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ORIGINAL ARTICLE

Electrical characterization of vacuum-deposited p-CdTe/n-ZnSe heterojunctions

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Abstract In this paper, we report a heterojunction of p-CdTe/n-ZnSe fabricated on a quartz substrate using thermal evaporation technique. The materials have a larger band gap difference in comparison to other II–VI heterojunctions-involving CdTe. The larger band gap difference is expected to increase diffusion potential and photovoltaic conversion efficiency. The electrical conduction mechanism involved, barrier height and band offset at the interface that are crucial to determine device performance are evaluated using electrical characterization of heterojunction. The junction exhibited excellent rectification behavior with an estimated barrier height of 0.9 eV.

Keywords Thin films · Electrical properties · Interfaces · Heterojunction

Introduction

II–VI compounds are of potential interest for photovoltaic and optoelectronic device application in UV to IR region owing to their direct band gap, which span over the entire visible region of the spectrum and high absorption coefficient (Fahrenbruch 1977; Chu and Chu 1995; Lour and Chang 1996; Neumark 1997; Le Meur et al. 1998; Chang and Lii 1998). Among II–VI compounds, CdTe is one of the extensively studied materials, particularly for photovoltaic (PV) application. It has a near optimum band gap to achieve maximum efficiency as required by Shockley and Queisser limit (1961). Thin-film PV cell fabricated with CdTe/CdS is the most efficient cell among the II–VI compounds, but efficiency is still far from its theoretical limit. The band gap difference and absorption beyond wavelength 500 nm limits its maximum achievable efficiency (Fahrenbruch 1977; Chu and Chu 1993, 1995). Replacing a CdS layer with wider band gap materials as the window layer is expected to enhance the efficiency of PV cells (Aranovich et al. 1978; Chu and Chu 1993; Spalatu et al. 2011). Hence, p-CdTe/n-ZnSe should have higher theoretical conversion efficiency (Bube et al. 1977). Very few works have reported the optical and photovoltaic properties of p-CdTe/n-ZnSe heterojunction prepared using close-spaced sublimation (Bube et al. 1977; Buch et al. 1977; Chu et al. 1992; Potlog et al. 2011; Spalatu et al. 2011). These works are based on band gap and alignment considerations. Further, for improvement of the efficiency of a CdTe-based device, detailed study of conduction mechanism and current limiting parameters which decides device efficiency is needed.

In this article, we report electrical properties of p-CdTe/n-ZnSe prepared by thermal evaporation. The results of current–voltage (*I*–*V*) and capacitance–voltage (*C*–*V*) characteristics are evaluated to understand the electrical conduction involved, barrier height, and the interface formed, as it is crucial to determine the device performance.

Experimental details

ZnSe and CdTe films were deposited on well-cleaned quartz substrates by vacuum evaporation method. High purity (99.99 %) ZnSe and CdTe powders were evaporated using resistive heated molybdenum boats. The films were deposited in a residual pressure of about 10^{-6} Torr while

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substrates were maintained at room temperature. Structural and compositional evaluation of the ZnSe and CdTe layers were done using XRD and EDX. The heterojunction was formed by successive deposition of ≅700-nm-thick ZnSe film on a silver (bottom contact)-deposited quartz substrate, followed by a ≅1-µm-thick CdTe layer and silver top contact through a shadow mask. Keithley-made Multimeter and Source Meter were used for current and voltage measurements and Agilent-made precision LCR meter was used for *C*–*V* measurement.

Results and discussion

Structural and compositional analysis

The properties of the heterojunction depend considerably on the crystalline quality and the composition of the compounds. The crystal structure of individual layers, ZnSe and CdTe was characterized using X-ray diffraction. The films exhibited zincblende structure with (111) preferred orientation as shown in Fig. 1. The composition analysis of the films indicated that the films were non-stoichiometric. ZnSe film was Se rich (Zn:Se ≅49:51 at %) and CdTe was Te rich (Cd:Te ≅48:52 at %). These A_{II} B_{VI} compounds dissociate while thermal evaporation under vacuum and B_{VI} components of the compounds have higher partial vapor pressure than the A_{II} components. Thus, thin films deposited at room temperature and at a high growth rate are commonly found to be rich in B_{VI}. They are normally found to have (111) direction perpendicular to the substrate surface (Rao et al. 2011).

