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ORIGINAL PAPER

Investigation of Electrical and Structural Properties of Ag/TiO_2/n-InP/Au Schottky Diodes with Different Thickness TiO_2 Interface

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Abstract

In this study, structural and electrical properties of Ag/TiO_2/n-InP/Au Schottky barrier diodes, constructed with sputtering method on n-InP wafer, are investigated. Particle size, d- spacing, micro-strain, ideality factor and barrier heights of two samples are determined for two different interfacial TiO_2 layer thickness. Thickness of TiO_2 interfacial layers are adjusted as 60 Å and 120 Å. X-ray diffraction (XRD) and current-voltage (I-V) measurements are employed for mentioned parameters. It is seen that sample with 60 Å TiO_2 interfacial layer is a more ideal diode. It is seen that as thickness of TiO_2 interface decrease Ag/TiO_2/n-InP Schottky diode becomes more ideal. This result is explained in main text in connection with series resistance, difference between d-spacings of interface and wafer. Comments on relation of lattice mismatch with series resistance are also made.

Keywords Schottky · Structural · Electrical · n-InP · TiO_2

1 Introduction

Investigation of electric and structural properties of solid-state materials started in the beginning of 1800 s. As a result of these investigations and experiments these materials are classified according to their electric conductivity. This classification is made in terms of carrier densities (holes and electrons) in valance and conduction bands of solid-state materials. Band gaps, regions without electrons, maintains data on type of material and helps to classify them as conductor, semiconductor or insulator. Band structure of a material gives light to its electric, magnetic and optic properties.

In semiconductors, forbidden region between valance and conduction bands is very narrow and current can be created with a small external energy. Conductivity of semiconductor material is dependent on electric field, impurity, temperature, magnetic field and intensity of luminance.

Because electric properties of semiconductors can be modified by doping impurities to crystal structure or applying external light and electric field, devices made up of semiconductors can be used for amplification, trigger circuits or energy conversion. By adding different type of materials and combining doped semiconductors with different properties, diodes and transistors are constructed. These devices are fundamentals of modern electronics.

Electronic technology today includes use of semiconductor materials. For instance, in laptops, scanners, cell phones etc. mass production of semiconductor integrated circuits is obliged. By high technology, in electronics industry semiconductors are investigated after combining with metals. Combination of semiconductor and metal is called as Schottky diode. Schottky diode is an electronic combination also known as barrier diode. It is used commonly as a rectifier in radio frequency and power applications. Schottky diode is a semiconductor diode which has a small voltage drop in forward bias. This small voltage drop gives opportunity to faster triggering and better system efficiency.

Also, Schottky barrier diodes form base of photodetectors, solar cells and metal-semiconductor transistors [1, 2]. Two of the fundamental properties of Schottky barrier diodes are barrier height (ϕ_B) and ideality factor (n). Value of ϕ_B is dependent on combination of metal and semiconductor [3].

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Metal-semiconductor contacts formed by using InP semiconductor have less stability level according to other contacts formed with different semiconductors because of low barrier height and large reverse bias leakage current[4]. In order to overcome this instability problem surface passivations are made with different solutions. As a result of these passivations more optimised surfaces are gained [5]. After these experiments contact studies with InP semiconductors are made by forming an interface layer between metal and semiconductor layers [6]. Korucu et al. noticed that in Au/n-InP Schottky barrier diodes ideality factor decrease and barrier height increase with increasing temperature. They attributed this result to inhomogenities in barrier height, interface states and effect of series resistance.

There are a few studies for both electrical and structural properties of Schottky structures. For example Reddy et al. investigated No/n-GaN Schottky diodes and found that interface could be the reason for degradation of Schottky diode [7]. Here No is Nobelium a synthetic chemical element with atomic number 102.

TiO_2 (Titanium di oxide) is a metal oxide formed by combination of Ti(Titanium) and oxygen. It is used in optic ϕ applications with its wide band gap (3 eV) and high refractive index ($n = 2.3$).It is frequently used in solar panels, self-cleaning surfaces, treatment of cancer, photovoltaic devices. One more advantage of TiO_2 is low cost and easy production. The photocatalytic properties of titania (TiO_2) have prompted research utilising its useful ability to convert solar energy into electron–hole pairs to drive novel chemistry[8–10].

