

SPECIALITY OF POISSON EQUATION SOLUTION AND CALCULATION OF BARRIER PROFILE ON THE INTERFACE TO NON-CRYSTALLINE SEMICONDUCTOR

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The Poisson equation is solved for obtaining space charge distribution and electrostatic potential profile depending upon location in depletion layer on the interface between metal and non-crystalline semiconductor. The calculation is performed taking into account the peculiarities of the electronic structure the non-crystalline semiconductor. The difference between the non-crystalline barrier and crystal barrier evidenced and discussed.

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1. Introduction

Non-crystalline semiconductors are widely used in different fields of electronics. However, until now there is not a generally accepted theory of metal – non-crystalline semiconductors contact phenomena. At present mathematical tools for crystalline semiconductors with empirical correction factor are used for calculations of device and electron processes. It does not account for the peculiar electronic properties of disordered materials.

The difference between the non-crystalline semiconductor and the crystalline one is the presence of deep localized states (DLS) in the mobility gap. It is a consequence of translation symmetry violation in crystal matrix. It determines difference between electro-physical properties of disordered semiconductors and crystals [1].

Non-crystalline semiconductors are similar to insulator if the crystal theory is used for the description of contact phenomena. However, it is in conflict with the experimental data [2,3]. This inconsistency between theoretical and experimental results is explained by the peculiarity of electronic properties of disordered materials.

Usually the internal field profile is obtained from experiments in the form of an exponential curve $F_1(x) = F_0 \exp(-\gamma x)$, where γ is determined from the approximation of experimental results. The coefficient γ changes from one sample to another. It does not contain information about material parameters, and, therefore, does not allow for the analysis of the correlation between processing parameters and the characteristics of the semiconductor.

A different way of getting the space charge distribution, electrostatic potential and internal field profile is the resolving of the Poisson equation. As a rule, some assumptions and calculus of approximations are used. In contrast to early works we consider that DLS are photo- and electrical active. DLS are distributed exponentially in the mobility gap (assumptions 2 and 6). We also count the coordinate from internal border of depletion layer to interface (boundary condition 1*).

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The aim of this work is to get the analytical expression for electrostatic potential distribution, which takes into account the semiconductor characteristics (distribution of DLS). It permits to solve both a direct problem – obtaining the potential profile from the known parameters of the semiconductor, and the reverse one – finding the characteristics of material from experimental measured data.

Solving is carried out for amorphous hydrogenated silicon (a-Si:H) as typical representative of non-crystalline semiconductors.

2. Assumptions and boundary conditions

The following assumptions are used for calculation.

1. In view of mobility edge uncertainty, the energy in band model is counted from vacuum level $E_0 = 0$ (Fig. 1).

2. DLS near Fermi level are photo- and electrical active. It may be either as n-type dopant (in the condition that energy be situated between Fermi energy and valence band ceiling) or as p-type dopant (in case that energy is situated between the bottom of the conduction band and Fermi energy) [4].

3. The influence of surface states in calculations is not taken into account.

4. Conductivity is monopolar n-type as hole mobility is two orders less than electron one [5].

5. The work function from metal is higher than that from a-Si:H, i.e. there is a depletion layer on the interface.

6. The density of DLS is so high that Fermi quasilevel couldn't change its position considerably. It permits to use exponential approximation of DLS distribution in the mobility gap:

$$g(E) = g_{F0} \exp(\beta(E - E_{F0})), \quad (1)$$

where g_{F0} is the density of DLS near Fermi level, β is the slope of approximating line in semilogarithmical coordinates; $[\beta] = eV^{-1}$ (Fig. 1) [4].

7. The model of complete depletion is used.

The following boundary conditions are used for calculation.

1*. Coordinate in depletion layer is counted from Me/a-Si:H interface deep into semiconductor. In auxiliary calculations [6] it is counted from internal border of space charge region (SCR).

2*. The Fermi function for electrons has the form [7]:

$$f_n(E, x) = \left[1 + \exp\left(\frac{E_{F0} - E + e\phi(x)}{kT}\right) \right]^{-1}, \quad (2)$$

where E_{F0} – Fermi energy in bulk of a-Si:H, $e\phi(x)$ – band bending depends upon location in depletion layer, kT – thermal energy, eV.