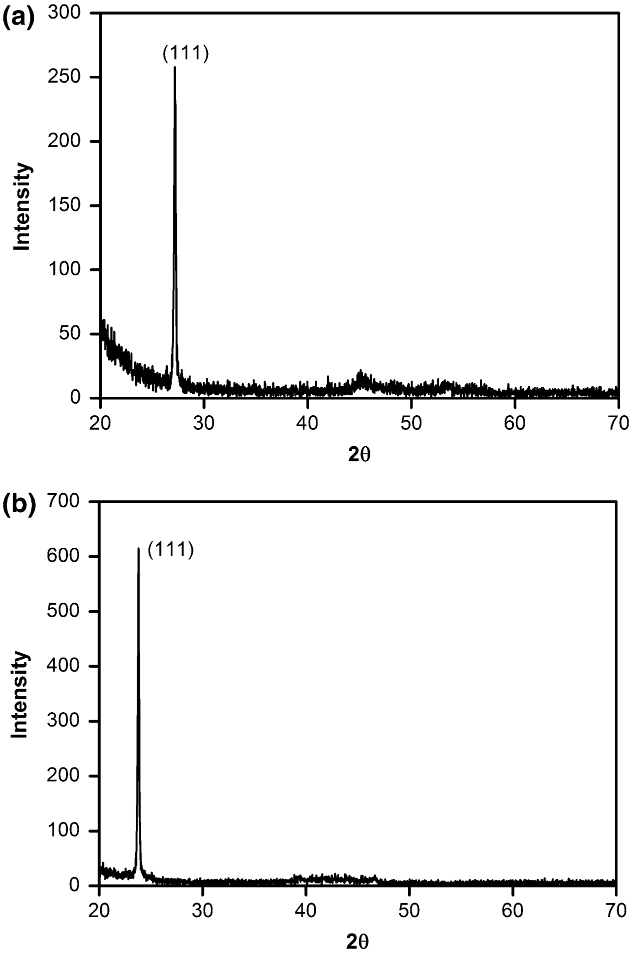

Fig. 1 XRD pattern of **a** ZnSe and **b** CdTe films deposited on quartz substrates

Electrical characterization

Electrical properties of the vacuum-deposited II–VI compounds thin films depend on the composition and structure of the films. Both ZnSe and CdTe layers used for forming heterojunctions were not intentionally doped and not treated chemically or thermally post-deposition. Such films deposited on unheated substrates will have very high electrical resistance due to self-compensating property inherited by these compounds (Rusu and Rusu 2000; Gowrish Rao et al. 2013). Figure 2a shows the I–V curves of p-CdTe/n-ZnSe heterojunction. The heterojunction shows the rectifying behavior, which is typical of p–n junction diode.

The current–voltage (*I*–*V*) characteristic of heterojunction provides essential parameters, such as the barrier height, parasitic resistances, which limits device performance. In heterojunctions, the barrier heights at the interface for electrons and holes are of different magnitude. Depending on the band alignment at interface, the current in a heterojunction consists of mostly electron or holes. In homojunctions, the diffusion of carriers is a significant contributor for the voltage dependence of the current. Whereas in heterojunctions, *I*–*V* characteristic depends also on thermionic emission across the interface in low doping level and the tunnel current in high-doped semiconductors. Several authors have proposed and verified models on conduction mechanism in heterojunctions (Chang 1965; Yang et al. 1993; Bhapkar and Mattauch 1993; Horio and Yanai 1990; Cavallini and Polenta 2008), which are similar to thermionic emission and diffusion model proposed by Sze and Crowell for a metal–semiconductor junction (Crowell and Sze 1966). Hence, the *I*–*V* characteristics of p-CdTe/n-ZnSe heterojunction have general form

$$I = I_s \exp\left(-\frac{qV_{bi}}{kT}\right)\left\{\exp\left(\frac{qV}{nkT}\right) - 1\right\} \tag{1}$$

where I_s is the reverse saturation current, k is Boltzmann's constant, n is a diode ideality factor, T is the temperature and q is the elementary charge. For higher forward bias voltages, Eq. (1) can be approximated as,

