HETEROJUNCTION SIMULATIONS OF WSe_2 SOLAR CELLS

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Abstract

In recent years much of the research has been directed toward identifying efficient, low cost earth-abundant semiconductors as absorber materials for next generation photovoltaic cells. Tungsten diselenide (WSe_2) has been identified as a little-studied material that has the potential to meet the aforementioned requirements [1].

Introduction

Literature has reported experimental and electronic measurements such as direct and indirect band gap (1.4eV, 1.5eV), mobility (30cm²/Vs), lifetime range (6-30ns) and absorption coefficient ($10^5 cm^{-1}$) with high carrier concentration (~$10^{17} cm^{-3}$) [1] that make WSe_2 a potential p-type model for solar cell (Fig 1) development.

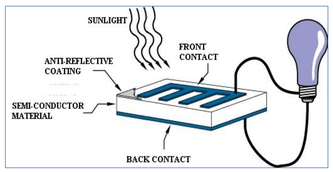

Figure 1 – Solar Cell Diagram[12]

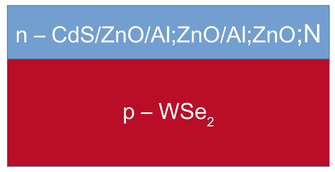

Figure 2 – Heterostructure Diagram

Heterojunction structure is a p-n junction formed between two closely matched semiconductors with different band gaps [2]. Fixing WSe_2 as a p-type layer, different n-type window materials (CdS, ZnO, Al;ZnO, Al;ZnO;N) were varied within the heterostructure simulations (Fig 2).

The software program used for simulations is AFORS-HET v2.5 which is an open source program made specifically for heterostructure simulations, having multiple features for layer specifications and input variable sweeping options.

WSe_2 Input Parameters

Table 1 shows the input parameters for WSe_2 p-type layer of the heterojunction used in solar cell simulations.

Parameter [units]	Value
Thickness [cm]	5E-5
Band Gap [eV]	1.42
Dielectric Constant [-]	20.5
Electron Affinity [eV]	4
Effective Conduction Band Density [cm^{-3}]	1.76E19
Effective Valence Band Density [cm^{-3}]	1.108E19
Effective Electron Mobility [cm^2/Vs]	23.68
Effective Hole Mobility [cm^2/Vs]	32.16
Acceptor Doping Concentration [cm^{-3}]	1E17

Table 1 – WSe_2 material parameters [1]

N-Type Window Materials

N-type window materials that were mentioned in the Introduction were selected based on compatibility of material properties to p-type WSe_2, as well as being accessible earth-abundant and easy to fabricate. Compatibility of the materials causes the forming of a heterostructure capable of utilizing the larger portion of the absorption spectrum, and Table 2 contains some of the important window material properties that were used in the simulations.

Parameter [units]	CdS	ZnO	Al;ZnO	Al;ZnO;N
Thickness [cm]	4E-6	4E-6	4E-6	4E-6
Band Gap [eV]	2.5[3]	3.27[5]	3.68[8]	3.1[11]
Dielectric Constant [-]	8.9[4]	8.66[6]	8.8[10]	8.8[10]
Electron Affinity [eV]	4.5[4]	4.5[6]	4.4[9]	3.6[9]
Effective Conduction Band Density [cm^{-3}]	2.24E18[4]	3.325E18[7]	3.72E18[1]	3.72E18[1]
Effective Valence Band Density [cm^{-3}]	1.47E19[4]	1.14E19[7]	1.14E19[1]	1.14E19[1]
Effective Electron Mobility [cm^2/Vs]	340[4]	17.7[5]	0.4[8]	0.4[8]
Effective Hole Mobility [cm^2/Vs]	50[4]	17.7[5]	0.4[8]	0.4[8]
Donor Doping Concentration [cm^{-3}]	1E18[4]	1E19[5]	1E19[1]	1E19[1]

Table 2 – Window material parameters

Band Structure and Efficiency

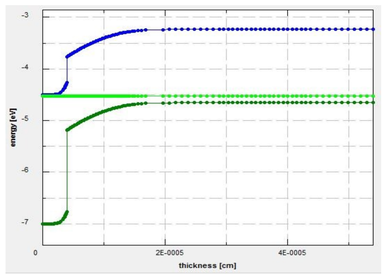

Figure 3 – WSe_2/CdS Band Structure

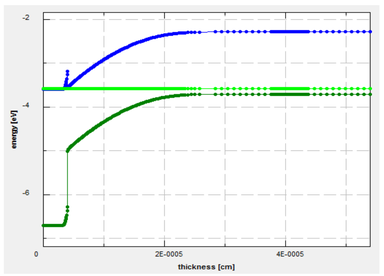

Figure 4 – WSe_2/Al;ZnO;N Band Structure

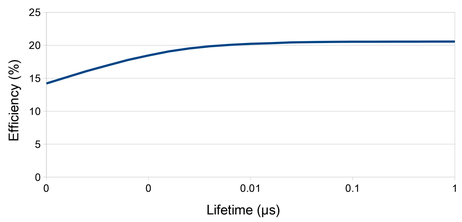

Figure 5 – WSe_2/CdS Efficiency Graph

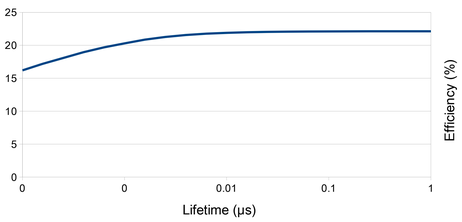

Figure 6 – WSe_2/ZnO Efficiency Graph

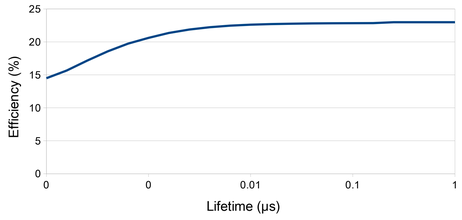

Figure 7 – WSe_2/Al;ZnO Efficiency Graph

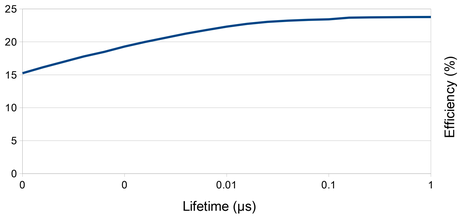

Figure 8 – WSe_2/Al;ZnO;N Efficiency Graph

Results

Figures 3-8 show the simulated results using parameters from Tables 1 and 2, along with measurements of the in house grown films of WSe_2, absorption spectra and refractive index and also different software features. Heterostructures simulated with Cds, ZnO and Al;ZnO show a type 2 band (Fig 3), while heterostructure with Al;ZnO;N (Fig 4) has a band where the E-field aides the carrier movement and increases the efficiency.

Fig 5-8 show the efficiencies of heterojunctions with previously discussed window materials as a function of carrier lifetime of WSe_2 p-type region (0.1ns to 1µs). It is shown that for conservative lifetime values the efficiency is in the range of 15%, while for optimistic, high lifetime values the efficiency ranges in the low 20%.

Conclusion

Obtaining high efficiencies of the heterojunction solar cells based on WSe_2 and various n-type window materials using both conservative and optimistic lifetime values within the simulation, confirms the potential for making an earth-abundant solar cell that has been the topic of discussion.

The fact that these high efficiencies have been produced by simulation using mostly generic and default values within the software shows that the heterostructures made from materials in Table 1 and 2 require additional attention and research.

Future work planned in the direction of examining heterostructures is looking into the effect that surface recombination has on effective lifetime, as well as the effect of the E-field, briefly mentioned for Al;ZnO;N band structure, and most importantly how and if electronic properties of n-type materials, along with various other parameters influence the performance of the heterojunction solar cells.

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