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Hopping conduction in amorphous superlattices

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Abstract. The effect of the intra-well hopping associated with an asymmetric interface charge distribution on the general hopping conductivity in amorphous superlattices is studied. It is found that the current density and hence the conductivity will be larger compared to that of an ordinary superlattice.

1. Introduction

Hopping conduction in superlattices has been studied theoretically (Esaki and Tsu 1970, Kazarinov and Suris 1972, Tsu and Döhler 1975, Calecki *et al* 1984) and experimentally (Esaki and Chang 1974). It is assumed that electrons may be initially localised in the z direction inside the quantum wells of the superlattice but they can move in the z direction by hopping from one quantum well to its neighbours when they interact with phonons.

In this work we describe a model that permits intra-well hopping as well as inter-well hopping. The reason for this is the observation of built-in electric fields (as large as 4×10^5 V cm^{-1}) associated with an asymmetric charge distribution in amorphous superlattices made from alternating layers of a-Si:H and a-SiO:H or from a-Si:H (Abeles and Tiedje 1984, Roxlo and Abeles 1986). Interface defect densities have been determined in these materials by using a number of spectroscopic techniques such as mid-gap optical absorption (Tiedje and Abeles 1984), electron-spin resonance (Wilson *et al* 1985), conductivity (Tiedje and Abeles 1984) and electro-absorption measurements (Roxlo and Abeles 1986). These techniques give estimates for the interface defect densities which vary from 10^{10} to 10^{12} cm^{-2}.

In the a-Si:H/a-SiO:H materials the charge distribution deduced from electro-absorption measurements is well described by an interface dipole model. Electro-absorption spectroscopy indicates that the interfaces are charged and asymmetrical. The built-in field associated with the asymmetrical charge distribution in the layer was observed to be as high as 4×10^5 V cm^{-1}. Our model is based on the asymmetric interface dipole model of Roxlo and Abeles (1986), where the interface dipole region has a finite thickness (figure 1). As a result of formation of large built-in fields, electrons will be localised at the edges of the wells. So we will have intra-well hopping as well as inter-well hopping.

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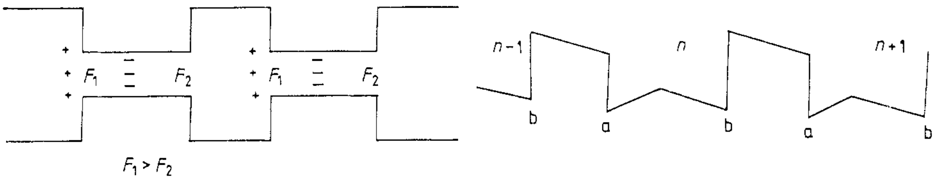

(a) (b)

Figure 1. (*a*) Charge distributions and (*b*) potentials for electrons in the asymmetric interface dipole model.

In § 2 we present a derivation of the electrical current expression for the asymmetric interface dipole model. In § 3 we compare the result with that of an ordinary superlattice with no built-in fields. It turns out that the current and hence the conductivity will be larger compared to that of an ordinary superlattice.

2. Derivation of the hopping current in the asymmetric interface dipole model

We consider an electron gas interacting both with a scattering system and an external field F. The total Hamiltonian is expressed as

$$H_T = H_e + H_s + H_i$$

where H_e is the one-electron Hamiltonian, H_s is the scattering system Hamiltonian and H_i is the interaction Hamiltonian between electrons and the scattering system.

The one-electron Hamiltonian H_e includes the effect of the applied field $\boldsymbol{F}$ in the z direction. The eigenstates $|\nu\rangle$ of H_e are assumed to be localised in the z direction. In Dirac notation we can write $H_e|\nu\rangle = \varepsilon_\nu|\nu\rangle$ where ε_ν are the eigenvalues of H_e.

To calculate the hopping current in the z direction we start from the usual expression for the current density J_z:

$$J_z = (-e/\Omega)\sum_{\nu\nu'} \tfrac{1}{2}(z_{\nu'} - z_\nu)[f_\nu(1-f_{\nu'})W_{\nu\nu'} - f_{\nu'}(1-f_\nu)W_{\nu'\nu}] \qquad (1)$$

where $(-e)$ is the electronic charge, z is the mean z coordinate of an electron in state $|\nu\rangle$ given by $\langle\nu|z|\nu\rangle$, f_ν is the occupation probability of the state $|\nu\rangle$, $W_{\nu\nu'}$ is the jump rate from the state $|\nu\rangle$ to the state $|\nu'\rangle$ and finally Ω is the volume of the system, which is defined as NSd (here N, S and d are number of wells, perpendicular area and period of the superlattice). Because of the two kinds of sub-wells in the system the localised states will be classified into two groups, $|\nu\rangle^a$ and $|\nu\rangle^b$, depending on whether the electron is in the a-type well or b-type well. Here the index ν corresponds to three indices (n, i, k) which specify the main well of localisation, the state number in the well and the two-dimensional momentum $(\hbar k)$ corresponding to the motion in the direction perpendicular to the z axis.