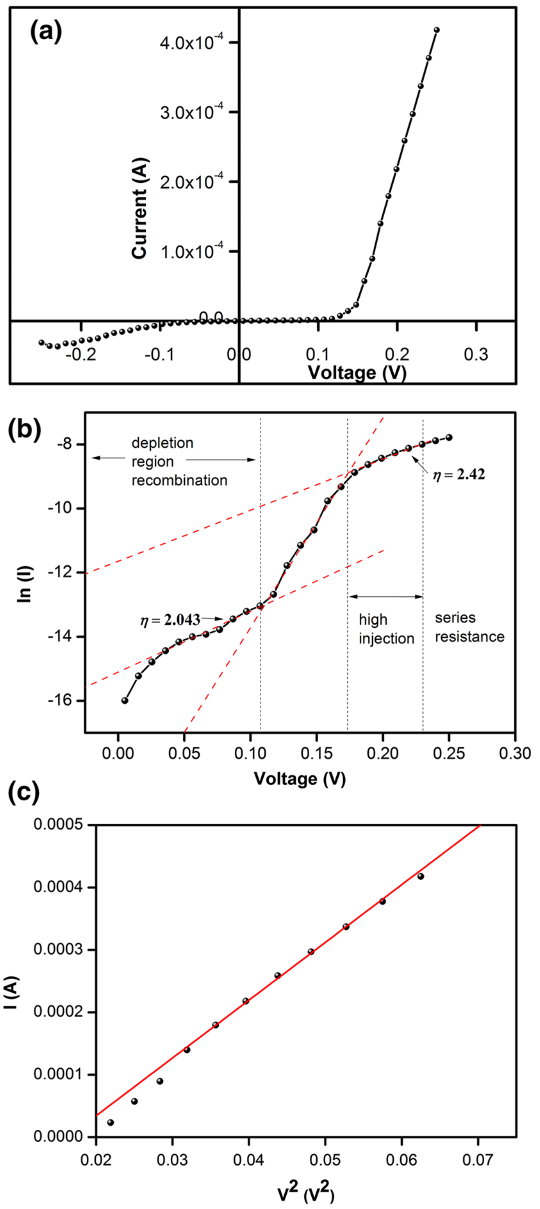

Fig. 2 **a** *I–V* characteristic, **b** ln *I* vs. *V* and **c** *I* vs. V^2 curve of p-CdTe/n-ZnSe heterojunction

$$I = I_s \exp\left(\frac{qV}{nkT}\right) \tag{2}$$

To analyze the conduction mechanism involved in the heterojunction the *I–V* characteristic was plotted in a semi-logarithmic scale as shown in Fig. 2b. The slope of the curve gives the ideality factor n; it can vary from 1 to 2 or above, depending on the conduction mechanism involved. The Fig. 2b shows the different regions corresponding to different values of n, which means that carrier transport in p-CdTe/n-ZnSe heterojunction is limited by various conduction mechanisms depending on the voltage. Such deviation from ideal *I–V* characteristic is common in the real diode involving defects and parasitic resistances. Current in real diode is generally expressed as follows,

$$I = I_0\left\{\exp\left[\frac{q(V - IR_s)}{nkT}\right] - 1\right\} + \frac{V - IR_s}{R_{SH}} \tag{3}$$

where R_s is the series resistance that arises from the bulk of the semiconductor involved and limits current significantly at higher voltages. R_{SH} is shunt resistance, plays major role in terms of leakage current in lower forward bias, and reverse bias voltages.

In Fig. 2b, the first part, up to 0.1 V, $n \cong 2$ indicates dominance of trap-assisted generation recombination current in the depletion region. In the second region, spanning from voltage 0.1–0.17, $n \cong 1$ implies ideal diode current in this region. Beyond 0.17 V, the ideality factor $n > 2$ suggests that conduction mechanism is other than diffusion or recombination current. High injection or series resistance may limit the current in this region. The linear dependence of the *I–V* characteristic at higher forward voltages can be approximated by,

$$I = \frac{V - V_0}{R} \tag{4}$$

where V_0 is the diffusion potential and R is the series resistance of the heterojunction. R is estimated from the inverse of the slope of the higher forward bias, which was ~253 Ω.

In Fig. 2c plot of I vs. V^2, drawn for higher bias voltage, was found to make a better linear fit corresponding to the shallow trap square law, a characteristic of space charge limited conduction, given by following Eq. (5), (Mathew 2003).

$$I = \left(\frac{AV^2 N_c \mu \varepsilon_0 \varepsilon_r}{8L^3 N_t}\right) \exp\left(\frac{-E_t}{kT}\right) \tag{5}$$

where ε_r is the relative permittivity, N_c is the effective density of the states in the conduction band, N_t is the concentration of traps with activation E_t, L the thickness of the film, μ carrier mobility. Thus, the analysis of *I–V* characteristics reveals that the parasitic resistance and defects in the diode limit current in heterojunction.

To determine the barrier height, the interface p-CdTe/n-ZnSe is characterized with *C–V*. Figure 3a, b show the voltage dependence of the capacitance and inverse squared of the capacitance of the heterojunction, respectively, measured at 100 kHz and 2 MHz signal frequency. In an ideal abrupt junction, the capacitance should decrease with increasing reverse voltage due to increase in depletion width with voltage and it should be independent of frequency. C^{-2} verses V curve should be a straight line given by the following Eq. (6),