3*. The values of electrostatic potential ϕ and internal electric field F_i on internal border of SCR are zero in the absence of the external voltage; on interface Me/a-Si:H they are, $-\phi_0$ and F_0 , respectively.

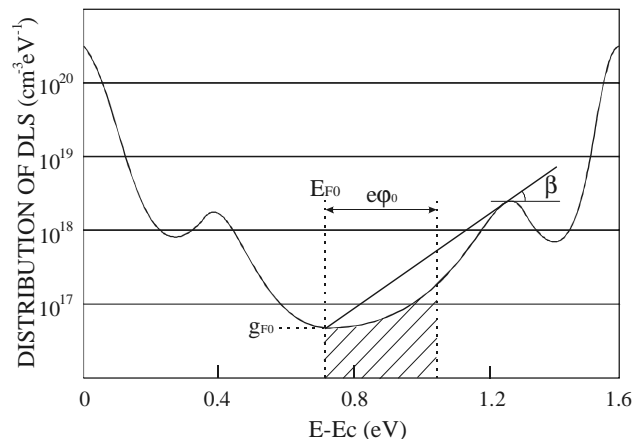


Fig. 1. Distribution of DLS in mobility gap of a-Si:H [4].

3. Calculation details

The Poisson equation establishes the correlation between density of space charge (DSC) $\rho(x)$ and electrostatic potential profile in SCR:

$$\frac{d^2\varphi(x)}{dx^2} = \frac{\rho(x)}{\epsilon\epsilon_0}. \quad (3)$$

DSC depends upon location in depletion layer (or electrostatic potential). It is defined by difference between mobile charges (electrons) and fixed ones (DLS):

$$\rho(x) = eN(x) - en(x) \quad (4)$$

or

$$\rho(\varphi) = eN(\varphi) - en(\varphi), \quad (5)$$

where e is electron charge, $N(x)$ or $N(\varphi)$ – distribution of ionized n-type dopant states concentration, $n(x)$ or $n(\varphi)$ - electrons ones.

The concentration of ionized states is evaluated within an exponential approximation of DLS distribution:

$$N(E) = \int_{E_{F0}}^E g(E)dE = \int_{E_{F0}}^E g_{F0} \exp(\beta(E - E_{F0}))dE. \quad (6)$$

Integration by energy in (6) is converted into electrostatic potential integration:

$$dE = E'(\varphi)d\varphi = (E_{F0} + e\varphi)'d\varphi = ed\varphi. \quad (7)$$

Then formula (6), considering (7) becomes:

$$N(\varphi) = \int_0^\varphi g_{F0} \exp(\beta e\varphi)ed\varphi = \frac{g_{F0}e}{\beta e} \exp(\beta e\varphi) \Big|_0^\varphi = \frac{g_{F0}}{\beta} [\exp(\beta e\varphi) - 1]. \quad (8)$$

The concentration of free electrons in SCR is:

$$n(\varphi) = n_0 \exp\left(-\frac{e\varphi}{kT}\right), \quad (9)$$

where n_0 is the concentration of free electrons in bulk of a-Si:H. Then, the expression (5) is written in the following way:

$$\rho(\varphi) = e \left[\frac{g_{F0}}{\beta} (\exp(\beta e\varphi) - 1) - n_0 \exp\left(-\frac{e\varphi}{kT}\right) \right]. \quad (10)$$

This is the basic expression for solving the Poisson equation. It is worked out in two stages as a function of band bending.

A. The case of small band bending

Let us take up SCR near inner boundary of the depletion layer. We suppose that band bending is negligible here, i.e. we postulate $e\varphi \sim kT$. The exponential is decomposed into Taylor series, and only two first two terms are retained [8]:

$$\exp(\beta e\varphi) = 1 + \beta e\varphi; \quad (11)$$

$$\exp\left(-\frac{e\varphi}{kT}\right) = 1 - \frac{e\varphi}{kT}. \quad (12)$$

In this case Poisson equation (3) could be written as:

$$\frac{d^2\varphi}{dx^2} = \frac{e^2 g_{F0}}{\epsilon\epsilon_0} \varphi - \frac{en_0}{\epsilon\epsilon_0}. \quad (13)$$