In this study TiO_2 is used as interface layer. Both structural and electric properties of *Ag/TiO_2/n-InP/Au* Schottky barrier diodes are investigated. The reason why TiO_2 is choosen as an interface is that it has transparent property and samples in this study may be examined in terms of photvoltaics for coming investigations.

2 Experimental

In this study Ag/TiO_2/n-InP/Au Schottky structure is constructed by using sputtering method on chemically cleaned n-InP semiconductor. The reason why sputtering technique is choosen is that it is more convenient to form TiO_2 by using this technique because of its condition of formation of such structures [11]. n type InP semiconductor crystal is used with (100) orientation, 500 µm thickness and 3.13×10^{18} cm^{-3} carrier density as a wafer. At first step n-InP crystal is cut with a diamond cutter and two wafers are formed. Ohmic contact is formed on rough side of the samples. TiO_2 thin film is grown on polished side of the wafers with 60 Å and 120 Å thicknesses and two different samples are gained. In the following sections of this study, samples with 60 Å and 120 Å thicknesses will be mentioned as sample A (S.A) and sample B (S.B), respectively (Fig. 1).

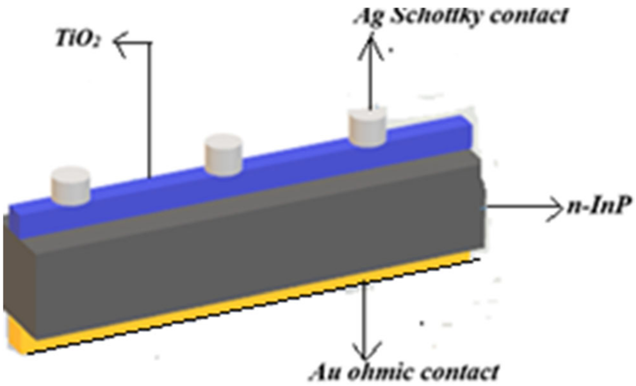

Fig. 1 Schematic diagram of Ag/TiO_2/n-InP/Au Schottky barrier diode

2.1 Cleaning Procedure

In order to construct a well optimised MS diode qualified and chemically well cleaned crystals should be used. Wafers are cleaned chemically in ultrasonic bath to remove organic and heavy metal impurities on their surfaces by following different steps. During cleaning of wafers deionised water (18.3 MΩ) (DIW) is used. Because cleaning of wafers and other experimental tools is very important to form a good performance Schottky diode all chemical operations are made very sensitively. In cleaning prosedure ordered steps are followed:

- All glass beakers and tweezers are cleaned with DIW and dried in high temperature oven.
- Steps during cleaning of iron mask, tweezers and wafers (n-InP) are given below:
- Washing in ultrasonic bath with triclor etile for 5 min.
- Rinsing with DIW.
- Washing in ultrasonic bath with acetone for 5 min.
- Rinsing with DIW.
- Washing in ultrasonic bath with methanole for 5 min.
- Rinsing with DIW.
- At the end of rinsing, in order to remove natural oxide layer on the surface wafers are waited in (1:10) HF + H_2O solution for 30 s.
- Rinsed with DIW.
- Tweezers, masks and wafers are dried in high purity N_2 atmosphere.

2.2 Formation of Ohmic Contact

After chemical cleaning and drying operations, in order to form Au ohmic contact on the rough side of wafers, samples are attached to sputtering system. System is vacumed to (2×10^{-6} Torr). Pure Au (%99.995) is sputtered on rough side of wafers with a thickness of 150 nm. During this sputtering operation temperature is kept constant at 80 ^{0} C. To form ohmic contact samples are annealed at 325 ^{0} C for 4 min.

Sputtering system operates as follows: wafers are put in sputtering system. Air in sputtering system is vacumed until desired pressure. Target metal is charged negatively. An electric field occurs with this negative charging resulting with a plasm medium. Positively charged gas ions comes out in this plasm medium and they hit the target metal with a big momentum. Atomic particles of target metal leaves it as a result of momentum transfer. These atomic particles pass through vacuum region and they stick on wafer surface.

2.3 Formation of Schottky Contact

In O_2 atmosphere Ti is sputtered on polished side of samples. 60 Å and 120 Å thick TiO_2 thin films are formed on polished sides of samples. Ag is coated on this interface with sputtering method with a thickness of 1500 Å to form Schottky contacts. During coating procedure an iron mask is used to gain 1mm radius diodes.

3 Results and Discussion

X-ray analysis of both samples are made with Bruker D8-Discover HRXRD device that contains Ge(220) oriented four crystal monocromator and X-ray source tube that produce 1.540 Å $CuK_{\alpha 1}$ wavelength X-rays. w- 2θ scanning of both samples are made for (002) plane. In Fig. 2 X-ray diffraction patterns for S.A and S.B can be seen.

In literature in classical calculations, 2θ angle is kept constant and rocking curve results are used by detecting θ angle [12–14]. But many factors are effective in optimising rocking curves. Surface bending, adjusting sample height, azimutual modifications are some of the modifications needed to be optimised. Making device adjustments crystolographically well, optimisation based errors can be reduced and parameters of samples can be gained accurately [15].

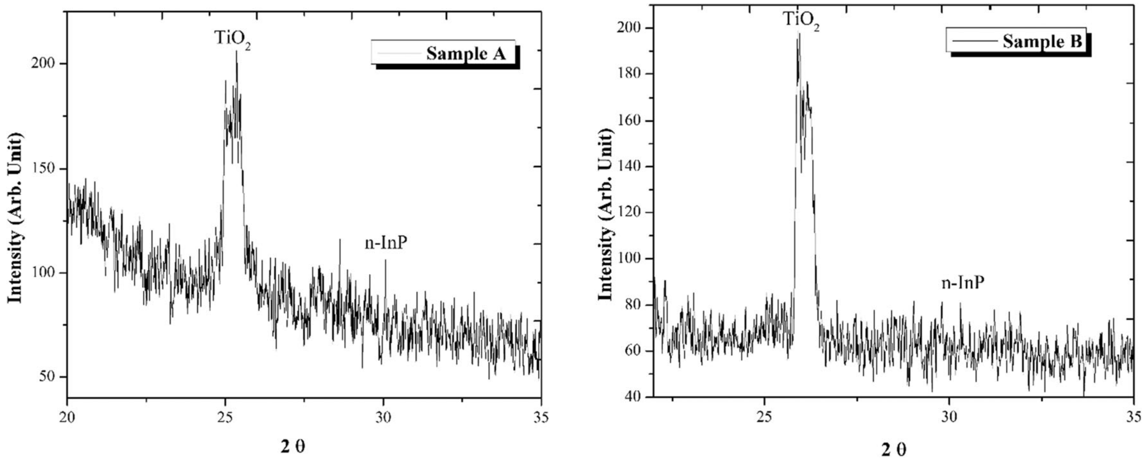

Fig. 2 XRD patterns for S.A and S.B

As can be seen in Fig. 2 for S.A peak positions of n-InP and TiO_2 are determined as 30.068 and 25.368 respectively. Full width at half maximum (FWHM) values are found as 0.02 for both layers in S.A. The same parameters for S.B are determined as 30.308 and 25.898. FWHM values for S.B are 0.04 and 0.089 for n-InP and TiO_2 layers respectively. FWHM values and peak positions are determined with peak analysis method by using a convenient software. As can be noticed if thickness of interface increase there is a positive shift in peak positions. So thickness of interface effects Bragg reflections. This situation may stem from lattice condensation with increasing thickness. Thickness of TiO_2 thin film interfaces are not determined with a private method. They are adjusted as growth conditions in sputtering device and aproximate values.

In Fig. 3 variation of FWHM versus 2-theta plot can be seen. As can be seen in Fig. 3 there is a shift in FWHM values dependent on 2-theta with increasing interface thickness. Shift in TiO_2 layers is larger than n-InP layers. This may be because n-InP wafer is a template.

Crystallite size and d-spacing of n-InP and TiO_2 layers are determined by using Bragg formula and Scherrer method. In order to apply Scherrer method safely, FWHM value should be determined accurately [16].

Crystallite size normal to reflective planes D can be gained by using Eq. (1)

$$D = \frac{k\lambda}{\beta_{hkl}\cos\theta} \rightarrow \cos\theta = \frac{k\lambda}{D}\left(\frac{1}{\beta_{hkl}}\right) \quad (1)$$

Here k is a coefficient, λ is wavelength of X-ray and θ is Bragg angle. d- spacing can be determined by using classic Bragg formula given in Eq. (2).

$$2d\sin\theta = n\lambda \quad (2)$$

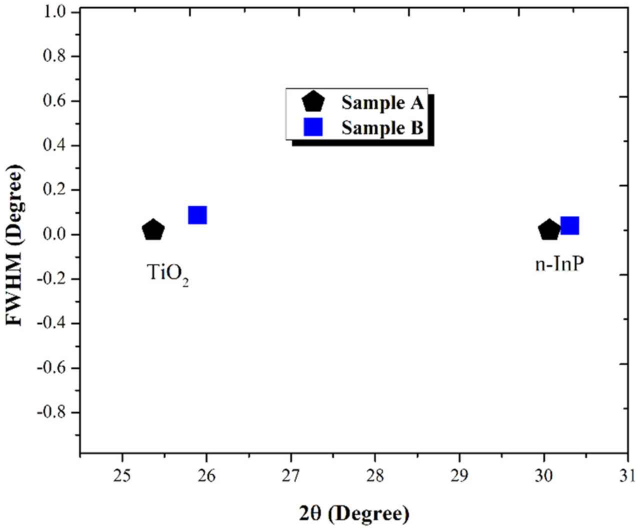

Fig. 3 Variation of FWHM with 2-theta for S.A and S.B

If we insert 1 in n we found d-spacing of atoms in lattice in other words we determine first degree reflection result. Results gained from these two equations are given in Table 1 for n-InP and TiO_2 layers.

All values gained for these two samples are in good accordance with previous works done by different researchers in literature. Also micro-strain values for both n-InP and TiO_2 layers are calculated for S.A and S.B by using Eq. (3) [16].

$$\varepsilon = \frac{\beta_{hkl}}{4\tan\theta} \tag{3}$$

Strain is a result of imperfect crystal structure. In Eq. (3) ε is root mean square (RMS) value of micro strain. Micro strain values are determined as 0.0086 and 0.0105 for n-InP and TiO_2 layers in S.A. For S.B micro strain values are determined as 0.017 and 0.045 for n-InP and TiO_2 layers respectively.

Here strain is assumed as uniform in all crystolographic orientations. It is assumed that crystal is isotropic and all parameters are independent of measured plane.

Dielectric (oxide) layer between metal and semiconductor converts metal-semiconductor (MS) structure to metal-insulator-semiconductor (MIS) structure. As thickness of this interfacial layer increase interface states starts to be in equilibrium with semiconductor. This situation effects structural parameters, interfacial layer, interfacial states and current-voltage (I-V) characteristics. Various current conduction mechanisms such as termionic emission (TE), diffusion, termionic field emission (TFE) may be effective in Schottky structures [17]. For this reason it may be difficult to explain I-V characteristics. I-V plot can be seen in Fig. 4.

Table 1 Particle size and d-spacings of n-InP and TiO2 layers in S.A and S.B

(nm)	Particle size	S.A d-spacing	Particle size	S.B d-spacing
n-InP	80.063	1.537	80.258	1.526
TiO_2	76.687	1.798	77.027	1.763

In ideal Schottky diodes, current conduction mechanism obeys TE model unless applied voltage is not too high. According to this model current can be defined as in Eq. (4).

$$I = I_o\left[\exp\left(\frac{qV_D}{kT}\right) - 1\right] \tag{4}$$

Here V_D is the potential difference on diode, k is Boltzman constant, T is temperature in Kelvin and I_o is saturation current. I_o can be defined as in Eq. (5).

$$I_o = AA^*T^2\exp\left[\frac{-q}{kT}\phi_B\right] \tag{5}$$

Here A is diode area, A* is effective Richardson constant and Φ_B is barrier height [17]. By using Eqs. (4) and (5) $Ln(I) = Ln(I_o) + V_D$ is gained. This is a mathematical definition of a line. Slope of this line gives ideality factor (n). In forward bias region of I-V plot slope of linear part is defined as $\tan\theta = q/nkT$, so ideality factor can be determined with Eq. (6).

$$n = \frac{q}{kT\tan\theta} \tag{6}$$

Saturation current can be gained from y axis intercept point of semi-logarithmic Ln(I)-V plot. Barrier height Φ_B can be calculated with Eq. (7) [17].

$$\phi_B = \frac{kT}{q}Ln\left(\frac{AA^*T^2}{I_o}\right) \tag{7}$$

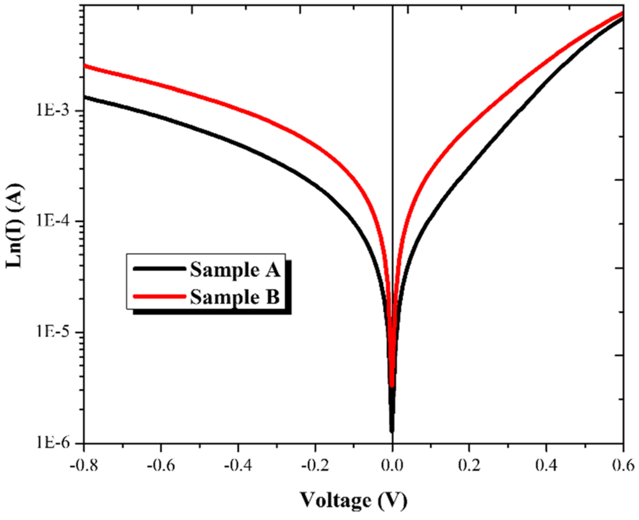

Fig. 4 Ln(I) vs. Voltage plot for S.A and S.B

Ideality factors (n) are determined as 1.39 and 1.41 and barrier heights (ϕ_B) are determined as 0.52 eV and 0.50 eV for S.A and S.B respectively at room temperature. It is desired that ideality factor is near 1 and barrier height is high for an ideal Schottky diode [9]. So S.A is a more optimised diode. In practice there is no diode with ideality factor equal to 1. Because of oxide layer at interface applied voltage effects barrier height [18–21]. Series resistance and shunt resistance are important parameters in Schottky barrier diodes. They are determined as 88 Ώ-1048 Ώ and 78 Ώ-4018 Ώ for 60 Å and 120 Å TiO_2 interface layer thickness, respectively by the help of Ohm's law from I-V measurements.

4 Conclusions

In this study, both structural and electrical properties of Ag/TiO_2/n-InP/Au Schottky barrier diodes are investigated. In structural terms, particle size, d-spacing and microstrain are determined by using data from XRD pattern. Results are given in Table 1 and in main text. In electrical terms from I-V plot ideality factors and barrier heights of samples are determined. It is seen that S.A is a more optimised diode. As thickness of TiO_2 interface decrease diode became more optimised. The reason for this may be series resistance effect that can be seen in bending of forward bias region in Fig. 4. Difference between d-spacings of TiO_2 and n-InP layers for S.A is 0.261 nm and 0.237 nm for S.B. This situation implies that there is larger lattice mismatch between TiO_2 and n-InP layers in S.A. Lattice mismatch may be responsible for decreasing or increasing series resistance along the sample. Vibrating atoms and electron cloud around them may produce extra electric fields on path-way of carriers and gives hand to inhomogeneous barrier height in Schottky structures.

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Declarations

Conflict of Interest We declare that there is no conflict of interest for this study.

Compliance with Ethical Standards During formation of this article we obeyed ethical standarts.

Consent to Participate All authors are consent to participate for this study.

Consent for Publication We declare that we are consent to publish this research article.

