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Screened potential of a charged step defect on a semiconductor surface

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Abstract
Following Gibbs' approach, a general electrostatic model of heterogeneous systems with non-homogeneous interfaces is proposed. The intrinsic surface polarization is taken into account through the introduction of a surface dielectric constant and the electrostatic boundary conditions are generalized as two-dimensional Poisson equations. This model is applied to analyse the electrostatic potential of a charged step defect on a semiconductor surface. The step line charge density, the surface charge density, and the surface dielectric permittivity are determined from the experimental data for the InP (110) surface.

1. Introduction

Many years ago Gibbs [1] proposed a model of heterogeneous systems. In this model, the nanoscopic transition zones between the bulk phases are replaced by fictitious surfaces. The real continuous behaviour of some bulk quantity is replaced by an idealized quantity which has a step-like behaviour across the phase boundary. The difference between the real and the idealized quantity is ascribed to the surface as a surface (excess) quantity. Originally, Gibbs [1] introduced the concept of excess quantities to restore the real amounts of matter, energy, charge, etc in the idealized system.

In [2, 3] the electrostatics of heterogeneous media have been studied. The intrinsic polarizability of the interface has been accounted for by introducing a surface dielectric constant. In this approach, the traditional boundary condition for the jump of the electric displacement field across the boundary has been generalized into a surface analogue of the bulk Maxwell equation for the surface electric displacement field. In [2] the nucleation of Langmuir monolayers at the air–water interface has been considered. The theory successfully described the suppression of the nucleation process with an increase in the water electrolyte concentration as a polarization effect analogous to the Thomson theory for three-dimensional (3D) phase transition [4].

In a previous paper [3], we calculated the electrostatic potential of a point charge on the interface between two bulk phases. The result has been compared with the experimental data

for the potential of charged defects on a semiconductor surface [5] and a good theoretical fit of the experimental data has been obtained. The fitting value of the surface dielectric constant has been found to be in good agreement with its theoretical estimation in the framework of the Gibbs approach.

In this paper we apply this approach to compute the electrostatic potential of a charged line on the boundary between two bulk phases. This problem is used as a model for a charged step on the InP(110) surface [6].

The paper is organized as follows. In section 2 we derive the complete system of equations describing the electrostatics of complex heterogeneous media with a new substantial element, namely the introduction of a surface dielectric constant, and we compute the electrostatic potential of a charged line on a phase boundary. In section 3 the field of a charged step on a semiconductor surface is obtained. The results of this calculation are used to interpret the experimental data [6].

2. Electrostatic potential of a charged line on a phase boundary

In [3], we considered an approach to the macroscopic electrostatics of a heterogeneous system consisting of two bulk phases divided by a phase boundary. It starts with the definition of the charge density and the electric displacement field [3, 7]:

$$\rho(z) = \rho_+(z)\theta(z) + \rho_-(z)\theta(-z) + \rho_s\delta(z) \quad (1)$$

$$D = D_+\theta(z) + D_-\theta(-z) + D_s\delta(z). \quad (2)$$

Here, we assume that the phase boundary surface is a plane situated at $z = 0$. Also, $\theta(z)$ is the Heaviside step-function and $\delta(z)$ is the Dirac function. The charge density and the electric displacement field in the bulk phases (situated at $z > 0$ and $z < 0$) are denoted by $\rho_\pm$ and $D_\pm$, respectively. Following Gibbs [1], the surface charge density ρ_s is defined as an excess quantity

$$\rho_s = \int_{-\infty}^{\infty} [\rho_{\mathrm{real}}(z) - \rho_+(z)\theta(z) - \rho_-(z)\theta(-z)]\,\mathrm{d}z \quad (3)$$

where $\rho_{\mathrm{real}}(z)$ is the real charge distribution in the heterogeneous system. Generally, $\rho_{\mathrm{real}}(z)$ is not known and the real continuous behaviour of the charge density is replaced by an idealized quantity which has a step-like behaviour across the phase boundary. The surface charge density is introduced in such a way that it restores the real amount of charge in the system which is not completely accounted for by the idealized charge distribution. The surface electric displacement field D_s is defined analogously to ρ_s. Finally, using $D = \varepsilon_0\varepsilon E$, where E is the electric field and ε_0 is the permittivity of vacuum, we define the dielectric constant ε in the system as

$$\varepsilon(z) = \varepsilon_+\theta(z) + \varepsilon_-\theta(-z) + \varepsilon_s\delta(z). \quad (4)$$

Here, ε_s is the surface dielectric constant and $\varepsilon_\pm$ are the dielectric constants for the two bulk phases.

