Thin Solid Films 519 (2011) 2015–2019

Contents lists available at ScienceDirect

Thin Solid Films

journal homepage: www.elsevier.com/locate/tsf

Two Gaussian distributions of the barrier height in chemical vapor deposition diamond/silicon junctions over a wide temperature range

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ARTICLE INFO

Article history:
Received 29 October 2009
Received in revised form 26 July 2010
Accepted 4 October 2010
Available online 14 October 2010

Keywords:
Diamond films
Electrical properties and measurements
Schottky diodes
Interface electronic properties
Field emission devices

ABSTRACT

Analysis of the current–voltage characteristics of a chemical vapor deposition diamond/n$^+$-Si junction for the temperature range 120–400 K revealed atypical temperature dependence for both the barrier height and the ideality factor and non-linearity in the Richardson plot at low temperatures. These results were interpreted according to model of Chand and Kumar. The junction revealed the existence of two Gaussian distributions of the barrier height, with mean barrier heights of 0.88 and 1.12 eV and standard deviations of 0.098 and 0.132 eV and Richardson constant of 0.5×10^6 and 0.9×10^6 A m^{-2} K^{-2} for the temperature intervals 120–200 and 200–400 K, respectively. The polycrystalline diamond matrix is composed of two distinct phases of microcrystals and amorphous carbon and each Gaussian distribution was related to one of these phases.

1. Introduction

Diamond has exceptional electrical, optical and thermal properties and is very attractive as an electronic material. There is currently great interest in carbon-based materials such as polycrystalline and nanocrystalline diamond, amorphous carbon and carbon nanotubes for diverse applications such as vacuum field-effect transistors, flat-panel displays, diodes, ion sources, scanning microscopes and energy conversion [1,2]. A variety of devices have been proposed with rectifying contacts using single-crystal diamond semiconductors, synthetic single-crystal diamond doped with boron, and homo- or heteroepitaxial diamond films [3–6]. Diamond film obtained by microwave plasma-assisted chemical vapor deposition (MPCVD) has attracted great interest as the active material in electronic devices such as field-emission devices. Owing to easy deposition on various types of substrate and over large surfaces at lower cost, chemical vapor deposition (CVD) films have been the focus of much interest in the field of diamond heteroepitaxy. Because of its biocompatibility and stability to many chemical agents, CVD diamond is also a very attractive candidate for chemical sensors and bioelectronics devices [7].

In the present study the electrical characteristics of a CVD diamond/n$^+$-Si junction was investigated for the temperature range 120–400 K using the method developed by Chand and Kumar [8–10] for non-homogeneous barriers. The diamond used in the junction was polycrystalline and was produced using the MPCVD technique [11,12]. It was composed of two different phases: diamond microcrystals and grain boundaries, which are regions located between crystals that contain others carbon structures such as graphite and diamond-like carbon (DLC). According to my results reported in the literature [11–13] experiments with diamond films, using a modified AFM demonstrated that electrical current flows mainly via grain boundaries and only some electrical carriers are transported through diamond microcrystals. In this device highly doped silicon was used, resulting in an abrupt asymmetric junction in which the depletion region is totally on the diamond side so that its behavior is very similar to a Schottky barrier [14]. An important application of this junction is in field emission devices. Studies of electronic emission from the diamond surface in similar junctions revealed that the diamond/silicon interface controls the supply of electrons to the diamond [11]. Thus, in addition to the influence of the structure, morphology and chemical composition of the diamond, is very important to understand charge injection at the interface and the surfaces states in the field emission process. Such knowledge can be used to control the concentrations and energy distributions in these states and consequently to improve the performance of electronic emission devices [15].

