japan Society of Applied Physics

Theoretical studies of L-electron effects on the AlAs–GaAs–AlAs double barrier structure (DBS) had been explored by us using the transfer-matrix method.[1)] However, this model does not take the boundary (or contact) interaction into account. This study uses a non-equilibrium Green's function (NEGF)[2–4)] framework to reformulate Kim's model[5,6)] and develop an alternative method to calculate the aforementioned effect.

The aim of this study is to develop an NEGF computational technique for solving ellipsoidal-valley quantum transport problems. The developed method is computationally efficient for semiconductor devices with an arbitrary potential profile and any growth direction.

Let the electron potential, $V(z)$, be a function of the growth-direction distance, z, then the Hamiltonian for the general ellipsoidal-valley can be expressed as

$$H_0 = \frac{\hbar^2}{2}\sum_{i,j=x,y,z} k_i W_{ij} k_j + V(z), \tag{1}$$

where W_{ij}, as shown in Appendix of ref. 1, is the 3×3 reciprocal effective mass tensor, (k_x, k_y) denotes the in-plane wave-vector $\mathbf{k}_\parallel$, and k_z denotes the wave-vector along the growth direction. Moreover, the time-independent Schrödinger equation, $H_0\Psi = E\Psi$, with constant potential, $V(z)$, has an eigenfunction of[1,5,6)]

$$\Psi = [A_+\exp(+ik_z z) + A_-\exp(-ik_z z)] \times \exp(ik_x x)\exp(ik_y y), \tag{2a}$$

or

$$\Psi = [A_+\exp(+ik' z) + A_-\exp(-ik' z)] \times \exp(-i\gamma z)\exp(ik_x x)\exp(ik_y y), \tag{2b}$$

where A_+ and A_- are the amplitudes of the propagation in the positive and negative directions along the z-axis, respectively. Furthermore,

$$\gamma = \frac{W_{xz}k_x + W_{yz}k_y}{W_{zz}}, \tag{3}$$

$$k' = \left\{\left(\frac{2}{\hbar^2}\right)\left(\frac{1}{W_{zz}}\right)\left[E - V(z) - \left(\frac{\hbar^2}{2}\right)(\beta_{xx}k_x^2 + 2\beta_{xy}k_x k_y + \beta_{yy}k_y^2)\right]\right\}^{1/2} \tag{4}$$

with

$$\beta_{ij} = W_{ij} - W_{iz}W_{jz}/W_{zz} \quad (i,j = x,y). \tag{5}$$

It is noted that the above expressions are instructive in that k_z is separated into two parts, namely $(-\gamma)$ and $(\pm k')$. So,

$$-\frac{\hbar^2}{2}W_{zz}\frac{d^2\zeta(z)}{dz^2} + \lambda(z)\zeta(z) = E\zeta(z) \tag{6}$$

with

$$\lambda(z) = \frac{\hbar^2}{2}\sum_{i,j=x,y}\beta_{ij}k_i k_j + V(z),$$

$$\zeta(z) = A_+\exp(+ik' z) + A_-\exp(-ik' z).$$

In this study, the Schrödinger equation for a potential profile with an arbitrary shape is solved using the NEGF method.[2–4)] Taking the boundary interaction term (Σ) into account, the Hamiltonian of the active device ($1,\ldots,N$ lattice sites) could be written as[4,7–9)]

$$[H_d + \Sigma]\{\zeta\} = E\hat{I}\{\zeta\} + \{s\}, \tag{7}$$

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where the source term $\{s\}$ is

$$\begin{bmatrix} -i2t\sin k_1' a \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \quad [H_d + \Sigma] = \begin{bmatrix} 2t - te^{ik_1' a} + \lambda_1 & -t & 0 & 0 & \cdots & 0 & 0 & 0 \\ -t & 2t + \lambda_2 & -t & 0 & \cdots & 0 & 0 & 0 \\ 0 & -t & 2t + \lambda_3 & -t & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -t & 2t + \lambda_{N-1} & -t \\ 0 & 0 & 0 & 0 & \cdots & 0 & -t & 2t - te^{ik_N' a} + \lambda_N \end{bmatrix},$$

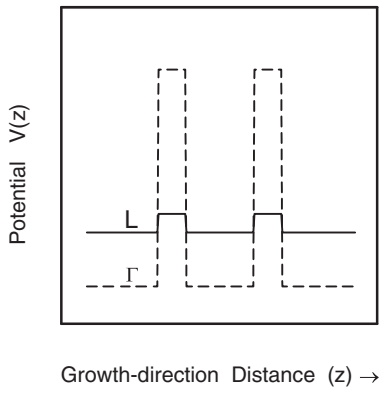

Fig. 1. Schematic potential profiles for AlAs–GaAs–AlAs DBSs at Γ- and L-points.

and the coupling term is $t = (\hbar^2/2a^2)W_{zz}$; in addition, the a denotes the lattice constant, and the k_1' and k_N' denote the k' parameters located at the lattice site 1 and N, respectively. Therefore, the broadening parameters at the left and right sides are $\Gamma_L(1,1) = 2t\sin k_1' a$ and $\Gamma_R(N,N) = 2t\sin k_N' a$, respectively. Once the Green's function G_d $(= [E\hat{I} - H_d - \Sigma]^{-1})$ is found, the transmission coefficient is followed by the trace of $T(E) = Tr[\Gamma_L G_d \Gamma_R G_d^+]$.[2–4)]

We now consider the transmission coefficients for the (001)-, (111)-, and (110)-oriented AlAs–GaAs–AlAs DBS samples with a 56-Å-thick GaAs well and 23-Å-thick AlAs barriers. The DBSs are sandwiched between two GaAs bulk regions. Throughout this study, the reference energy is located at the conduction band edge of the bulk GaAs (0 eV for Γ-band and 0.29 eV for L-band). For an arbitrarily oriented AlAs–GaAs–AlAs multilayer, a double-barrier configuration of the conduction band edge exists not only at the Γ-point, but also at the L-point, as shown in Fig. 1. The band offsets at both the Γ- and L-points are approximately 1 and 0.1 eV, respectively. Calculating at the in-plane wave vector $(k_x, k_y) = (1,1)\pi/a$ and $(1.08, 1.08)\pi/a$, Figs. 2(a) and 2(b), 3(a) and 3(b), and 4(a) and 4(b) show the transmission coefficient (T) spectrums generated by the incident L-electrons for the (001)-, (111)-, and (110)-oriented DBS samples, respectively. Four equivalent L-valleys exist along the [111], [$\bar{1}$11], [1$\bar{1}$1], and [11$\bar{1}$] directions, respectively. From a symmetrical perspective, it is clear that the transmission spectrum generated by the incident electron located at one of the L-valleys may, or may not, be identical to those of the other three L-valleys. Furthermore, it is evident that the L-electron transmission spectrum is strongly ellipsoidal-orientation dependent. Consequently, the resonant tunneling current generated by the

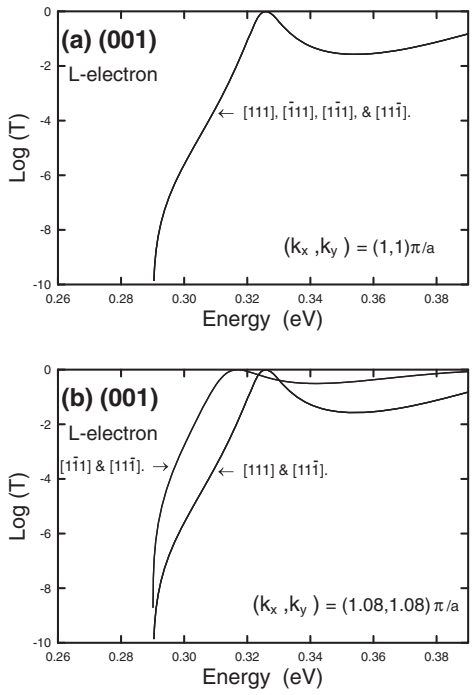

Fig. 2. Calculated transmission coefficients in (001)-oriented AlAs–GaAs–AlAs DBS generated by incident electrons derived from four L-valleys with in-plane vector (k_x, k_y) = (a) $(1,1)\pi/a$ and (b) $(1.08, 1.08)\pi/a$.

incident L-electrons will vary significantly for different growth directions and different L-valleys.

Notably, the present calculations mainly apply the framework of eq. (2b) [but not via (2a)] throughout this study. Furthermore, the framework of eq. (2a) results in the form as:

$$-\frac{\hbar^2}{2} W_{zz} \frac{d^2\phi(z)}{dz^2} - i\hbar^2 (W_{xz}k_x + W_{yz}k_y) \frac{d\phi(z)}{dz} + \left[\frac{\hbar^2}{2} \sum_{i,j=x,y} W_{ij}(z) k_i k_j + V(z) \right] \phi(z) = E\phi(z), \quad (8)$$

with $\phi(z) = A_+ \exp(+ik_z z) + A_- \exp(-ik_z z)$. Importantly, the calculating framework of eq. (2a) yields the unauthentic and singular figure shape of the transmission coefficients. The reason is the existence of the first-order derivative term in eq. (8) [i.e., $i\hbar^2(W_{xz}k_x + W_{yz}k_y)(d\phi(z)/dz)$]. It is instructive that k_z is separated into two parts, namely $(-\gamma)$ and $(\pm k')$, so that the first-order derivate term does not exist in eq. (6). Moreover, k_z is dependent of the momentum in the transverse (x and y) direction due to the γ parameter [see eq. (3)], but not for k'. The coupling of the longitudinal motion to the transverse motion exists in the ellipsoidal valleys via the off-