Assuming that the Maxwell equations are valid for the above-defined fields, the equations for the electrostatic potential and the corresponding boundary conditions are obtained in the form

$$\varepsilon_-\Delta\varphi_- = -\frac{\rho_-}{\varepsilon_0}, \quad (5)$$

$$\varepsilon_+\Delta\varphi_+ = -\frac{\rho_+}{\varepsilon_0}, \quad (6)$$

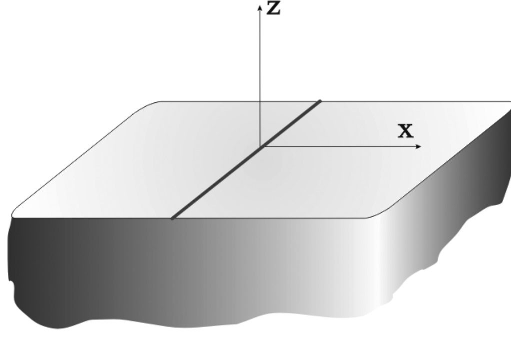

Figure 1. Schematic of the system under consideration in the text.

$$\varepsilon_+ \frac{\partial \varphi_+}{\partial z}\bigg|_{z=0} - \varepsilon_- \frac{\partial \varphi_-}{\partial z}\bigg|_{z=0} + \varepsilon_s \Delta_s \varphi_s = -\frac{\rho_s}{\varepsilon_0}, \tag{7}$$

$$\varphi_-|_{z=0} = \varphi_+|_{z=0} = \varphi_s. \tag{8}$$

Here, the indexes 's', '+' and '−' are used to denote the electrostatic potential at $z = 0$, $z > 0$, and $z < 0$, respectively. Equation (7), the classical boundary condition for the jump of the normal component of the electrostatic displacement field at the surface, is generalized as a Poisson equation on the surface, as it is modified by the term $\varepsilon_s \Delta_s \varphi$, which takes into account the surface polarization. The laplacian Δ_s is taken only with respect to the surface coordinates.

Let us point out that the form of the equations strongly depends on the geometry of the various phase boundaries in the system under consideration. Therefore, one has to derive the particular set of boundary conditions for every given problem.

One can estimate the value of ε_s to be

$$\varepsilon_s = \int_{-\infty}^{\infty} [\varepsilon_{\text{real}}(z) - \varepsilon_{\text{ideal}}(z)]\, \mathrm{d}z \sim \varepsilon_{\text{bulk}}\delta, \tag{9}$$

where $\varepsilon_{\text{bulk}} = (\varepsilon_+ + \varepsilon_-)/2$ is the average bulk dielectric constant and δ is the width of the transition zone, which is of the order of the average interparticle distance.

Now we apply this theory to the problem of computing the electrostatic potential of a uniformly charged line on the interface between two bulk phases (figure 1). Let us take the y axis to coincide with the charged line. We denote the electrostatic potentials and the surface dielectric constants for $x > 0\,(x < 0)$ by $\varphi_{s+}(\varphi_{s-})$ and $\varepsilon_{s+}(\varepsilon_{s-})$, respectively. The surface charge density is given by

$$\rho_s(x) = \rho_{s+}(x)\theta(x) + \rho_{s-}(x)\theta(-x) + \rho_l\delta(x) \tag{10}$$

where ρ_l = constant is the line charge density introduced as an excess of the surface charge density. The equation (7) becomes

$$\varepsilon_+ \frac{\partial \varphi_+}{\partial z}\bigg|_{z=0} - \varepsilon_- \frac{\partial \varphi_-}{\partial z}\bigg|_{z=0} + \varepsilon_{s\pm} \frac{\mathrm{d}^2 \varphi_\pm}{\mathrm{d}x^2} = -\frac{\rho_{s\pm}}{\varepsilon_0}. \tag{11}$$

The boundary condition for the jump of the normal to the line component of the surface dielectric field is given by

$$\varepsilon_{s+} \frac{\mathrm{d}\varphi_{s+}}{\mathrm{d}x}\bigg|_{x=0} - \varepsilon_{s-} \frac{\mathrm{d}\varphi_{s-}}{\mathrm{d}x}\bigg|_{x=0} = -\frac{\rho_l}{\varepsilon_0}. \tag{12}$$

