TEMPERATURE DEPENDENT PARAMETERS OF SINGLE WALLED CARBON NANOTUBES / Si HETEROJUNCTIONS

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In this study, the forward bias *I-V* characteristics of SWCNT/*n*-Si heterojunctions were studied in the wide temperature range of 20–315 K in order to get detailed information on the barrier heights distribution (φ_B). Schottky barrier height (SBH) and η, values and their dependencies on temperature were obtained by using Cheung-Cheung method, considering the presence of the interface native oxide layer. 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.

Key words: single wall carbon nanotube thin film; floating catalyst chemical vapor deposition; Schottky barrier height; barrier inhomogeneity; photodetector.

INTRODUCTION

Single-walled carbon nanotubes (SWCNTs) are the subject of intense research activities due to their outstanding physical and chemical properties, such as ultrahigh carrier mobility, diameter-dependent bandgaps, ultrabroad spectral absorption, large specific surface area, and good chemical stability [1]. In addition, SWCNT arrays and films are of great interest for applications such as a transparent conductive contact in photodetectors due to the facile process, controlled optical absorption and good device reliability [2–3].

At the same time, the efficiency of such a photodetector depends largely on the quality of the contact between SWNTs and the substrate material. *I-V* measurements are an efficient way for evaluating the quality of contacts and for the extraction of fundamental parameters such as the Schottky barrier height (SBH), ideality factor η and the series resistance R_s. Also, it is well known that the electrical measurements performed only at room temperature does not give detailed information about the nature of barrier at metal/semiconductor interface. In this regard, it becomes important to carry out measurements over a wide range of temperatures *T*, down to cryogenic ones.

To date, most research activity has been dealing with SWNT/Si junctions at room temperature, while few detailed studies have been focused on the transport properties of the SWNT-based SB diodes under wide range of temperatures. Because of this, there is a lack of data describing the behavior of the SBH and η as a function of temperature for SWCT/Si SB.

MATERIALS AND METHODS

The SWCNT films were deposited *directly* on the Si substrate by floating catalyst chemical vapor deposition (FCCVD) using argon (99.99 % purity) as a carrier gas and ferrocene ($Fe(C_5H_5)_2$, 98 % purity) and ethanol (C_2H_5OH, 99.8 % purity) as the hydrocarbon and catalytic sources at 1050 °C [3]. After the deposition was completed, a drop of ethanol was dropped on the samples and the photodetector was thermally annealed in vacuum (10^{-3} Pa) at 400 °C for 3 h to form a good contact between the SWCNT film and Si. The area of the heterojunction A formed was $A = 0.087$ cm^2. More details about samples fabrication and characterization can be found elsewhere [3].

The micro-morphology of SWCNT film was characterized at room temperature under ambient conditions using a scanning laser confocal micro-Raman spectrometer, Confotec NR 500 equipped with 473 nm excitation wavelength and diffraction grating 600 lines/mm. Several maps at various positions were collected in a point-by-point mode with a scanning area of 48 μm × 48 μm with 1.6 μm steps, including about 900 spectra for each map on the sample (Figure 1a,b). Subsequently, each spectrum in the maps was fitted by a set of Lorentzian line shapes and the information on the main Raman peaks position, intensity, and widths (full width at half maximum) were collected for subsequent statistical analysis.

Figure 1, *a* shows statistical evolution of the full width at half maxima ($FWHM_{G+}$) of the G+ mode as a function of the G+ position. The deviation from the mean G+ frequencies values and its FWHM (see figure 1, *a*, *b*) vary significantly within the same region, indicating the presence of inhomogeneity in the film properties, such as built-in strain or nonzero initial doping due to the ambient atmosphere. The variations in all of these parameters across the surface of the film samples lead to the formation of clusters, as shown in the $FWHM_{G+}$ vs G+ frequency plots (Figure 1a, where each point represents a single measurement). Within each cluster, the standard deviations from the mean values of the G+ mode frequency and $FWHM_{G+}$ constitute on average 2.5 and 6.2 cm^{-1}, respectively.

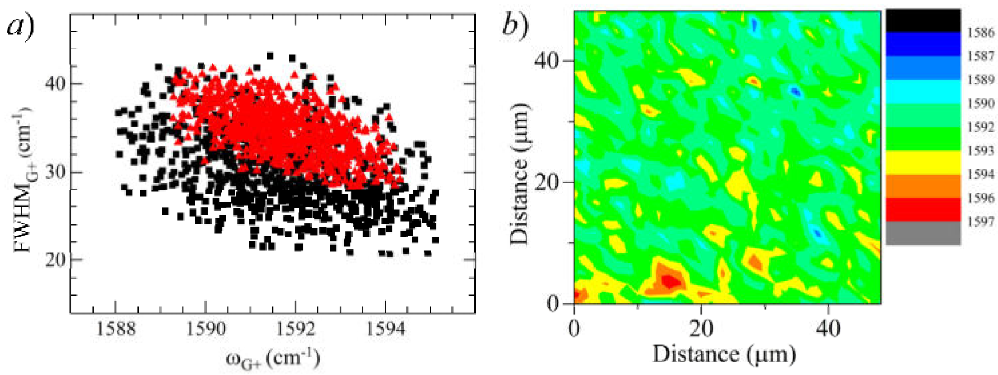

Fig. 1. a – Correlation between the FWHM of the G+ and its position obtained from Raman mapping measured at various positions of SWCNT film; *b* – a point-by-point Raman map displaying the variation of the G+ peak position as a function of coordinates on the surface of the SWCNT film sample

The *I-V* measurements in the wide range of temperature 20–315 K and voltage range of –3 V…+3 V (10 mV steps) were performed using a Keithley 2602A source-meter and a temperature-controlled cryogenic probe station at the pressure under the dark. Semilogarithmic plot of the forward biased *J-V* characteristics of the SWCNT/Si heterojunction measured from 20 to 315 K are shown in Figure 2, *a*. The experimental forward biased *J-V-T* curves at low voltages were analyzed at each temperature within the Cheung-Cheung method, considering the presence of the interface native oxide layer [4] to determine the Schottky diode parameters. In this case, the forward biased *J-V* characteristic can be expressed according to the following expression,

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

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

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

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]:

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

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

RESULTS AND DISCUSSION

The Schottky diode parameters (φ_B, η) were calculated for the region where the change of $\frac{dV}{d(\ln J)}$ is linear, using equations (2, 3) for the different temperatures and the results are graphically shown in Figure 2, *b*.

The analysis of the measured temperature-dependent *J-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 (insert in Fig. 2, *b* where η_0 and T_0 was calculated as 0.49 and 500 K respectively). Such temperature dependencies of both η and SBH have already been reported in several studies, in which the aforementioned unusual temperature dependence in the heterojunction characteristics indicate that spatial inhomogeneities are effective at the heterojunction interface [5, 6].

The most complete explanation for spatial inhomogeneity of the barrier height in Schottky contacts was proposed by Werner and Güttler [5] by assuming the Gaussian distribution of the barrier amplitude with a mean value φ_{Bm} and standard deviation from the mean σ_B. As per this method, the Gaussian distribution expression of the barrier heights with a mean value of φ_{Bm} and standard deviation σ_B has the form

$$P(\varphi_B) = \frac{1}{\sigma_B\sqrt{2\pi}}e^{\left[-\left(\frac{(\varphi_B-\varphi_{Bm})^2}{2\sigma_B^2}\right)\right]}, \tag{4}$$

where φ_{Bm} and σ_B, can be used to model the inhomogeneities and, for thermionic current, leads to an apparent barrier height being lower than the mean barrier height [7].

$$\varphi_{ap} = \varphi_{Bm} - \frac{q\sigma_B^2}{2kT} + kTln\left[1 + erf\left(\frac{\varphi_{Bm}}{\sqrt{2}\sigma_B}\right)\right] - kTln\left[1 + erf\left(\frac{\varphi_{Bm} - \frac{\sigma_B^2}{kT}}{\sqrt{2}\sigma_B}\right)\right]. \quad (5)$$

The plot of φ_B versus $q/2kT$ of studied heterojunction is shown in Figure 3, *a*. From figure 3, *a*, the presence of three different linear fits indicates that there are effective three-fold Gaussian distribution barrier heights. From the fitting procedure, the φ_{Bm} values and their corresponding σ_B were obtained for each temperature region.

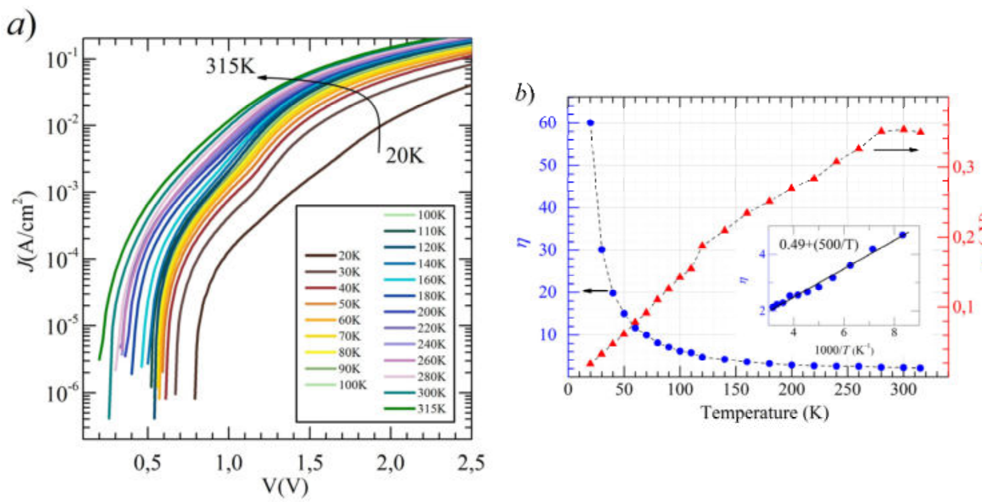

Fig. 2. a – Forward biased *J-V* characteristics of the SWCNT/Si junction under dark conditions measured in the *T* range of 20–315 K; *b* – Ideality factor (circles, left Y-axis) and SBH (triangles, right Y-axis) as a function of *T* obtained using Cheung's method. Insert demonstrate η as a function of 1000/*T* characteristics of SWCNT/Si junction