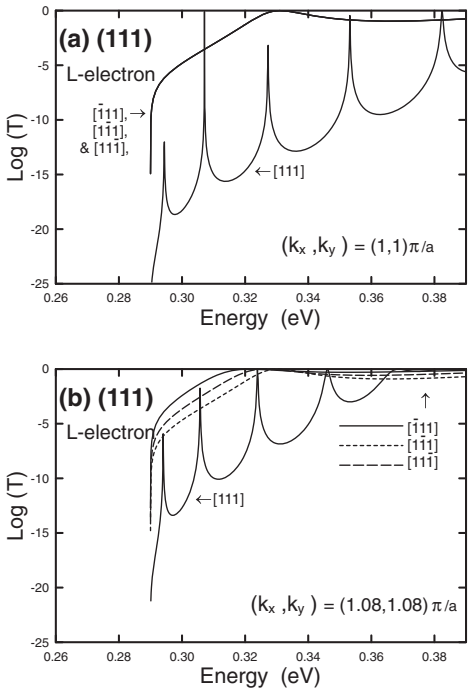

Fig. 3. Calculated transmission coefficients in (111)-oriented AlAs–GaAs–AlAs DBS generated by incident electrons derived from four L-valleys with in-plane vector $(k_x, k_y) =$ (a) $(1, 1)\pi/a$ and (b) $(1.08, 1.08)\pi/a$.

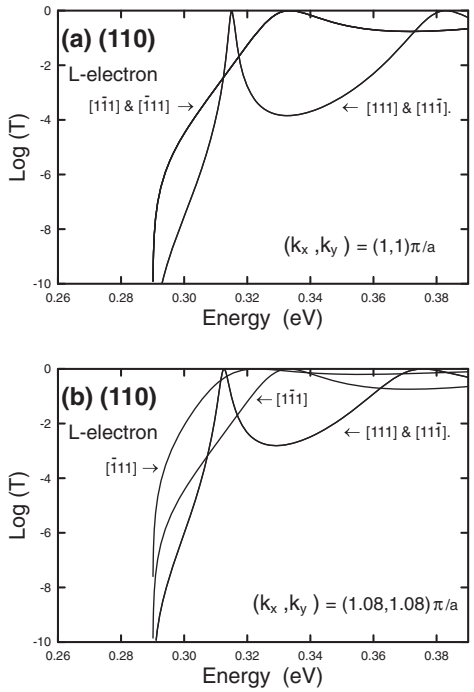

Fig. 4. Calculated transmission coefficients in (110)-oriented AlAs–GaAs–AlAs DBS generated by incident electrons derived from four L-valleys with in-plane vector $(k_x, k_y) =$ (a) $(1, 1)\pi/a$ and (b) $(1.08, 1.08)\pi/a$.

diagonal effective-mass tensor elements, which are valley and growth-direction dependent. Furthermore, the total kinetic energy and transverse momentum must be conserved.

The theoretical calculations only from the Γ-valley electrons have well explained the peak current densities of AlAs–GaAs–AlAs DBS, but those theoretical results yielded much smaller valley current than the experimental results.[10–14] From the previous articles,[1,15] they have demonstrated that the L-valley electrons should have significant contributions to the valley current in the AlAs–GaAs–AlAs DBS, and that is also implied by the results of the present study.

The band-bending effect is not taken into account in our calculations, either. Including band-bending effect in our calculations may significantly enhance the current (or transmission coefficients) contributed from the L-valley electrons. The boundary (or contact) interaction effects in the NEGF framework have been formulated and specified in refs. 3 and 9 in details.

Finally, the treatment of ellipsoidal-valley quantum transport along arbitrary growth direction is a difficult problem to solve due to presence of first-order derivatives in effective mass equation. The present operation on the kinetic energy H_z cause the first-order derivative term in eq. (8) to drop out, which can also be done by a canonical transformation method.[16]

In conclusion, an effective non-equilibrium Green's function method has been presented. Moreover, this method could be applied to the ellipsoidal-valley calculation for a multilayer heterostructure having not only various growth directions but also arbitrary potential profiles. Importantly, it should be noted that k_z must be separated into two parts, namely $(-\gamma)$ and $(\pm k')$, so that the wrong figure shape of the transmission coefficients does not exist.

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