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ANALYTIC PROPERTIES AND SELF-CONSISTENCY IN A SCHOTTKY BARRIER MODEL*

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We apply a one-dimensional model to studies of intrinsic Schottky barriers. The semiconductor possesses two bands (s and p) and the metal has one conduction band. For the first time explicitly analytic formula for the density of states is given. An extremely accurate analytic formula (compared to numerical results) for the Fermi level position is proposed. It is shown that the Fermi level of the (covalent) semiconductor–metal interface is independent of the metal bulk parameters. Also self-consistent numerical results are presented.

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Although the metal–semiconductor interface is a very active area of research it seems that there is no fully satisfactory theory [1–8], because of the enormous complexity of this structure. This work adheres to the following philosophy. We consider the simplest model (that hopefully retains some physics of the original problem) and try to solve it as accurately as possible.

Following our previous works [9–10] we present here new fully analytic results that shed light on the nature of the charge transfer across the interface.

In the model we study, the semi-infinite crystal is formed by cleaving the infinite crystal. The Green's functions for the cleaved crystal can be described in terms of the infinite crystal Green's function and the scattering potential introduced by the cleavage. Finally, two semi-infinite crystals are joined to form an interface.

The Hamiltonian of the one-dimensional semiconductor is given elsewhere [11]. Here we only quote the following notation for energies, hopping integrals and auxiliary quantities:

$$\epsilon_L = \frac{\epsilon_{pp,L} - \epsilon_{ss,L}}{2}, \quad \epsilon_{pp,L} + \epsilon_{ss,L} = 0, \quad \epsilon_R = \epsilon_{ss,R},$$

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$$\beta_{ss,L} = \beta_L(1+\delta_L),\ \beta_{pp,L} = \beta_L(1-\delta_L),\ 0 \le \delta_L \le 1,\ \beta_{sp,L} = \sqrt{\beta_{ss,L}\beta_{pp,L}},$$

$$\alpha_L = \frac{1}{2\lambda_L}[(E-\epsilon_L)(E+\epsilon_L) - 4\beta_{ss,L}\beta_{pp,L}],\ \lambda_L = (E-\epsilon_L)\beta_{ss,L} - (E+\epsilon_L)\beta_{pp,L},$$

$$\gamma_L = \begin{cases} \pm\sqrt{\alpha_L^2 - 1}, & \text{for } \alpha_L > 1,\ \alpha_L < -1 \text{ respectively;} \\ \mathrm{i}\sqrt{1-\alpha_L^2}, & \text{for } |\alpha_L| \le 1, \end{cases}$$

$$g_L(m) = \frac{(-\alpha_L + \gamma_L)^{|m|}}{\gamma_L},$$

$$\beta_{ss,R} = \beta_R(1+\delta_R),\ 0 \le \delta_R \le 1,\ \alpha_R = \frac{E-\epsilon_R}{2\lambda_R},\ \lambda_R = \beta_{ss,R}.$$

The junction coupling operators are assumed in the form

$$H_{LR}^{-1,0} = \begin{pmatrix} -\alpha \mid -1, s >< 0, s \mid \\ -\beta \mid -1, p >< 0, s \mid \end{pmatrix}.$$

In the next part of the work G^0 and ρ^0, G and ρ, G' and ρ' are used as quantities specifying the bulk, surface and the junction, respectively.

We assume that the valence band of the semiconductor is completely full and contains two electrons per atom while the semiconductor conduction band is completely empty. Before forming the interface the metal conduction band is half-filled and contains one electron per atom.

If there is no surface state then for energies in the gap we obtain fully analytic formulae for the densities of states

$$\rho'^{s}_L(n,E) = \rho_R(0,E)\frac{e^{2|n+1|x}}{\Delta\Delta^*}\left[\alpha\left(\frac{\beta_{pp}}{\lambda_L}\delta^{-1n} + G_{ss}^{-1,-1}\right) + \beta\left(\frac{-\beta_{sp}}{\lambda_L}\delta^{-1n} + G_{sp}^{-1,-1}\right)\right]^2, \tag{1}$$

$$\rho'^{p}_L(n,E) = \rho_R(0,E)\frac{e^{2|n+1|x}}{\Delta\Delta^*}\left[\alpha\left(\frac{\beta_{sp}}{\lambda_L}\delta^{-1n} + G_{sp}^{-1,-1}\right) + \beta\left(\frac{-\beta_{ss}}{\lambda_L}\delta^{-1n} + G_{pp}^{-1,-1}\right)\right]^2, \tag{2}$$

$$\rho'^{s+p}_L(n,E) = \rho'^{s}_L(n,E) + \rho'^{p}_L(n,E), \quad \text{because } \mathrm{Im}G_{LL} = 0, \tag{3}$$

where

$$x(E) = \ln(|\alpha_L(E)| - \sqrt{\alpha_L^2 - 1}), \tag{4}$$

$$\delta^{mn} = \begin{cases} 0 & \text{if m = n} \\ 1 & \text{otherwise} \end{cases} \rightarrow \text{complement of the } \textit{Kronecker symbol}, \text{ and}$$

$$\Delta = 1 - G_{RR}^{0,0}[\alpha^2 G_{ss}^{-1,-1} + 2\alpha\beta G_{sp}^{-1,-1} + \beta^2 G_{pp}^{-1,-1}]. \tag{5}$$

