Optical Phonons in Metal-Semiconductor Tunnel Junctions

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A calculation of the conductance of a metal-semiconductor tunnel junction for which interactions with optical phonons occur in the semiconductor electrode is given. The calculation is based upon a Green's-function theory of Appelbaum, Brinkman, and Zawadowski. The conductance is found for a uniform self-energy and a spatially dependent self-energy. Although there is qualitative agreement between the present results and the main features of the transfer Hamiltonian formalism given by Davis and Duke, further analysis of the data on p-Si indicates that barrier effects occur in addition to the electrode effects. On the basis of the doping dependence of the reverse-bias line shape in p-Si, it is suggested that a region of strong interaction with the optical phonons occurs in the barrier near the metal electrode at low doping levels.

I. INTRODUCTION

One of the prominent many-body effects in tunneling is the self-energy effect due to optical phonons in degenerate-semiconductor electrodes.[1] The interpretation[2] of this effect has been based upon the transfer Hamiltonian formalism.[3]

In this formalism, the conductance of the tunnel junction is thought to give information about the bulk spectral-weight function

$$A(\xi_k, \epsilon) = (1/\pi) \mid \mathrm{Im}G(\xi_k, \epsilon) \mid$$

of the electrode in which the many-body interactions occur. Agreement between theory and experiment for the self-energy effect due to optical phonons in highly doped p-Si is satisfactory.[2] However, several developments have occurred since the interpretation was given. First, Appelbaum and Brinkman[4] have derived a theory of tunneling which does not involve a transfer matrix element but instead involves the Green's functions for the so-called left-hand and right-hand problems. Zawadowski[5] had previously derived a similar theory, but Appelbaum and Brinkman[6] went on to examine the effects of the interface between an electrode and the tunnel barrier. In particular, they found that when the interface was accounted for, the self-energy $\Sigma(z, \epsilon)$ shows spatial oscillations near the barrier similar to Friedel oscillations.

The second development was the derivation of a wave-function approach to inelastic tunneling[7,8] which made use of an orthogonal-basis set instead of the usual non-orthogonal-basis set.[3] It might have been thought that any theory such as the Green's-function theory of Appelbaum, Brinkman, and Zawadowski[9] (ABZ) which uses a nonorthogonal basis set gives incorrect answers for interface effects. This is because the interface effects occur in the region where the nonorthogonal basis states are ill defined. However, by comparing the results of the wave-function approach to the Green's-function theory (ABZ), we have found no disagreement and we must conclude the Green's function theory is correct. Further, either of these theories (the wave-function approach or the Green's-function approach) can give structure in the conductance due to the interaction with a phonon (or any other energy-loss mechanism) in the barrier region which resembles the self-energy effect discussed by Davis and Duke.[2]

Third, additional data[10] on lower doped semiconductor electrodes show that the structure in the conductance is strikingly sensitive to doping, an effect which does not appear to be due to the bulk spectral-weight function. Also, an analysis of the magnetic field dependence of these functions[11] indicates that some of the structure in the conductance must be due to interactions in or near the barrier region.

The purpose of the present paper is, therefore, to examine the effects of interactions with phonons in a semiconductor electrode with the ABZ theory since this theory correctly treats many-body interactions in all regions of the tunnel junction. Specifically, we wish to determine how important the spatial variation of the self-energy is for semiconductor electrodes since, as noted above, some discrepancies do exist between the results of the transfer Hamiltonian formalism (which omits interface effects) and experiment.

In Sec. II, we derive the conductance for a uniform self-energy using the Green's-function theory of ABZ. The results of this calculation are then compared with the results of the transfer Hamiltonian formalism. In Sec. III, we examine the spatial dependence of the self-energy for semiconductor electrode for a square barrier and for a Schottky barrier. We then find the conductance for a model self-energy which approximates the spatial dependence found for a square barrier and a Schottky barrier satisfactorily. In Sec. IV, we give a summary of our results.

