Investigation of Optimum Transparent Conductive Oxides (TCOs) for CdS:O/CdTe Thin Film Solar Cells (TFSCs) from Numerical Analysis.

M S Sadek.
Dept. of Information and Communication Engineering, Southeast University.

Abstract

Transparent Conductive Oxides (TCOs) are an increasingly important component of solar cells, where they act as front electrode elements. The structural templates, diffusion barriers and their work function controls the open circuit voltage ($V_{oc}$). In this paper, various transparent conductive oxide materials have been studied which are used as the front surface contacts of CdS:O/CdTe based thin film solar cells. Various electrical and optical parameters like work function, thickness, temperature etc., of some common transparent conductive oxides materials such as ZnO, FTO, SnO$_2$, AMPS-1D, Efficiency, Temperature, are studied. The main idea was to find an optimum conductive oxide layer for CdTe solar cell which shows the great potential in thin film area of solar cell. All the analysis was done by using the widely used simulator Analysis of Microelectronic and Photonic Structures (AMPS 1D). It was observed that both SnO$_2$ and ZnO show similar performance under various conditions. Indium Tin Oxide (ITO) has shown the worst performance among them in all conditions. Fluorinated Tin Oxide (FTO) looked promising match for CdTe solar cells in some conditions.

Introduction:

Cadmium Telluride (CdTe) is a promising material for solar cells as it has an ideal energy band gap ($E_g$) of 1.45 eV and larger absorption coefficient (>5×10$^7$/cm) [M. Hadrich et al., J. Britt et al.]. The polycrystalline CdS was found to be the best-suited hetero-junction n-type partner with p-type CdTe absorber for CdS/CdTe solar cell. Small-area CdTe cells already achieved efficiency of 16.5% in laboratory and commercial modules have achieved efficiency of 10% [X. Wu et al.]. CdTe solar cells use Transparent Conductive Oxides (TCO) as the front contact which is optically transparent and electrically conductive materials. [Hecht, D. S et al.]

Major considerations in the choice of the TCO for the solar cell, besides the conductivity and transparency, are electronic compatibility with the adjacent layers in the cell, processing requirements, and stability under environmental conditions. A carrier concentration on the order of 10$^{20}$ cm$^{-3}$ or higher and a band gap energy above 3eV are usually for high conductivity. As with all transparent conducting films, a tradeoff must be done between the conductivity and transparency, since increasing thickness and the carrier concentrations will increase the conductivity, but decreases the transparency.

Features of TCO:

TCO for solar cell applications have been fabricated from both inorganic and organic materials. In case of organic solar cells, the TCO is made up of a layer of mostly Indium Tin Oxide (ITO), Fluorine doped Tin Oxide (FTO), doped Zinc Oxide (ZnO), SnO$_2$ etc.

In order to be employed for large scale PV design, the basic characteristic features of a TCO material should be –

- High transparency in visible light and more than that to enhance efficiency.
- High conductance.
High carrier mobility.
- Excellent long term stability.
- Low cost.
- High throughput deposition.
- Capable of some sorts of light trapping.
- Some may require device specific properties.

**Different TCOMaterials:**

There are many different materials which are extensively used in solar cells as the front contact. Among them Indium Tin Oxide (ITO) is most widely used for different devices because of its two main properties, its electrical conductivity and optical transparency as well as the ease of deposition methods like Physical Vapor Deposition, Electron beam evaporation and sometimes sputter diffusion. ITO is a heavily doped n-type semiconductor with a bandgap of around 4eV. [Kim, H.; Gilmore et al.]

The distinguishable property of ITO is its chemical resistance of moisture. Because of its bandgap, it is mostly transparent in the visible part of the spectrum and its extinction coefficient in this wavelength range is zero. In the UV region, it is opaque, so it has non-zero k due to band to band absorption, similar as NIR and IR region of the spectrum.

ITO has some inherent drawbacks due to which novel alternative materials are searched for. High costs, limited resource of Indium in the earth’s crusts, the fragility and also the lack of flexibility puts a limit on the uses of ITO. Moreover, costly fabrication techniques requiring vacuum arrangements are added limitations of ITO. [Fortunato, E. et al.] So cheaper alternatives such as SnO₂, ZnO, Fluorine doped Tin Oxide (FTO) are most widely used for thin film solar cells.

Doped zinc oxide (ZnO) and SnO₂ films have received increasing interest in recent years since they combine the common properties of TCO, i.e. high conductivity and excellent transparency, with low cost, low toxicity, easy fabrication and patterning [Granqvist, C.G et al., Klinshirm, C.F et al.]. In particular, doped ZnO has become a valid alternative to the commonly used indium tin oxide (ITO) as TCO layer for silicon thin-film solar cells, being highly stable in a hydrogen plasma environment [Illiberi, A et al, Banerjee, R. et al., Minami, T]. SnO₂ is one of the best alternatives of ITO. In spite of their popularity, SnO₂ as well as ZnO has major drawbacks, the limited transparency in the infrared and the brittleness are the main concerns [Minami, T, Van Deelen, J. et al.].

![Transmittance spectrum of ZnO film deposited at 250°C and a DEZ partial pressure of 4.58 mbar. Inset: band gap as a function of carrier concentration.](image)

**Overview of CdS/CdTe Solar Cell:**

The polycrystalline CdS was found to be the best-suited hetero-junction n-type partner with p type CdTe absorber for CdS/CdTe solar cell but it has three main issues that limit device performance by limits the values of Vₜ₉ and FF [T.L. Chu et al.]
There is a crucial need for a higher band gap window material to further improve and overcome the limitations associated with the CdTe heterojunction solar cells. Oxygenated cadmium sulfide (CdS:O) seems to be a better candidate in this regard. However, the advantage of CdS:O window layer over the CdS has been reported elsewhere [Aminul Islam et al.]. Nano crystalline CdS:O is a promising window material as it has higher optical band gap (2.5-3.1 eV), a better lattice match with CdTe absorber and reduce inter-diffusion tendency at the PN junction [X. Wu, R. et al.]. Moreover, the formation of stable, low resistance back contact to p-CdTe is another well-known major challenge associated with the fabrication of efficient CdTe based solar cells. [Vinod K. Jain, et al.].

In this paper different CdS:O/CdTe cell structures with different transparent conducting oxides layers are simulated to find the optimum structure of CdTe based solar cells. Various factors associated with front contact such as the thickness, carrier concentrations, etc. are studied.

**Modelling and Simulation:**

In this work, one-dimensional Analysis of Micro-Electronics and Photonic System (AMPS-1D) simulator has been used to investigate the effect of different transparent conductive oxide layers, their thickness, temperature sensitivity, mobility are discussed in case of CdS:O and CdTe based solar cells. It is well known that the AMPS program has been developed to pragmatically simulate the electrical and optical characteristics of the thin film hetero-junction solar cells. It has been proven to be a very powerful tool in understanding device physics operation and physics for single crystal, poly-crystal and amorphous structures. To date, more than 200 groups worldwide have been used AMPS-1D for solar cell design [Hong Zhu, et al.].

A three-layer device model of a TCO/CdS:O/CdTe solar cell are investigated. The starting device structure was ITO/CdS:O/CdTe. Then I have changed the TCO layers to find out the optimum structure of the CdTe based solar Cell.

![Fig. 2 Simulated structure of CdS:O/poly-CdTe solar cell](image)

Then the TCO layers are changed by using different materials like ITO, FTO etc., and tries to find out the optimum TCO layers that best suit for the poly-crystalline CdTe based solar cell. Table 1 shows the description of all the parameters used in this analysis, these parameters were selected based on literature, theory, experimental data, or in some cases, reasonable estimation.

| parameters | TCOs | n-CdS:O | p-CdTe |
|------------|------|----------|--------|
| W (μm)     | ITO  | FTO      | SnO₂   | ZnO    | 0.1 | 1 |
| ε/ε₀       | 2    | 10       | 9      | 9      | 9   | 9.4 |
| μₐ(cm²/Vs) | 50   | 100      | 100    | 100    | 350 | 500 |
| μₔ(cm²/Vs) | 25   | 25       | 25     | 25     | 50  | 60  |
| n, p (/cm³) | 1.7e18 | 1.7e18  | 1.7e18 | 1.7e18 | 1e17 | 5e14 |
| Eₐ (eV)    | 3.60 | 4.20     | 3.35   | 3.35   | 2.75 | 1.50 |
| Nₑ (/cm³)  | 2.2e18 | 2.2e18 | 2.2e18 | 2.2e18 | 1.8e19 | 7.5e17 |
| Nᵥ (/cm³)  | 1.8e19 | 1.8e19  | 1.8e19 | 1.8e19 | 2.4e18 | 1.8e18 |
| ε (eV)     | 4.10 | 4.50     | 4.35   | 4.35   | 4.50 | 4.28 |
The band gap of CdS:O film is depends on the O<sub>2</sub>/Ar ratio in the film growth process, band gap increase with increase of O<sub>2</sub>/Ar ratio. X.wu and others have shown that band gap of CdS:O film increased from 2.42 eV to 3.17 eV for different O2 and Ar ratio as shown in Table-2.[X.wu, et al.].

| O<sub>2</sub>/Ar (%) | Optical band gap (eV) |
|---------------------|-----------------------|
| 0                   | 2.42                  |
| 1                   | 2.52                  |
| 2                   | 2.65                  |
| 3                   | 2.80                  |
| 5                   | 3.17                  |

In this work, the band gap of CdS:O window layer has been taken 2.75 eV to be in the middle of the range.

Results and Discussion:

The numerical analysis has been performed with the envision to detect the best suited transparent conductive oxides layers for polycrystalline CdTe based solar cell. The dependency of different TCO materials on the performance of the solar cell are investigated first by using AMPS-1D. Fig -3 shows the simulated efficiency of the solar cell design using different TCO layers, whose specification was given to the Table-I.

| TCO Material | J<sub>sc</sub> | V<sub>oc</sub> | FF | Efficiency (%) |
|--------------|----------------|--------------|-----|----------------|
| SnO<sub>2</sub> | 13.49          | 1.038        | 0.883 | 11.233        |
| ITO          | 11.33          | 1.035        | 0.883 | 9.856         |
| FTO          | 13.75          | 1.038        | 0.883 | 11.226        |
| ZnO          | 11.189         | 1.038        | 0.882 | 11.189        |

From the results, it is clear that SnO<sub>2</sub> is the best suited transparent conductive oxides for polycrystalline CdTe based solar cell in terms of efficiency is concern. It is worth noting that the open circuit voltage (V<sub>oc</sub>) and Fill Factor (FF) remains almost constant for every TCO materials. The short circuit current (J<sub>sc</sub>) changes significantly as the TCO material changes.
The most interesting fact is, indium tin oxide (ITO) which is the most usable conductive oxides, but it exhibits the worst performance according to the simulation results.

In real cases operating temperature plays a very vital part which affects the performance of the solar cells. At higher operating temperature, parameters such as the effective density of states, absorption coefficients, electron and hole mobility, carrier concentrations and band gaps of the materials are affected. An investigation has been done on $V_{oc}$ and $\eta$ of the final cell to understand the effect of temperature on CdS:O/CdTe cell with operating temperature range. The most prominent three TCO materials namely FTO, SnO$_2$, and ZnO are investigated and there are no significant changes are noticed.

In this simulation, operating temperature are varied from 273K to 333K. It is evident from the Fig -5 that the efficiency ($\eta$) shows the linear decreases at the gradient of $-0.25$/°K, with increase of operating temperature. This is the indicator of higher degree of stability of the cell at higher operating temperature or in stressed conditions. These results are in good agreement with related works [M. A. Matin, etal. D. Bonnet & H. Raben horst, M. Gloeckler, et al., Nowshad Amin, et al.].

Fig. 5 Temperature effect on the efficiency (%) of different TCO layers

Fig -6 shows the decrease of open circuit voltage of different TCO layers and similar types of linearly decreasing curves are obtained, which shows temperature stability of the cell. But both SnO$_2$ and ZnO shows better resistance against temperature. It is clear that, the open circuit voltage has a strong dependency on temperature because, if temperature increases, the band-gap of the material decrease and eventually leakage current is increased, which eventually decreases the open circuit voltage.
The thickness of different TCO layers are also investigated. In this case, three conductive oxides are taken and their thickness are varied from 100 nm to 800 nm. There is no significant change is observed as shown in the following figure.

**Fig. 7 Efficiency with the change of TCO layer thicknesses**

**Conclusion:**
In this numerical analysis, Cadmium Telluride (CdTe) based design of thin film solar cell which is the most prominent and most widely used thin film solar cell are taken with CdS being the window layer having lattice matched with the CdTe absorber. Different materials are used as the transparent conductive oxides (TCO) layers in order to find the maximum performance from the cell. It is obvious from the simulated results that, SnO$_2$ is the most suitable oxide layer for the cell providing the maximum efficiency about 11.233%. FTO and ZnO oxide layers also shows good performance resulting efficiency about 11.226% and 11.181% respectively. Temperature dependency of the open circuit voltage value is also a great concern. Because the device’s fill factor (FF) is a function of both open circuit voltage($V_{oc}$) and short circuit current density ($J_{sc}$) All of the oxides layers shows great resistance againstoperating temperature changes, which is the basic criteria for a good conductive oxide. The efficiency did not alter too much by thickness variation within a limited range.
References:

1. Aminul Islam, M. A. Matin, Yusuf Sulaiman and Nowshad Amin: In Proceeding of 1st International Conference on the Developments in Renewable Energy Technology (ICDRET) (2009), p.181.
2. Banerjee, R., Ray, S., Basu, N., Batabyal, A.K., Barua, A.K., “Degradation of tin-doped indium-oxide film in hydrogen and argon plasma,” J. Appl. Phys. 62, 912-916 (1987).
3. D. Bonnet & H. Raben horst, 9th IEEE PVSC, 1972, IEEE, NewYork, 1972, p 129.
4. Fortunato, E.; D. Ginley; H. Hosono; D.C. Paine (March 2007). "Transparent Conducting Oxides for Photovoltaics". MRS Bulletin 32: 242–247.
5. Granqvist, C.G., “Transparent conductors as solar energy materials: A panoramic review,” Solar Energy Mater.Solar Cells 91, 1529-1598 (2007).
6. Hecht, D. S; Hu, I. Irvin, G. "Emerging Transparent Electrodes Based on Thin Films of Carbon Nanotubes, Graphene and Metallic Nanostructures, 2011, Advanced Materials, 23, 1482"
7. Hong Zhu, Ali KaanKalkan, JingyaHou and Stephen J. Fonash: AIP Conf. Proc., vol. 462 (1999), p. 309.
8. Illiberi, A., Sharma, K., Creatore, M., van de Sanden, M.C.M., “Novel approach to thin film polycrystallinesilicon on glass”, Materials Letters 63 (21), 1817-1819 (2009).
9. J. Britt, C. Ferekides: Applied Physics Letters, vol. 62 (1993), p. 2851.
10. Kim, H.; Gilmore, C. M.; Piqué, A.; Horwitz, J. S.; Mattoussi, H.; Murata, H.; Kafafi, Z. H.; Chrisey, D. B. (1 December 1999). "Electrical, optical, and structural properties of indium–tin–oxide thin films for organic light-emitting devices". Journal of Applied Physics 86 (11): 6451. doi:10.1063/1.371708. Retrieved 29 July 2014."
11. Klinshirn, C.F., Meyer, B.K., Wang, A., Hoffmann, A., Geurts, J., [Zinc Oxide: From Fundamental Properties to Novel Applications] Springer Series in Materials Science 120 (2010)
12. M. Hadrich, C. Kraft, C Loffler, H. Metzner, U. Reisloehner, W. Witthuhn: Thin Solid Films, vol. 517 (2009) , p. 2282.
13. Minami, T. “Present status of transparent conductive oxide thin-film development for Indium-Tin-Oxide (ITO) substitutes,” Thin Solid Films 516, 5822-5828 (2008).
14. Minami, T “Substitution of transparent conducting oxide thin films for indium tin oxide transparent electrode applications” Thin Solid Films 516, 1314 - 1321 (2008).
15. M. A. Matin, Nowshad Amin and KamaruzzamanSopian, “Ultra-Thin High Efficiency CdS/CdTe Thin Film Solar Cells from Numerical Analysis” The 3rd International Conference on RENEWABLE ENERGY SOURCES (RES'09), Canary Islands, Spain, July 1-3, 2009.
16. M. Gloeckler, A. L. Ferenbruch, and J. R. Sites, "Proceedings of the 3rd World Conf. on Photovoltaic Energy Conversion (2003), p. 491.
17. Nowshad Amin, Mahmud A. Matin and KamaruzzamanSopian, Prospects of Novel Front and Back Contacts for High Efficiency Cadmium Telluride Thin Film Solar Cells from Numerical Analysis, 18th International Photovoltaic Science and Engineering Conference - PVSEC-18, Kolkata, India, January 21-25, 2009.
18. T.L. Chu, S.S. Chu, N. Schultz, C. Wang, C.Q. Wu: J. Electrochem. Soc. 139 (9) (1992), p. 2443
19. Van Deelen, J., Rendering, H., het Mannetje, H., Huis in ’t Veld, B., Theelen, M., Vroon, Z., Poodt, P., Hovestad, A., “Highly improved transparent conductors by combination of TCOs and metallic grids” Proc. 37th IEEE Photovoltaic Specialists Conference 992 - 994 (2010) and refs. Therein.
20. Vinod K. Jain, C. R. Jalwania, S. K. Mehta & S. Ganesan: Solar Cells, vol. 23 (1988), p. 181.
21. X. Wu et al., Proc. 0f 17th European PVSC (2001)
22. X. Wu, R. G. Dhere, Y. Yan, M. J. Romero, Y. Zhang, J. Zhou, C. Dehart, A. D., C. P. and B. To: NREL report (2002), p.1
23. X. Wu, R. G. Dhere, Y. Yan, M. J. Romero, Y. Zhang, J. Zhou, C. Dehart, A. D., C. P. and B. To, High efficiency polycrystalline CdTe thin film solar cells with an oxygenated amorphous CdS (a-CdS:O) window layer., NREL, USA, pp1-4, 2002.