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## The influence of spatial dispersion of the bulk dielectric function on surface screening

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**Abstract.** The effect of spatial dispersion of the bulk dielectric function of a semiconductor on the surface potential barrier is studied with the help of a few different surface screening models.

The transmission coefficients for field-emitted electrons calculated using the Miller–Good approximation for both transmission over and tunnelling through the barrier are much smaller than those predicted by the dispersionless theory.

### 1. Introduction

The purpose of this paper is to study the influence of the spatial dispersion of the bulk dielectric function of a semiconductor on the shape of the surface potential barrier and on field emission.

Field emission is the phenomenon during which the electrons from a solid tunnel into the vacuum through the surface barrier owing to the presence of an external electric field.

Usually in semiconductors this barrier is approximated by

$$B(z) = -e^2(\epsilon_0 - 1)/4(\epsilon_0 + 1)z - eFz \quad (1)$$

where it is assumed that the semiconductor occupies the  $z < 0$  region and the electric field  $F$  is perpendicular to its surface, i.e. the  $z = 0$  plane. In a typical experiment,  $F$  is  $10^7$ – $10^8$  V cm<sup>-1</sup>. The first term in (1) represents the image-force potential and  $\epsilon_0$  is the dielectric constant of the semiconductor.

Since the semiconductor is characterised by the dielectric function rather than by a constant, it is expected that the spatial dispersion of the dielectric function involves changes in the shape of the barrier (1) and what follows affects the emission.

Field emission from semiconductors has been investigated experimentally since the early 1960s (see the reviews in [1, 2]) but until now there has been no exhaustive description to account for this phenomenon. It is explained qualitatively only (see, e.g., [3, 4]) by the Stratton [5] theory combined with the effective-mass approximation. Recently the problem of the influence of the form of the semiconductor dielectric function on field emission was raised again in [6, 7] where the so-called specular electron reflection model [8, 9] (see also [10]) was used to describe the surface screening. This model, however, is based on the plane-wave character of the electron wavefunctions

and we think that it is more effective for a semi-infinite jellium than for a semi-infinite semiconductor. In the present paper, we study the tunnelling of the electrons through the surface barrier using some new screening models which are applicable most of all to semiconductors.

## 2. Surface screening

To find the potential energy of a point charge  $Q_{\text{ext}}$  near a semi-infinite semiconductor, we recall that this energy is the product of  $Q_{\text{ext}}/2$  and the induced potential at the point-charge position. In the dispersionless model, this energy is simply  $-Q_{\text{ext}}^2(\epsilon_0 - 1)/4(\epsilon_0 + 1)z$ , where  $z$  is the distance from the vacuum–dielectric interface, i.e. the  $z = 0$  plane.

Generally, according to the linear response theory, the induced potential  $V_{\text{ind}}$  is related to the total potential  $V$  through  $\Delta V_{\text{ind}}(\mathbf{r}) = 4\pi \int d^3r' \chi(\mathbf{r}, \mathbf{r}')V(\mathbf{r}')$ , where  $\chi$  is the polarisability function. It will be more convenient in our case to write down this equation in terms of the Hankel transform with respect to  $\rho = \sqrt{x^2 + y^2}$ :

$$\left(\frac{d^2}{dz^2} - q_{\parallel}^2\right)V_{\text{ind}}(q_{\parallel}, z) = \frac{8\pi^2}{q_{\parallel}} \int dz' \chi(q_{\parallel}, z, z')V(q_{\parallel}, z'). \quad (2)$$

$V = V_{\text{ind}} + V_{\text{ext}}$ , where  $V_{\text{ext}}$  is due to the point charge located say at the distance  $z_0$  from the  $z = 0$  plane. Since we are interested in the value of  $V_{\text{ind}}$  at the point-charge site, we substitute in our expressions  $z_0 = z$ .