Finally, there is the boundary condition

$$\varphi_{s-}|_{x=0} = \varphi_{s+}|_{x=0}\,. \tag{13}$$

3. Charged line on the semiconductor surface

We apply the theory formulated in equations (5), (6), (8) and (11)–(13) to compute the potential of a charged step on III–V compound semiconductor surfaces [6]. The authors of [6] have observed, by scanning-tunnelling microscopy, the appearance of a vacancy-denuded zone around steps on InP(110). They attributed this behaviour to the charge repulsion between the charged step and the charged P vacancies. The step potential has been roughly estimated by summing the potentials of aligned point charges. The potential of the point charge on the semiconductor surface has been approximated by a screened Coulomb potential [5, 6]. The distribution of the charged vacancies around the step has been calculated from the expression

$$c(x) = c_\infty \exp\left(-\frac{e\varphi_s(x)}{kT}\right) \tag{14}$$

where c_∞ is the vacancy concentration on step-free surfaces, e is the elementary charge, k is the Boltzmann constant, and T is the temperature. The authors of [6] have fitted the experimentally inferred width of the vacancy-denuded zone and the charge of the step has been estimated to be in the range $+1e$ to $- + 3e$ per lattice spacing.

The main assumptions in our approach are as follows: (i) the approach is applicable to distances that exceed the atomic scale, i.e. only the macroscopic parameters of the semiconductor are needed; (ii) the charged step is modelled by a uniformly charged line on the semiconductor surface; (iii) the defects are treated as point charges with charge $+e$ [5]; (iv) an unspecified local relationship between the chemical potential and the surface charge density is assumed; (v) both bulk and surface charges are taken into account in the calculation of the screening of the additional charge.

In the semiconductor ($z < 0$), the equilibrium density of free carriers with effective mass m is given by the well-known expression [8, 9]

$$c(\mu) = 2N\Phi_{1/2}(\mu^*) \tag{15}$$

where N is the effective density of states

$$N = 2\left(\frac{2\pi mkT}{(2\pi\hbar)^2}\right)^{1/2}. \tag{16}$$

$\Phi_{1/2}(\mu)$ is the Fermi–Dirac integral

$$\Phi_{1/2}(\mu^*) = \frac{2}{\pi}\int_0^\infty \frac{\sqrt{u}}{1+\exp(u-\mu^*)}\mathrm{d}u \tag{17}$$

with $\mu^* = \mu/kT$. The charge density ρ_- is

$$\rho_- = e[c(\mu+\varphi_-) - c(\mu)]. \tag{18}$$

We assume that the linear approximation holds and develop the expression for ρ_- in powers of φ_-, retaining only the linear term

$$\rho_- = -\varepsilon_0\varepsilon_-\kappa_-^2\varphi_- \tag{19}$$

where the inverse bulk screening length κ_- is defined by the expression

$$\kappa_-^2 = \frac{e^2N}{\varepsilon_0\varepsilon_- kT}\Phi'_{1/2}(\mu^*). \tag{20}$$

In the bulk of the semiconductor, the free carriers are holes with concentration p. The holes form a non-degenerate gas and, according to [8, 9],

$$\kappa_-^2 = \frac{e^2p}{\varepsilon_0\varepsilon_- kT}. \tag{21}$$

The surface carrier concentration Γ is introduced as a Gibbs excess, analogously to equation (1). Consequently, the surface charge density is defined as

$$\rho_s = e[\Gamma(\varphi_s + \varphi_{s,\infty}) - \Gamma(\varphi_{s,\infty})] \tag{22}$$

where $\varphi_{s,\infty}$ is the so-called surface potential [8]. In linear approximation, we obtain

$$\rho_s = -\varepsilon_0\varepsilon_s\kappa_s^2\varphi_s \tag{23}$$

and κ_s^{-1} is the surface screening length. The expression for κ_s is given by

$$\kappa_s^2 = \frac{e^2\alpha c_P}{\varepsilon_0\varepsilon_s kT} \tag{24}$$

where c_P is the surface concentration of the phosphorus vacancies and α is a factor between 0 and 1 which measures the number of free surface carriers per phosphorus vacancy.

