Cost benefit modeling of AB$_2$X$_4$ (A= Cd; B= Ga; X= S, Se) solar photovoltaic (PV) materials

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Abstract
Present paper focus towards implementation and commercialization of emerging solar PV technology with cost effective manner. Energy band gap, absorption coefficients and module implementation cost for 1KW solar power plant for ternary AB$_2$X$_4$ (A= Cd; B= Ga; X= S, Se) solar photovoltaic (PV) system is investigated here. All the material related calculations are carried out using density functional theory [1] and cost related calculations by using mathematical expressions. By performing a comparative cost study between proposed materials based solar photovoltaic module and crystalline based solar photovoltaic module we concluded that present material will be cost effectively commercialized as compare to Crystalline Si.

Index Terms: Solar PV, Cost, DFT

1. Introduction

With increasing gap between global energy supply and demand due to limited conventional energy resources, it is mandatory to harness maximum energy from renewable energy resources. To full fill above requirements researchers must pay their attention towards developments of emerging renewable energy harnessing techniques. It is found that out of all available renewable energy sources solar energy is worldwide authorized and having great potential to fulfill the gap between energy supply and demand. In this present paper our focus is towards investigation of such emerging solar collector materials. Ternary chalcogenides materials AB$_2$X$_4$ (A= Cd; B= Ga; X= S, Se) show excellent attractional properties as a suitable solar collector materials. Full potential linearized augmented plane wave (FP-LAPW) based density functional theory (DFT) approach have been implemented here to study electronic and optical behavior of proposed materials [1]. At last a cost comparative analysis between present material based solar PV module and Crystalline Si based PV module are done and on the basis of that we concluded about suitability and economical benefit of present ternary chalcogenides AB$_2$X$_4$ (A= Cd; B= Ga; X= S, Se) materials.

Regarding previous literatures available, Maestro et al.2016 [2] presents the optimization of three solar PV compounds to provide the sufficient electricity as per requirement of typical household (10 kWh/day). A systematic study has been carried out by Chandel et al.2014 [2] to achieve energy demand (2.5 MW capacity solar PV plant) for garment zone in Jaipur. Pavlovic et al. 2013 [3] has been studied about generation of electricity from 1 MW capacity of solar PV plant in Serbia. Dale et al.2013 [4] has analyzed the meta-analysis result related to wind, PV and CSP like renewable energy technologies. Srivastava et al.2013 [5] explore their idea on the impact of solar PV technology and their upcoming effects on Indian economy. Pandey et al.2012 [6] has been studied the role of solar PV technology in the development of Rajasthan as well as for western India. The potential requirement for solar PV recycling policies is analyzed by Donald et al.2010 [7] for major types of solar PV materials.
Kalowekamo et al.2009 [8] evaluates manufacturing costs of OSC that lies between $48.8 and $138.9/m². Muneer et al.2005 [9] has been studied about how the electricity obtained from solar PV systems become major part of the future energy solution. The economic viability of a stand-alone solar photovoltaic system has been analyzed by Kolhe et al.2009 [10]. Prasanna et al. [11] have been presented the financial feasibility of 100 KW roof top solar PV power based on life cycle cost of energy. The basic problem behind the costs of PV systems has been studied by Smested et al. [12].

2. Theoretical Methodology

The electronic band gap and absorption coefficient spectra are obtain by full-potential linearized augmented plane wave (FP-LAPW) as embodied in WIEN2k software package. mBJ exchange potential are used to investig ate the required calculations [13] by using density functional theory (DFT). The cost of AB₂X₄ (A = Cd; B = Ga; X = S, Se) solar photovoltaic (PV) materials are expressed on per-unit-area basis, whereas the same for solar PV module are based upon cost per watt that obtained under peak solar radiation.

3. Result and Discussion

The energy band gap value calculated from FP-LAPW investigation is presented in Table 1. Both the compounds showing direct band gap nature. The integrated area under the absorption curve near solar visible spectrum from 1-6eV is presented in table 2.

Efficiency of proposed chalcopyrite’s materials are around 10% for S based and 20% for Se based compounds [19, 20] as indicated in table 2. For future comparison also 15% efficiency [21] of crystalline silicon is taken. The cost investigation has been organized by calculating the manufacturing amount of CdGa₂X₄(X = S, Se) materials per square meter area. We use bottom-up cost estimation for the materials, overhead, and labor costs.

The PV modules cost ($/Wp) has been obtained by dividing the fabrication cost per square meter by the output of the equal space, in this case 1000 Wp/m² times efficiency. The reported amount in $/Wp because it carries efficiency, cell and module yield, and it empower the opinion to be similar with another solar PV technologies. For initiation of cost calculation first we start with elemental composition calculation [14] of proposed CdGa₂X₄(X = S, Se) compounds. The elemental composition calculated value along with density (gm/cm³) [15] and cost ($/100gm) [16] of each element which are taken from various online resources are mention in table 3.