In the models that we are going to apply the polarisability function  $\chi$  of the semi-infinite semiconductor is expressed in terms of the functions which characterise the bulk. The model used in [7] is described in detail for the example in [10]. Sometimes it is called the specular electron reflection model. It is based on the assumption that

$$\chi(q_{\parallel}, z, z') = \vartheta(-z)\vartheta(-z')[\chi_b(q_{\parallel}, z - z') + \chi_b(q_{\parallel}, z + z')] \quad (3)$$

where  $\chi_b$  is the bulk polarisability. Note that  $\chi_b(q_{\parallel}, z) = (q_{\parallel}^2 - d^2/dz^2)\alpha_b(q_{\parallel}, z)$ , where  $\alpha_b$  is the susceptibility which is related to the bulk dielectric function through (Fourier transform)  $\alpha_b(q) = [\epsilon_b(q) - 1]/4\pi$ .

Two other descriptions of surface screening have been introduced in [11] (hereafter referred to as model I) and [12] (hereafter referred to as model II). Model I is based on the assumption that  $\alpha(q_{\parallel}, z, z') = \vartheta(-z)\vartheta(-z')\alpha_b(q_{\parallel}, z - z')$  and according to the discussion in [11] is applicable to semiconductors and dielectrics rather than to metals. The idea behind the development of model II lies in the following. In [12] it was shown that the susceptibility  $\alpha$  of a semi-infinite semiconductor can be expressed approximately in terms of envelope wavefunctions which in contrast with Bloch functions have the plane-wave character. Since the assumption about specular electron reflection concerning polarisability  $\chi$  (equation (3)) was originally made for jellium and was based on the plane-wave character of electron wavefunctions, we believe that in the case of semi-infinite semiconductors it should be made concerning susceptibility  $\alpha$  [12]. If we introduce the parameter  $p$  in order to distinguish between models I and II, then the Hankel transform of the function  $\chi$  in these models has the form

$$\begin{aligned} \chi(q_{\parallel}, z, z') = & \vartheta(-z)\vartheta(-z')[(q_{\parallel}^2 - d^2/dz^2)\alpha_b(q_{\parallel}, z - z') \\ & + p(q_{\parallel}^2 + d^2/dz^2)\alpha_b(q_{\parallel}, z + z' - a)] \end{aligned}$$

$$\begin{aligned}
 & + \delta(z)\delta(z')[\alpha_b(q_{\parallel}, z - z') + p\alpha_b(q_{\parallel}, z + z' - a)] \\
 & - \delta(z)\vartheta(-z')[-\alpha'_b(q_{\parallel}, z - z') + p\alpha'_b(q_{\parallel}, z + z' - a)] \\
 & - \vartheta(-z)\delta(z')[\alpha'_b(q_{\parallel}, z - z') + p\alpha'_b(q_{\parallel}, z + z' - a)]
 \end{aligned} \tag{4}$$

where  $\alpha'_b(q_{\parallel}, \xi) = (d/d\xi)\alpha_b(q_{\parallel}, \xi)$ . Here  $p$  is 0 and 1 for models I and II, respectively. Introducing parameter  $a$ , we distinguish in model II the position of specular plane for electron wavefunctions from the position of the electron density step at the surface [12].

The potential  $V$  is continuous at  $z = 0$ . The jump of  $\partial V/\partial z$  at  $z = 0$  depends on the model and is 0 for the specular electron reflection model. For the remaining models, we have

$$\begin{aligned}
 \left[ \frac{\partial V}{\partial z} \right]_{z=0^-}^{z=0^+} & = \frac{8\pi^2}{q_{\parallel}} \left( [\alpha_b(q_{\parallel}, 0) + p\alpha_b(q_{\parallel}, -a)]V(q_{\parallel}, 0) \right. \\
 & \left. - \int_{-\infty}^0 [-\alpha'_b(q_{\parallel}, -z') + p\alpha'_b(q_{\parallel}, z' - a)]V(q_{\parallel}, z') dz' \right).
 \end{aligned} \tag{5}$$

Now to solve for the potentials the only input required in all the methods just mentioned is the susceptibility or, what is equivalent, the dielectric function for the bulk semiconductor. We choose the form of the dielectric function suggested by Schulze and Unger [13] (see the discussion in [7] in connection with this choice):

$$\epsilon(q) = 1 + (\epsilon_0 - 1)/[1 + (\epsilon_0 - 1)q^2/k_{TF}^2](1 + 3q^2/4k_F^2) \tag{6}$$

where  $k_{TF}$  and  $k_F$  are the Thomas–Fermi wavenumber and the Fermi wavenumber, respectively. The Schulze–Unger equation characterises an intrinsic semiconductor.

