Transmission coefficient of a metal-metal interface in the tight-binding model

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We present a tight-binding-model calculation of the transmission coefficient for electrons incident upon the interface between two metals. The role of the coupling produced by overlap of wave functions of the two metals is elucidated. The existence of a critical angle analogous to the optical critical angle is demonstrated. The relevance of these results to proximity-effect tunneling experiments is discussed.

There is much current interest in inhomogeneous metallic sytems such as double layers as employed in proximity-effect tunneling experiments,[1] or bimetallic superlattices,[2] also known as layered ultrathin coherent structures (LUCS).[3] In such systems, the metal-metal interface presumably plays a crucial role in determining the anisotropy of various transport properties. It is therefore necessary to consider the transmission coefficient of an interface between two metals for Fermi-surface electrons incident upon the interface. The purpose of this Report is to present the results of a calculation of the transmission coefficient for a single intermetallic interface.

It will be assumed that the interface is ideal in the sense that it is perfectly planar, that the metallic layers adjacent to it are characterized by equal lattice constants, and that the two metals are simple cubic, aligned along a common direction in the cubic unit cell (such as the [100] direction). The recent report of the epitaxial growth of Nb-Ta single-crystal superlattices with a high degree of crystalline perfection[2] indicates that this ideal system may be, in fact, an experimentally realizable situation.

The model adopted here for the metallic band structures is the tight-binding model. This model is most appropriate for transition metals, but the conclusions reached below should be qualitatively applicable to other metals, as well. The parameters of the model are as follows:

(1) The ratio R of the tight-binding bandwidths.

(2) The difference v between the Fermi energies of the two metals in units of the bandwidth of one of the two metals.

(3) The effective overlap integral T, coupling atoms of one metal to atoms of the other across the interface.

The translational symmetry in planes parallel to the interface, combined with the tight-binding model assumption, leads to a quasi-one-dimensional problem involving electron propagation in the presence of a local potential confined to the interface region. This problem may be solved exactly by the techniques elucidated by Kalkstein and Soven.[4] Yaniv[5] has shown how to apply these techniques to calculate the exact Green's function $G(m,n)$, for two semi-infinite metals with an interface between metallic layers of index $i=0$ and -1. The techniques of Refs. 4 and 5 are mathematically equivalent to those employed by Maradudin and Wallis[6] to the Montroll-Potts model[7] of lattice vibrations. Indeed, the results that will be described below have been used to determine the transmission coefficient for *phonons* incident upon an interface between two different crystals.[8]

If atoms of metal a occupy all lattice planes $m \leq -1$, and atoms of metal b occupy all planes $m \geq 0$, then Yaniv finds that the diagonal Green's function for $m \leq -1$ (i.e., in metal a) is

$$G(m,m)=\frac{i}{2T_a}\frac{1}{\sin(\phi_a)} \times[1+r(\phi_a,\phi_b)\exp(2im\phi_a)] , \tag{1}$$

where

$$\sin(\phi)=\begin{cases}\left[1-\left[\dfrac{\omega}{2T}\right]^2\right]^{1/2}, & \left[\dfrac{\omega}{2T}\right]^2 \leq 1 \\ i\,\mathrm{sgn}(\omega)\left[\left[\dfrac{\omega}{2T}\right]^2-1\right]^{1/2}, & \left[\dfrac{\omega}{2T}\right]^2 > 1\end{cases} \tag{2}$$

$$\omega=E-W(k_{||}) , \tag{3}$$

and

$$r(\phi_a,\phi_b) = -\frac{[\exp(i\phi_a)-u_a][\exp(-i\phi_b)-u_b]-\gamma}{[\exp(-i\phi_a)-u_a][\exp(-i\phi_b)-u_b]-\gamma}, \tag{4}$$

$$\gamma = T^2/(T_a T_b) . \tag{5}$$

The quantities $W_{a,b}(k_{||})$ and T_a, T_b are related to matrix elements of the bulk Hamiltonians in the Bloch-Wannier representation[3,4]:

$$W_{a,b}(k_{||}) = \langle nk_{||} \mid H_{a,b} \mid nk_{||} \rangle , \tag{6}$$

$$T_{a,b}(k_{||}) = \mid \langle nk_{||} \mid H_{a,b} \mid n+1,k_{||} \rangle \mid . \tag{7}$$

The quantities $u_{a,b} = U_{a,b}/T_{a,b}$, where $U_{a,b}$ is the *change* in the self-consistent potential of electrons near the interface relative to the bulk. The matrix element $T = T(k_{||})$ is given by an equation analogous to (7) for $n = -1$, except that it is a matrix element of the full, two-layer Hamiltonian.