II. OPTICAL PHONONS—UNIFORM SELF-ENERGY

Let the tunnel junction consist of a degenerate-semiconductor electrode in the region $z<0$, a square

barrier of height V_0 in the region $0<z<b$, and a free-electron metal in the region $z>b$. For simplicity, we assume that the semiconductor carriers are electrons with effective mass m^* and these carriers occupy states up to the Fermi level, a distance μ above the band edge at $T=0°$K. In the semiconductor electrode, we assume that the electrons interact via a deformation-potential coupling to optical phonons of energy $\hbar\omega$.[2] We also assume that the mass of the electrons is m_b in the barrier and m_0 in the metal.

As discussed in the Introduction, the nonorthogonality of the basis states used by Appelbaum and Brinkman[4] does not introduce any error into the Green's-function theory (through second order in the tunneling amplitude T). Therefore, we conclude the theory of ABZ is correct and we make use of their results. In their theory, the current per unit area is given by

$$\begin{aligned} I=(-2\pi e/\hbar)(\hbar^2/2m_b)^2(2/\pi^2) &\times\int d^3r\int d^3r'\delta(z-\bar z)\delta(z'-\bar z)\\ &\times\int_0^{-eV}d\epsilon\int_{-\infty}^{+\infty}d\epsilon'\delta(\epsilon'-\epsilon-eV)\\ &\times\{\mathrm{Im}G^L(\mathbf{r},\mathbf{r}',\epsilon)(\partial^2/\partial z\partial z')\,\mathrm{Im}G^R(\mathbf{r},\mathbf{r}',\epsilon')\\ &-[(\partial/\partial z')\,\mathrm{Im}G^L(\mathbf{r},\mathbf{r}',\epsilon)](\partial/\partial z)\,\mathrm{Im}G^R(\mathbf{r},\mathbf{r}',\epsilon')\\ &-[(\partial/\partial z)\,\mathrm{Im}G^L(\mathbf{r},\mathbf{r}',\epsilon)](\partial/\partial z')\,\mathrm{Im}G^R(\mathbf{r},\mathbf{r}',\epsilon')\\ &+[(\partial^2/\partial z\partial z')\,\mathrm{Im}G^L(\mathbf{r},\mathbf{r}',\epsilon)]\,\mathrm{Im}G^R(\mathbf{r},\mathbf{r}',\epsilon')\}. \end{aligned}\tag{2.1}$$

The bias voltage V is defined so that negative voltage corresponds to electrons flowing into the semiconductor in accordance with the convention used by Davis and Duke.[2] The point $\bar z$ can be taken as any point in the barrier region, $0<z<b$, since all many-body interactions occur to the left in the region $z<0$.[4] $G^L(\mathbf{r},\mathbf{r}',\epsilon)$ is the retarded Green's function for the left-hand problem and $G^R(\mathbf{r},\mathbf{r}',\epsilon')$ is similarly defined for the right-hand problem. [We will denote right-hand quantities, such as ϵ', by a prime and left-hand quantities, such as ϵ, without a prime.]

Since we have translational symmetry parallel to the junction (i.e., perpendicular to z), we can write for both G^L and G^R that

$$G(\mathbf{r},\mathbf{r}',\epsilon)=\int[d^2p_t/(2\pi)^2]\times\exp[i\mathbf{p}_t\cdot(\mathbf{r}-\mathbf{r}')]G(z,z',\mathbf{p}_t,\epsilon).\tag{2.2}$$

For optical phonons with a deformation-potential coupling, the self-energy is local,[12] i.e., $\Sigma(\mathbf{r},\mathbf{r}',\epsilon)=\Sigma(\mathbf{r},\epsilon)\delta(\mathbf{r}-\mathbf{r}')$.

Hence, we find that G^L obeys

$$[-(\hbar^2/2m)(d^2/dz^2)+V(z)-\epsilon-\mu+\hbar^2p_t^2/2m+\Sigma(z,\epsilon)]G^L(z,z',\mathbf{p}_t,\epsilon)=-\delta(z-z'),\tag{2.3}$$

where

$$V(z)=0,\quad z<0;\qquad =V_0,\quad z>0.\tag{2.4}$$

We take $m=m^*$ for $z<0$ and $m=m_b$ for $z>0$. The spatially dependent self-energy $\Sigma(z,\epsilon)$ is given approximately by[6]