Assuming that $f_\nu \ll 1$ (which corresponds to a low concentration of carriers) we can neglect the Pauli factors in the square brackets. Further, for simplicity we make the following assumptions, which can easily be justified for moderate external fields:

$$\Delta = \varepsilon_b^0 - \varepsilon_a^0 \gg kT \qquad (2a)$$

$$\Delta \gg eFd \qquad (2b)$$

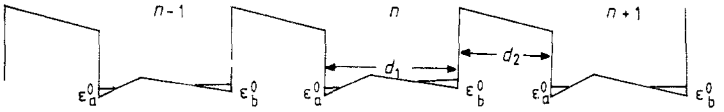

Figure 2. Potentials and ground states for electrons.

where $d = d_1 + d_2$ is the lattice period in the z direction. As a result of the assumption (2*b*) we can drop the indices i: this means that electrons always hop between the ground states of the wells (figure 2). In the nearest-neighbour approximation where we have only non-zero transition rates like $W_{n:n}^{\mathrm{a}\to\mathrm{b}}$, $W_{n:n-1}^{\mathrm{a}\to\mathrm{b}}$, $W_{n:n+1}^{\mathrm{a}\to\mathrm{a}}$ and $W_{n:n+1}^{\mathrm{b}\to\mathrm{b}}$, J_z becomes

$$\begin{aligned}
J_z = (-e/\Omega) \sum_n \sum_{k,k'} [&\tfrac{1}{2}(z^{\mathrm{b}}_{n,k'} - z^{\mathrm{a}}_{n,k})(f^{\mathrm{a}}_{n,k} W^{\mathrm{a}\to\mathrm{b}}_{n,k:n,k'} - f^{\mathrm{b}}_{n,k'} W^{\mathrm{b}\to\mathrm{a}}_{n,k':n,k}) \\
&+ \tfrac{1}{2}(z^{\mathrm{a}}_{n,k'} - z^{\mathrm{b}}_{n,k})(f^{\mathrm{b}}_{n,k} W^{\mathrm{b}\to\mathrm{a}}_{n,k:n,k'} - f^{\mathrm{a}}_{n,k'} W^{\mathrm{a}\to\mathrm{b}}_{n,k':n,k}) \\
&+ \tfrac{1}{2}(z^{\mathrm{b}}_{n-1,k'} - z^{\mathrm{a}}_{n,k})(f^{\mathrm{a}}_{n,k} W^{\mathrm{a}\to\mathrm{b}}_{n,k:n-1,k'} - f^{\mathrm{b}}_{n-1,k'} W^{\mathrm{b}\to\mathrm{a}}_{n-1,k':n,k}) \\
&+ \tfrac{1}{2}(z^{\mathrm{a}}_{n+1,k'} - z^{\mathrm{b}}_{n,k})(f^{\mathrm{b}}_{n,k} W^{\mathrm{b}\to\mathrm{a}}_{n,k:n+1,k'} - f^{\mathrm{a}}_{n+1,k'} W^{\mathrm{a}\to\mathrm{b}}_{n+1,k':n,k}) \\
&+ \tfrac{1}{2}(z^{\mathrm{a}}_{n+1,k'} - z^{\mathrm{a}}_{n,k})(f^{\mathrm{a}}_{n,k} W^{\mathrm{a}\to\mathrm{a}}_{n,k:n+1,k'} - f^{\mathrm{a}}_{n+1,k'} W^{\mathrm{a}\to\mathrm{a}}_{n+1,k':n,k}) \\
&+ \tfrac{1}{2}(z^{\mathrm{a}}_{n-1,k'} - z^{\mathrm{a}}_{n,k})(f^{\mathrm{a}}_{n,k} W^{\mathrm{a}\to\mathrm{a}}_{n,k:n-1,k'} - f^{\mathrm{a}}_{n-1,k'} W^{\mathrm{a}\to\mathrm{a}}_{n-1,k':n,k}) \\
&+ \tfrac{1}{2}(z^{\mathrm{b}}_{n+1,k'} - z^{\mathrm{b}}_{n,k})(f^{\mathrm{b}}_{n,k} W^{\mathrm{b}\to\mathrm{b}}_{n,k:n+1,k'} - f^{\mathrm{b}}_{n+1,k'} W^{\mathrm{b}\to\mathrm{b}}_{n+1,k':n,k}) \\
&+ \tfrac{1}{2}(z^{\mathrm{b}}_{n-1,k'} - z^{\mathrm{b}}_{n,k})(f^{\mathrm{b}}_{n,k} W^{\mathrm{b}\to\mathrm{b}}_{n,k:n-1,k'} - f^{\mathrm{b}}_{n-1,k'} W^{\mathrm{b}\to\mathrm{b}}_{n-1,k':n,k})]
\end{aligned} \tag{3}$$

