Short-wavelength phonon emission from a metal-semiconductor interface

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We believe that short-wavelength phonons (the phonons whose wave vectors correspond to the edge points of the Brillouin zone) may be emitted by electrons when crossing the interface if it is abrupt. To show this, we have obtained the exact solution of the Schrödinger equation for an electron whose effective mass is a smooth steplike function of distance from the interface, where an electrostatic potential is supposed to be unchanged. We then analyzed the matrix element of the electron-phonon interaction and find it is exponentially small if the interface is smooth, so that the mean width of the step is much greater then the phonon wavelength. This smallness should disappear if the interface becomes abrupt.

It is well known that short-wavelength phonons (phonons whose wave vectors correspond to the edge points of the Brillouin zone) are emitted under tunneling in metal-oxide-metal structures and are not emitted in metal–direct-band-semiconductor structures.[1] To understand the difference between these two situations, we have considered the emission of such phonons and showed that it occurs only if the potential barrier profile is abrupt, so that the mean scale for it deviation is about the phonon wavelength.[2] This condition is satisfied in metal-oxide-metal barriers, which are usually thin (20–50 Å) and high (a few eV). In regard to metal-semiconductor structures, the barriers are wide (more then 100 Å), but low (a few tenths of an eV), and they usually become smooth for tunneling electron at a metal surface due to an electrical image.[3] Experiments[4] where the short-wavelength phonons were observed in Au–superthin oxide–p-InAs structures and not observed in Au–InAs structures support this assertion.

In the present paper we show that short-wavelength phonons should be emitted as well at the interface where the potential profile is smooth, but the effective mass of the electron has a discontinuity. To understand the necessity of such a discontinuity let us consider the transfer matrix element corresponding to the electron-phonon interaction at the interface,

$$T = g\int_{-\infty}^{+\infty} \psi_f^* e^{iqz} \psi_i \, dz. \tag{1}$$

It becomes exponentially small if the phonon wave vector q is of the order of π/a (a is the lattice constant), whereas the envelopes of the electron wave functions before, ψ_i, and after, ψ_f, are smooth, so that they do not contain high-frequency Fourier components. We suppose the interface between the two materials under study to be flat, so it is possible to reduce the problem to the one-dimensional one. Thus in (1) z is the coordinate along the normal to the interface, where $z = 0$, q is the wave vector component along the z axis, and g is the constant of the electron-phonon interaction. If the exact Bloch-like wave functions $u_k(r)e^{ikr}$ were to replace ψ_i and ψ_f in (1) this result would not change essentially, if the mean scale for the Bloch amplitude $u_k(r)$ is of atomic size and so is much less than the lattice constant.

For ψ_i and ψ_f, which have jump discontinuities, integral (1) is not so small. The main contribution to it in this case comes from the vicinity (about the phonon wavelength) of the break points. If we suppose the semiclassical approximation to be valid, then these discontinuities may be associated with breaks in momentum $p(z) = \sqrt{2m(z)[E - U(z)]}$. They arise from singularities of the potential $U(z)$ (at the surface or near the short-range impurities) or from discontinuities of the effective mass $m(z)$ near the surface. The first possibility was studied in detail in Ref. 2; the latter is the subject of the present paper.

We shall consider only the variation of the effective mass, supposing $U(z)$ to be unchanged through the interface. Such an assumption can hardly be realized in experiment. Nevertheless, the situation is quite practicable when $U(z)$ become sufficiently smooth, so that it may be regarded as unchanged on the scale of about a. It may occur, for instance, in metal-semiconductor contacts due to electrical image charge.[3] In fact, if it happens, one can regard the interface as a surface where only the effective mass has a discontinuity, but not the potential. This is the reason for calling it an effective-mass interface.

In the present paper we propose the exact solution of the model problem where $m(z)$ is a smooth steplike function of z, with a mean half-width of the step w. We shall examine the matrix element (1) and show that it is exponentially small if $qw \gg 1$, and this is not the case if $qw \leq 1$.