$$\Sigma(z,\epsilon)=-g^2\rho(z)\theta(-z)[\ln|(\epsilon+\hbar\omega)/(\epsilon-\hbar\omega)|+i\pi\theta(|\epsilon|-\hbar\omega)],\tag{2.5a}$$

$$\rho(z)=(\rho_t/\pi)\int_0^{k_F}dk_z\,|\chi_{k_z}(z)|^2,\tag{2.5b}$$

$$\rho_t=m^*/2\pi\hbar^2.\tag{2.5c}$$

The coupling constant g is assumed to be equal to its bulk value throughout the region $z<0$, and

$$\theta(z)=1,\quad z>0;\qquad =0,\quad z<0.$$

The wave functions $\chi_{k_z}(z)$ are solutions of Schrödinger's equation for the unperturbed left-hand problem. More elaborate versions of the bulk Σ corresponding to Eq. (2.5) were given by Davis and Duke, but Eq. (2.5) is sufficiently accurate for the purposes of this paper. To include the effects of acoustic phonons and impurity scattering, we can use the prescription given by Davis and Duke [their Eq. (A2.5)].[2]

In this section we approximate $\rho(z)$ by its bulk value $\rho(-\infty)=\rho_tk_F/\pi$. (Corrections to this approximation will be taken up in Sec. III.) The resulting expression for $\Sigma(z,\epsilon)$ is

$$\Sigma(z,\epsilon)=\Sigma_B(\epsilon)\theta(-z),\tag{2.6}$$

where $\Sigma_B(\epsilon)$ is the bulk value of the self-energy.

Substituting Eqs. (2.4) and (2.6) into Eq. (2.3), we find that

$$G^L(z,z',\mathbf{p}_t,\epsilon)=(-m_b/\hbar^2K)\{\alpha\exp[-K(z'+z)]+\exp[-K|z-z'|]\},\quad 0<z,z'\tag{2.7a}$$

$$=(-m_b/\hbar^2K)[2/(1-i\gamma)]\times\exp(-i\lambda z-Kz'),\quad z<0<z'\tag{2.7b}$$

where

$$\alpha=(1+i\gamma)/(1-i\gamma),\tag{2.8a}$$

$$\gamma=m_b\lambda/m^*K,\tag{2.8b}$$

$$\lambda=\{(2m^*/\hbar^2)[\epsilon+\mu-\Sigma_B(\epsilon)]-p_t^2\}^{1/2},\tag{2.8c}$$

and

$$K=[(2m/\hbar^2)(V_0-\epsilon-\mu)+p_t^2]^{1/2}.\tag{2.8d}$$

A similar expression holds for G^R except that there are no many-body effects to be accounted for.

Substituting the above expression for G^L and a similar expression for G^R into Eq. (2.1), we obtain the current after some manipulation,

$$I=\frac{-8e}{\pi\hbar}\int_0^{-eV}d\epsilon\int\frac{d^2p_t}{(2\pi)^2}\exp(-2Kb)\,\frac{\gamma'}{1+\gamma'^2}\,\mathrm{Im}\alpha, \tag{2.9}$$

where

$$\gamma'=m_b k_z'/m_0 K \tag{2.10a}$$

and

$$k_z'=[(2m_0/\hbar^2)(\mu'+\epsilon)-p_t^2]^{1/2}. \tag{2.10b}$$

(Recall that primed quantities refer to the right-hand electrode.) Making use of Eq. (2.8), we find

$$I=\frac{-e}{\pi\hbar}\int_0^{-eV}d\epsilon\int\frac{d^2p_t}{(2\pi)^2}D(\mathbf{p}_t,\epsilon), \tag{2.11}$$

where

$$D(\mathbf{p}_t,\epsilon)=\frac{16\gamma_1\gamma'\exp(-2Kb)}{[(1+\gamma_2)^2+\gamma_1^2][1+\gamma'^2]} \tag{2.12a}$$

and

$$\gamma=\gamma_1+i\gamma_2. \tag{2.12b}$$

To compare the above results with the results of the transfer Hamiltonian formalism,[2] it is simplest to consider them in the quasiparticle approximation, in which

$$\mathrm{Im}\Sigma_B(\epsilon)\to 0. \tag{2.13}$$

Then from Eqs. (2.8b), (2.8c), (2.12a), and (2.12b), we see that $D(\mathbf{p}_t,\epsilon)$ is nonzero only when