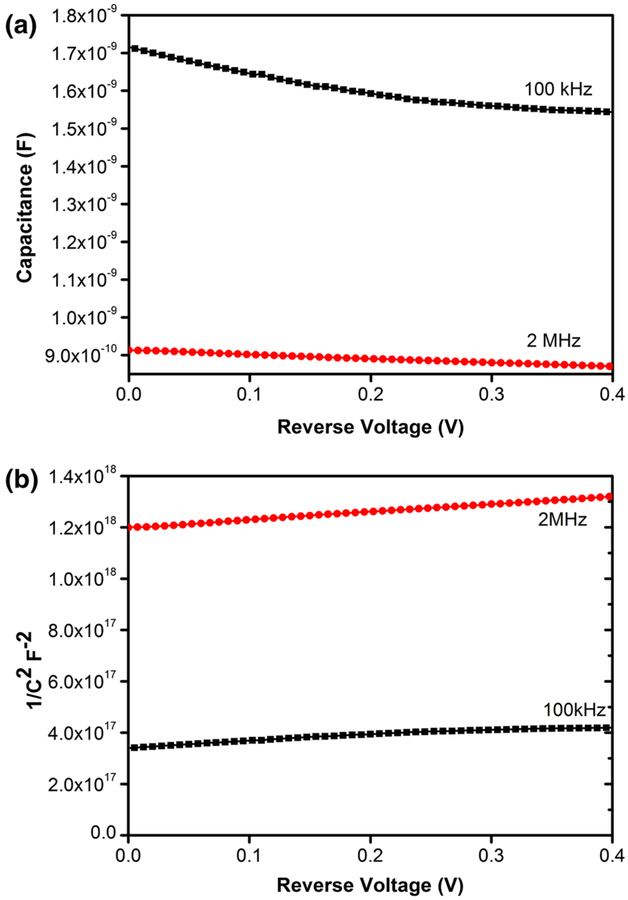

Fig. 3 **a** Junction capacitance and **b** C^{-2} as function of voltage of p-CdTe/n-ZnSe heterojunction

$$\frac{1}{C^2} = 2\left[\frac{\left(V - V_b + \frac{kT}{q}\right)}{q\varepsilon_o\varepsilon_r NA^2}\right] \tag{6}$$

where ε_r is the dielectric constant, V is applied voltage, V_b is built-in potential, N doping density and A is the effective area of the diode. Slope of C^{-2} verses V is commonly used to determine the carrier density or doping density and intercept at C^{-2} is zero to find V_b of the junction. As can be seen from the Fig. 3a C–V does depend on the frequency, indicating the presence of electrically active traps at interface (Hoffman et al. 2001). The voltage intercept of the $C^{-2}(V)$ in Fig. 3b is also too large to say it as a built-in potential. This indicates the existence of insulating layer at the interface, formed due to inter-diffusion of components at the interface (Buch et al. 1977; Mauk et al. 1990). In such cases the built-in potential can be calculated from Eq. (7)

$$qV_{bi} = E_g - E_f(\mathrm{CdTe}) - E_f(\mathrm{ZnSe}) - \Delta E_c \tag{7}$$

where E_g is the energy band gap of CdTe, E_f (CdTe) and E_f (ZnSe) are Fermi levels in respective compounds, ΔE_c is the energy difference between conduction bands of CdTe and ZnSe. The $qV_{bi} \sim 0.9$ eV was calculated using Eq. (7).

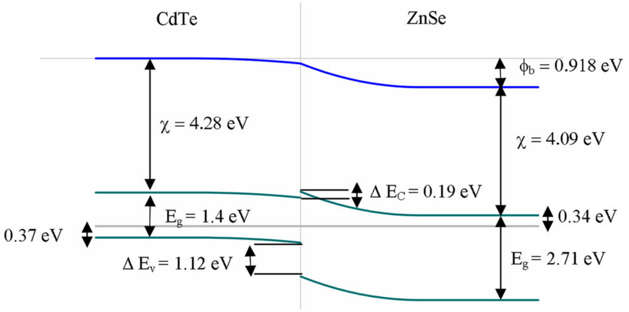

Fig. 4 Band profile of p-CdTe/n-ZnSe heterojunction

Based on the results of the electrical characterization band profile for p-CdTe/n-ZnSe heterojunction is drawn, as shown in Fig. 4, using electron affinity rule. The band alignment shows the conduction band offset ΔE_c is 0.19 eV and valence band offset ΔE_v is 1.12 eV. The junction offers small barrier for electrons and large barrier for holes, hence blocking from crossing junction. Thus, compared to CdS/CdTe, the band offset of CdTe/ZnSe favors the higher conversion efficiency.

Conclusions

A heterojunction of p-CdTe/n-ZnSe is fabricated using thermal evaporation method. Structural and compositional analysis showed that both the layers had cubic structure and were non-stoichiometric. The rectifying nature of the junction was found from the *I*–*V* characteristic. Current conduction was dominated by the trap-assisted recombination and high injection current. Capacitance measurement revealed presence of traps and insulating interfacial layer controlling the current transport across the junction. However, larger band gap of ZnSe and valence band offset are favorable for better performance.

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