wherein the indices i have been dropped.

From the form of equation (3) it is noted that the second term is exactly equal to the first term. On the other hand, if we replace $n \to n+1$ in the third, sixth and eighth terms we find the fourth, fifth and seventh terms respectively. If we look at figure 2 we can immediately write down:

$$\begin{aligned}
&z^{\mathrm{b}}_{n,k'} - z^{\mathrm{a}}_{n,k} = d_1 \qquad && z^{a}_{n,k} - z^{\mathrm{b}}_{n-1,k'} = d_2 \\
&z^{\mathrm{a}}_{n,k} - z^{\mathrm{a}}_{n-1,k'} = d \qquad && z^{\mathrm{b}}_{n,k} - z^{\mathrm{b}}_{n-1,k'} = d(=d_1 + d_2).
\end{aligned}$$

Then J_z becomes:

$$\begin{aligned}
J_z = (-e/\Omega) \sum_n \sum_{k,k'} [&d_1(f^{\mathrm{a}}_{n,k} W^{\mathrm{a}\to\mathrm{b}}_{n,k:n,k'} - f^{\mathrm{b}}_{n,k'} W^{\mathrm{b}\to\mathrm{a}}_{n,k':n,k}) \\
&+ d_2(f^{\mathrm{b}}_{n,k} W^{\mathrm{b}\to\mathrm{a}}_{n,k:n+1,k'} - f^{\mathrm{a}}_{n+1,k'} W^{\mathrm{a}\to\mathrm{b}}_{n+1,k':n,k}) \\
&+ d(f^{\mathrm{a}}_{n,k} W^{\mathrm{a}\to\mathrm{a}}_{n,k:n+1,k'} - f^{\mathrm{a}}_{n+1,k'} W^{\mathrm{a}\to\mathrm{a}}_{n+1,k':n,k}) \\
&+ d(f^{\mathrm{b}}_{n,k} W^{\mathrm{b}\to\mathrm{b}}_{n,k:n+1,k'} - f^{\mathrm{b}}_{n+1,k'} W^{\mathrm{b}\to\mathrm{b}}_{n+1,k':n,k})].
\end{aligned} \tag{4}$$

If we denote the total number of electrons in the nth well by n, we can write $n = n_{\mathrm{a}} + n_{\mathrm{b}}$

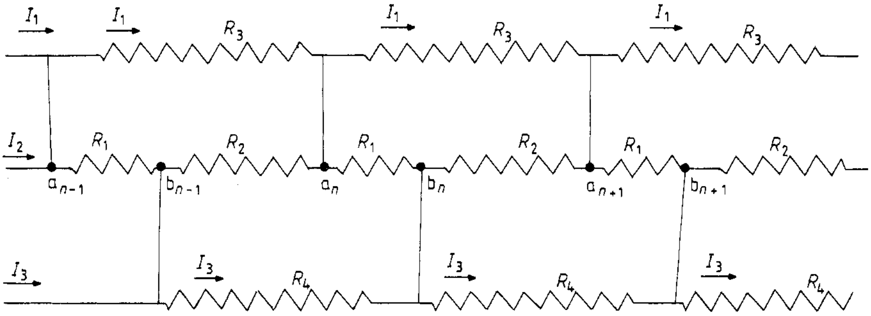

Figure 3. The resistivity network of the system.

where n_a and n_b are the number of electrons in wells a and b, respectively. Then we can define the normalisation such that

$$f_n^{a} = \sum_k f^{a}_{n,k} = \sum_k f^{a}_{n+1,k} = Sn_a$$

$$f_n^{b} = \sum_k f^{b}_{n,k} = \sum_k f^{b}_{n+l,k} = Sn_b \qquad (l \text{ integer}).$$