We shall first examine the above Green's function in a situation for which the number of parameters is *minimal*. Hence, we set $u_a = u_b = 0$.

If the interface is perpendicular to the [100] directions of both lattices, then we find a further simplification:

$$\frac{\omega_a}{2T_a} = \frac{E}{2T_a} + v - 3 + \cos(k_y) + \cos(k_z) , \tag{8}$$

$$\frac{\omega_b}{2T_b} = R\frac{E}{2T_a} - Rv - 3 + \cos(k_y) + \cos(k_z) , \tag{9}$$

$$v = \frac{E_{Fa} - E_{Fb}}{4T_a} , \tag{10}$$

$$R = \frac{T_a}{T_b} , \tag{11}$$

and T, T_a, and T_b, are independent of $k_{||}$, $E_{F_{a,b}}$ being the Fermi energy in a or b. The lattice constants of a and b are assumed to be equal, so we may use dimensionless wave vectors.

Now, along the real axis, ϕ_a is restricted to the closed interval

$$0 \le \phi_a \le \pi/2 .$$

Along the imaginary axis, $\mathrm{Im}\phi_a$ can be positive or negative, depending in the sign of ω_a. Because $m < 0$ in (1), we see that allowed values (nonexponentially increasing) of the second term in (1) require $\omega_a < 0$. Hence, if ϕ_a is imaginary, then $\omega_a < -2T_a$ (for $T_a > 0$).

However, if ϕ_a is imaginary, then the corresponding E value is *not* that of a propagating electron in metal a. Of course, there may exist interface bound states,[4] that have imaginary ϕ_a, but these correspond to excitations that are *confined* to the near vicinity of the interface. When we consider the reflection coefficient, we envision a situation in which an incoming electron from a distant region of metal a approaches the interface and is reflected, subsequently being detected in a region far removed from the interface. If one restricts consideration to this case, one thus obtains the reflection probability appropriate to a given interface.

In the limit of bulk metal a, where we take $\phi_a = \phi_b$, $u_a = u_b = 0$, and $\gamma = 1$ in (4), r vanishes and the resulting Green's function reduces to that of bulk metal a, as required. One may therefore identify the second term in brackets in (1) as being due to reflection from the interface, the exponential factor representing the interference between incident and reflected electron waves.

Thus, the reflection coefficient is $\mid r(\phi_a,\phi_b) \mid^2$. For the "minimal parameter" case introduced above, one has

$$\mid r(\phi_a,\phi_b) \mid^2 = \left| \frac{\exp[i(\phi_a - \phi_b)] - \gamma}{\exp[-i(\phi_a + \phi_b)] - \gamma} \right|^2 , \tag{12}$$

where ϕ_a is *real*, and so $\mid \omega_a \mid \le 2T_a$. Using arguments analogous to those presented above for $\mathrm{Im}\phi_a \neq 0$, we find that $\mathrm{Im}\phi_b < 0$ so that $\mid r \mid^2$ approaches unity exponentially for ϕ_b moving away from zero on the negative imaginary axis. Since the energy values corresponding to such a ϕ_b represent an exponentially decaying electron state in metal b, this result is as expected.

To appreciate the results presented below, it helps to represent the maximum range of allowed energies in metals a and b as subbands. To obtain the appropriate subband width, consider the bulk electron energies as a function of (dimensionless) wave vector, and vary the component of this wave

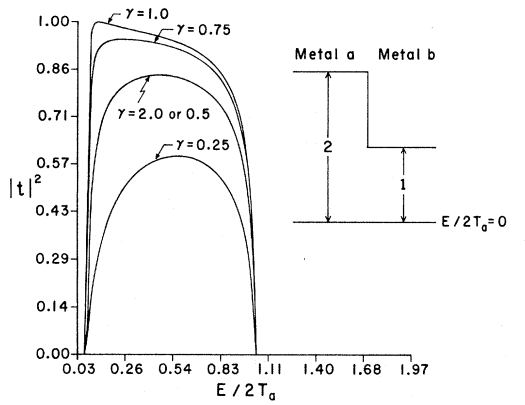

FIG. 1. Transmission coefficient vs $E/2T_a$ for electrons normally incident upon interface between metal a and metal b from metal a side. The bandwidth of metal a is twice that of metal b ($R=2.0$), and $v=0.03$ so that subband bottoms are nearly coincident (inset). Results for several values of intermetallic coupling γ are shown.