$$0<p_t^2<(2m/\hbar^2)[\epsilon-\mathrm{Re}\Sigma_B(\epsilon)+\mu]. \tag{2.14}$$

(For p_t^2 outside this range γ is pure imaginary so γ_1 vanishes and consequently, D vanishes.) Neglecting any bias dependence of D, we find

$$\frac{dI}{dV}=\frac{e^2}{\pi\hbar}\rho_t\int_0^{-eV-\mathrm{Re}\Sigma_B(-eV)+\mu}dE_t D(E_t,-eV), \tag{2.15a}$$

where

$$E_t=\hbar^2p_t^2/2m^*. \tag{2.15b}$$

Further assuming $D=D_0\exp(-E_t/E_0)$ (uniform-field approximation) gives agreement with Davis and Duke [their Eqs. (1.11), (2.1), and (2.2) with $Z(\epsilon)=1$ since the self-energy does not depend upon $\mathbf{k}$]. Equation (2.15) is also in agreement with a previous Green's-function calculation.[12]

Although no detailed analysis of the conductance has been made when the imaginary part of $\Sigma_B(\epsilon)$ is nonzero, it appears that the qualitative features are quite similar to the numerical results of Davis and Duke. Hence, we conclude that if $\Sigma(z,\epsilon)$ does not deviate significantly from $\Sigma_B(\epsilon)$ near the electrode-barrier interface, the transfer Hamiltonian formalism gives reliable results.

III. OPTICAL PHONONS—NONUNIFORM SELF-ENERGY

A. $\Sigma(z,\epsilon)$ near Interface

Instead of assuming the form (2.6) for $\Sigma(z,\epsilon)$, let us now explicitly calculate it from (2.5). For the square barrier of the previous section, the wave functions $\chi_{k_z}(z)$ are of the form

$$\chi_{k_z}(z)=2^{1/2}\sin(k_z z+\theta_{k_z}),\qquad z<0 \tag{3.1}$$

where

$$\sin\theta_{k_z}=(-k_z/K_z)[1+(k_z/K_z)^2]^{-1/2} \tag{3.2a}$$

and

$$K_z=[(2m^*/\hbar^2)(V_0-\hbar^2k_z^2/2m^*)]^{1/2}. \tag{3.2b}$$

[We take $m_b=m^*$ since the form (2.5b) is strictly valid only for this case.] To a good approximation, we find upon substituting Eq. (3.1) into Eq. (2.5) that

$$\Sigma(z,\epsilon)=\theta(-z)\Sigma_B(\epsilon)[1-\sin 2k_F(z-z_0)/2k_F(z-z_0)], \tag{3.3}$$

where

$$\sin 2k_F z_0/2k_F z_0\simeq 1-\tfrac{2}{3}(\mu/V_0). \tag{3.4}$$

(Typically, $k_F z_0\sim 0.1$ for semiconductor electrodes.) In the limit of $V_0\to\infty$, $z_0\to 0$ and Eq. (3.3) becomes exact. Numerical integration of Eq. (2.5b) gives results which can be satisfactorily fit by Eq. (3.3).

We have also calculated $\Sigma(z,\epsilon)$ for a Schottky barrier using the results of previous studies[13,14] of the one-electron conductance through this barrier. We assume that for $-d<z<0$, the potential barrier is of the form

$$V(z)=(2\pi e^2 n_D/\epsilon_s)(z+d)^2, \tag{3.5}$$

where d is the width of the depletion region, n_D is the number of donors for n-type semiconductors (or number of acceptors for p-type), and ϵ_s is the static dielectric constant of the semiconductor. For $z<-d$, we take $V(z)=0$. The form of $V(z)$ for $z>0$ is of little importance for the calculation of $\Sigma(z,\epsilon)$, so we extend the form (3.5) into the region $z>0$. The wave functions are then given by