With the above definitions equation (4) can be written as

$$\begin{aligned} J_z = (-e/\Omega) \sum_n \, & [d_1(Sn_a\langle W\rangle^{a\to b}_{n:n} - Sn_b\langle W\rangle^{b\to a}_{n:n}) \\ & + d_2(Sn_b\langle W\rangle^{b\to a}_{n:n+1} - Sn_a\langle W\rangle^{a\to b}_{n+1:n}) \\ & + d(Sn_a\langle W\rangle^{a\to a}_{n:n+1} - Sn_a\langle W\rangle^{a\to a}_{n+1:n}) \\ & + d(Sn_b\langle W\rangle^{b\to b}_{n:n+1} - Sn_b\langle W\rangle^{b\to b}_{n+1:n})]. \end{aligned} \qquad (5)$$

Here ⟨ ⟩ simply means the thermal average, which is defined such as

$$\begin{aligned} \langle W\rangle^{a\to b}_{n:n} &= \Big(\sum_{k,k'} f^{a}_{n,k} W^{a\to b}_{n,k:n,k'}\Big)\Big/\Big(\sum_k f^{a}_{n,k}\Big) \\ \langle W\rangle^{b\to a}_{n:n} &= \Big(\sum_{k,k'} f^{b}_{n,k'} W^{b\to a}_{n,k':n,k}\Big)\Big/\Big(\sum_{k'} f^{b}_{n,k'}\Big) \end{aligned} \qquad (6)$$

and so on.

To proceed further we consider the resistivity network of this system, which is shown in figure 3. From symmetry arguments, the currents in the resistances R_3 will be the same, which is denoted I_1. Also the currents in the resistances R_4 will be the same, denoted I_3. Therefore the currents in the resistances R_1 and R_2 will be the same and will be called I_2:

$$I_2 = -e(f_a\langle W\rangle^{a\to b}_{n:n} - f_b\langle W\rangle^{b\to a}_{n:n}) = -e(f_b\langle W\rangle^{b\to a}_{n:n+1} - f_a\langle W\rangle^{a\to b}_{n+1:n}) \qquad (7)$$

with $f_a = Sn_a$ and $f_b = Sn_b$. Substituting equation (7) in (5) and doing the summation over n, with the definition $\Omega = NSd$, we write

$$\begin{aligned} J_z = -e(n_a\langle W\rangle^{a\to b}_{n:n} - n_b\langle W\rangle^{b\to a}_{n:n}) - e(n_a\langle W\rangle^{a\to a}_{n:n+1} - n_a\langle W\rangle^{a\to a}_{n+1:n}) \\ - e(n_b\langle W\rangle^{b\to b}_{n:n+1} - n_b\langle W\rangle^{b\to b}_{n+1:n}). \end{aligned} \qquad (8)$$

In equation (8) the first term corresponds to J_2, and the second and the third terms correspond to J_1 and J_3 respectively ($J_z = J_1 + J_2 + J_3$). To calculate these current density components we need to calculate n_a and n_b separately (the transition rates are assumed to be known). The concentrations n_a and n_b are calculated in Appendix 1. Using the Miller and Abraham formula for the transition rates (Miller and Abraham 1960) we can write

$$W_{ij} = \nu_\mathrm{ph} J(r_{ij}) \frac{1}{1 - \exp(-\Delta_{ij}/kT)} \simeq \nu_\mathrm{ph} J(r_{ij}) \exp(-|\Delta_{ij}|/kT) \tag{9}$$

for transitions upwards in energy, and

$$W_{ij} = \nu_\mathrm{ph} J(r_{ij}) \tag{10}$$

for transitions downwards in energy. Here ν_ph is the phonon frequency and

$$J(r_{ij}) = \exp(-2r_{ij}/a) \tag{11}$$

is the usual overlap integral.

Equations (9) and (10) are derived with the aid of Fermi's golden rule, using the electron–phonon interaction in the deformation potential approximation for the perturbation Hamiltonian V. The factor $\exp(-2r_{ij}/a)$ comes from the square of the transition matrix element of V, which is proportional to the overlap between the local wavefunctions on sites i and j (here a is the lattice parameter). In Appendix 2 the transfer integrals will be calculated for this particular problem.