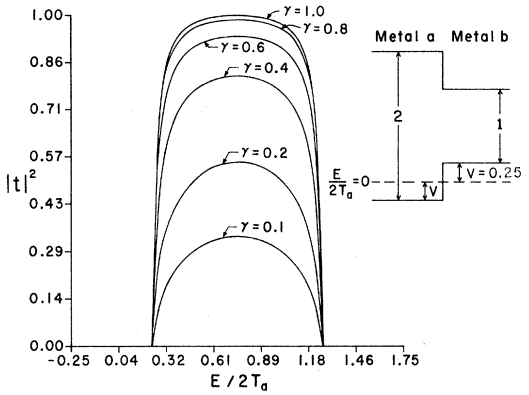

FIG. 2. Transmission coefficient vs $E/2T_a$ for electrons normally incident on metal-a — metal-b interface (as in Fig. 1.) for $v=0.25$ and several γ values. Inset depicts subband configuration.

vector $\vec{k}\cdot\hat{n}$ (where $\hat{n}$ is the unit normal to the interface) over its entire range of values. The resulting range of energies yields the subband width.

In our minimal parameter case, the subband widths are $4T_a$ and $4T_b$. For the moment, we consider only *normal* incidence ($k_y=k_z=0$). If we measure energy on the scale where $2T_a=1$, then these bandwidths are 2 and $2/R$, respectively. When the metals are in contact, the Fermi levels in the subband equalize, so that the bottom of the subband of metal b is located at a distance v from the origin. $E/2T_a=0$, while the bottom of the subband of metal a is located at $-v$ relative to the origin.

We now fix R, the ratio of metal a bandwidth to that of metal b, at a particular value ($R=2$) and vary γ, $E/2T_a$, and v. The parameter $\gamma=(T^2/T_aT_b)$ measures the coupling of the two metals, while v $[=(E_{F_a}-E_{F_b})/4T_a]$ is a measure of the difference in Fermi energies. Results for the transmission coefficient $|t|^2=1-|r|^2$ for two values of v are displayed in Figs. 1 and 2. In these plots, $E/2T_a$ is varied over the entire allowed range in the metal a subband, $-v$ to $2-v$.

In Fig. 1, the bottoms of the subbands nearly coincide ($v=0.03$). In this case $E_F/2T_a$, the common Fermi level, must lie between 0 and 1. Using (12), it is easy to show that, as a function of γ, $|t|^2$ is always largest for all E when $\gamma=1$. Also, if $\gamma>1$, then $|t|^2$ has the same values as are found for $1/\gamma$. For example, in Fig. 1 the curves for $\gamma=2$ and 0.5 coincide. For γ deviating from unity, the average $|t|^2$ decreases, although the average for $\gamma=0.75$ does not deviate from that for $\gamma=1$ by as much as the average for $\gamma=0.25$ deviated from that for $\gamma=0.5$. Also note the rapid increase in $|t|^2$ just above the subband minima.

The results that one obtains when the *tops* of the two subbands nearly coincide ($v=0.47$) are the mirror reflection of the $v=0.03$ results, obtained by reflecting about $E/2T_a=0$ and shifting the whole curve up by 1.5 along the $E/2T_a$ axis.

In Fig. 2 are the results for the symmetrical case ($v=0.25$) where the centers of the subbands coincide. Note that the $|t|^2$ curves are also symmetrical. Again, the average $|t|^2$ decreases as γ deviates from unity, but the *rate* of decrease is rather slow at first, *accelerating* as γ deviates further from unity. thus $|\partial|t|^2/\partial\gamma|$ is an increasing function of $|1-\gamma|$.