| Table 1 Band gap (in eV) for CdGa₂S₄ and CdGa₂Se₄ compounds |
|---------------------------------|-----------------|-----------------|
| Method | Approach | CdGa₂S₄ | CdGa₂Se₄ |
| FP-LAPW | DFT-mBJ | 3.22 | 2.36 |

| Material | IAC | η(%) |
|----------|-----|------|
| CdGa₂S₄ | 77.99 | 10[20] |
| CdGa₂Se₄ | 135.81 | 20[20] |
| Crystalline Si | _ | 15[21] |
Table 3 CdGa2S4 and CdGa2Se4 elemental composition along with density (gm/cm³) and cost ($/100gm)

| Elemental Composition | Density (gm/cm³) | Cost ($/100gm) | Elemental Composition | Density (gm/cm³) | Cost ($/100gm) |
|-----------------------|------------------|----------------|-----------------------|------------------|----------------|
| Cd (29.57%)           | 8.65             | 46             | Cd (19.8%)            | 8.65             | 46             |
| Ga (36.69%)           | 5.907            | 220            | Ga (24.56%)           | 5.907            | 220            |
| S (33.74%)            | 2.07             | 24             | Se (55.64%)           | 4.79             | 61             |

Now first we start with cost calculation of each element of CdGa2S4 compound according to their elemental composition percentage and after that combined all individual obtained elemental cost to get CdGa2S4 compound cost.

Since 29.57% of Cd in 8.65gm/cm³ = (29.57*8.65)/100 = 2.55gm/cm³

As from table 3 the cost of 100gm/cm³ Cd is $46

Hence 2.55gm/cm³ Cd cost = ($46* 2.55)/100 = $1.173

Similarly

Since 36.69% of Ga in 5.907gm/cm³ = (36.69*5.907)/100 = 2.16gm/cm³

As from table 3 the cost of 100gm/cm³ Ga is $220

Hence 2.16gm/cm³ Ga cost = ($220* 2.16)/100 = $4.752

Similarly

Since 33.74% of S in 2.07gm/cm³ = (33.74*2.07)/100 = 0.69gm/cm³

As from table 3 the cost of 100gm/cm³ S is $24

Hence 0.69gm/cm³ S cost = ($24* 0.69)/100 = $0.165

Hence total cost ($/100gm) of CdGa2S4 compound = ($1.173 + $4.752 + $0.165) = $6.09

Similarly we calculate cost of CdGa2X4(X= S, Se) compounds as indicated in table 4.

Now once the proposed material cost is calculated we are are in position to calculate over all module cost of solar photovoltaic system. We know very well that bulk semiconductor thickness lies between 200- 300 micron [17] hence an assumption is made for current proposed material thickness is 200 microns. Therefore, semiconductor material quantity required is 200g/m² and the cost of 200gm proposed materials are shown in table 4.

After the bulk material cost estimation, the calculation of the photovoltaic module cost ($/m²) is needed. The module cost estimation includes semiconductor material cost, electrical interconnections, glass substrate, protective cover, packaging material cost, absorbing dye, catalyst, electrolyte and labor cost [8], [12]. Kalowekamo et al.2009 [8] is taken as cost reference from literature for electrical interconnections, glass substrate, protective cover, packaging material cost, absorbing dye, catalyst, electrolyte cost and for labor cost reference taken are Smestad et al. 2008 [12]. Including all the cost components we estimate the PV module cost ($/m²) as indicated in table 5.

Table 4 Material Cost of CdGa2X4(X= S, Se) compounds

| Compound | Cost ($/100gm) | Cost ($/200gm) |
|----------|----------------|----------------|
| CdGa2S4  | 6.09           | 12.18          |
| CdGa2Se4 | 5.529          | 11.18          |
Table 5 PV module Cost ($/m²) of CdGa₂X₄(X=S, Se) compounds

| Cost Component | CdGa₂S₄-Cost($/m²) | CdGa₂Se₄-Cost($/m²) |
|----------------|---------------------|----------------------|
| Semiconductor Compound | 12.18 | 11.18 |
| Electrical Contact & Interconnection | 6.84 | 6.84 |
| Substrate | 45.50 | 45.50 |
| Protective cover | 45.58 | 45.58 |
| Packaging Material | 4.35 | 4.35 |
| Other(absorbing dye, Catalyst, Electrolyte) | 14.50 | 14.50 |
| Labor | 5 | 5 |
| **Total** | **133.95** | **133.95** |

Table 6 $/Wp and $/KWp cost of PV module

| Compounds | Cost $/Wp | Cost $/KWp |
|-----------|-----------|------------|
| CdGa₂S₄   | 1.343     | 1343       |
| CdGa₂Se₄  | 0.669     | 669        |
| Crystalline | 0.7589[18] | 758.90[18] |

The PV module cost per square meter area is calculated, and further it is required for dollar per watt and dollar per kilo watt cost calculation of PV module. For CdGa₂S₄ compound $/Wp cost

\[
\frac{S}{Wp} = \frac{s/m^2}{\eta \times 1000W_p/m^2} = \frac{133.95s/m^2}{0.10 \times 1000W_p/m^2} = 1.3398/Wp
\]

Here \(\eta\) indicates efficiency of the module. Hence $/KWp cost of CdGa₂S₄ compound = 1000* 1.3398/Wp = 1339 $/KWp

Similarly calculate $/Wp and $/KWp cost of all the proposed compounds along with crystalline PV module are indicated in table 6. From table 6 it is clear that Se based PV modules require less cost compare to other modules.

4. Conclusion

The energy band gap and absorption coefficient spectra of ternary chalcogenides materials AB₂X₄ (A= Cd; B= Ga; X= S, Se) using FP-LAPW methods are computed here. The present calculation shows that CdGa₂Se₄ poses ideal band gap value for maximum absorption of solar incoming radiation. From the cost point of view CdGa₂Se₄ is comparatively less expensive and more efficient compare to other compounds.

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