$$\chi_{k_z}=2^{1/2}\sin[k_z(z+d)+\theta_{k_z}],\qquad z<-d \tag{3.6a}$$

$$=2^{1/2}[U^2(a,0)-a^{-1}U'^2(a,0)]^{-1}U(a,\eta),\qquad z>-d \tag{3.6b}$$

where

$$a=-\lambda_0^2k_z^2, \tag{3.7a}$$

$$\eta=(z+d)/\lambda_0, \tag{3.7b}$$

$$\lambda_0=(\hbar^2\epsilon_s/16\pi m^*e^2n_D)^{1/4}, \tag{3.7c}$$

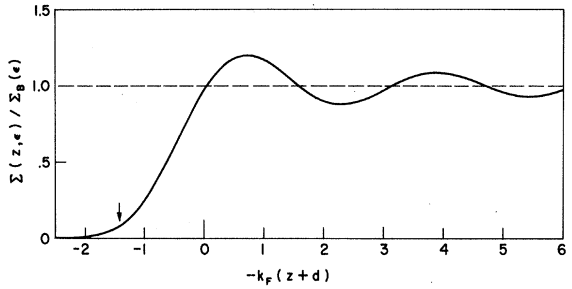

FIG. 1. Self-energy $\Sigma(z, \epsilon)$ near a Schottky barrier. The arrow marks the turning point for electrons at the Fermi level. Parameters were chosen for heavy holes in Si ($p=1.2\times10^{20}$ cm^{-3}).

and

$$\theta_{k_z}=\arctan[\sqrt{(-a)}U(a, 0)/U'(a, 0)]. \quad (3.7d)$$

$U(a, \eta)$ is a parabolic cylindrical function which is exponentially decreasing as $\eta\to\infty$.[15]

Results of numerical calculations of $\Sigma(z, \epsilon)/\Sigma_B(\epsilon)$ for parameters appropriate to heavy holes in p-Si for an acceptor concentration of 1.2×10^{20} are shown in Fig. 1. (Similar results are obtained for light holes.) In the electrode region, the form of $\Sigma(z, \epsilon)$ is satisfactorily approximated by Eq. (3.3) if the origin is taken at the turning point of electrons at the Fermi level. Consequently, we shall consider the form (3.3) as adequate for the purposes of this paper. We regard k_Fz_0 as a parameter, whose approximate magnitude can be determined by fitting Eq. (3.3) to the results of numerical calculations of $\Sigma(z, \epsilon)$.

B. Current Calculated with Nonuniform $\Sigma(z, \epsilon)$

To find the current with a nonuniform $\Sigma(z, \epsilon)$ in the left-hand electrode (semiconductor) we must solve Eq. (2.3) with $\Sigma(z, \epsilon)$ given by Eq. (3.3). Unfortunately, we have not found a solution to the differential equation. Therefore, we resort to perturbation theory in which G^L is given by (through order g^2)

$$G^L(z, z', \mathbf{p}_t, \epsilon)=G_0^L(z, z', \mathbf{p}_t, \epsilon) + \int dz''G_0^L(z, z'', \mathbf{p}_t, \epsilon)\Sigma(z'', \epsilon)G_0^L(z'', z', \mathbf{p}_t, \epsilon), \quad (3.8)$$

where the unperturbed G_0^L is given by Eq. (2.7) with $\Sigma_B(\epsilon)$ set equal to zero. We note that we can write [see Eq. (3.3)]

$$\Sigma(z, \epsilon)=\Sigma_B(\epsilon)\theta(-z)+\delta\Sigma(z, \epsilon), \quad (3.9a)$$

where

$$\delta\Sigma(z, \epsilon)=-\Sigma_B(\epsilon)\theta(-z)\sin2k_F(z-z_0)/2k_F(z-z_0). \quad (3.9b)$$

Let us first find the contribution of $\delta\Sigma(z, \epsilon)$ to G^L which we write as

$$\delta G^L(z, z', \mathbf{p}_t, \epsilon)=(-m_b/\hbar^2K)(\delta\alpha)\exp[-K(z+z')]. \quad (3.10)$$