References

1. Ates A, Saglam M, Guzeldir B, Yildirim MA, Astam A (2010) The electrical characteristics of cu/cus/p-si/al structure: An Experimental study. J Optoelectron Adv Mater 12(7):1466–1471
2. Aydogan S, Saglam M, Turut A (2005) Current-voltage and capacitance-voltage characteristics of polypyrrole/p-inp structure: An Experimental study. Vacuum 77(3):269–274
3. Tung RT (2000) Comment on numerical study of electrical transport in homogeneous schottky diodes: An Experimental study. J Appl Phys 88(12):7366–7367
4. Cakici T, Guzeldir B, Saglam M (2015) Temperature dependent of electrical characteristics of au/n-gaas/in schottky diode with in2s3 interfacial layer obtained by using spray pyrolysis method: An experimental study. J Alloy Compd 646:954–965
5. Iyer R, Lile DL (1991) Role of polysulfides in the passivation of the inp surface: An experimental study. Appl Phys Lett 59(4):437–439
6. Ayyildiz E, Cetin H, Horvath ZJ (2005) Temperature dependent electrical characteristics of sn/p-si schottky diodes: An Experimental study. Appl Surf Sci 252(4):1153–1158
7. Reddy R, Ramesh K, Choi C (2006) Structural and electrical properties of Mo/n-GaN Schottky diodes: An Experimental study. Pss Appl Mater Sci 203(3):622–627
8. Ben I, Chaabouni F, Ranguis A (2020) Cr doping effect on the structural, optoelectrical and photocatalytic properties of RF sputtered TiO_2 thin films from a powder target: An Experimental study. J Alloys Compd 825. https://doi.org/10.1016/j.jallcom.2020.153988
9. Güzelçimen F, Tanören B, Çetinkaya Ç, Kaya M, Efkere H, Özen Y, Bingöl D, Sirkeci M, Kınacı B, Ünlü M, Özçelik S (2020) The effect of thickness on surface structure of rf sputtered TiO_2 thin films by XPS, SEM/EDS, AFM and SAM: An experimental study. Vacuum 182. https://doi.org/10.1016/j.vacuum.2020.109766
10. Daughtry J, Alotabi S, Fabretto H, Andersson G (2021) Composition and properties of RF-sputter deposited titanium dioxide thin films: An Experimental study. Nanoscale Adv 3(4):1077–1086
11. Kars İ, Çetin S, Kınacı B, Sarıkavak B, Bengi A, Altuntaş H, Öztürk M, Özçelik S (2010) Influence of thermal annealing on the structure and optical properties of d.c. magnetron sputtered titanium dioxide thin films: an Experimental study. https://doi.org/10.1002/sia.3373
12. Öztürk MK, Yu H, Sarıkavak B, Korçak S, Özçelik S, Özbay E (2010) Structural analysis of an InGaN/GaN based light emitting diode by X-ray diffraction: an experimental study. J Mater Sci Mater Electron 21(2):185–191
13. Öztürk MK, Altuntaş H, Çörekçi S, Hongbo Y, Özçelik S, Özbay E (2011) Strain-stress analysis of AlGaN/GaN heterostructures with and without an AlN suffer and Interlayer: an experimental study. Strain 47(s2):19–27
14. Kisielowski C (1999) Strain in GaN thin films and heterostructures. Semicond Semimetals 57(GaN II):275–317
15. Baş Y (2015) $In_xGa_{1-x}N$ (x = 0,075; 0,090; 0,100) Mavi LED'lerin Mikroyapısal Kusurlarının Ters Örgü Uzay Haritası İle İncelenmesi: Doctoral thesis. Gazi Üniversitesi Fen Bilimleri Enstitüsü, Ankara, 1, 2, 9, 12, 14, 15, 16, 24, 25, 28, 34, 35, 45, 46, 55

16. Singla G, Singh K, Pandey O (2013) Williamson–Hall study on synthesized nanocrystalline tungsten carbide (WC): An Experimental study. Appl Phys A 113(1):237–242
17. Bilgili AK, Güzel T, Özer M (2018) Current-voltage characteristics of Ag/TiO2/n-InP/Au Schottky barrier diodes: an experimental study. J Appl Phys 125:035704. https://doi.org/10.1063/1.5064637
18. Sze SM (1981) Physics of semiconductor devices: a book, 2nd edn. Willey, New York, pp 245–300
19. Cowley AM, Sze SM (1965) Surface state and barrier height of metal-semiconductor systems: a book. J Appl Phys 36:3212–3216
20. Brillson LJ (1982) The surface and properties of metal-semiconductor interfaces: a book. Surf Sci Rep 2:123–326
21. Passlack M, Hunt NE, Schubert E, Zydzik G, Hong JP (1994) Dielectric properties of electron-beam deposited Ga2O3 films: a letter. Appl Phys Lett *l* 64:20