### 3. Surface barrier

#### 3.1. Specular electron reflection model

In this case (see [6, 7] or [10];  $z \geq 0$ )

$$V_{\text{ind}}(\rho, z, z_0) = -Q_{\text{ext}} \int_0^{\infty} dq_{\parallel} \frac{1 - q_{\parallel}a(q_{\parallel})}{1 + q_{\parallel}a(q_{\parallel})} J_0(\rho q_{\parallel}) \exp[-q_{\parallel}(z + z_0)] \tag{7}$$

where

$$a(q_{\parallel}) = \frac{1}{\pi} \int \frac{dq_{\perp}}{(q_{\perp}^2 + q_{\parallel}^2)\epsilon(q)}. \tag{8}$$

When  $\epsilon$  is given by (6), then

$$\begin{aligned}
 a(q_{\parallel}) & = 1/\epsilon_0 q_{\parallel} + [(\epsilon_0 - 1)/\epsilon_0](1/|q_1|^2) \\
 & \quad \times \{\text{Re } q_1 - [(\alpha^2 + \beta^2)/\sqrt{4\epsilon_0\alpha^2\beta^2 - (\alpha^2 + \beta^2)^2}] \text{Im } q_1\}.
 \end{aligned} \tag{9}$$

Here  $\alpha^2 = 4k_F^2/3$ ,  $\beta^2 = k_{TF}^2/(\epsilon_0 - 1)$ ,  $|q_1|^2 = [q_{\parallel}^4 + (\alpha^2 + \beta^2)q_{\parallel}^2 + \epsilon_0\alpha^2\beta^2]^{1/2}$ ,  $\text{Re } q_1 = (2|q_1|^2 + q_{\alpha}^2 + q_{\beta}^2)^{1/2}/2$ ,  $\text{Im } q_1 = -(2|q_1|^2 - q_{\alpha}^2 - q_{\beta}^2)^{1/2}/2$ , where  $q_{\alpha}^2 = q_{\parallel}^2 + \alpha^2$  and  $q_{\beta}^2 = q_{\parallel}^2 + \beta^2$ .

The potential  $B(z)$  experienced by an electron ( $Q_{\text{ext}} = e$ ) is equal to  $eV_{\text{ind}}$  ( $\rho = 0, z, z_0 = z$ )/2 and can be calculated numerically.

### 3.2. Models I and II

In order to find the potential in the framework of models I and II, we followed the method of solution of the equations suggested in connection with model I [11]. Finally the expression for the potential becomes

$$V(\rho, z) = \int_0^\infty V(q_{\parallel}, z_0, z) J_0(\rho q_{\parallel}) dq_{\parallel} \quad (10)$$

where ( $z_0 > 0$ , i.e. the external charge  $Q_{\text{ext}}$  is in the vacuum)

$$V(q_{\parallel}, z_0, z) = Q_{\text{ext}} \exp(-q_{\parallel}|z - z_0|) + V_4(q_{\parallel}, z_0) \exp(-q_{\parallel}z) \quad (11)$$

for  $z \geq 0$  (vacuum) and

$$\begin{aligned} V(q_{\parallel}, z_0, z) &= V_1(q_{\parallel}, z_0) \exp(q_{\parallel}z) + V_2(q_{\parallel}, z_0) \\ &\quad \times \exp(q_1 z) + V_3(q_{\parallel}, z_0) \exp(q_2 z) \\ &= V_1(q_{\parallel}, z_0) \exp(q_{\parallel}z) + 2 \operatorname{Re}[V_2(q_{\parallel}, z_0) \exp(q_1 z)] \end{aligned} \quad (12)$$

for  $z < 0$  (semiconductor). Here  $q_2 = q_1^*$ . Functions  $V_i(q_{\parallel}, z_0)$  are the solutions of the set of the algebraic equations

$$\begin{bmatrix} a_{11} & a_{12} & a_{12}^* & 0 & V_1 \\ Pa_{11} & Pa_{12} & Pa_{12}^* & 0 & V_2 \\ 1 & 1 & 1 & -1 & V_3 \\ a_{41} & a_{42} & a_{42}^* & 0 & V_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 2q_{\parallel} \end{bmatrix} Q_{\text{ext}} \exp(-q_{\parallel}z_0). \quad (13)$$