Substituting Eq. (3.9b) into Eq. (3.8) (Σ is replaced by $\delta\Sigma$), we find upon making use of Eq. (2.7)

$$\delta\alpha=(-im_b/\hbar^2K)[1/(1-i\gamma)^2]\Sigma_B(\epsilon)\exp(-2i\lambda z_0) \times[E_1(-2i(\lambda+k_F)z_0)-E_1(-2i(\lambda-k_F)z_0)], \quad (3.11)$$

where now (we take into account scattering by acoustic phonons and impurities with a phenomenological parameter Γ_a)

$$\lambda=[(2m^*/\hbar^2)(\epsilon+\mu+i\Gamma_a)-p_t^2]^{1/2} \quad (3.12a)$$

and

$$\gamma=m_b\lambda/m^*K. \quad (3.12b)$$

The function $E_1(z)$ is defined as[16]

$$E_1(z)\equiv\int_z^\infty\frac{e^{-t}}{t}dt, \qquad |\arg z|<\pi \quad (3.13a)$$

$$=-0.57721\cdots-\ln z-\sum_{n=1}^{\infty}\frac{(-1)^nz^n}{nn!}. \quad (3.13b)$$

Substituting Eq. (3.11) into Eq. (2.9) (α is replaced by $\delta\alpha$), we find the current δI due to $\delta\Sigma(z, \epsilon)$:

$$\delta I=\frac{8e}{\pi\hbar}\int_0^{-eV}d\epsilon\int\frac{d^2p_t}{(2\pi)^2}\exp(-2Kb)\frac{\gamma'}{1+\gamma'^2}\frac{m_b}{\hbar^2Kk_F} \times\mathrm{Re}\{[\Sigma_B(\epsilon)/(1-i\gamma)^2]\exp(-2i\lambda z_0) \times[E_1(-2i(\lambda+k_F)z_0)-E_1(-2i(\lambda-k_F)z_0)]\}. \quad (3.14)$$

In a similar manner, we can obtain the current $\bar{\delta}\bar{I}$ due to the $\Sigma_B(\epsilon)\theta(-z)$ term in Eq. (3.9a). [Of course, we could use the results of the previous section to calculate $\bar{\delta}\bar{I}$, but to facilitate comparison with Eq. (3.14), we use perturbation theory, Eq. (3.8).] The results are

$$\bar{\delta}\bar{I}=\frac{8e}{\pi\hbar}\int_0^{-eV}d\epsilon\int\frac{d^2p_t}{(2\pi)^2}\exp(-2Kb)\frac{\gamma'}{1+\gamma'^2}\frac{m_b}{\hbar^2Kk_F} \times\mathrm{Re}\{[\Sigma_B(\epsilon)/(1-i\gamma)^2](2k_F/\lambda)\}. \quad (3.15)$$

To simplify the above expressions, we make the approximations

$$\exp(-2Kb)\simeq\exp(-2K_0b)\exp(-E_t/E_0), \quad (3.16a)$$

where K_0 and E_0 are constants and

$$1/(1-i\gamma)^2\simeq[1/(1+\gamma_F^2)]\exp(2i\Phi_F), \quad (3.16b)$$

where

$$\gamma_F=m_bk_F/m^*K_0 \quad (3.16c)$$

and

$$\tan\Phi_F=\gamma_F. \quad (3.16d)$$

For the parameters of interest, $\Phi_F \simeq k_F z_0$. [This result is obtained by expanding both Eqs. (3.4) and (3.16d) to lowest order and setting $m_b = m^*$.] We also evaluate γ' at $\epsilon = 0$, $p_t = 0$.

Combining Eqs. (3.14)–(3.16) we find the conductance (above background) is given by

$$dI/dV_{\text{phonon}} = -G_0 \times \mathrm{Re}\{[\Sigma_B(-eV)/\mu](\mathfrak{L}(-eV)+\bar{\mathfrak{L}}(-eV))\}, \quad (3.17)$$

where

$$G_0 = \frac{e}{\pi\hbar}\rho_t \frac{16\gamma'\gamma_F \exp(-2K_0 b)}{(1+\gamma'^2)(1+\gamma_F^2)} = \text{const}, \quad (3.18a)$$

$$\mathfrak{L}(-eV) = \frac{1}{4\mu}\int_0^\infty dE_t \exp(-E_t/E_0)\{\exp(2i\Phi_F - 2i\lambda z_0) \times [E_1(-2i(\lambda+k_F)z_0) - E_1(-2i(\lambda-k_F)z_0)]\}, \quad (3.18b)$$

and

$$\bar{\mathfrak{L}}(-eV) = \frac{1}{4\mu}\int_0^\infty dE_t \exp(-E_t/E_0)[\exp(2i\Phi_F)2k_F/\lambda]. \quad (3.18c)$$

