UDC 621.396.677

ANALYSIS OF TEMPERATURE DEPENDENT PARAMETERS OF GRAPHENE/n-Si HETEROJUNCTION

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Abstract: In this study, the forward bias *I-V* characteristics of graphene/n-Si heterojunctions were studied in the wide temperature range of 10–320 K in order to get detailed information on the barrier heights distribution (φ_B). The Schottky parameters (φ_B, η) are estimated in the framework of the thermoelectron emission theory using Cheung-Cheung method considering the presence of the interface native oxide layer. At room temperature, we obtain an ideality factor of about 2.5 and a Schottky barrier height of ~0.22 eV, which reduces at lower temperatures. A quantitative analysis of the inhomogeneity in Schottky barrier heights is presented using the potential fluctuation model proposed by Werner and Guttler.

Keywords: graphene, chemical vapor deposition, Schottky diode parameters, barrier heights distribution.

I. INTRODUCTION

Graphene has been widely studied as a promising next generation optoelectronic material due to potential advantages such as ultrahigh carrier mobility, ambipolar behavior, inherent good chemical stability and good compatibility with other semiconductor materials [1].

At the same time, *I-V* measurements performed in a wide temperature range are an effective way to evaluate the quality of contacts and for the extraction of fundamental parameters such as the Schottky barrier height (SBH) and ideality factor (*η).*

Also, the accuracy of determining the main parameters of the heterojunction in a wide temperature range is determined by an adequate choice of the method of elaboration of the experimental data, taking into account the quality of the metal/semiconductor interface. For graphene/silicon heterojunctions, this is especially relevant, since the charge states arising at the interface, surface roughness, loose contact of graphene with the material, and natural inhomogeneity of the oxide introduce distortions into the ideal picture of graphene contact with another material.

II. RESULTS AND DISCUSSION

For the device fabrication, graphene growth was performed through the atmospheric pressure chemical vapor deposition using methane as a precursor. After the growth graphene was transferred onto structured n-Si substrates with metallic contacts by a wet-chemical process without using polymeric frame. The area of the heterojunction *A* formed was *A* = 0.087 cm^2. More details about samples fabrication and characterization can be found elsewhere [2,3].

Figure 1 shows the dark *I-V* characteristics of the graphene/Si heterojunctions under a voltage bias from –5 to +5 V (40 mV steps) plotted in a semilogarithmic scale. The experimental data follows the typical Schottky heterojunction dependency (inset to Fig. 1).

To determine the Schottky heterojunction parameters over wide temperature range, the experimental forward biased *I-V* curves at low voltages were analyzed at each temperature within the Cheung-Cheung method, considering the presence of the interface native oxide layer [4]. In this case, the forward biased *I-V* characteristic can be expressed according to the following expression,

$$I = AA^{*}T^{2}e^{-\sqrt{\chi}\delta}e^{-\frac{\varphi_B}{kT}}\left[e^{\frac{q(V-IR_S)}{\eta kT}}-1\right], \qquad (1)$$

where A^{*} is the Richardson constant (≈ 112 A·cm^{-2}·K^{-2} for *n*-Si), *k* is the Boltzmann constant, q is an elementary charge, χ (in eV) is the mean tunneling barrier height and δ (in Å) is the interface oxide thickness which was assumed to be 2–3 nm. For $V - IR_S \gg \eta kT/q$ Eq. (1) provides

$$\frac{dV}{d\,(\ln J)} = R_S AJ + \frac{\eta kT}{q}. \qquad (2)$$

where $J = I/A$ is the current density. From Eq.(2) it follows that the derivative $dV/d(\ln J)$ should be directly proportional to the current density J. From the fitting procedure the R_S and the η values are obtained.

Employing the estimated from Eq. (2) the η values, the SBH (φ_B) and again the R_S can be deduced by an additional Cheung's equation, defined as [4]:

$$H(J) \equiv V - \frac{\eta kT}{q}\ln\left(\frac{J}{A^{*}T^{2}e^{-\sqrt{\chi}\delta}}\right) = R_S AJ + \eta\varphi_B/q. \tag{3}$$

Obviously, plot $H(J)$ also obeys a straight linear relationship.