$P$  denotes here the permutation  $\alpha \rightleftharpoons \beta$ .

$$\begin{aligned} a_{12} &= (1/q_{\beta})[\beta^2/(q_1 - q_{\beta}) - p \exp(-q_{\beta}a) \\ &\quad \times (q_{\parallel}^2 + q_{\beta}^2)/(q_1 + q_{\beta})] + 1 + p \exp(-q_{\beta}a) \end{aligned} \quad (14)$$

$$\begin{aligned} a_{42} &= Aq_1\{[1 + p \exp(-q_{\beta}a)]/q_{\beta}(q_1 + q_{\beta}) \\ &\quad - [1 + p \exp(-q_{\alpha}a)]/q_{\alpha}(q_1 + q_{\alpha})\} + q_1 + q_{\parallel}. \end{aligned} \quad (15)$$

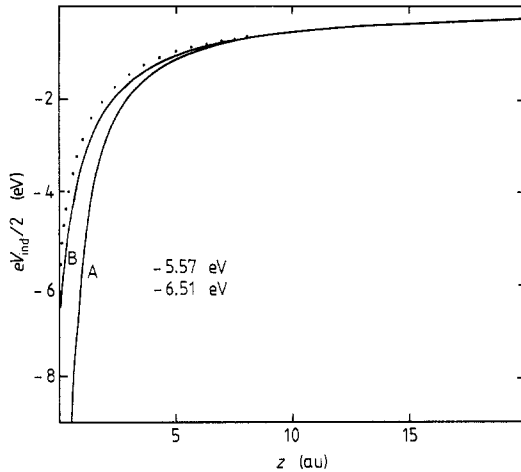
$A = (\epsilon_0 - 1)\alpha^2\beta^2/2(\alpha^2 - \beta^2)$ . When we replace  $q_1$  by  $q_{\parallel}$  in  $a_{12}$  (equation (14)) and in  $a_{42}$  (equation (15)), we obtain  $a_{11}$  and  $a_{41}$ , respectively.

Solving (13) for  $V_4$ , we get

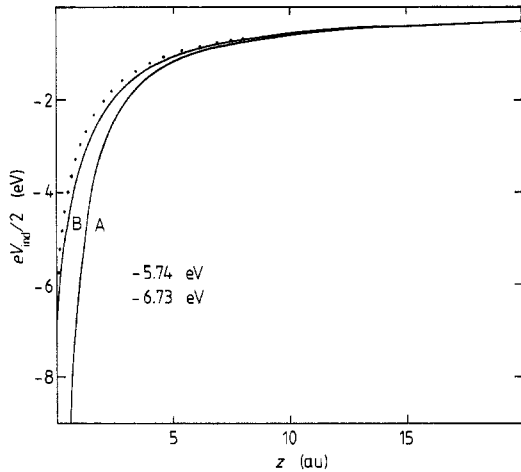
$$\begin{aligned} V_4(q_{\parallel}, z_0) &= \{2q_{\parallel}(1 - P)[(a_{11} - \operatorname{Re} a_{12}) \operatorname{Im} a_{22}]/(1 - P) \\ &\quad \times [a_{11} \operatorname{Im}(a_{42}^* a_{22}) - a_{41} \operatorname{Re} a_{12} \operatorname{Im} a_{22}] - 1\} Q_{\text{ext}} \exp(-q_{\parallel}z_0). \end{aligned} \quad (16)$$

As already mentioned, the potential  $B(z)$  experienced by an electron ( $Q_{\text{ext}} = e$ ) is  $eV_{\text{ind}}(\rho = 0, z, z_0 = z)/2$ . In order to obtain the induced potential  $V_{\text{ind}}$  outside the semiconductor ( $z \geq 0$ ), we must drop the Coulombic term  $Q_{\text{ext}} \exp(-q_{\parallel}|z - z_0|)$  in (11). In the case of field emission,  $B(z)$  contains an additional term  $-eFz$  due to the externally applied electric field  $F$ . Finally ( $J_0(0) = 1$ )

$$B(z) = \frac{e}{2} \int_0^\infty V_4(q_{\parallel}, z) \exp(-q_{\parallel}z) dq_{\parallel} - eFz. \quad (17)$$