The solution of this differential equation with boundary conditions consideration leads to the result:

$$\varphi(x) = \frac{n_0}{eg_{F0}} \left[1 - \operatorname{ch}\left(\frac{W-x}{L_D}\right) \right], \quad (14)$$

where W is the width of the quasi-neutral region, L_D is Debye length near inner boundary of SCR:

$$W = \sqrt{\frac{\epsilon\epsilon_0}{g_{F0}e^2}} \operatorname{arcch}\left(1 + \frac{kTg_{F0}e}{n_0}\right), \quad (15)$$

$$L_D = \sqrt{\frac{\epsilon\epsilon_0}{e^2g_{F0}}}. \quad (16)$$

B. The case of strong band bending

Let us make an analysis of SCR in strong band bending condition, i.e. let us assume $e\varphi \gg kT$. In this case $\exp(\beta e\varphi) \gg 1$; $\exp(-e\varphi/kT) \rightarrow 0$. Then the Poisson equation (3) could be re-written as:

$$\frac{d^2\varphi}{dx^2} = \frac{eg_{F0}}{\beta\epsilon\epsilon_0} \exp(\beta e\varphi). \quad (17)$$

This differential equation is solved by separating the variables taking into account the boundary conditions. The electrostatic potential depends on distance in SCR, and, therefore:

$$\varphi(x) = -\frac{2}{\beta e} \ln \left| \cos\left(\frac{W-x}{\sqrt{2}L_D}\right) \right|, \quad (18)$$

where W is defined from (19), L_D – from (16):

$$W = \sqrt{\frac{2\epsilon\epsilon_0}{e^2g_{F0}}} \arccos \left[\exp\left(-\frac{\beta e\varphi_0}{2}\right) \right]. \quad (19)$$

4. Results and discussion

The analysis of (14) shows that SCR width in typical undoped a-Si:H films extend more than 2 – 3 μm (Fig. 2). It overcomes the films thickness, commonly used. Therefore, in case of contact phenomena in non-crystalline semiconductors we have to say about quasi-neutral region instead of neutral one. The electrostatic potential profile depends on the density of DLS near Fermi level g_{F0} and on the concentration of free electrons, n_0 .

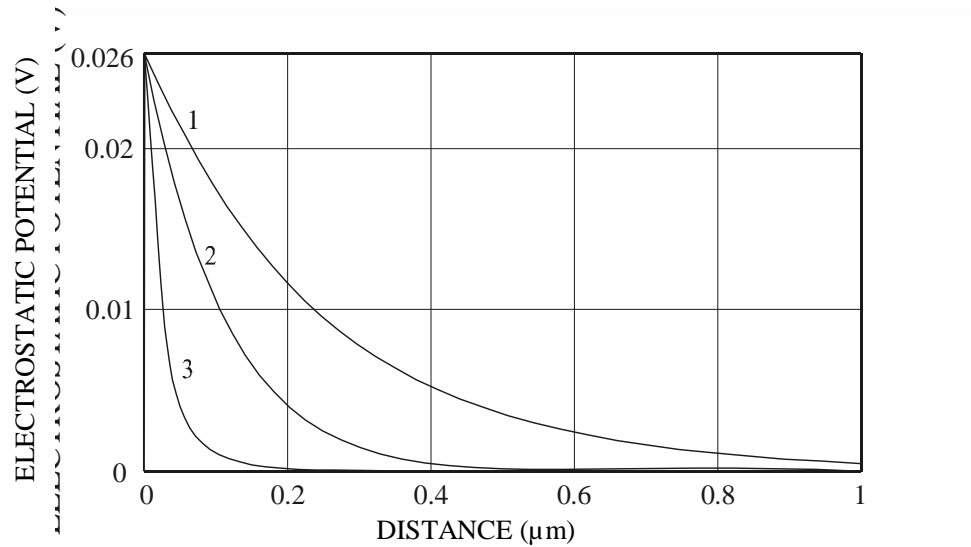


Fig. 2. Distribution of electrostatic potential in quasi-neutral region. Approximated parameters: 1 - $g_{F0} = 10^{16} \text{ cm}^{-3}\text{eV}^{-1}$, $\beta = 5.76 \text{ eV}^{-1}$; 2 - $g_{F0} = 10^{17} \text{ cm}^{-3}\text{eV}^{-1}$, $\beta = 5.18 \text{ eV}^{-1}$; 3 - $g_{F0} = 10^{18} \text{ cm}^{-3}\text{eV}^{-1}$, $\beta = 4.32 \text{ eV}^{-1}$ [9].

