Contents lists available at ScienceDirect

Thin Solid Films

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

Studies on In-pWSe₂ Schottky diode by current-voltage-temperature method

Achamma John Mathai*, K.D. Patel, R. Srivastava

Department of Physics, Sardar Patel University, Vallabh Vidyanagar-388120, Gujarat, India

ARTICLE INFO

Article history: Received 1 April 2009 Received in revised form 9 January 2010 Accepted 21 January 2010 Available online 29 January 2010

Keywords: In-pWSe₂ Schottky diodes Current-Voltage measurements Metal-semiconductor contacts Tunneling Thermionic emission

1. Introduction

Although great efforts have gone into providing a systematic study of Schottky barrier system over the years, a complete determination of the detailed mechanisms responsible for Schottky barriers is still quite elusive due to difference in the characteristics of the real system with that of the ideal one [1–13]. Perhaps the reason may be due to the multiplicity of charge transport mechanisms that come into play at the interface instead of a single mechanism along with other physical and chemical interface situations that arise in practical diodes. This makes the interface a very complex region, which in turn reflects on their terminal physical characteristics. Significant amount of work is still being made on ways and means to arrive at a more realistic interpretation of the characterizing parameters of real Schottky diodes [14–17].

Regarding WSe₂ Schottky interfaces, various studies have been carried out in the past with different goals [18–30]. Investigations on In-*p*WSe₂ Schottky diodes by photoemission spectroscopy and scanning electron microscopy to investigate the lateral inhomogeneity aspects as well as the interface reaction with the deposited metal revealed that there is no such reaction at the interface with indium [18,29]. Most of these studies have been focused on the efforts to find out device parameters at room temperature and at one or two low temperatures. But the extraction of device parameters by current-voltage (I-V) measurements based on thermionic emission model only at room temperature or at a few low temperatures may not give

E-mail address: achammajohn@yahoo.com (A.J. Mathai).

ABSTRACT

Two types of $In-pWSe_2$ Schottky barrier diodes were fabricated, one on as grown (uncleaved) and the other on cleaved WSe₂ surface. Current–voltage characteristics of these diodes have been analyzed over a wide span of temperature ranging from 140 K to 300 K on the basis of thermionic emission theory with Gaussian distribution model of barrier height. Below 200 K, a model has been considered where the total current is assumed to be the sum of thermionic emission, generation recombination and tunneling components. The observed deviation in barrier height, ideality factor and Richardson plot below 200 K are interpreted in terms of the contribution of these multiple charge transport mechanisms across the interface of the fabricated diodes. © 2010 Elsevier B.V. All rights reserved.

precise values. The analysis and interpretation with few experimental data can also lead to incorrect results even if more complex models are used. On the other hand, the characteristics measured in a wide temperature range will give much more experimental data, which allows the determination of the parameters of Schottky structure with a higher degree of precision. Besides, the *I–V* investigations of the diodes on wide temperature range will also be useful to study the dominant conduction mechanisms in different temperature regions. The chemical inertness of the basal plane of WSe₂ and its ideal property for the fabrication of Schottky barrier devices prompted the study of In-*p*WSe₂ systems [29,30].

2. Experimental details

Semiconducting crystals of p type WSe₂ were grown by direct vapour transport technique with an acceptor density of 10¹⁶/cm³. Mostly the as grown crystal surfaces may not be plane and have spirals, steps, kinks, voids etc. For a detailed investigation on more homogeneous surfaces, the crystals were cleaved with adhesive tape so that large terraces of non-reactive van der Waal's plane were available for metal deposition. Thus to make comparative studies, Schottky devices were fabricated on both uncleaved and cleaved surfaces separately. Both cleaved and uncleaved crystals were cleaned thoroughly with acetone and were mounted on the substrate holder in the vacuum chamber (HHV BC-300). Pure indium metal (Aldrich 99.9%) was evaporated onto the semiconductor surface by thermal evaporation method at a vacuum level of the order of 1.333×10^{-7} Pa. Thickness of the evaporated In metal was 500 Å with a deposition rate of 0.2 Å per second. Schottky contact was taken with low strain Ag alloy wires and silver paste (Eltec-1228 °C) from the evaporated In



^{*} Corresponding author. C/o Dr. Bobby Antony, Department of Applied Physics, ISM University, Dhanbad, 826 004-Jharkhand, India. Tel.: +91 947 019 4795.

^{0040-6090/\$ –} see front matter s 2010 Elsevier B.V. All rights reserved. doi:10.1016/j.tsf.2010.01.027

regions. The ohmic contact was taken with the same type of silver paste and Ag alloy wires from the WSe₂ surface.

The current–voltage–temperature (I–V–T) data were acquired from 300 K down to 140 K at an interval of 20 K using Keithley 2400 Source Measurement Unit (SMU) along with Lakeshore temperature controller (Model 340), which balanced the cooling power provided by a Closed Cycle Refrigerator (CCR 75014) against two heater circuits. Keithley Lab-Tracer software coordinated the measurement and sourcing activities at once.