In the presence of the applied electric field $\boldsymbol{F}$, the energies are modified: $E = \varepsilon + eFz$ (the electronic charge is $-e$). If we calculate the energy differences for the above transitions we find

$$E^\mathrm{a}_{n+1} - E^\mathrm{a}_n = (\varepsilon_\mathrm{a} + eFz^\mathrm{a}_{n+1}) - (\varepsilon + eFz^\mathrm{a}_n) = eFd > 0$$

$$E^a_{n+1} - E^\mathrm{b}_n = (\varepsilon_\mathrm{a} + eFz^\mathrm{a}_{n+1}) - (\varepsilon_\mathrm{b} + eFz^\mathrm{b}_n) = \varepsilon_\mathrm{a} - \varepsilon_\mathrm{b} + eFd_2 < 0$$

$$E^\mathrm{b}_n - E^\mathrm{a}_n = (\varepsilon_\mathrm{b} + eFz^\mathrm{b}_n) - (\varepsilon_\mathrm{a} + eFz^\mathrm{a}_n) = \varepsilon_\mathrm{b} - \varepsilon_\mathrm{a} + eFd_1 > 0$$

$$E^\mathrm{a}_{n+1} - E^\mathrm{b}_n = (\varepsilon_\mathrm{a} + eFz^\mathrm{a}_{n+1}) - (\varepsilon_\mathrm{b} + eFz^\mathrm{b}_n) = \varepsilon_\mathrm{a} - \varepsilon_\mathrm{b} + eFd_2 < 0.$$

Accordingly the transition rates are

$$W^{\mathrm{a}\to\mathrm{a}}_{n:n+1} = W^{\mathrm{b}\to\mathrm{b}}_{n:n+1} = \nu_\mathrm{ph} J(d) \exp(-eFd/kT) \tag{12a}$$

$$W^{\mathrm{b}\to\mathrm{a}}_{n:n+1} = \nu_\mathrm{ph} J(d_2) \tag{12b}$$

$$W^{\mathrm{a}\to\mathrm{b}}_{n:n} = \nu_\mathrm{ph} J(d_1) \exp[-(\Delta + eFd_1)/kT] \tag{12c}$$

and for the inverse transitions

$$W^{\mathrm{a}\to\mathrm{a}}_{n+1:n} = W^{\mathrm{b}\to\mathrm{b}}_{n+1:n} = \nu_\mathrm{ph} J(d) \tag{12d}$$

$$W^{\mathrm{a}\to\mathrm{b}}_{n+1:n} = \nu_\mathrm{ph} J(d_2) \exp[-(\Delta - eFd_2)/kT] \tag{12e}$$

$$W^{\mathrm{b}\to\mathrm{a}}_{n:n} = \nu_\mathrm{ph} J(d_1). \tag{12f}$$

Here we dropped the angular brackets because for this particular problem the J and therefore the W do not depend on k. Substituting the transition rates from equations

(12*a*)–(12*f*) and the values of n_a and n_b from Appendix 1 into equation (8), we can calculate the total current density:

$$J_z = \frac{-enJ(d)[\exp(-eFd/kT) - 1]J(d_1)\{\exp[-(\Delta + eFd_1)/kT] + 1\}\nu_{ph}}{J(d_1)\{\exp[-(\Delta + eFd_1)/kT] + 1\} + J(d_2)\{\exp[-(\Delta - eFd_2)/kT] + 1\}}$$
$$- \frac{enJ(d)[\exp(-eFd/kT) - 1]J(d_2)\{\exp[-(\Delta - eFd_2)/kT] + 1\}\nu_{ph}}{J(d_1)\{\exp[-(\Delta + eFd_1)/kT] + 1\} + J(d_2)\{\exp[-(\Delta - eFd_2)/kT] + 1\}}$$
$$- \frac{enJ(d_1)J(d_2)\{\exp[-(\Delta + eFd_1)/kT] - \exp[-(\Delta - eFd_2)/kT]\}\nu_{ph}}{J(d_1)\{\exp[-(\Delta + eFd_1)/kT] + 1\} + J(d_2)\{\exp[-(\Delta - eFd_2)/kT] + 1\}}. \tag{13}$$

In Appendix 2 we show that $J(d_1) \gg J(d_2)$, which is larger than $J(d)$. Therefore we can easily neglect $J(d)/J(d_1)$ and $J(d_2)/J(d_1)$. So (13) becomes

$$J_z = -enJ(d)[\exp(-eFd/kT) - 1]\nu_{ph} - enJ(d)\exp(-\Delta/kT)\nu_{ph}\frac{\exp(-eFd_1/kT) - \exp(eFd_2/kT)}{\exp[-(\Delta + eFd_1)/kT] + 1}. \tag{14}$$

3. Results and discussion

In Appendix 3 we calculate the current density for an ordinary superlattice with no built-in field. If we compare (14) with (A3.6), we see that the first term in (14) is the current density in the absence of the built-in field and the second term is the increase in the hopping current due to the built-in field. Let us denote this term by J_{bi}. To estimate the order of magnitude of this current we set $d_1 = d_2 = d/2$. In this case J_{bi} becomes

$$J_{bi} = neJ(d)\nu_{ph}\frac{\exp(-\Delta/kT)}{\exp[-(\Delta + eFd/2)/kT] + 1} 2\sinh(eFd/2kT). \tag{15}$$

