EFFECT OF AN ELECTRIC FIELD IN THE SPACE CHARGE REGION ON SURFACE STATES

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The quantization of the current carriers and the effect of an electric field in the space charge region on Tamm surface states are investigated within the framework of the Kronig–Penney model and in the effective mass approximation.

The quantization of the current carriers in the surface layers of space charge and the effect of an external electric field on surface states have been investigated by means of various models. For instance, in the works [1-3], the effective mass approximation was used to quantize the energy spectrum of current carriers in the space charge region (SCR) for germanium and silicon. It was shown that the quantization of the energy spectrum leads to significant changes in all quantities that must be taken into account when establishing the voltage-capacitance curve, interpreting the field effect experiments, and analyzing the surface transport phenomena. The effect of an external electric field on surface states was considered in the framework of the simple one-dimensional Kronig–Penney and Mathieu model in [4, 5], and with the two-zone Maue–Antonchik model in [6]. The calculations showed that applying a voltage at the metal–semiconductor contact to enhance the electron emission from the semiconductor leads to an increased localization of the surface wave function of the surface state at the surface and to the appearance of a surface barrier of instability.

In this work, first by using the Kronig–Penney model and then in the effective mass approximation, we consider the quantization of the energy spectrum of the current carriers in the SCR and the effect of zone bending on the Tamm surface states.

The Kronig–Penney Model. For the sake of simplicity, we shall assume that the electric field in SCR is uniform and penetrates down to a depth Na, where a is the lattice constant, N is an integer, and we shall neglect the image forces. The potential energy \( v(x) \) of an electron can then be written as (Fig. 1)

\[
v(x) = \begin{cases} 
V_0 + eU & \text{for } x < -aN; \\
\frac{\hbar^2}{2m} \sum_{n=1}^{1-N} \delta(x - na) - eU x/(Na) & \text{for } -aN \leq x < 0; \\
\frac{\hbar^2}{2m} \sum_{n=1}^{\infty} \delta(x - na) & \text{for } x > 0,
\end{cases}
\]  

(1)

where \( V_0 \) is the height of the barrier, U is the voltage between the surface and the bulk of the crystal, \( m \) and \( e \) are the electron mass and charge magnitude, respectively, \( 2\hbar = h \) is Planck's constant, \( \delta(x) \) the Dirac function, and \( \Omega \) the impenetrability coefficient [7].

In the first region, \( (x < -aN) \), the wave function at an energy \( W \) smaller than \( V_0 + eU \) is

\[
\psi(x) = A \exp[\lambda(x+Na)],
\]

(2)

where

\[
\lambda = \left[2m(V_0 + eU - W)\right]^{1/2}/\hbar.
\]

The third region, \( (x > 0) \), is divided into subdomains of width \( a \) and numbered such that the subdomain at the right of a delta-function has the same number as the number \( n \) which appears in the argument of the delta-function. The wave function in the subdomain \( n \) is then [8]
\[ \psi(x) = \left\{ e^{i\kappa(x-na)} - (Q - e^{i\kappa a}) e^{-i\kappa(x-na)}/(Q - e^{-i\kappa a}) \right\} Q^n B_1 + \]
\[ + \left\{ e^{i\kappa(x-na)} - (1 - Qe^{i\kappa a}) e^{-i\kappa(x-na)}/(1 - Qe^{-i\kappa a}) \right\} Q^{-n} B_1, \]

where

\[ \kappa = \left( \frac{2mV}{\hbar} \right)^{1/2}; \]
\[ Q = \text{sign}(\Lambda) \exp(-qa); \]
\[ \Lambda = \cos(\kappa a) + \frac{V}{2\kappa} \sin(\kappa a); \]
\[ \exp(-qa) = |\Lambda| - (\Lambda^2 - 1)^{1/2}. \]

If \(|\Lambda| > 1\), \(q\) is real and \(|Q| < 1\). To satisfy the natural boundary condition at \(x \to \infty\) for surface states, one must take \(B_2 = 0\).

The second region, \((-aN < x < 0)\), can also be divided in subdomains of width \(a\) and numbered in the same manner as in the third region. The wave function in the subdomain \(-n\) is thus

\[ \psi(x) = C_1(n)A_i(\xi) + C_2(n)B_i(\xi), \]

where

\[ \xi = -\left[ x + aNW/(eU) \right]/x_0; \]
\[ x_0 = \left[ h^2aN/(2meU) \right]^{1/3}; \]

\(A_i(z)\) and \(B_i(z)\) are the Airy functions [9].

The coefficients \(C_1(n)\) and \(C_2(n)\) for \(N - 1 \leq n \leq 1\) satisfy the recurrence relations

\[ C_1(n + 1) = \left[ 1 + \pi \xi x_0 A_t(\xi(n)) B_t(\xi(n)) \right] C_1(n) + \pi \xi x_0 B_t^2(\xi(n)) C_2(n); \]

\[ C_2(n + 1) = -\pi \xi x_0 A_t^2(\xi(n)) C_1(n) + \left[ 1 - \pi \xi x_0 A_t(\xi(n)) B_t(\xi(n)) \right] B_t(\xi(n)) C_2(n) \]

in which

\[ \xi(n) = a[n - NNW/(eU)]/x_0. \]

From (6) and (7) it follows that the coefficients \(C_1(n)\) and \(C_2(n)\) cannot vanish simultaneously for any \(n\).

The continuity of wave functions and of their derivatives at the points \(x = 0\) and \(x = -aN\) implies that

\[ A = A_t(\xi(N)) C_1(N) + B_t(\xi(N)) C_2(N); \]

\[ B_t = \left[ Q - e^{-i\kappa a} \right] \left[ A_t(\xi(0)) C_1(1) + B_t(\xi(0)) C_2(1) \right]/(2i \sin(\kappa a)) \]

and two more conditions: