IJESRT
INTERNATIONAL JOURNAL OF ENGINEERING SCIENCES & RESEARCH TECHNOLOGY

THE EFFECT OF CHANGING MASS DENSITY OF IMPURITIES ADDED TO TIO2-MEH ON CURRENT AND ENERGY GAP VALUES

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DOI: 10.5281/zenodo.843926

ABSTRACT

TiO_2-MEH thin filmhas been grown onto glass substrate at room temperatureby spin coating and doped with $CaSO_4$, $CuCO_3$ and La_2O_3. The current – voltage relation for the four samples were studied. It was found that at a certain voltage the current decreases as the density increases. This may be due to the fact that the density increasing, increases resistance and decreases current. The energy gap is also shown to be affected by the density. When the impurities were added the increase of free charge carriers causes the Fermi level to move and jump from the energy gap 2.216 to 3.721 eV. Then upon increasing the mass density to be 2.69, 4.35 and 6.51 g/cm^3 the energy gap decreases to be 3.721, 3.295 and 2.15 respectively. This decreasing may be related to the fact that, according to tight binding approximation, the density increases, increases the width of energy band, which in turn decreases the energy gap

KEYWORDS: Mass density, energy gap, Fermi level, tight binding, approximation, energy band.

I. INTRODUCTION

In general terms, there are three different types of PV devices: the organic,inorganic and the organic-inorganic hybrids(combination of the conjugated polymer and inorganic nanoparticles). As none of these kindof PV cells completely matches the solar spectrum. Blending polymer is useful to control the electrical properties, increasing the photo luminance efficiency and the charge transport properties can also be enhanced [1]. The term "band gap" refers to the energy difference between the top of the valence band to the bottom of the conduction band The measurement of the band gap of materials is important in the semiconductor, nanomaterial and solar industries.The bandgap is important as it determines theportion of the solar spectrum a photovoltaic cell absorbs. To improve the efficiency of solar cells one can use layers of different materials with different bandgap properties.The optical band gap E_g can be experimentally obtained from absorption coefficient[2].Spin coating is a technique employed to coating a flat surface by a thin liquid film facilitated by a fast rotation of the surface. Several processing parameters involved in the spinning process such as spin speed, final film thickness, solution viscosity, spin time, etc. [3]. Faced with high and rising energy prices, limitations in energy supply, and growing concerns about climate changes and their environmental- and health-related effects,

currently the total global energy consumption of oil, coal, natural gas, nuclear and hydropower, etc., is estimated to be about some 12000 million ton oil equivalents per year. To put this number in perspective, one could note that it is about twelve times larger than the total value of the all renewable energy market. The economics of renewable energy and energy savings is a challenging subject, fraught with risks but also noteworthy for its new opportunities. . Solar energy is one of the renewable energy resources. About 8.6× 10^{16} watts of solar radiation

ISSN: 2277-9655
Impact Factor: 4.116
CODEN: IJESS7

reaches lands and oceans, illuminating and heating the earth. If we could capture only 0.02 percent of that energy, we could solve energy problems. solar cells were mostly used to supply energy for space satellite or to provide power for small electronic devices Polymer solar cells have a potential advantage, which is much thinner than traditional silicon solar cells and their ability to be produced from solution. This means that they can be printed or coated on glass, metal foils or plastics, instead of using expensive vacuum deposition as for traditional silicon solar cells. The optical absorption coefficient of organic molecules is high, so a large amount of light can be absorbed with a small amount of materials, usually on the order of hundreds of nanometers.

In this work TiO_2-MEH is deposited and doped with different impurities. The materials used are exhibited in section two, result and discussion is in section three and conclusion is in section four.