If the effective mass of the electron $m(z)$ is a smooth function of z, then Schrödinger's equation may be written as[5]

$$\frac{d}{dz}\left(\frac{1}{m(z)}\frac{d\psi}{dz}\right) + 2E\psi = 0. \tag{2}$$

Here E is the energy of the electron (the potential energy term is supposed to be constant and included in E), and ψ is its wave function. We have adopted units where $\hbar = 1$. Let $\psi = \frac{d\varphi}{dz}$.[6] Then φ should obey the equation

$$\frac{d^2\varphi}{dz^2} + 2m(z)E\varphi = 0, \tag{3}$$

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which is similar to the usual Schrödinger one, and so it could be solved in the semiclassical approximation, were $m(z)$ sufficiently smooth. However, we shall use another way.

Let $m(z)$ be of the form

$$m(z) = \frac{m_1 + m_2 e^{\frac{z}{w}}}{1 + e^{\frac{z}{w}}}. \tag{4}$$

Then Eq. (3) could be solved exactly. Its particular, linear independent solutions are

$$\varphi_1 = e^{ik_1 z} F(\alpha, \beta, \gamma, -e^{\frac{z}{w}}) , \tag{5}$$
$$\varphi_2 = e^{-ik_1 z} F(\alpha - \gamma + 1, \beta - \gamma + 1, 2 - \gamma, -e^{\frac{z}{w}}) = \varphi_1^*.$$

Here F is the hypergeometric function

$$k_1 = \sqrt{2m_1 E}, \quad k_2 = \sqrt{2m_2 E},$$
$$\alpha = i(k_1 + k_2)w, \quad \beta = i(k_1 - k_2)w,$$
$$\gamma = 1 + 2ik_1 w = \alpha + \beta + 1.$$

The wave functions ψ_i and ψ_f can be found as linear combinations of $\psi_1 = \frac{d\varphi_1}{dz}$ and $\psi_2 = \frac{d\varphi_2}{dz}$, satisfying the asymptotic conditions far from the interface. ψ_i is a superposition of incident wave and divergent scattering wave and ψ_f is a superposition of transmitted wave and convergent wave,[7] i.e., $\psi_i \propto e^{ik_2 z}$ for $z \to +\infty$ and $\psi_f \propto e^{ik_1 z}$ for $z \to -\infty$. Then from (5) we find

$$\psi_i = A(\psi_1 + B\psi_2), \quad \psi_f = C\psi_1,$$
$$B = -\frac{\Gamma(\gamma)\Gamma(\alpha^*)\Gamma(1+\alpha^*)}{\Gamma(\gamma^*)\Gamma(\beta)\Gamma(1+\beta)} . \tag{6}$$

Coefficients A and C are determined from the normalization conditions. For matrix element (1) we obtain

$$T = AC^* g \int e^{iqz} \psi_1^* (\psi_1 + B\psi_2)\, dz . \tag{7}$$

To analyze integral (7), at first let us suppose that $qw \gg 1$. It is convenient to evaluate (7) for the complex variable z. The integration contour can then be shifted to the half plane where the integrand is decaying; then $|z| \to \infty$ due to the factor $e^{i(q \pm k_{1,2} \pm k_{1,2})z}$. This is the upper half plane, if $q > k_1 + k_2$ (Fig. 1). The magnitude of T is then determined by singularities of the functions ψ_1 and ψ_2 in the upper half plane. They are singularities of the hypergeometric functions F, which have only logarithmic branch points at $e^{\frac{z}{w}} = -1$ [i.e., $z_n = i\pi w(2n+1)$, $n = 0, \pm 1, \pm 2, \ldots$], if $\alpha + \beta - \gamma$ is an integer, as in our case.[8] Thus the integrand in (7) is an analytical function on the whole z plane except the cut, which should be done along the imaginary axis from z_0 (the point nearest to the real axis) to infinity (Fig. 1). Integral (7) then turns into that along the cut. The main contribution to (7) comes from the vicinity (of the order of q^{-1}) of $z_0 = i\pi w$. Then for $qw \gg 1$ z_0 is far enough from the real axis so that $T \propto e^{-\pi q w}$. If $q \gg k_{1,2}$, then

$$T = gAC^*(B_1 \ln qw + B_2)\frac{e^{-\pi q w}}{q}, \tag{8}$$

where B_1 and B_2 are independent of q. Thus the matrix element (1) for too smooth interfaces becomes exponentially small. This is not the case only if by chance $q \pm k_{1,2} \pm k_{1,2} = 0$ and the equation for energy conservation is satisfied simultaneously.