To interpret the results of numerical evaluations of $\mathfrak{L}$ and $\bar{\mathfrak{L}}$, we write Eq. (3.17) in the form

$$dI/dV_{\text{phonon}} = -(G_0/\mu)[C_r(-eV) \times \mathrm{Re}\Sigma_B(-eV) + C_i(-eV)\,|\,\mathrm{Im}\Sigma_B(-eV)\,|\,], \quad (3.19)$$

where

$$C_r(-eV) = \mathrm{Re}[\mathfrak{L}(-eV)+\bar{\mathfrak{L}}(-eV)] \quad (3.20a)$$

and

$$C_i(-eV) = \mathrm{Im}[\mathfrak{L}(-eV)+\bar{\mathfrak{L}}(-eV)]. \quad (3.20b)$$

Since $\mathfrak{L}$ and $\bar{\mathfrak{L}}$ are slowly varying functions of eV [compared with $\Sigma_B(-eV)$], we evaluate the coefficients of $\mathrm{Re}\Sigma_B(-eV)$ and $\mathrm{Im}\Sigma_B(-eV)$ at $-eV = \pm\hbar\omega$, using $C_r(\hbar\omega)$ and $C_i(\hbar\omega)$ for $eV \sim -\hbar\omega$ (reverse bias) and $C_r(-\hbar\omega)$ and $C_i(-\hbar\omega)$ for $eV \sim +\hbar\omega$ (forward bias). (Through order g^2, the results of Davis and Duke can also be represented in the above manner.)

We take the following values of the parameters appearing in $\mathfrak{L}$ and $\bar{\mathfrak{L}}$: $\mu = 0.14$ eV, $\hbar\omega = 0.064$ eV, $\Gamma_a = 0.002$ eV, $E_0 = 0.4$ eV, and $\Phi_F = k_F z_0 = 0.1$. These values are reasonable for p-Si (1.2×10^{20} cm^{-3}).[2,10] Numerical integration of Eqs. (3.18b) and (3.18c) gives

$$C_r(\hbar\omega) = 0.18, \quad (3.21a)$$

$$C_i(\hbar\omega) = 0.26, \quad \text{(reverse bias)} \quad (3.21b)$$

$$C_r(-\hbar\omega) = 0.55, \quad (3.21c)$$

$$C_i(-\hbar\omega) = -0.03, \quad \text{[forward bias; nonuniform } \Sigma(z,\epsilon)\text{]}. \quad (3.21d)$$

To compare to the results of Davis and Duke, we can compare the above results to the values of C_r and C_i obtained for the case where it is assumed that $\Sigma(z,\epsilon) = \Sigma_B(\epsilon)\theta(-z)$. This corresponds to setting $\mathfrak{L}(-eV) = 0$ in Eqs. (3.20a) and (3.20b). In this case we find

$$C_r(\hbar\omega) = 1.03, \quad (3.22a)$$

$$C_i(\hbar\omega) = -0.71, \quad \text{(reverse bias)} \quad (3.22b)$$

$$C_r(-\hbar\omega) = 0.88, \quad (3.22c)$$

$$C_i(-\hbar\omega) = -1.08, \quad \text{[forward bias; uniform } \Sigma(z,\epsilon)\text{]}. \quad (3.22d)$$

In both instances above, we have considered coupling to the optical phonons only in the region $z<0$, i.e., outside the barrier, and we have taken the coupling constant g and the phonon frequency ω to be constant throughout the electrode (region $z<0$).

The results of these model calculations indicate that including the spatial variation of $\Sigma(z,\epsilon)$ in the calculation of the conductance reduces the magnitude of the contribution from $\mathrm{Re}\Sigma_B(\epsilon)$ (also called "odd"[6]), in both forward and reverse bias, with a larger reduction in reverse bias than in forward [as compared with the uniform $\Sigma(z,\epsilon)$ conductance]. The contribution from $\mathrm{Im}\Sigma_B(\epsilon)$ (also called "even"[6]) is found to be quite small in forward bias and of the opposite sign [as compared with the uniform $\Sigma(z,\epsilon)$ case] in reverse bias.