Analysis of the current–voltage (I–V) characteristics of CVD diamond/n$^+$-Si junctions on the basis of thermionic emission–diffusion (TED) theory revealed an atypical decrease in barrier height and increase in ideality factor with decreasing temperature [11]. Non-linearity of the Richardson plot at low temperature can be a consequence of this decrease in barrier height. These results cannot be explained adequately by incorporating an interfacial oxide layer or interface states, tunneling, image force lowering, or generation and recombination of currents in the depletion region [11,12,15]. Chand and Kumar [8–10] established a model for electrical conduction based on a TED mechanism and supposition of the existence of Gaussian distributions of barrier height for non-homogeneous systems to

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0040-6090/$ – see front matter © 2010 Elsevier B.V. All rights reserved.
doi:10.1016/j.tsf.2010.10.003

explain the nature and origin these effects. The system is described as a set of parallel junctions with different barrier heights within the Gaussian distribution boundary, for which each contributes independently to the current. The numerical simulation method of Chand and Kumar demonstrates the possibility of the existence of single or multiple Gaussian distribution(s) at the contact, depending on the type of Schottky diode. Chand and Kumar [8–10] applied the model to a Pd_2Si/n-Si Schottky diode [9] and proved the existence of two Gaussian distributions of the barrier height. Current–voltage–temperature (*I–V–T*) measurements using the Chand–Kumar method confirmed that this is a very practical tool for studying the nature of the barrier formed in Schottky diodes in general, and particularly for non-homogeneous interfaces. Experimental data for other devices have also been interpreted using this method [16,17].

2. Experimental procedure

Diamond film was grown on a heavily doped n-type silicon (100) substrate, with bulk resistivity of 1 Ω cm in an MPCVD system. The silicon substrate was pre-treated by polishing with diamond powder of 0.25 mμ grain size and cleaned in an ultrasonic cleaner before deposition. The gas was composed of hydrogen (99%) and methane (1%), the substrate temperature was 800 °C and the pressure was 40 Torr. In a time of 14 h at microwave power of 4 kW, films of 5 μm in thickness were obtained, as confirmed by infrared interference measurements. The film quality was assessed by micro Raman spectroscopy using a Renishaw system. Additional information on the deposition conditions and substrate preparation is reported elsewhere [11,12,15]. Atomic force microscopy revealed that the surface morphology was relatively rough and comprised microcrystals with a predominant ⟨111⟩ orientation. The samples were chemically treated with H_2SO_4–CrO_3 solution to remove graphite from the surface to improve device performance. To fabricate diamond/n^+-Si diodes, circular gold contacts with a diameter of ~2 mm were deposited on the diamond surface via thermal evaporation [11,12]. The silicon was considered to be one of the electrodes and the diamond/gold contact was ohmic. Some degree of oxidation will occur and generate a thin interfacial oxide layer between a metal and diamond unless special processing conditions to prevent this are implemented. CVD diamond does not contain a native oxide but it can be oxidized at elevated temperature (started at ~700 K) in air. In these films the oxidation rate depends on the crystallographic orientation, the growth conditions, and the conditions for metal evaporation. Further studies are needed for a complete understanding of the oxidation process in diamond films.

The devices were placed in a steel vacuum chamber at a pressure of ~1 mPa. A Keithley 487 picoammeter/voltage source was used for *I–V* measurements. The temperature was measured with a platinum resistor. Electrical measurements were performed in the Center for Electronics, Optoelectronics and Telecommunications, University of Algarve.

3. Results and discussion

Various aspects of the conduction mechanisms of a diamond/silicon interface can be studied in terms of the *I–V–T* characteristics. The important constant adjustment is the ideality factor, $n=1$. This number characterizes the slope of a current–voltage plot as measured on a semi-logarithmic scale. The *I–V* characteristics of CVD diamond/silicon devices at forward bias for the temperature range 120–400 K are presented in Fig. 1. Analysis of these results using TED theory revealed an abnormal decrease in barrier height and increase in ideality factor with decreasing temperature [11] and non-linearity in the activation energy plot at low temperature. In barrier height versus ideality factor plot [11] was suppose a linear variation, but extrapolation of this plot to an ideality factor of $n=1$ showed a barrier height