The lower qw is, the closer is z_0 to the real axis, so that for $qw \sim 1$ the factor $e^{-\pi q w}$ becomes not so small. We shall examine now the opposite limiting case, $qw \ll 1$. Then $\frac{|z|}{w} \gg 1$ in the major part of the integration region, so it is possible to replace the hypergeometric functions in (5), supposing $e^{-\frac{|z|}{w}} = 0$. If we suppose also $k_{1,2} w \ll 1$, then

$$\psi_1 = ik_1 e^{ik_1 z}, \quad \psi_2 = -ik_1 e^{-ik_1 z} \quad \text{for } z < 0$$

and

$$\psi_1 = \tfrac{1}{2} i(k_1 - k_2) e^{-ik_2 z} + \tfrac{1}{2} i(k_1 + k_2) e^{ik_2 z},$$
$$\psi_2 = -\tfrac{1}{2} i(k_1 + k_2) e^{-ik_2 z} - \tfrac{1}{2} i(k_1 - k_2) e^{ik_2 z}$$
$$\text{for } z > 0. \tag{9}$$

For ψ_i and ψ_f we obtain

$$\psi_i = \begin{cases} e^{ik_1 z} + C_1 e^{-i(k_1 + i\delta)z} & \text{if } z < 0 , \\ C_2 e^{i(k_2 + i\delta)z} & \text{if } z > 0 , \end{cases} \tag{10}$$
$$\psi_f = \begin{cases} C_3 e^{i(k_1' - i\delta)z} & \text{if } z < 0 , \\ e^{ik_2' z} + C_4 e^{-i(k_2' - i\delta)z} & \text{if } z > 0 . \end{cases}$$

There

$$C_1 = -\frac{k_1 - k_2}{k_1 + k_2}, \quad C_2 = \frac{2k_2}{k_1 + k_2} ,$$
$$C_3 = \frac{2k_1'}{k_1' + k_2'} , \quad C_4 = \frac{k_1' - k_2'}{k_1' + k_2'} ,$$
$$k_{1,2}' = \sqrt{2m_{1,2}(E - \omega_q)},$$

and ω_q is the phonon energy. We also assume

$$A = -\frac{i}{k_1} , \quad C = -\frac{2i}{k_1' + k_2'} ,$$

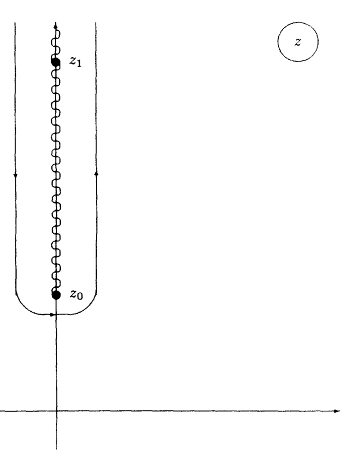

FIG. 1. Integration contour used to evaluate Eq. (7).

in order that the coefficients of the incident and transmitted waves become unity, and introduce an infinitesimal attenuation $\delta \to +0$ for scattering waves to provide convergence of (7) at $z \to \pm\infty$. Then

$$T = g\left(\frac{iC_2}{q+k_2-k_2'} - \frac{iC_3}{q+k_1-k_1'} - \frac{iC_1C_3}{q-k_1-k_1'} + \frac{iC_2C_4}{q+k_2+k_2'}\right) . \tag{11}$$

We see that (11) does not contain any exponentially small factor connected with the interface as in (8).

Expressions (9) and (10) could be obtained if we impose the appropriate matching conditions at $z = 0$, instead of solution of (2). These matching conditions are

$$\psi(-0) = \psi(+0),$$
$$\frac{1}{m_1}\psi'(-0) = \frac{1}{m_2}\psi'(+0). \tag{12}$$

Equations (12) immediately ensue from (2). They are necessary for the derivatives in (2) to exist.

It is important to note that Eq. (2) holds in the effective-mass approximation only. It means that the inequality $w \gg a$ should be satisfied. Otherwise, more complicated matching conditions have to be imposed. Such conditions depend on the material under study and imply a jump discontinuity in the envelope wave function as well (see Ref. 9 and references therein). Nevertheless, the matching conditions may affect the coefficients C_1–C_4 for the plane waves in (10) only, so that the result (11) remains valid.