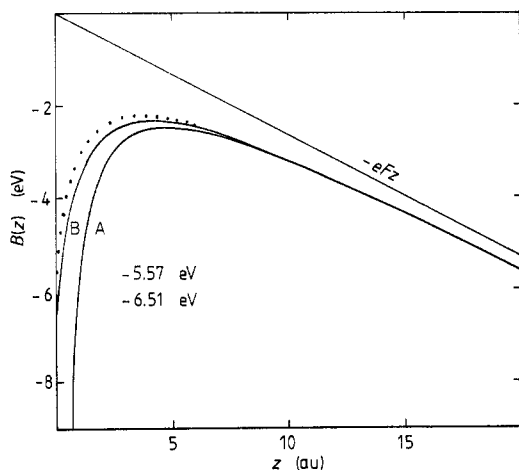
**Figure 1.** Electrostatic potential energy of an electron located in the vacuum as a function of the distance from the surface of semi-infinite semiconductor for silicon: curve A, dispersionless model; curve B, model I;  $\cdots$ , specular electron reflection model.



**Figure 2.** Electrostatic potential energy of an electron located in the vacuum as a function of the distance from the surface of semi-infinite semiconductor for GaAs: curve A, dispersionless model; curve B, model I;  $\cdots$ , specular electron reflection model.

### 3.3. Results

After numerical integration once, we obtain the results for  $B(z)$  which are presented in figures 1–3. Figures 1 and 2 show the dependence of the electrostatic energy of an electron image-force potential  $eV_{\text{ind}}/2$  on the distance  $z$  from the surface of the semi-infinite semiconductor for silicon ( $\epsilon_0 = 11.94$ ,  $k_F = 0.96$  and  $k_{\text{TF}} = 1.1$  in atomic units) and GaAs ( $\epsilon_0 = 13$ ,  $k_F = 0.98$  and  $k_{\text{TF}} = 1.12$  [14]). Figure 3 illustrates the shape of the surface barrier  $B(z) = eV_{\text{ind}}(z)/2 - eFz$  for silicon when  $F = 5 \times 10^7 \text{ V cm}^{-1}$ . In all the three figures the full curves which are divergent at  $z = 0$  represent the dispersionless approximation. The other full curves correspond to the calculations in the framework of model I. The full circles indicate the dependence of the potentials on  $z$  according to the specular electron reflection model. The results obtained with model II ( $a = 6.64$  au for silicon) do not differ very much from those calculated according to model I and for simplicity are not shown in the figures.



**Figure 3.** The shape of the surface barrier for silicon when the external electric field  $F$  is  $5 \times 10^7 \text{ V cm}^{-1}$ ; curve A, dispersionless model; curve B, model I;  $\cdots$ , specular electron reflection model.

The  $B(z)$  curves can be simply approximated by

$$B(z) = -f/[z + f/|B(0)|] - eFz \quad (18)$$

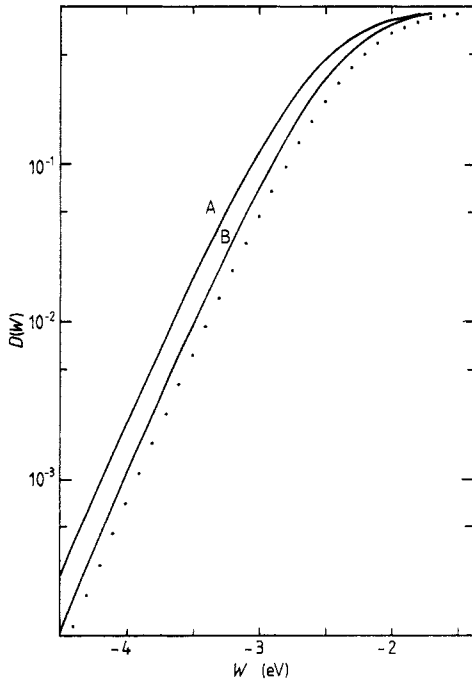
where  $B(0)$  equals  $eV_{\text{ind}}(0)/2$  and for silicon, when the Schulze–Unger dielectric function (equation (6)) is used, is  $-5.57 \text{ eV}$  and  $-6.51 \text{ eV}$  for the specular electron reflection model and model I, respectively. The first value disagrees with that given in [7], where the specular electron reflection model is used. When we use the Penn dielectric function [15] instead of the Schulze–Unger dielectric function, these values are  $-6.2 \text{ eV}$  and  $-7.4 \text{ eV}$ , respectively [16]. Model II leads to the result  $-6.56 \text{ eV}$  for equation (6).