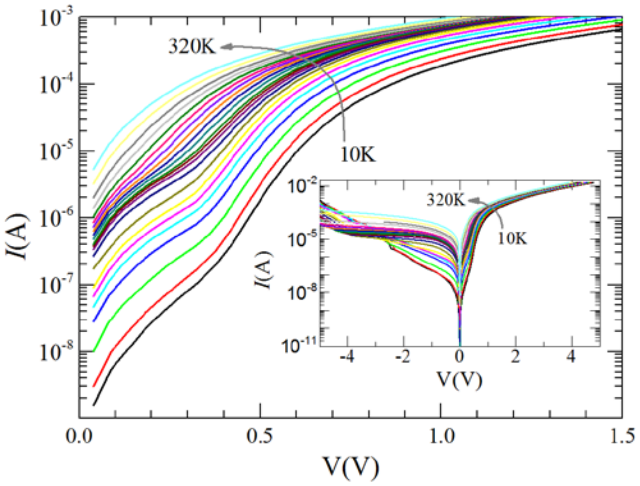

Figure 1. Forward biased *I-V* characteristics of the graphene/Si heterojunction under dark conditions measured in the *T* range of 10 – 320 K. The inset shows the experimental data of the graphene/Si heterojunction under a voltage bias from –5 to +5 V plotted in a semilogarithmic scale

The analysis of the measured temperature-dependent *I-V-T* characteristics of the heterojunctions by using the thermionic emission theory reveals a decrease in the zero-bias SBH and an increase in the η with the decrease of the temperature (Figure 2a). Such temperature dependencies of both η and SBH indicate the influence of inhomogeneities at the graphene/n-Si interface, which are also mentioned in several studies [5,6]. In order to explain the origin of anomalous temperature behavior of SBH and η, the temperature dependent barrier inhomogeneities were evaluated assuming the Gaussian distributions of the SBH [5]. As per this method, the total forward bias current flowing over all possible barrier heights is then given by

$$J(V) = \int_0^{+\infty} J(\varphi_B, V)P(\varphi_B)d\varphi_B, \tag{4}$$

Gaussian distribution expression of the barrier heights with a mean value of φ_{Bm} and standard deviation σ_B has the form

$$P(\varphi_B) = \frac{1}{\sigma_B\sqrt{2\pi}}e^{\left[-\left(\frac{(\varphi_B-\varphi_{Bm})^2}{2\sigma_B^2}\right)\right]}, \tag{5}$$

The apparent barrier height (φ_{ap}) has the form [7]

$$\varphi_{ap} = \varphi_{Bm} - \frac{\sigma_B^2}{2kT} + kT\ln\left[1 + \mathrm{erf}\left(\frac{\varphi_{Bm}}{\sqrt{2}\sigma_B}\right)\right] - kT\ln\left[1 + \mathrm{erf}\left(\frac{\varphi_{Bm}-\frac{\sigma_B^2}{kT}}{\sqrt{2}\sigma_B}\right)\right], \tag{6}$$

where erf denotes the error function.

The plot of φ_{ap} versus 1/2*kT* of studied heterojunction is shown in Figure 2b. Utilizing a model tailored to thermionic emission over a Gaussian distribution of barriers, both the mean barrier height (φ_{Bm}) and the standard deviation (σ_B) in the distribution were extracted from experimental data via multiple linear regression (Figure 2b). The obtained graphene/Si heterojunction parameters are summarized in Table 1.

To obtain more accurate values, the conventional activation energy equation can be modified under the assumption of Gaussian distribution of barrier heights, as follows

$$\ln\left(\frac{I_0}{T^2 AA_{eff}^{*}}\right) = -\frac{\varphi_B}{kT} + \left(\frac{\sigma_B^2}{2k^2T^2}\right), \tag{7}$$

where saturation current (I_0) can be extracted from the experiment by linear fitting of the forward *I-V-T* characteristics.

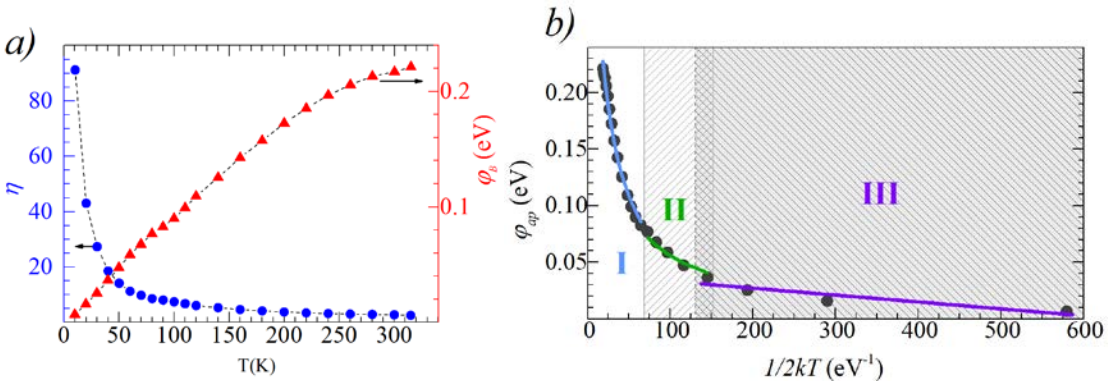

Figure 2. *a*) Ideality factor (circles, left Y-axis) and SBH (triangles, right Y-axis) as a function of *T* obtained using Cheung's method. *b*) Apparent SBH as a function of 1/2*kT* of the graphene/Si heterojunction

The modified Richardson plot for the graphene/Si heterojunction is shown in Figure 3b. From the fitting procedure the values of φ_{Bm} and effective Richardson constant (A^*_{eff}) were extracted. It should be noted that in the calculations of the effective Richardson constant (A^*_{eff}) the full contact area between graphene and Si was taken as a constant (A = 0.087cm^2).