An interesting question arises when $qw \sim 1$ and $w \sim a$. This means that the main contribution in (1) comes from a region, of size about a, so an applicability of any matching conditions and envelope wave functions is not clear in this case.

We believe the effective-mass interface could be realized in Schottky barriers with Ag as the metal. Unlike other noble or transition metals Ag produces an abrupt interface with A_3B_5 semiconductors.[10] An interesting situation arise in the contact metal–p-InAs. The Fermi level at the interface in this case is pinned 0.13 eV above the bottom of the conduction band (Fig. 2). Tunneling through the gap, where $p(z)$ is a smooth function, could not result in emission of short-wavelength phonons. Nevertheless, such phonons could be emitted at the interface if it was sufficiently abrupt.

Emission of short-wavelength phonons at the effective-mass interface has an additional advantage in the absence of a potential barrier there (or if it is too low). Indeed, only an electron whose momentum is normal to the barrier plane could tunnel effectively. This makes difficult the emission of phonons with nonzero wave vector, implying an additional condition for q [i.e., $|p_{\|} + q_{\|}| \ll \hbar(\lambda d)^{-1/2}$, where $p_{\|}$ and $q_{\|}$ are the components of the wave vectors in the direction parallel to the interface, λ is the subbarrier wavelength, and d is the width of the barrier]. Such restrictions disappear if emission occurs at an interface without any tunneling. This is possible for an electron which had been excited before. It seems to us that the downshift of the threshold in the energy distribution of emitted electrons which has been observed in photocathodes[11] is connected with the mechanism of phonon emission discussed here.

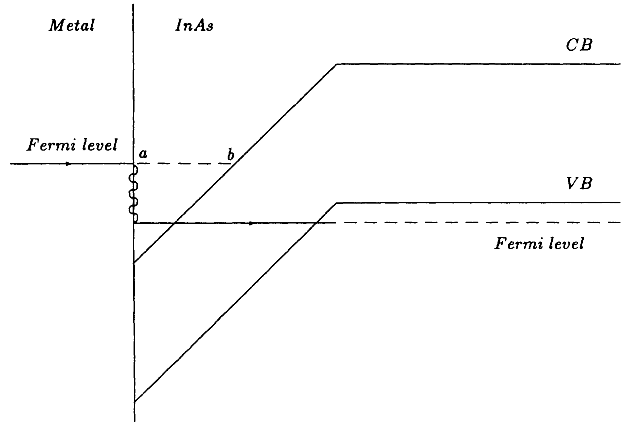

FIG. 2. Schematic potential versus distance diagram for metal–p-InAs contact. The arrows schematically indicate the tunneling path of an electron which emits a short-wavelength phonon at the abrupt interface (point a), but not at the turning point b, where $p(z)$ is smooth. CB and VB denote the bottom of the conduction and the top of the valence bands, respectively.

In conclusion, we have shown that an abrupt interface makes the short-wavelength phonon emission more effective. This may be understood from the following qualitative argument. From the point of view of an electron as a quasiparticle, the interface is the place where the effective parameters of the energy bands have a discontinuity. The sharper this break, the larger is the classical force acting on the electron from the crystalline lattice. It should increase the momentum, which could be transferred to the phonon emitted when an electron is crossing the interface. This qualitative argument is verified by the exact solution of the problem. We have shown that the transfer electron-phonon matrix element for large q is increased due to the high-frequency components of the wave function arising when the interface becomes abrupt. The mean range of this sharpness should be of the order of or less than the phonon wavelength. Otherwise the probability of phonon emission becomes exponentially small. We propose a possible experimental test of the effect.

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[6]This substitution leads to an increase of the order of the differential equation, and so an additional constant has to be involved in its general solution. Nevertheless, the solution of the input equation should not depend on the choice of this constant. In our case such an extra constant arises after integration of Eq. (2) with respect to z and leads to the term independent of z in the expression for $\varphi(z)$. It has no influence on $\psi = \frac{d\varphi}{dz}$. We suppose this constant to be equal to zero.

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