So the correction will be small for small external electric fields and larger for higher fields. Further if we remember that $\Delta \gg eFd, kT$, we neglect the exponential term in the denominator of (14) and (15). So in the ohmic limit (14) becomes

$$J_z = [ne^2J(d)Fd\nu_{ph}/kT][1 + \exp(-\Delta/kT)]. \tag{16}$$

Therefore the correction will be $\exp(-\Delta/kT)$ times the current density of an ordinary superlattice with no built-in field. Since we have assumed that $\Delta \gg kT$, we can find an upper limit for the correction term: the maximum value of the correction will be $e^{-1} \simeq 0.37$ times the current density of an ordinary superlattice.

4. Conclusions

We have investigated the effect of the intra-well hopping and an asymmetric interface charge distribution on general hopping conductivity in superlattices. We have found that the current density and hence the conductivity will be larger compared to that observed in an ordinary superlattice. The upper limit of the enhancement is found to be about 37%. It should be emphasised that our formulation is based on the assumption that electrons always hop between the ground states of the sub-wells. Further work should focus on incorporating the excited states.

Acknowledgments

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Appendix 1. Calculation of n_a and n_b

As we stated earlier (equation (7)) the current from a_n to b_n over the resistance R_1 is equal to the current from b_n to a_{n+1} over R_2:

$$-e(f_a\langle W\rangle_{n:n}^{a\to b} - f_b\langle W\rangle_{n:n}^{b\to a}) = -e(f_b\langle W\rangle_{n:n+1}^{b\to a} - f_a\langle W\rangle_{n+1:n}^{a\to b}).$$

If we divide each side of (7) by S we get

$$e(n_a\langle W\rangle_{n:n}^{a\to b} - n_b\langle W\rangle_{n:n}^{b\to a}) = e(n_b\langle W\rangle_{n:n+1}^{b\to a} - n_a\langle W\rangle_{n+1:n}^{a\to b}). \tag{A1.1}$$

On the other hand the normalisation condition for n_a and n_b is

$$n_a + n_b = n. \tag{A1.2}$$

In equations (A1.1) and (A1.2) the transition rates are assumed to be known (equations (12*a*)–(12*f*)). The only unknowns are n_a and n_b. If we solve n_a and n_b from (A1.1) and (A1.2) we find

$$n_a = \frac{n[J(d_1) + J(d_2)]}{J(d_1)\{\exp[-(\Delta + eFd_1)/kT] + 1\} + J(d_2)\{\exp[-(\Delta - eFd_2)/kT] + 1\}} \tag{A1.3}$$

$$n_b = \frac{n\{J(d_1)\exp[-(\Delta + eFd_1)/kT] + J(d_2)\exp[-(\Delta - eFd_2)/kT]\}}{J(d_1)\{\exp[-(\Delta + eFd_1)/kT] + 1\} + J(d_2)\{\exp[-(\Delta - eFd_2)/kT] + 1\}}. \tag{A1.4}$$

Appendix 2. Calculation of the transfer integrals

Assuming that the built-in fields are uniform, we can write (figure A1):

$$V(z) = eF_1 z \qquad 0 < z < z_1 \tag{A2.1}$$

$$V(z) = -eF_2(z - d) \qquad z_1 < z < d_1 \tag{A2.2}$$

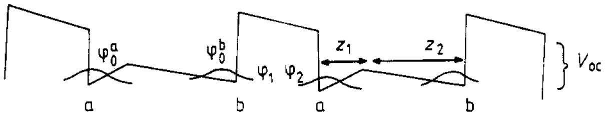

Figure A1. Potentials and the appropriate wavefunctions for electrons.

$$V(z) = V_{oc} - eF_2(z - d_1) \qquad d_1 < z < d. \tag{A2.3}$$

The ground-state wavefunctions associated with these potentials (Zawadzki 1983) are

$$\varphi_0^a = BA_0^a z \exp(-\alpha_0^a z) \qquad A_0^a = 4(\alpha_0^a)^3 \qquad \alpha_0^a = (3m^* eF_1/2\hbar^2)^{1/3} \tag{A2.4}$$

$$\begin{aligned}&\varphi_0^b = BA_0^b(d_1 - z)\exp[-\alpha_0^b(d_1 - z)]\\ &A_0^b = 4(\alpha_0^b)^3 \qquad \alpha_0^b = (3m^* eF_2/2\hbar^2)^{1/3}\end{aligned} \tag{A2.5}$$

$$\varphi_1 = B' \exp(-Kz) \tag{A2.6}$$

$$\varphi_2 = B' \exp[-K(d_2 - z)] \qquad K = [2m^*(V_{oc} - \varepsilon)/h]^{1/2}. \tag{A2.7}$$

Here the coefficients B and B' are to be found from the normalisation over the distance d.