Increasing the values of E_0 or $\Phi_F = k_F z_0$ somewhat [in the calculation of Eq. (3.21)] has the general effect of increasing both $C_r(\hbar\omega)$ and $C_r(-\hbar\omega)$, whereas $C_i(\hbar\omega)$ decreases with increasing E_0 and increases with increasing $\Phi_F = k_F z_0$. The coefficient $C_i(-\hbar\omega)$ can change sign, but remains small. The results are not sensitive to the value chosen for Γ_a.

In addition, we have examined the coefficients $C_r(\hbar\omega)$ and $C_i(\hbar\omega)$ (reverse bias) for μ down to 0.048 eV ($p = 2\times10^{19}$), and have not found any strong doping dependence. In particular, we have *not* found that $C_r(\hbar\omega)$ changes sign as indicated by the data of Cullen, Wolf, and Compton.[10]

We draw the following conclusions. First, although the magnitude of the principal self-energy effect, namely, the term due to $\mathrm{Re}\Sigma_B(\epsilon)$, is probably not as strong as predicted by the transfer Hamiltonian formalism, certainly such an effect must be present in p-Si and other degenerate materials.[2] Since g is not known accurately, however, one cannot reliably estimate the absolute magnitude. Effects due to $|\,\mathrm{Im}\Sigma_B(\epsilon)\,|$ are probably masked by phonon emission in the barrier.[6]

Second, in addition to the essentially electrode type of an effect discussed above, barrier effects (e.g., from interactions in the region $z>0$ in the square-barrier model or for $z>-d$ in the Schottky barrier) must also be present. The large step increase[1,10] in forward bias observed in p-Si must be from the barrier region since

$C_i(-\hbar\omega)\simeq 0$. This is in agreement with Duke and Kleiman's[11] analysis of the magnetic field dependence. In addition, the structure in the conductance in reverse bias for low doped p-Si[10] is of the form of a $\ln|eV+\hbar\omega|$ term, but with a sign opposite to that found in Eq. (3.19) for an electrode effect.

Third, to account for the structure in reverse bias for low doped p-Si, we suggest a strong interaction with the optical phonons in the barrier region adjacent to the metal electrode. The reason that we suggest this position for the interaction is that the results of the wave-function calculation for inelastic processes in the barrier[8] showed that a $\ln|eV+\hbar\omega|$ term in the conductance can arise from interactions near the edges of the barrier, with the sign of the effect being determined by the edge at which the interaction occurs. In the case of low doped p-Si, the sign of the effect then dictates the metal-barrier edge.

Finally, it appears that both bulk and barrier effects can occur simultaneously in degenerate semiconductor units. The only clear way to distinguish them is to consider a case where a difference between the frequencies of the bulk and the barrier phonons exists. For example, *if* k_F is small compared with the Fermi-Thomas screening momentum k_s in a polar semiconductor, the barrier effect would show the unscreened LO phonon, whereas the bulk effect would show the screened LO phonon with a frequency near the TO phonon. In the experiments published thus far, k_F has always been larger than k_s and no such difference has been detected.[17]

IV. SUMMARY

In this paper we have calculated the conductance of a metal-semiconductor tunnel junction for which interactions with optical phonons occur in the semiconductor using the Green's-function theory of ABZ. We found that if it is assumed that the self-energy is uniform throughout the electrode, the theory agrees with the transfer Hamiltonian approach in the quasiparticle approximation. When the spatial variation of the self-energy is included, the magnitude of the principal self-energy effect [arising from $\mathrm{Re}\Sigma(z,\epsilon)$] is found to be smaller than for the case of a uniform $\Sigma(z,\epsilon)$. The qualitative features are not changed appreciably, though, and such electrode effects must be important in the interpretation of experimental data.

To account for the large increase in the conductance in forward bias observed in p-Si[1,10] and for the doping-dependent behavior observed in reverse bias,[10] however, we conclude that barrier effects must also be included. Based upon the nature of the reverse-bias line shape in low doped p-Si,[10] we suggest that a strong interaction with the optical phonons is occurring in the region of the barrier near the metal electrode at low doping levels.

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