The parameter  $f$  is determined by the condition that  $B(z)$  defined by (18) approaches the same maximum as the exact  $B(z)$  does. This means that  $f$  depends on the applied electric field  $F$  in the suggested approximation. For silicon characterised by (6) and for  $F = 5 \times 10^7 \text{ V cm}^{-1}$ ,  $f = 5.83 \text{ eV au}$  and  $6.33 \text{ eV au}$  for the specular electron reflection model and for model I, respectively. Model II gives  $6.37 \text{ eV au}$ .

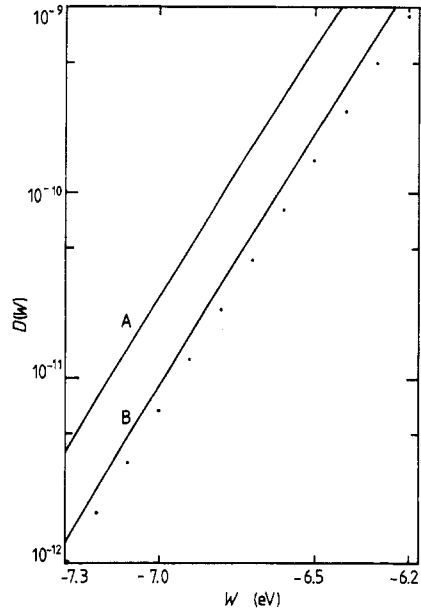
Apart from  $-eFz$  the leading term in an asymptotic expansion of  $B(z)$  for large  $z$  is  $-e^2(\epsilon_0 - 1)/4(\epsilon_0 + 1)z$  for all the discussed models, which is in accordance with the result for classical dielectric. The first few quantum corrections to  $B(z)$  in the specular electron reflection model combined with (6) can be seen from the following asymptotic expansion:

$$\begin{aligned} B(z) = & -[e^2(\epsilon_0 - 1)/4(\epsilon_0 + 1)z][1 - [\epsilon_0/(\epsilon_0 + 1)] \\ & \times \{[1 + (\alpha^2 + \beta^2)/\sqrt{\epsilon_0\alpha\beta}]/\sqrt{2\sqrt{\epsilon_0\alpha\beta} + \alpha^2 + \beta^2}\}(1/z) \\ & + [\epsilon_0(\epsilon_0 - 1)/(\epsilon_0 + 1)^2] \\ & \times \{[1 + (\alpha^2 + \beta^2)/\sqrt{\epsilon_0\alpha\beta}]^2/(2\sqrt{\epsilon_0\alpha\beta} + \alpha^2 + \beta^2)\} \\ & \times (1/z^2) + \dots] - eFz. \end{aligned} \quad (19)$$

For the remaining models I and II the formulae for quantum corrections to  $B(z)$  are long and complicated and so we give the values only. Generally, these corrections form an expansion in inverse powers of  $z$ :  $b/z^2 + c/z^3 + \dots$ . When  $z$  is given in atomic units and the potential energy  $B(z)$  in electronvolts, then the coefficients  $b$  and  $c$  are as follows:



**Figure 4.** The transmission coefficient as a function of the energy  $W$  of the tunnelling electron for silicon when  $F = 5 \times 10^7 \text{ V cm}^{-1}$ : curve A, dispersionless model; curve B, model I;  $\cdots$ , specular electron reflection model.



**Figure 5.** The transmission coefficient as a function of the energy  $W$  of the tunnelling electron for GaAs when  $F = 4.4 \times 10^7 \text{ V cm}^{-1}$ : curve A, dispersionless model; curve B model I;  $\cdots$ , specular electron reflection model.

for silicon, 1.8607, 3.4352 and 1.5817, 3.9320 for models I and II, respectively. For GaAs, one obtains 1.7935 and 3.4205 for model I.