3. Results and discussions

The nature of the I-V characteristics of the two sets of uncleaved and cleaved $In-pWSe_2$ Schottky diodes at different temperatures are shown in Fig. 1a,b. According to thermionic emission theory, the observed current '*T* passing through the barrier is related to the applied voltage '*V*' in a manner expressed by the equation [31,32]:

$$I = I_0 exp\left[\frac{q(V - IR_s)}{nkT}\right] \left[1 - exp\left(\frac{-q(V - IR_s)}{kT}\right)\right]$$
(1)

Here ' I_0 'is the saturation current, 'n' is the ideality factor and ' R_s ' is the series resistance of the diode. *T* represents the absolute temperature in *K*, *k* the Boltzmann's constant and *q* the electronic charge. The values of I_0 , *n* and R_s were extracted from a series of iterations using SigmaPlot 5.0 software. The best fit to the experimental *I–V* curves of these diodes in the forward bias region is shown in Fig. 2a,b. The zero bias barrier height ' ϕ_{b0} ' and flat band barrier height ' ϕ_{bf} ' were calculated by the following equation [1,3,33]:

$$\Phi_{b0} = \frac{kT}{q} ln \left[\frac{AA^* T^2}{I_0} \right] \tag{2}$$

and

$$\phi_{bf} = n\phi_{b0} - (n-1)\frac{kT}{q} ln \left[\frac{N_V}{N_A}\right]$$
(3)

Here *A* is the diode area, which is 3.6×10^{-3} cm² and *A*^{*} is the Richardson constant, which is 27.6 A/cm²/K² for WSe₂ [22,34]. 10¹⁶ is the net acceptor density *N*_A for both cleaved and uncleaved WSe₂ crystal. Similarly 10¹⁸ is the effective density of states *N*_V for both cleaved and uncleaved WSe₂ crystal. So it is quite natural that the barrier heights are closer for both the cleaved and uncleaved diodes.

The variation of zero bias barrier height ϕ_{b0} , flat band barrier height ϕ_{bf} and ideality factor n as a function of temperature for the two types of diode is shown in Fig. 3a,b. It shows both ϕ_{b0} and ϕ_{bf} decrease whereas n increase with the fall in temperature. The reported value of ϕ_{b0} at room temperature for cleaved In-*p*WSe₂ diode is 0.55 eV by photoemission spectroscopy [30]. In the present case the room temperature values of ϕ_{b0} are 0.58 eV and 0.61 eV for uncleaved and cleaved diodes respectively. Fig. 4a,b shows the variation of series resistance R_s with temperature. The values of R_s are found to be around several hundred ohms at 300 K, though it increases rapidly below 200 K. Similarly the value of *n* also increases considerably at low temperature. Eq. (2) can be rewritten in the form,

$$\ln\left[\frac{I_0}{T^2}\right] = \ln\left(AA^*\right) - \frac{q\phi_{b0}}{kT} \tag{4}$$

known as the Richardson equation. Based on this equation a plot of ln (I_0/T^2) vs. 1000/*T* were made and is shown in Fig. 5(a,b). The plot should be a straight line which will give the values of ϕ_{b0} and A^* from its slope and intercept respectively for a known diode area *A*. However, in our case we can see that the points at low temperatures are deviated from the straight line. Considering the linear region, the values of ϕ_{b0} (E_a) and A^* were evaluated by the slope and intercept and are tabulated in Table 1. The values of E_a are very low and the values of A^* are considerably away from the known theoretical value of 27.6. The deviation in Richardson plot at low temperatures, low values of A^* , E_a and the high magnitude of ideality factor n can be considered as an indication of non-ideal nature which may be attributed to: a) inhomogeneous nature of the fabricated diode [7,8,12,35–38], b) multiplicity of operative transport mechanisms [1,3,15,31], and c) a combination of both (a) and (b).

Inhomogeneities can be readily expected in WSe₂ based Schottky diodes because of the specific nature of its surfaces, which may contain defects, kinks, voids, steps, chalcogen vacancies etc. The non-idealities in the deposited metal overlayer morphology (grain boundaries, clusters etc) would also strongly influence the development of Schottky barriers. Thus interfaces may contain potential fluctuations in the lateral plane on a length scale smaller than the width of space charge region making the interface electrically inhomogeneous in nature. The deviation in the *I–V* characteristics based on thermionic emission diffusion (TED) model of real Schottky diodes with ideal one has been explained by many authors [39–54] as the presence of such barrier height inhomogeneties. Under these circumstances, we assume here also that the distribution of the Schottky barrier height (SBH) ' $P(\phi_b)$ ' is Gaussian in character with a



Fig. 1. I-V characteristics of In-pWSe₂ Schottky diodes at different temperatures.

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