The transfer integral $J(d_1)$ is

$$J(d_1) = \int_0^{d_1} \varphi_0^a(z) V(z) \varphi_0^b[-(z - d)]\,\mathrm{d}z. \tag{A2.8}$$

Now defining

$$A_0^a = AF_1 \qquad A_0^b = AF_2 \qquad \text{with } A = 6m^* e/\hbar^2 \tag{A2.9}$$

$J(d_1)$ becomes

$$\begin{aligned}J(d_1) = {}& A^2B^2eF_1^2F_2 \int_0^{z_1} z^2(d_1 - z)\exp(-A^{1/3}F_1^{1/3}z)\exp[-A^{1/3}F_2^{1/3}(d_1 - z)]\,\mathrm{d}z\\ &- A^2B^2eF_1F_2^2 \int_{z_1}^{d_1} z(d_1 - z)(z - d)\exp(-A^{1/3}F_1^{1/3}z)\\ &\times \exp[-A^{1/3}F_2^{1/3}(d_1 - z)]\,\mathrm{d}z.\end{aligned} \tag{A2.10}$$

Further with the definitions

$$C = A^2B^2eF_1F_2\exp(-A^{1/3}F_2^{1/3}d_1) \qquad \text{and} \qquad \alpha = A^{1/3}(F_1^{1/3} - F_2^{1/3}) \tag{A2.11}$$

we can write

$$\begin{aligned}J(d_1) = C\biggl(&F_1 \int_0^{z_1} (d_1z^2 - z^3)\exp(-\alpha z)\,\mathrm{d}z\\ &- F_2 \int_{z_1}^{d_1} [-d_1d_2z + (d_1 + d)z^2 - z^3]\exp(-\alpha z)\,\mathrm{d}z\biggr).\end{aligned} \tag{A2.12}$$

To proceed further we have to know the value of z_1. Let us assume that $F_1 = 2F_2$. The condition

$$\oint F\,\mathrm{d}z = 0$$

requires that $F_1 z_1 = F_2(d - z_1)$, which gives $z_1 = d/3$. We can also take $d_1 = d/2$, so $J(d_1)$ becomes

$$J(d)_1) = CF_2\{(d^2/\alpha^2)[-(7/18)\exp(-\alpha d/3) + (1/4)\exp(-\alpha d/2)]\} + CF_2\{(d/\alpha^3)[-\exp(-\alpha d/3) - 2] + (1/\alpha^4)[18\exp(-\alpha d/3) - 6\exp(-\alpha d/2) - 12]\}. \tag{A2.13}$$

Taking $F_1 = 2F_2 = 2 \times 10^6\ \mathrm{V\,m^{-1}}$, $m^* = 0.014m_0$ and $d_1 = d_2 = 50$ Å, we show that $\alpha \simeq 3 \times 10^7\ \mathrm{m^{-1}}$ (A2.17) and $B \simeq 10^{-10}$ (A2.19). Substituting the above values in (A2.13) we find

$$J(d_1) \simeq 10^{-17}\ \mathrm{meV}. \tag{A2.14}$$

On the other hand $J(d_2)$ is

$$J(d_2) = \int_{d_1}^{d} \varphi_1 V(z) \varphi_2\, \mathrm{d}z = (B')^2 \exp(-Kd_2)(V_{\mathrm{oc}} d_2 - eF_2 d_2^2/2). \tag{A2.15}$$

Taking $m^* = 0.014m_0$ and $V_{\mathrm{oc}} - \varepsilon \simeq 200$ meV we find $K \simeq 2.5 \times 10^8$ and for $d = 100$ Å we show that $B' = \sqrt{5} \times 10^4$ (A2.21). So for $F_2 = 10^6\ \mathrm{V\,m^{-1}}$, $J(d_2)$ becomes

$$J(d_2) = 2 \times 10^{-20} + 4 \times 10^{-23} \simeq 2 \times 10^{-20}\ \mathrm{meV}. \tag{A2.16}$$

Calculation of α:

$$\alpha = A^{1/3}(F_1^{1/3} - F_2^{1/3}) = (6m^* e/h)^{1/3}(F_1^{1/3} - F_2^{1/3}).$$