The presence of three different linear fits indicates that there are effective three Gaussian distributions of barrier heights. These values are listed in Table 1. The variations in the values of effective Richardson constants (A^*_{eff}) for three temperature regions are lower than the known value for *n*-Si, that is assumed to be ≈ 112 A·cm^{-2}·K^{-2}.

Table 1. Temperature-dependent parameters of graphene/n-Si heterojunction

Temperature range, *T*(K)	Cheung's method		Werner and Guttler method		Modified Richardson plot	
	η	φ_B (eV)	φ_{Bm} (eV)	σ_B (eV)	A^*_{eff} (A·cm^{-2} ·K^{-2})	φ_{Bm} (eV)
III (10–40)	91-18.6	0.0067-0.037	0.039	0.008	0.00012	0.048
II (40–80)	18.6-8.5	0.037-0.077	0.160	0.038	29.500	0.275
I (90–320)	8.0-2.5	0.08-0.22	0.385	0.095	67.823	0.736

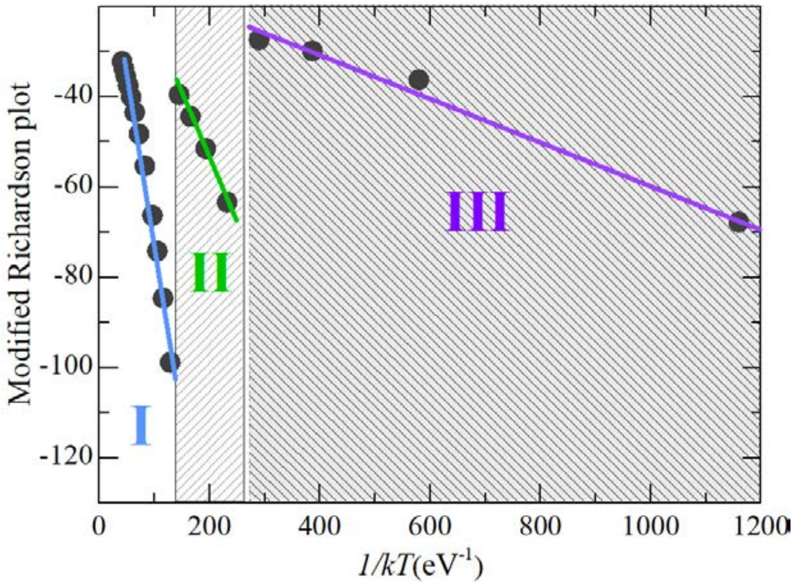

Figure 3. Modified Richardson plot for graphene/Si heterojunction. The solid lines represents the best fit to the experimental data in each region.

III. CONCLUSIONS

The parameters of graphene/Si heterojunction, such as ideality factor, Schottky barrier height and effective Richardson constant values over a wide temperature range of 10–320 K are presented. The obtained results, which were based on thermoelectron emission theory, exhibited an increase of η and a decrease of φ_B with the decreasing temperature and A^*_{eff} was found to be much lower than its theoretical value (for *n*-Si ≈ 112 $A{\cdot}cm^{-2}{\cdot}K^{-2}$). The differences in the A^*_{eff} values can be caused by spatially inhomogeneous SBHs and potential fluctuations at the interface that consist of low and high barrier areas. In this case, inhomogeneities of SBH can be caused by poor interface quality, inhomogeneity of surface states and dislocations, as well as inhomogeneous thickness of the dielectric interfacial layer. Besides, inhomogeneities and/or residual contamination in the interfacial region may be introduced during the copper etching and subsequent transfer process of the graphene film onto *n*-Si substrates.

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АНАЛИЗ ТЕМПЕРАТУРНЫХ ЗАВИСИМОСТЕЙ ПАРАМЕТРОВ ГЕТЕРОПЕРЕХОДА ГРАФЕН/n-Si

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Аннотация: В данной работе исследовались прямые темновые вольтамперные характеристики гетероперехода графен/n-Si в широком температурном диапазоне 10-320 K с целью получения детальной информации о распределении высоты барьеров (φ_B). Основные параметры диода Шоттки (φ_B, η) оценены в рамках теории термоэлектронной эмиссии по методу Чунгов с учетом наличия межфазного оксидного слоя. Установлено, что при комнатной температуре коэффициент неидеальности достигает значения ~2,5, а высота барьера Шоттки ~0,22 эВ. Количественный анализ неоднородности высоты барьера Шоттки представлен с использованием модели предложенной Вернером и Гуттлером.

Ключевые слова: графен, химическое парофазное осаждение, параметры диода Шоттки, распределение высоты барьеров.