Next, we solve the system equations (5), (6), (8) and (11)–(13) with the corresponding expressions for the charge densities obtained above. The solution for the potentials of the bulk phases and of the charged line on the semiconductor surface ($z_0 = 0$) is cast into the form

$$\varphi_+(x, z) = \int_0^\infty \hat{\psi}_s e^{-\xi z}\cos(\xi x)\,d\xi, \tag{25}$$

$$\varphi_-(x, z) = \int_0^\infty \hat{\psi}_s e^{\sqrt{\xi^2+\kappa_-^2}z}\cos(\xi x)\,d\xi, \tag{26}$$

$$\varphi_s(x) = 2\int_0^\infty \hat{\psi}_s\cos(\xi x)\,d\xi, \tag{27}$$

where

$$\hat{\psi}_s = \frac{\rho_l}{2\pi\varepsilon_0}\frac{1}{\xi + \varepsilon_-\sqrt{\xi^2+\kappa_-^2} + \varepsilon_s\left(\xi^2+\kappa_s^2\right)}. \tag{28}$$

The numerical computations were performed with the following set of parameters. The bulk hole concentration is 1.3–2.1 $\times$ 10^{18} m^{-3} [5, 10]. The surface density of the phosphorus vacancies is $c_P = 1.87 \times 10^{16}$ m^{-2} [6]. For the bulk screening length $R_- = 1/\kappa_-$ (at 297 K and with $\varepsilon_- = 12.5$) we used the value 3.2 nm. The surface dielectric constant ε_s, the parameter α, and the line charge density ρ_l were used as fitting parameters.

The results of our calculation are shown on figure 2. The points are obtained using equation (14) from the experimental results for the vacancy concentration $c(x)$ taken from figure 3 in [6]. The best fit gives the values $\varepsilon_s = 7$ nm, $\alpha = 0.33$, and $\rho_l = +0.172e$ per lattice spacing; the standard deviation is 0.009 952. In fact, the fitting procedure results in a rather shallow minimum—the standard deviation is less than 0.01 for ε_s = 5–12 nm, α = 0.3–0.4, and $\rho_l = +0.15$ to $+0.25e$ per lattice spacing. If we use the estimation (9) for the ε_s, the value obtained for the width of the transition zone δ is of the order of one to two lattice constants (for InP—0.6 nm) which is a reasonable result. We must point out that the authors of [6] have estimated ρ_l to be in the region of $+1e$ to $+3e$ per lattice spacing, that is, our approach predicts a drastically lower line charge density of the charged step.

An important feature of our approach is the behaviour of the surface potential as x tends to 0. From equations (27) and (28) one sees that as $x \to 0$ the surface potential goes to a constant and is not diverging. The surface screening charge is not felt very close to the charged line and the potential tends to the *two-dimensional* potential of a charged line, which is a constant. One should compare this result with the well-known behaviour of the potential of a uniformly charged plane in *three dimensions*, which is also a constant. In our previous work [3] we have shown that the surface electrostatic potential of a point charge on the interface between

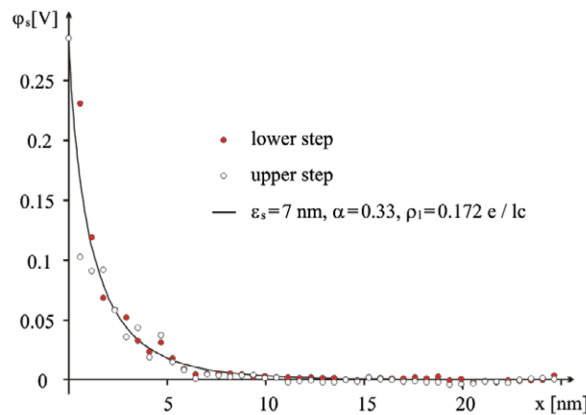

Figure 2. Surface potential φ_s of a charged step on the surface computed for $\varepsilon_s = 7$ nm, $\alpha = 0.33$, and $\rho_l = +0.172e$ per lattice spacing. The points are obtained using equation (14) from the experimental results for the vacancy concentration $c(x)$ taken from figure 3 in [6].

(This figure is in colour only in the electronic version)

two bulk phases diverges as $\ln r$ and not as $1/r$ as $r \rightarrow 0$ (r is the distance to the point charge on the surface). This behaviour is not surprising—φ_s is obtained as a solution of a two-dimensional Poisson equation and it is well known that the two-dimensional Coulomb potential is logarithmic.

In conclusion, we have applied the theory for the electrostatics of heterogeneous systems with non-homogeneous phase boundaries based on the Gibbs approach to compute the potential of a charged line on the phase boundary. The surface dielectric constant is introduced in order to take into account the intrinsic surface polarizability of the phase boundary. The potential of a charged step on a semiconductor surface is computed within this framework. The surface dielectric constant is determined by fitting to the existing experimental results for the potential of charged steps on a semiconductor surface. Its value is found to be of the expected order of magnitude. The theory predicts a much smaller line charge density than the one obtained in the traditional approach to the electrostatics of the system.

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