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Theoretical consideration of charge transport through the nanoindentor/GaAs junction

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Abstract. The process of indentation of GaAs single crystal by the conductive nanoindentor has been analyzed theoretically. The diode formed by the nanoindentor tip and small area of GaAs platelet has been considered. The evolution of local mechanical stress during the nanoindentation cycle and an appropriate transformation of electric potential difference inherent in tip/GaAs junction are described qualitatively. The non-monotone variation of the mechanical stress and electric potential difference during the indentation cycle has been disclosed. The current spike experimentally registered in the moment of abrupt penetration of indentor tip into the GaAs platelet has been attributed to the non-monotone variation of potential difference during the indentation cycle.

Keywords: nanoindentor, GaAs single crystal, charge transport.

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1. Introduction

A nanoindentation technique is widely used for the local mechanical stressing of solid and determination of its microhardness [1]. The nanoindentor is a small probe with the sharp hard tip. During the nanoindentation cycle the tip is pressed into the solid-state specimen by an increasing mechanical force (see Fig. 1). At the first stage of the cycle, the tip moves down smoothly and elastically deforms the specimen of solid. When the pressing force reaches certain critical value, the tip abruptly penetrates into the specimen. This effect is called a "pop-in event".

The manufacturing of different elements in nanoelectronics is accompanied by the appearance of mechanical stresses inside these elements. These technological stresses vary in nanometer scale. The sharply variable/local stresses also exist in the systems with quantum dots, which attract common attention now. The experimental study of the influence of these local stresses on physical properties of semiconductor structures is a topical but very complicate problem. The possible approach to the problem solution is the modeling of technological local stresses by the stress, which is induced by a nanoindentor probe: a comprehensive study of physical effects that accompany nanoindentation cycle can help to foresee the consequences of technological stressing.

In the experimental work [2], a 1 μm epitaxial GaAs layer with Si dopant concentration $N_D = 10^{16}$ cm^{-3} has been grown by the molecular beam epitaxy on 350 μm thick GaAs (100) substrate. A conductive nanoindentation system has been used to study an electric response of doped GaAs epilayer on a local mechanical stressing. The experimental technique used in Ref. [2] involves the standard nanoindentation hardware, conductive indentor probe, electric voltage source, and nanoammeter. This technique enables the study of correlation between the force acting on GaAs specimen, displacement of nanoindentor, and electrical current flow through the nanoindentor tip/GaAs junction. During the nanoindentation test, the constant voltage and increasing mechanical force have been applied to the tip/GaAs contact, and the magnitude of current running through this contact has been monitored. In this way, a sharp current spike was registered just before the pop-in event [2].

In the present article, the theoretical study of diode properties of tip/GaAs junction is carried out, and the explanation of current spikes arising in the course of nanoindentation cycle is proposed.

2. Diode properties of nanoindentor tip/GaAs junction

To study the variation of diode properties of tip/GaAs junction during the nanoindentation cycle, the evolution of electron energy bands under the axial compressive stress was considered using the set of programs PWscf. The computations showed the linear increase of the energy gap between the valence and conductivity bands in Γ-point during the compression cycle:

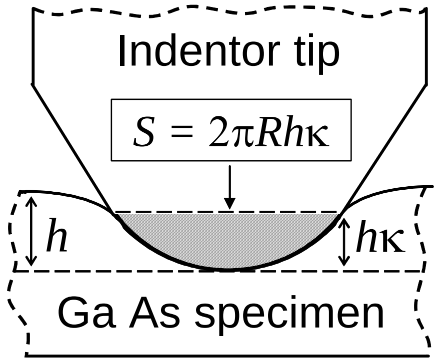

Fig. 1. Nanoindentor acting on GaAs platelet (schematically).