The effects of off-normal incidence are readily evaluated by defining

$$v_a(k_{||})=v-[2-\cos(k_y)-\cos(k_z)]$$
$$=v-\Delta v_a \tag{13}$$

and

$$v_b(k_{||})=v+[2-\cos(k_y)-\cos(k_z)]/R$$
$$=v+\Delta v_b\ . \tag{14}$$

For $R>1$, one finds that the metal a subband, defined by

$$-v_a(k_{||})<E/2T_a<2-v_a(k_{||})$$

(so that ϕ_a is real) moves rigidly upward relative to the metal b subband,

$$v_b(k_{||}) < E/2T_a < 2/R + v_b(k_{||}) , \tag{15}$$

because for $R > 1$, as $k_{||}$ $[=(k_y^2+k_z^2)^{1/2}]$ increases from 0, the change in v_a (Δv_a) is greater than the change in v_b (Δv_b). When $2/R + v + \Delta v_b = -v + \Delta v_a$, one is at a critical value for $k_{||}$ above which there is *no transmission.* The corresponding angle of incidence is analogous to the optical critical angle. This occurs because, at the critical $k_{||}$, the bottom of the subband of metal a coincides with the top of the subband of metal b (cf. Fig. 3). However, there may be values of v for which no critical $k_{||}$ exists. For example, for $R = 2$, $v > 0.5$ there are no critical $k_{||}$ values. In general, for $v > 2 - 3/R$ or $v < -1/R$ and $R > 1$, there are no critical $k_{||}$ values.

Similarly, for $R < 1$, there may occur critical $k_{||}$ values for which the top of the subband of metal a coincides with the *bottom* of the subband of metal b, so that there is no transmission for larger $k_{||}$ values. The condition necessary for this is

$$v_b = 2 - v_a$$

or (16)

$$\Delta v_b - \Delta v_a = 2 - 2v ,$$

so that there are no critical $k_{||}$ values only when $v < 2(1/R - 1)$ or $v > 1$.

In Fig. 3 we display the transmission coefficient versus $E/2T_a - \Delta v_a$ for $R = 2$, $\gamma = 1$, and $v = 0.25$. For $\Delta v_a = 0.8$, the shape of the curve is quite similar to that for $\gamma = 1$ in Fig. 1. Indeed, for $\Delta v_a = 0.88$, the curve for $v = 0.25$, $\gamma = 1$ would coincide with the $\gamma = 1$ curve in Fig. 1, because at this value of Δv_a, the subband bottoms are separated by 0.06, as they are for Fig. 1. The decay of $|t|^2$ as the critical $k_{||}$ value is approached is also clearly evident in Fig. 3. The critical value of Δv_a in this case is 3.0.

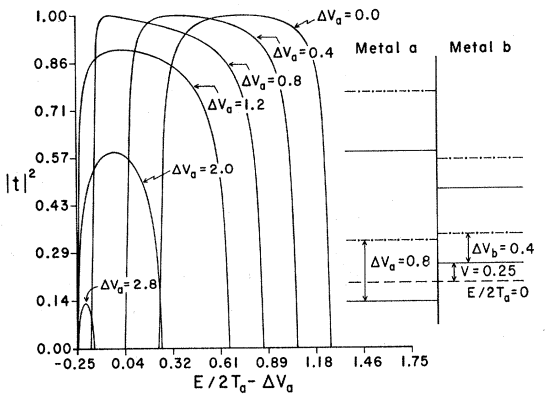

FIG. 3. Transmission coefficient vs $E/2T_a - \Delta v_a$ for $\gamma = 1.0$, $v = 0.25$, $R = 2.0$, and several values of Δv_a. Inset depicts change in relative subband configuration as Δv_a increases from 0 (solid lines) to 0.8 (dash-dot lines).

The model we have presented ignores several conditions which may be present in a realistic situation. It does not consider the effects of a mismatch in lattice constants. It does not treat the effects of having the two metals in different orientations, e.g., metal a having [111] direction aligned with the [100] direction of metal b. This can occur if there is a lattice-constant mismatch. Perhaps the weakest point of the model is its assumption that the interface is perfectly planar.

Despite these shortcomings, the essential physics of the transmission of electrons through a metal-metal interface emerges from this model in its description of electron transmission between subbands of two metals. The subband diagram in Figs. 1–3 will continue to be relevant even after the features enumerated above are included in the model.

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[1]E. L. Wolf and B. Arnold, Phys. Rep. (in press).
[2]S. M. Durbin, J. E. Cunningham, M. E. Mochel, and C. P. Flynn, J. Phys. F. 11, L223 (1981).
[3]I. K. Schuller, Phys. Rev. Lett. 44, 1597 (1980).
[4]David Kalkstein and P. Soven, Surf. Sci. 26, 85 (1971).
[5]Avishay Yaniv, Phys. Rev. B 17, 3904 (1978).
[6]A. A. Maradudin and R. F. Wallis, Phys. Rev. 148, 945 (1966).
[7]E. W. Montroll and R. B. Potts, Phys. Rev. 102, 72 (1956).
[8]Gerald B. Arnold and M. Menon J. Phys. (Paris) C6, Supp. 12, 377 (1981).