II. MATERIALS AND METHOD

The first simulation structure procedure used in this work is a double layer device; typically consisting of the poly[2-methoxy-5-(2'ethylhexyloxy)-1,4-phenylenevinyl-ene] (MEH-PPV) polymer sandwiched between an anode usually TiO_2 substrate, and Ag as cathode, in the second structure procedure ; we replaced MEH by MEH+$CaSO_4$, MEH+$CuCO_3$ andMEH+La_2O_3[4]. The samples were prepared using the spin coating method.The films deposited on a glass slides, which were cleanedwith distilled water and acetone .Firstly TiO_2 was deposited on the glass substrates and then the layers of MEH and MEH blending with $CaSO_4$, $CuCO_3$and La_2O_3were deposited on to TiO_2.The UV-VisSpectrophotometer was used to measure the absorption for prepared thin films, the optical parameters were calculated such as,band gap andabsorption.Organic polymer light emitting diodes have potential impact in solid state lighting and flat panel display because of their advantage of low power consumption, low cost and easymanufacturing impure[9].Titanium dioxide (TiO_2) is considered very close to an ideal semiconductor for photo catalysis becauseof its high stability, low cost and safety toward both humans and the environment [5]. MEH-PPVit'ssoluble in common organic solvents, in conjunction with a low operating voltage for light emission and relatively high conversion efficiency [6]. La_2O_3 is Rare earth oxide. It's a semiconductor material with a band bap of 4.3 eV. It has the lowestlattice energy[7]. $CaSO_4$ is one of the well-known compoundsemiconductors suitable to be used as host matrix forlarge variety of dopants[8].

III. RESULTS AND DISCUSSION

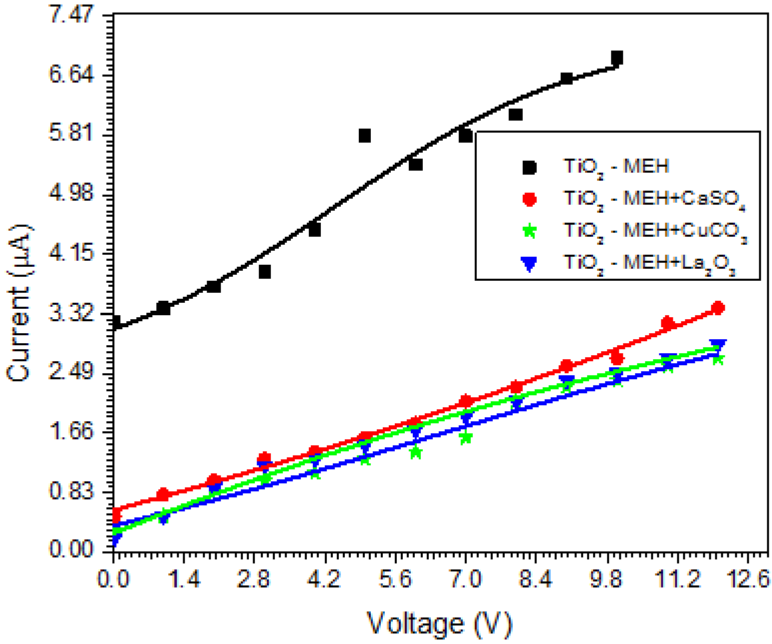

Fig. (1):I-V for TiO_2-MEH alone and when doped

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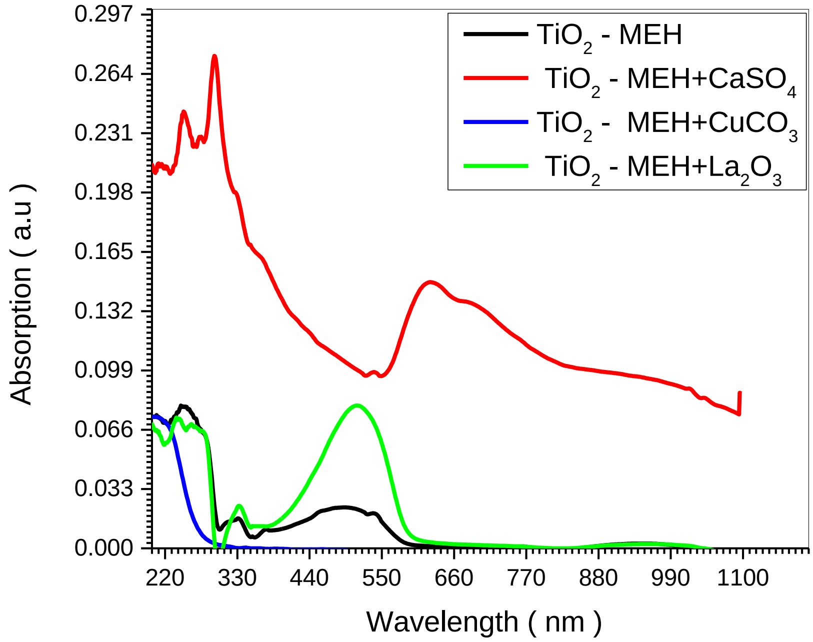

Fig.(2) : Absorption against wavelength for TiO_2-MEH alone and when doped

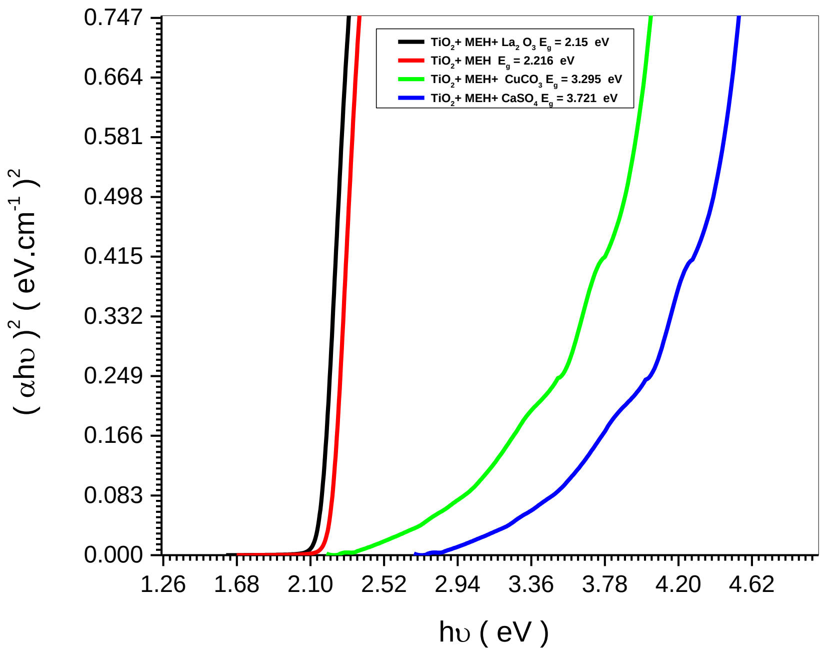

Fig. (3) : $(\alpha h\nu)^2$Vs. $h\nu$ for TiO_2-MEH alone and when doped

TheI-V characteristic curve for TiO_2 – MEH binary layer when it is alone and when doped with $CaSO_4$, $CuCO_3$ and La_2O_3 with densities 2.69, 4.35 and 6.51 g/cm^3. For a given voltage the current decreases up on increasing the density of impurities. For zero density of impurities the current is very high then decreases up on increasing the density. This may be attributed to the fact that increasing density increasing ohmic resistance (R), thus decreases the current (I), according to the relation[9]:

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$I = \frac{V}{R}$ (1)

The increase of resistance due to density increase can be found by treating the medium through which free carriers move as a fluid of viscosity (η) and by treating charges as droplets of radius (a) and speed (v), the equation of motion of charges for uniform motion under the action of electric field intensity (E) is given by:

$m\ddot{x} = eE - 6\pi\eta av = 0$ (2)

Thus

$v = \frac{e}{6\pi\eta a}E$ (3)

The current density (J) is thus given by:

$J = nev = \frac{ne^2}{6\pi\eta a}E = \sigma E$ (4)

The viscosity can be given in terms of matter density$\rho_\circ$, velocity v and mean free path $L_\circ$ to be

$\eta = \frac{\rho_\circ}{2}L_\circ v$ (5)

Thus the resistance R takes the form :

$R = \frac{\rho L}{A} = \frac{1}{\sigma}\frac{L}{A} = \frac{6\pi a\eta}{ne^2} = \frac{3\pi aL_\circ v\rho_\circ}{ne^2} = c_\circ\rho_\circ$ (6)

This indicates clearly that increasing matter density increases resistance, which decreases current according to equation (1) where

$I = \frac{V}{c_\circ\rho_\circ}$ (7)

This equation can easily explain Fig(1) where increasing density by an amounts 0, 2.69, 4.35 and 6.51 g/cm^3 decreases the current (I).

The absorption spectra and the energy gap curves in figures (2) and (3) shows that increasing the density of the bulk doped TiO_2-MEH due to the increase of $CaSO_4$, $CuCO_3$and La_2O_3 concentrations which are 2.69 , 4.35 and 6,51 g/cm^3 respectively causes the energy gap E_g to decrease to take the values 3.721, 3.295 and 2.25 eV respectively. This may be explained by using light binding approximation, where the energy E_n of electrons in band n is given by[10,11]:

$E_n = \alpha_n + \gamma_n \cos ka$ (8)

The maximum electron energy E_+ and the minimum values E_- are given by:

$$E_+ = \alpha_n + \gamma_n \quad E_- = \alpha_n - \gamma_n \qquad (9)$$

For cos = ± 1 (10)

Thus the band width of band n is given by :

$\Delta E_n = E_+ - E_- = 2\gamma_n = 2\langle\emptyset_i|H_{cry}|\emptyset_m\rangle$ (11)

Where H_{cry} is the crystal field energy which can be affected by the concentration and density of the impurities which are in the form of ions. Thus increasing density so increasing the electric field generated by it which increases the crystal field energy H_{cry}, which in in turn increases γ and ΔE_n respectively i-e

$\Delta E_n \sim \gamma_n \sim H_{cry} \sim \rho_\circ$ (12)

If one assume the center of the bands are at constant distances E in the energy space. Thus

$$E = \Delta E_{n1} + \Delta E_{n2} + E_g$$

$E_g = E - \Delta E_{n1} - \Delta E_{n2} = E - 2\gamma_{n1} - 2\gamma_{n2}$ (13)

This means according to equations (12) and (13) that

$Eg \sim E - 4\rho_\circ$ (14)

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Impact Factor: 4.116
CODEN: IJESS7

This means that increasing the density decreases the energy gap. The fact that introducing doping TiO_2-MEH with impurities increases $E_g$from 2.216 eV to3.721 eV may be due to the fact that these impurities increases free carriers concentrations (n),which increases Fermi energy E_F, where[12,13]

$$E_F = \frac{h^2}{2m}\left(\frac{3n}{\gamma\pi}\right)^{2/3} \quad (15)$$

For conductors, and it takes the form

$$E_F = \frac{E_1+E_2}{2} + \frac{KT}{2}\ln\frac{4nd}{c_\circ} \quad (16)$$

For semiconductors. This means that introducing impurities in TiO_2-MEH causes E_F to increase and jump from one narrow forbidden band E_g ~ 2.216 eV to a wider one 3.721 eV but once E_F jump to the wider one it tend to decrease up on increasing $\rho_\circ$ according to tight binding model .

IV. CONCLUSION

The TiO_2-MEH binary layer electric characteristics are affected by different massdensity of impurities. The mass density increasing; decreases current and energy gap values.

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CITE AN ARTICLE

Abdallah, M. D., Elmahdi Said, T. M., H, A. S., & Elhouri Ahmed, S. A. (2017). THE EFFECT OF CHANGING MASS DENSITY OF IMPURITIES ADDED TO TIO2-MEH ON CURRENT AND ENERGY GAP VALUES. *INTERNATIONAL JOURNAL OF ENGINEERING SCIENCES & RESEARCH TECHNOLOGY*, *6*(8), 258-562. Retrieved August 16, 2017.