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

$$\ln\left(\frac{J_0}{T^2}\right) - \left(\frac{q^2\sigma_B^2}{2k^2T^2}\right) = \ln\left(A_{\text{eff}}^*\right) - \frac{q\varphi_B}{kT}. \quad (6)$$

The linear fitting procedure of the forward *J-V* characteristics was applied to extrapolate the current density J_0.

The modified Richardson plot of $\ln\left(\frac{J_0}{T^2}\right) - \left(\frac{q^2\sigma_s^2}{2k^2T^2}\right)$ versus q/kT for the SWCNT SBD 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 SWCNT and Si was taken as a constant (A = 0.087cm^2).

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 $\approx 112\ \text{A·cm}^{-2}\text{·K}^{-2}$.

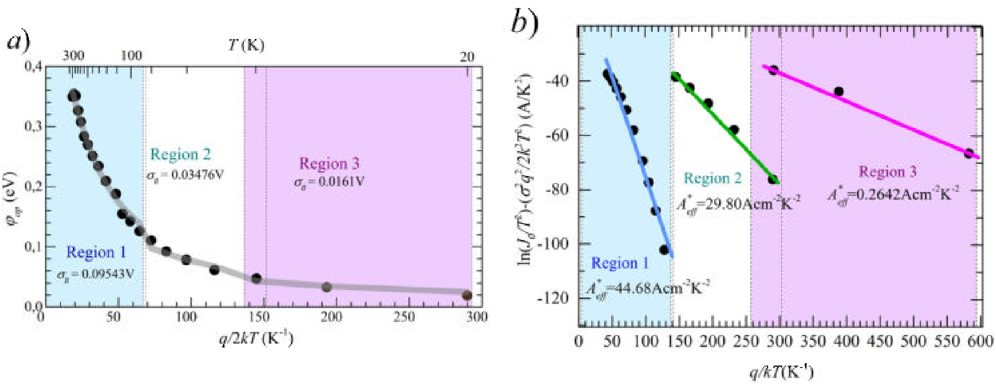

Fig. 3. a – Apparent SBH as a function of temperature of the SWCNT/Si heterojunction;
b – Modified Richardson's plots for SWCNT/Si heterojunction.
The solid lines represents the best fit to the experimental data in each region

CONCLUSIONS

The parameters of SWCNT/Si heterojunction, such as ideality factor (η), Schottky barrier height (φ_B) and effective Richardson constant values (A^*_{eff}) over a wide temperature range of 20–315 K are presented. 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. The inhomogeneities of SBH, in turn, 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 deposition process of the SWCNT film. It also should be noted that A^*_{eff} is possibly underestimated because the actual effective contact area ($A = 0.087\ \text{cm}^2$), between the mesh of nanotubes making up the porous SWCNT film and the Si substrate, used in A^*_{eff} calculations is usually much smaller than the nominal area due to incomplete surface coverage, consistent with the rough morphology of the films.

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ТЕОРЕТИЧЕСКОЕ ИССЛЕДОВАНИЕ ПРИБОРНЫХ ГЕТЕРОСТРУКТУР НА ОСНОВЕ 2D-МАТЕРИАЛОВ С ИСПОЛЬЗОВАНИЕМ ФИЗИКО-МАТЕМАТИЧЕСКИХ МОДЕЛЕЙ

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В докладе проведено теоретическое исследование приборных гетероструктур на основе 2D-материалов, а именно: полевых транзисторов (ПТ) на двухслойном графене (ДГ), а также многобарьерных гетероструктур на основе MoS_2/WSe_2 и GaN/SiC/графен с вертикальным транспортом с помощью разработанных физико-математических моделей, входящих в состав системы моделирования наноэлектронных приборов NANODEV.

Ключевые слова: двухслойный графен; 2D-материалы; моделирование; полевой графеновый транзистор; гетероструктура с вертикальным транспортом.

THEORETICAL INVESTIGATION OF DEVICE HETEROSTRUCTURES BASED ON 2D-MATERIALS WITH THE USING OF PHYSICO-MATHEMATICAL MODELS

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In the paper theoretical investigation of device heterostructures based on 2D-materials, namely field-effect transistors based on bilayer graphene and heterostructures based on MoS_2/WSe_2 and GaN/SiC/graphene with vertical transport has been carried out with the using of developed models included in simulation system of nanoelectronic devices NANODEV.

Key words: bilayer grapheme; 2D-materials; simulation; modeling; graphene field-effect transistor; heterostructures with vertical transport.