$$E_\Gamma(\sigma) = E_\Gamma(0) + \alpha_\Gamma \sigma \,, \qquad (1)$$

where σ is an absolute stress value, $E_\Gamma(0)$ = 1.43 eV [3], $\alpha_\Gamma \approx$ 0.045 eV/GPa is a computed value. This value is rather close to the value 0.055 eV/GPa reported in the early work [4]. In contrast to this, the energy gap in X-point decreases during the axial stressing as

$$E_X(\sigma) = E_X(0) - \alpha_X \sigma \,, \qquad (2)$$

where $E_X(0)$ = 1.9 eV [3], $\alpha_X \approx$ 0.083 eV/GPa is a computed value. As a consequence, the inequality

$$E_X(\sigma) < E_\Gamma(\sigma) \qquad (3)$$

is valid when $\sigma > 3.7$ GPa .

In the simplest approach to the problem solution the axial stress may be related to the applied force $F(h)$ by the simple formula

$$\sigma(h) = (2\pi R h \kappa)^{-1} F(h) \,, \qquad (4)$$

where $R \approx 234$ nm is the radius of indentor tip, h is the displacement of tip during the nanoindentation cycle, and κ is a dimensionless adjusted parameter introduced in view of the misfit between the shapes of indentor tip and specimen surface (see Fig. 1). Thus, the value $h\kappa$ is the depth of penetration of tip into the specimen and $S(h) = 2\pi R h \kappa(h)$ is the area of tip/GaAs contact.

Let $\kappa = \kappa_1$ before the pop-in event. Fig. 1 and elementary calculation shows that after the event

$$\kappa_2 = \frac{\kappa_1 + \Delta h / h_s}{1 + \Delta h / h_s} \;, \qquad (5)$$

where $\Delta h = h_f - h_s$, the values h_s and h_f correspond to the start and finish of the pop-in event. In the case when the area $S(h)$ of nanoindentor-semiconductor contact varies linearly in the interval $h_s < h < h_f$, the expression

$$\kappa(h) \equiv \kappa_1 + (\kappa_2 - \kappa_1)(h - h_s)/\Delta h \qquad (6)$$

is valid.

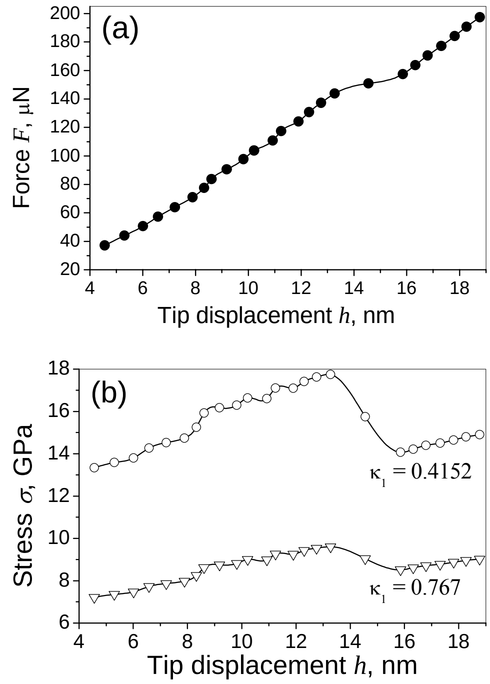

Fig. 2. Reported in Ref. [2] experimental values of the force applied to the specimen (a), and the correspondent values of the mechanical stress (b) computed from Eqs. (4)-(6).

Fig. 2a shows the monotonous dependences of the compressive force on the tip displacement measured in Ref. [2] during the nanoindentation cycle for doped specimen with $N_D = 10^{16}$ cm^{-3}. The experimental points shown in Fig. 2a and Eqs. (4)-(6) enabled the computation of the mechanical stress versus tip displacement. The graphs of stresses created by the nanoindentor tip are shown in Fig. 2b for two different values of the parameter κ. The choice of κ values shown in Fig. 2b will be explained below.