If we put $m^* = 0.014m_0$, $F_1 = 2 \times 10^6\ \mathrm{V\,m^{-1}}$ and $F_2 = 10^6\ \mathrm{V\,m^{-1}}$ we find

$$\alpha = 3 \times 10^7\ \mathrm{m^{-1}}. \tag{A2.17}$$

Calculation of B: from the normalisation condition

$$\int_0^d \varphi_0^{\mathrm{a}*} \varphi_0^{\mathrm{a}}\, \mathrm{d}z = 1$$

which gives

$$B^2 A^2 \int_0^d z^2 \exp(-2\alpha_0^{\mathrm{a}} z)\, \mathrm{d}z = 16B(\alpha_0^{\mathrm{a}})^6\{[d^2/2\alpha_0^{\mathrm{a}} - 2d/4(\alpha_0^{\mathrm{a}})^2 - 2/8(\alpha_0^{\mathrm{a}})^3]\exp(-2\alpha d) - 2/8(\alpha_0^{\mathrm{a}})^3\} = 1. \tag{A2.18}$$

Here we put $A_0^2 = 16(\alpha_0^{\mathrm{a}})^6$. If we put $\alpha_0^{\mathrm{a}} \simeq \alpha = 3 \times 10^7\ \mathrm{m^{-1}}$ and $d = 100$ Å in (A2.18) we find

$$B \simeq 10^{-10}. \tag{A2.19}$$

Calculation of B': from the normalisation condition

$$\int_0^d \varphi_1^* \varphi_1\, \mathrm{d}z = 1$$

we find

$$B' = 1\Big/\int_0^d \exp(-2Kz)\, \mathrm{d}z = 2K/[1 - \exp(-2Kd)] \tag{A2.20}$$

with $K = [2m^*(V_{\mathrm{oc}} - \varepsilon)/\hbar^2]$. Taking $m^* = 0.014m_0$ and $V_{\mathrm{oc}} - \varepsilon = 200$ meV we find $K = 2.5 \times 10^8\ \mathrm{m^{-1}}$ and for $d = 100$ Å

$$B' = \sqrt{5} \times 10^4. \tag{A2.21}$$

Appendix 3. Calculation of the hopping current for an ordinary superlattice with no built-in fields

When there is no built-in field we will have only inter-well hopping. So in this case in the nearest-neighbour approximation equation (1) becomes

$$J = (-e/\Omega) \sum_n \sum_{k,k'} [\tfrac{1}{2}(z_{n+1,k'} - z_{n,k})(f_{n,k} W_{n,k:n+1,k'} - f_{n+1,k'} W_{n+1,k':n,k}) + \tfrac{1}{2}(z_{n-1,k'} - z_{n,k})(f_{n,k} W_{n,k:n-1,k'} - f_{n-1,k'} W_{n-1,k':n,k})]. \qquad (A3.1)$$

If we replace $n \rightarrow n+1$ in the second term we find the first term. Remembering that $z_{n+1,k'} - z_{n,k} = d$ we can write (A3.1) as

$$J_z = (-ed/\Omega) \sum_n \sum_{k,k'} (f_{n,k} W_{n,k:n+1,k'} - f_{n+1,k'} W_{n+1,k':n,k}). \qquad (A3.2)$$

If we denote the total number of electrons in the nth well by n we can define the normalisation such that $f_n = f_{n+1} = Sn$. By this definition (A3.2) becomes

$$J = (-endS/\Omega) \sum_n (\langle W \rangle_{n:n+1} - \langle W \rangle_{n+1:n}). \qquad (A3.3)$$

Here $\langle\ \ \rangle$ means the thermal average, which is defined as

$$\langle W \rangle_{n:n+1} = \left(\sum_{k,k'} f_{n,k} W_{n,k:n+1,k'} \right) \Big/ \left(\sum_k f_{n,k} \right)$$

and so on. Using the Miller and Abraham formula we can write

$$\langle W \rangle_{n:n+1} = \nu_{\mathrm{ph}} J(d) \exp(-eFd/kT) \qquad (A3.4)$$

$$\langle W \rangle_{n+1:n} = \nu_{\mathrm{ph}} J(d). \qquad (A3.5)$$

To go further we define $\Omega = NSd$, substitute (A3.4) and (A3.5) into (A3.3) and do the summation over n. So the current density becomes

$$J_z = -en\nu_{\mathrm{ph}} J(d)[\exp(-eFd/kT) - 1]. \qquad (A3.6)$$

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