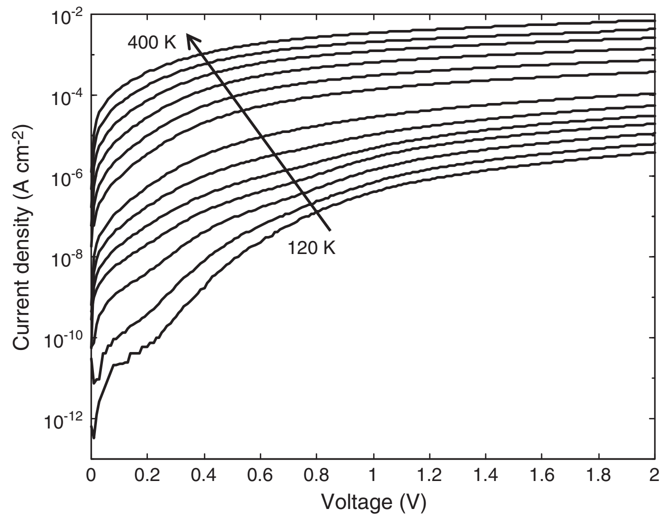

Fig. 1. Experimental forward bias current–voltage characteristics of the CVD diamond/silicon junction at various temperatures.

of ~1.8 eV, which is unrealistic because it is higher than the theoretical value of ~1.1 eV. Experimental data for CVD diamond/silicon revealed a barrier height of $\Phi_b<1$ eV [11]. Different factors can contribute to a reduction in barrier height with decreasing temperature, such as diamond non-homogeneity, the effect of the image force, generation and recombination currents in the space-charge region, an elevated internal field due to application of electrical voltage, the narrow depletion region of diamond at low temperature, the tunneling process and assisted tunneling [11].

Fig. 2 shows a plot of the experimental barrier height versus the inverse ideality factor at various temperatures. In accordance with the Chand–Kumar model [8–10] the nature and origin of the decrease in barrier height and increase in ideality factor with decreasing temperature are assumed to be associated with non-homogeneity of the material, which can involve, for example, differences in phases, orientation, interface quality, and electrical charges. The model also assumes the existence of a Gaussian distribution of barrier heights around a mean value at the interface. This Gaussian distribution represents a large number of non-interacting parallel diodes, each of which has a different barrier height [8].

In accordance with TED theory, the total current across a junction at forward bias *V* can be expressed as:

$$I(V) = \int i(\Phi_b, V)G(\Phi_b)d\Phi_b, \quad (1)$$

where $i(\Phi_b,V)$ corresponds to the current at bias *V* for barrier height Φ_b and can be written as:

$$i(\Phi_b, V) = AA_RT^2 exp\left(-\frac{q\Phi_b}{kT}\right)\left[exp\left(\frac{-q(V-ir_s)}{kT}-1\right)\right], \quad (2)$$

where *A* is the effective diamond junction area (3.1×10^6 m^2), A_R is the Richardson constant (theoretical value 1.2×10^6 $A m^{-2} K^{-2}$), *q* is the electron charge, *k* is the Boltzmann constant, *T* is the absolute temperature and r_S is the series resistance. The term $G(\Phi_b)$ is the Gaussian distribution of the barrier height with mean value $\overline{\Phi}_b$ and standard deviation σ over the contact region. This has the form:

$$G(\Phi_b) = \frac{1}{\sigma\sqrt{2\pi}} exp\left(-\frac{(\Phi_b-\overline{\Phi}_b)^2}{2\sigma^2}\right), \quad (3)$$

where the factor $\frac{1}{\sigma\sqrt{2\pi}}$ is a normalization constant.

The expressions for $i(\Phi_b,V)$ (based on TED theory) and $G(\Phi_b)$ are introduced in Eq. (1) and integrated [8–10]. Assuming that the