The graphs presented in Fig. 2b exhibit the non-monotonous variation of stress versus the tip displacement. The non-monotony appears because the tip/GaAs junction area $S = 2\pi R h \kappa$ arises during the nanoindentation cycle: the stress increases first because the force increases quicker then the area, but decreases when because the graph of force reaches the "plateau" (see Fig. 2a). It is seen from Fig. 2b that the pop-in event takes place at the maximal stress value. If κ = 0.767, this event is accompanied by the 15 % stress relaxation. The reduction of an unknown κ value results in the increase of stress values computed from the experimental values of the force and makes the stress relaxation more pronounced.

The indentor tip and contiguous spatial domain of the semiconductor platelet form a Schottky barrier diode. For the reverse bias voltage the current flows through the diode are

$$\begin{aligned} J_\Gamma(h) &= j_0 S(h) \exp(-|e|\varphi_\Gamma / k_B T), \\ J_X(h) &= j_0 S(h) \exp(-|e|\varphi_X / k_B T), \end{aligned} \qquad (7)$$

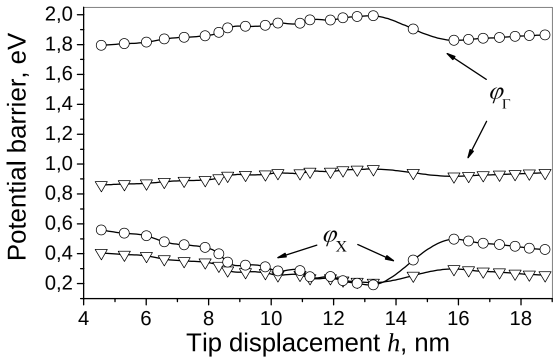

Fig. 3. Potential barriers versus tip displacement computed for the GaAs specimen using the couples of values $\kappa_1 = 0.767$, $\varphi_0 = 0.86$ eV (triangles) and $\kappa_1 = 0.4152$, $\varphi_0 = 0.2$ eV (circles).

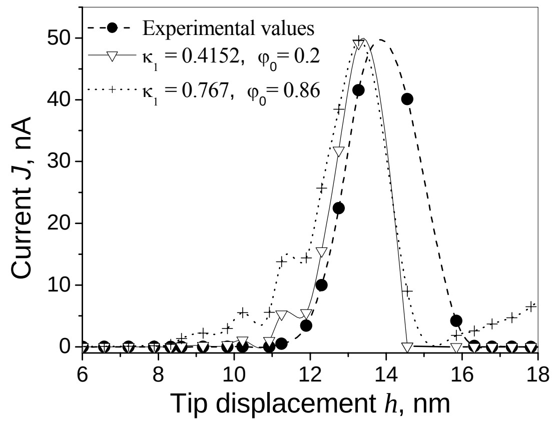

Fig. 4. Theoretical (triangles and crosses) and experimental (closed circles) values of current flow obtained for GaAs specimens with $N_D = 10^{16}$ cm^{-3}.

where the subscripts Γ and X mark the current flows created by the carriers corresponding to Γ- and X-points of the Brillouin zone, j_0 is the saturation current density, e is the electron charge, T is temperature, and k_B is the Boltzmann constant [5].

The non-monotonous dependence of stresses causes the non-monotonous variation of potential barriers inherent to the diode structure

$$\varphi_{\Gamma,X} = E_{\Gamma,X} - \varphi_0 - \Delta\varphi_{\Gamma,X}\,, \tag{8}$$

where φ_0 is a potential induced by the surface charges,

$$\Delta\varphi = (|\,e\,|\,E\,/\,4\pi\,\varepsilon_S)^{1/2} \tag{9}$$

is the potential barrier reduction caused by the Schottky effect, and the parameter E that have the dimension of electric field is introduced as

$$E = [2N_D(|\,e\,|U + |\,e\,|U_{bi} - k_B\,T\,)]^{1/2}\,\varepsilon_S^{-1/2} \tag{10}$$

where N_D is the silicon concentration, U is the bias voltage, $|\,e\,|U_{bi}$ is the built-in electric potential, $\varepsilon_S = 12\varepsilon_0$ is the dielectric constant of GaAs [5], ε_0 is the dielectric constant of vacuum.