We also derive an analytic result for ρ'^{s+p}_L in the case of existence of the surface state (E_{Surf} exists if $\epsilon_L < 2\beta_L$ and then $E_{\mathrm{Surf}} = \epsilon_L \delta_L$),

$$\rho'^{s+p}_L(n, E = E_{\mathrm{Surf}}) = \rho_R(0, E) \frac{\exp(2|\, n+1 \,|\, x) 2}{|\, G^{0,0}_{RR}(E) \,|^2} \frac{2}{(\alpha\sqrt{1-\delta_L} + \beta\sqrt{1+\delta_L})^2} \quad (6)$$

and

$$\rho'_R(n, E = E_{\mathrm{Surf}}) = \rho_R(0, E)\{1 - \cos[2n \arccos(|\, \alpha_R \,|)]\}, \quad (7)$$

where

$$x = \ln |\, \epsilon_L / 2\beta_L \,| \,. \quad (8)$$

After forming the interface there is a charge flow across the junction. The Fermi levels E_{F} is determined by the global charge neutrality $\delta\rho_{\mathrm{sem}} + \delta\rho_{\mathrm{met}} = 0$. This assures partial self-consistency in the Friedel sense.

The derived formulae give important exact results (within the model) that provide new insight into the physics of semiconductor–metal junction:

(a) exponential decay of states (in n variable) on the semiconductor side starting from the -2 site,

(b) the decay constants $x(E)$ and x depend only on parameters of a semiconductor.

If we assume that

$$\alpha = \sqrt{\beta_{ss,L}\beta_{ss,R}}, \quad \beta = \sqrt{\beta_{ss,R}\beta_{pp,L}}, \quad (9)$$

then if there is no surface state $E_{\mathrm{F}} = 0.5 E_{\mathrm{g}} \delta_L$, where $E_{\mathrm{g}} = (E^b_c - E^t_v)/2$, $E^t_v = \epsilon_{ss,L} + 2\beta_L(1+\delta_L)$, $E^b_c = \epsilon_{pp,L} - 2\beta_L(1-\delta_L)$. This postulated relation agrees with numerical results with the accuracy of at least four decimal figures. The Fermi level position depends only on ratio of conduction to valence band widths of a semiconductor, $w_c/w_v = (1-\delta_L)/(1+\delta_L)$, and is completely independent of the metal parameters (this last fact is well known experimentally). Finally, a sign of δ_L governs the direction of the charge transfer. We verify numerically that

$$\sum_{i=-1}^{-\infty} \Delta n^L_i = \begin{cases} > 0, & \text{for } \delta_L > 0; \\ \leq 0, & \text{otherwise.} \end{cases}$$

In Fig. 1 we present the Fermi level position and polarization of a junction for a selected set of parameters.

The fully self-consistent procedure should include potential change due to a charge redistribution upon the junction formation. For a discrete model this potential on a given site is due to (a) a change of charge on other sites, (b) a change of charge on the same site. In the (b) case one has to introduce the Coulomb repulsive potentials U_L (semiconductor) and U_R (metal) under assumption that these quantities do not depend on the site label with respect to the interface position.

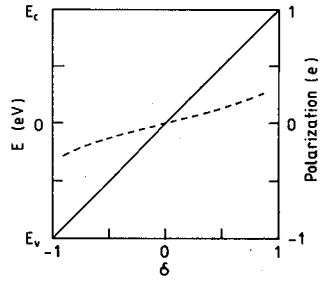

Fig. 1. Fermi energy as a function of δ_{sem} (solid line, left axis) for the following bulk parameters: $\epsilon_{s,\mathrm{sem}} = -\epsilon_{p,\mathrm{sem}} = -2.5$ and $\epsilon_{s,\mathrm{met}} = E_{\mathrm{F}}$. Values of $\beta_{\mathrm{sem}} = 1$, $\beta_{\mathrm{met}} = 1$ and $\delta_{\mathrm{met}} = 0$. Eq. (9) is employed. Also polarization of the junctions, labelled on right axis, in units of number of electrons transferred, is displayed as a broken curve.

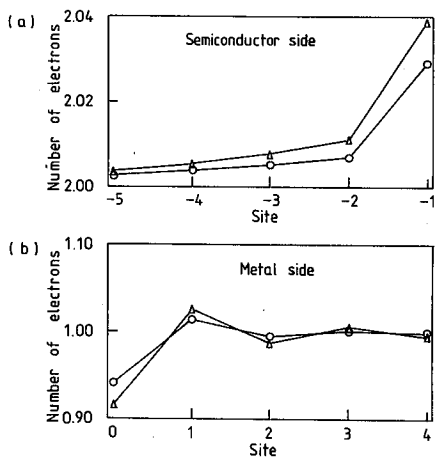

Fig. 2. Site charge distribution (for $U = 1$ eV – a self-consistent case, diamonds and for $U = 0$, triangles). Bulk parameters (except δ_{sem}) as in Fig. 1. These parameters together with $\delta_{\mathrm{sem}} = 0.5$ correspond to the following widths of the bands: $w_{s,\mathrm{met}} = 4$, $w_{s,\mathrm{sem}} = 6$, and $w_{p,\mathrm{sem}} = 2$.

As regards to the tight-binding models, it is extremely difficult to achieve convergence in the case (a) unless it is postulated that the charge can change only an extremely small number of sites next to interface.

Similarly as Masri [12] we achieved convergence when only the case (b) was assumed, for $U_L = -U_R = U$ using the Friedel sum rule. In Fig. 2 we present results for $U = 1$ eV.

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