#### 4. Transmission through the surface barrier

We calculate the transmission coefficient  $D(F, W)$  for the surface barrier according to the methods in [17, 18] (see also [19]).  $W$  is here the so-called  $z$ -directed energy (i.e. the part of the energy for motion normal to the surface) of the tunnelling electron:

$$D(F, W) = \left[ 1 + \exp\left(-i \frac{\sqrt{8m}}{\hbar} \int_{z_1}^{z_2} \sqrt{W - B(z)} dz\right) \right]^{-1}. \quad (20)$$

Here  $z_1$  and  $z_2$  are the points at which the integrand has zeros.

When  $W$  is above the peak of the barrier, we suggest a better approximation than  $D(F, W) = 1$  used in [7]. In this region ( $0.5 \leq D \leq 1$ ), we approximate the shape of the barrier with (18) and we adopt the analytical formula in [19] to evaluate  $D(F, W)$ .

Finally, for  $W \geq B_{\max}$ , we put

$$D(F, W) = \left[ 1 + \exp\left\{\frac{16}{3}(f/e^2)^{3/4}(m^2 e^5/F\hbar^4)^{1/4}[v(y)/y^{3/2}]\right\} \right]^{-1} \quad (21)$$

when  $W \leq W_1 = -\sqrt{2feF} + eFf/|B(0)|$ , and  $D(F, W) = 1$  when  $W > W_1$ . Here  $y = \sqrt{4feF/(W - eFf/|B(0)|)}$  and  $v(y)$  is the function defined in [19].



The results for  $D(F, W)$  are presented in figures 4 and 5. Curves A correspond to the dispersionless approximation, and curves B illustrate the results obtained within the framework of model I. The dotted curves represent the calculations according to the specular electron reflection model. Model II leads to similar results to those of model I. One can see that the models of surface screening which we have discussed lead to results which differ considerably from those predicted by the dispersionless theory.

## 5. Conclusions

We studied the effect of the spatial dispersion of the semiconductor dielectric function on the surface potential barrier. This study was limited to semiconductors in which valence band electrons play the major role in the screening and we did not take into account, for example, the screening due to the surface states.

We employed two models of surface screening which are more appropriate for semiconductors and dielectrics than the specular electron reflection model used in previous calculations [6, 7].

We confirm previous conclusions that the surface potential barrier is broader than predicted by the dispersionless theory. This broadening leads to considerable reduction in the emission of electrons. However, the above effects are not as strong as those obtained in the framework of the specular electron reflection model.

In conclusion, we would like to comment on the behaviour of the transmission coefficient  $D$  as a function of the energy  $W$  as displayed in figures 4 and 5. This problem has not yet been discussed. The graphs of  $D$  against  $W$  (logarithmic scale) can be represented by almost straight and parallel lines in a wide energy range  $W$ , say, characteristic of the field emission from valence or conduction bands. From this, it follows that the functions  $D(W)$  obtained within various surface-screening models (including the dispersionless theory) differ only in the proportionality factors which are almost independent of  $W$ . This means that the total energy distribution curves of field-emitted electrons  $p_T(E) \propto \int D(E - E_\perp) dE_\perp$  [5] calculated with the help of the methods discussed have the same relative shapes. For example, for field emission from the valence band in GaAs [3] (see also figure 5 in the present paper) the shape of the total energy distribution curve (i.e. the curve normalised to unit peak value) will not be affected by the changes in surface screening due to dispersion of the bulk dielectric function. This conclusion remains true for different values of the electric field  $F$  applied in the field emission experiments.

For a given energy  $W$  the variation in  $F$  does not change very much the ratio of the transmission coefficients first obtained within dispersionless theory and second calculated within the framework of one of the models discussed (see figure 2 in [6] for the specular electron reflection model). This explains the result of the calculations done in [7] with the help of the specular model. Compared with the dispersionless theory the magnitude of the field-emitted current was reduced but the character of the Fowler-Nordheim law was unchanged.

We believe that the results of our considerations are of practical value to later work on an improved theory of field emission from semiconductors. The present theory is not as satisfactory as it is for metals and it must be further developed.

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