The potential barriers φ_Γ and φ_X computed from Eq. (8) are shown in Fig. 3. The computations were carried out for $j_0 = 10^{10}$ A/m^2, $T = 300$ K, $U_{bi} = 0.591$ V [3] and the reverse bias voltage $U = 3$ V, which was maintained in the course of experiments. Two different couples of values κ_1, φ_0 were used for computations. The choice of φ_0 will be explained below. It is of importance that φ_Γ is substantially higher than φ_X in the high-pressure range, and therefore, in this range the current flow J_Γ can be disregarded.

3. Explanation of the electric current spikes observed during nanoindentation of the GaAs specimen

To explain the experimentally observed spikes of electrical current, the theoretical dependences of current flow J_X on the tip displacement were computed from the Eqs. (4)-(10). These dependences are presented in Fig. 4. The current values were computed for the discrete collection of tip displacements shown in Figs. 2, 3. The computations were carried out for maximal and minimal values of the potential ($\varphi_0 = 0.53 \pm 0.33$ eV [5]). The curves were plotted using the "spline" tool involved in standard MathSoft Apps. The amplitudes of theoretical spikes were equalized to the experimental one by the adjustment of parameter κ_1 values.

Fig. 4 illustrates a satisfactory agreement between the theoretical current values and experimental spike obtained in Ref. [2]. Therefore, the stress relaxation accompanying the pop-in event is sufficient for the substantial reduction of current flow and formation of the spike at the $J(h)$ curve. However, the additional reasons for the abrupt current reduction after the pop-in event may exist, and we can point out two of them now. First, the pop-in event may be accompanied by the substantial changes in the parameters involved in the Eqs. (1), (2), because in the case under consideration this event is caused by the jump-like transformation of the crystal lattice [6]. Second, the experimentally observed during pop-in event deflection at the $F(h)$ curve may be less pronounced than the real one due to the apparatus effects. The latter statement is supported by the computer experiments carried out in Ref. [6].

4. Discussion and summary

It may be summarized that the spikes observed in the course of measuring the current flow through the junction formed by the indentor tip and thin GaAs platelet is caused by superposition of two physical effects: i) the linear decrease of the energy gap in X-point of the Brillouin zone; ii) the non-monotonous dependence of the mechanical stress induced during the nanoindentation cycle on the tip displacement. These effects result in the non-monotonous variation of the electric potential barrier inherent to the tip/GaAs junction. As far as the barrier value is involved in the exponential describing the variation of current flow (see Eq. (7)), the current spike appears.

It should be emphasized that the current spikes are described above in the frame of simplest theoretical approach. Additional physical mechanisms of the affect of the pop-in event on the current flow may also be present; among them the reconstruction of crystal lattice accompanied by the radical change of the electron band structure should be mentioned.

The experimentally observed correlation between the appearance of the current spike and presence of epilayer doped by silicon points to the diffusive nature of current, because in this case the saturation current density is proportional to $N_D^{1/2}$.

The affect of mechanical nanostressing on the charge transport in semiconductors is an intriguing problem. The theoretical aspect of the problem may be subdivided into the "electronic" and "mechanical" parts. The electronic part includes (i) the theoretical study of the energy band structure of semiconductor both before and after the transformation of crystal lattice caused by the pop-in event; (ii) the elucidation of physical peculiarities of the current flow through the tip/specimen junction. The point (i) means that the parameters $E_{\Gamma,X}(0)$ and $\alpha_{\Gamma,X}$, which are involved in the Eqs. (1), (2), must be computed not only for the elastically deformed cubic lattice but also for the lattice that is transformed by the indentor tip. The point (ii) is topical because the charge transport through the junction with diode-like characteristic drastically depends on the structural, physical and chemical features of the junction and its material.

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