Analysis of (18) shows that electrostatic potential profile is more “abrupt” than early data (Fig. 3) [2, 3]. It is determined by value of g_{F0} and approximate parameter β .

The results differ substantially from the calculations for crystal semiconductors [8] and from the data on a-Si:H [2,3]. They are characterized by high accuracy. This follows from the following reasons. Firstly, the approximate curve is based on Fermi energy instead band tail as in [7]. Secondly, the terms in (14 – 16) and (18, 19) are defined by the electronic structure of disordered material. It determines the electro-physical parameters of the semiconductor. Thirdly, the mathematical simulation curves are in good agreement with the experimental data [6,10], and the theory of barrier formation between metal and non-crystalline semiconductor [4].

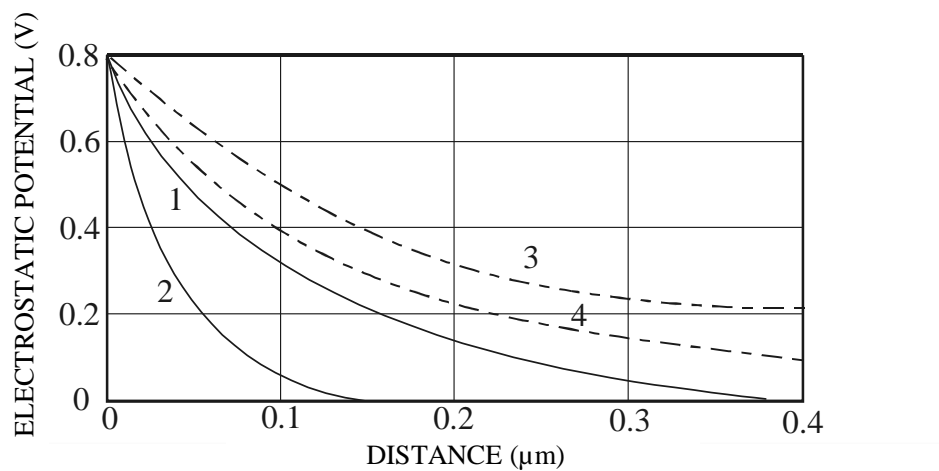


Fig. 3. The distribution of the electrostatic potential in SCR. Approximated parameters for curves 1 and 2 are like those in Fig. 2. Curves 3 and 4 are calculated by [3] for the same approximated parameters.

5. Conclusions

The internal electrical field profile in non-crystalline semiconductors differs from the linear one specific to crystals with uniform distribution of shallow dopant. This is explained by the participation of DLS in the process of formation of contact barrier between metal and semiconductor.

The potential profile differs from commonly accepted exponential curve. It is interconnected with the imperfection of the experimental methods. At the first examination of transient photocurrent the influence of contacts is not taken account [2]. The modified time of flight technique neglects charge loss during drift process [3]. The consideration of these weaknesses allows for getting more precise results [6].

However, divergences between theoretical and experimental results still are present. These are due to several reasons. Firstly, everything methods are physically limited [10]. Secondly, we use the assumptions of negligible and strong band bending. If the value of potential is between 0.26 V and 0.026 V the calculation becomes inaccurate. But this does not reduce the importance of this work. The potential profile near interface is more unable for the analysis of contact characteristics.

The field is concentrated near the interface between metal and non-crystalline semiconductor. In connection with such field distribution the effective height of barrier may be lower than that calculated. As a result of contact fields overlapping in thin films, the displacement of Fermi energy at the borders of the mobility gap can be observed [9].

The findings have to be considered in subsequent calculations of current-voltage and capacity-voltage diagrams of contact metal – disordered semiconductor. Also, it must be taken into account the simulation of electronic devices like thin-film transistors, solar cells, optoelectronic sensors, etc.

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