Modeling high efficiency multi-junction solar cell design integrating III-V and I-III-VI semiconductors

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Introduction

- Photovoltaic systems are a renewable source of energy that converts energy from the sun directly into electrical energy.
- Solar cells are typically compose of semiconductors that are described predominantly by their bandgap (E_g).
- A single junction solar cell only absorbs photon energies higher than its bandgap; sub-bandgap energy photons are transmitted and therefore lost.
- As the bandgap of a single junction solar cell increases, the short-circuit current (J_{sc}) of the cell decreases; conversely, the open-circuit voltage (V_{oc}) increases. The ideal single junction solar cell bandgap is therefore an optimization between J_{sc} and V_{oc} to achieve maximum power.
- Detailed balance calculations of a single junction solar cell predict a maximum power conversion efficiency of 33% [1].
- Multi-junction solar cell (MJSC) are capable of surpassing the single junction solar cell efficiency. MJSC consists of several single junction solar cell connected in series via tunnel junction, where each sub-cell has a bandgap tailored to absorb a specific portion of solar spectrum (see Fig.1).
- The standard triple-junction solar cell consisting of GaInP/InGaAs/Ge has achieved an efficiency greater than 40% under concentrated illumination [2].
- However, this standard design is not optimal: we wish to explore an alternative bandgap combination via the integration of I-III-VI with III-V semiconductor materials.

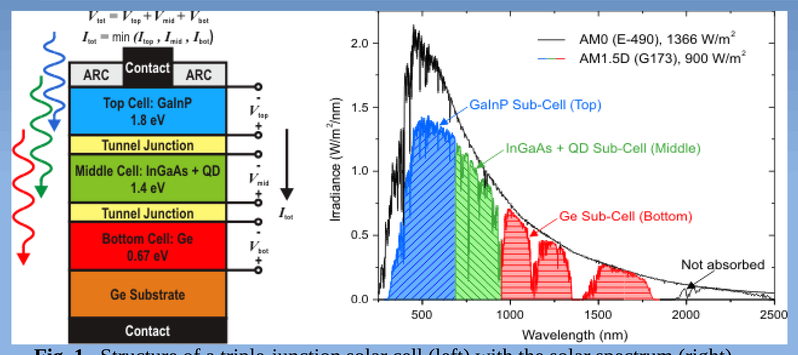

Fig. 1. Structure of a triple-junction solar cell (left) with the solar spectrum (right).

Multi-junction solar cells

A. MJSC structure

- Current matching of the sub-cells is achieved by choosing the right bandgap for each sub-cell.
- In a standard triple-junction solar cell design (GaInP/InGaAs/Ge), the bottom Ge sub-cell significantly overproduces current (50%).
- Detailed balance predictions target a bottom sub-cell with E_g=1.0 eV.
- The I-III-VI semiconductor material Cu(In,Ga)Se_2 is a promising material to replace germanium in the triple junction solar cell design because of its strong absorption characteristics in combination with its tuneable bandgap.
  - Growth of Cu(In,Ga)Se_2 on a GaAs substrate has been shown in the literature [3].

B. Numerical Model

- Semiconductor device simulation software package TCAD Sentaurus is used to simulate the optical and electrical properties of the solar cell.
  - This has been shown to successfully model MJSC for concentrator applications [4].
- Modeling the CIGS/GaAs interface is the main challenge since Cu(In,Ga)Se2 is lattice mismatched to GaAs:
  - A gradient region of CIGS near the interface to GaAs is implemented to account for inter-diffusion of Ga and In from substrate and CIGS respectively.
  - Includes a molar fraction dependent bandgap, electron affinity and the effects of a changing lattice constant by considering the formation of strained induced defects and threading dislocation densities (TDD). The effects of TDD are modeled using an effective Shockley-Read-Hall (SRH) minority carrier recombination lifetime.

$$\frac{1}{\tau_{SRH,TDD}} = \frac{1}{\tau_{SRH}} + \frac{\pi^3 D[TDD]}{4}$$

$$D = \frac{\mu\, k_b\, T}{q}$$

$$\frac{1}{\tau_{eff}} = \frac{1}{\tau_{rad}} + \frac{1}{\tau_{Aug}} + \frac{1}{\tau_{SRH,TDD}}$$

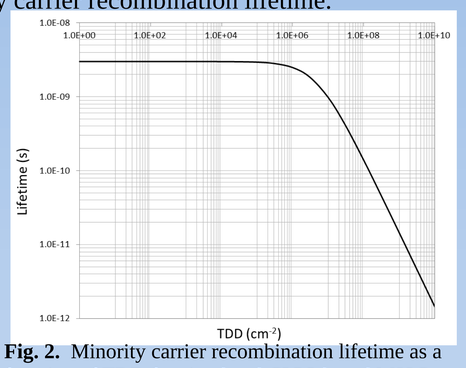

Fig. 2. Minority carrier recombination lifetime as a function of TDD for simulated CIGS-based MJSC.

Numerical Simulations

A. Cu(In,Ga)Se_2 single junction solar cell

- Study the performance of a Cu(In,Ga)Se_2 single junction solar cell compared to data in the literature for a similar structure.
- Figures 3a and 3b show the simulated external quantum efficiency and the current – voltage characteristics respectively.
  - Good agreement between experiment and simulation based on [5] for a molar fraction of x=0.3.

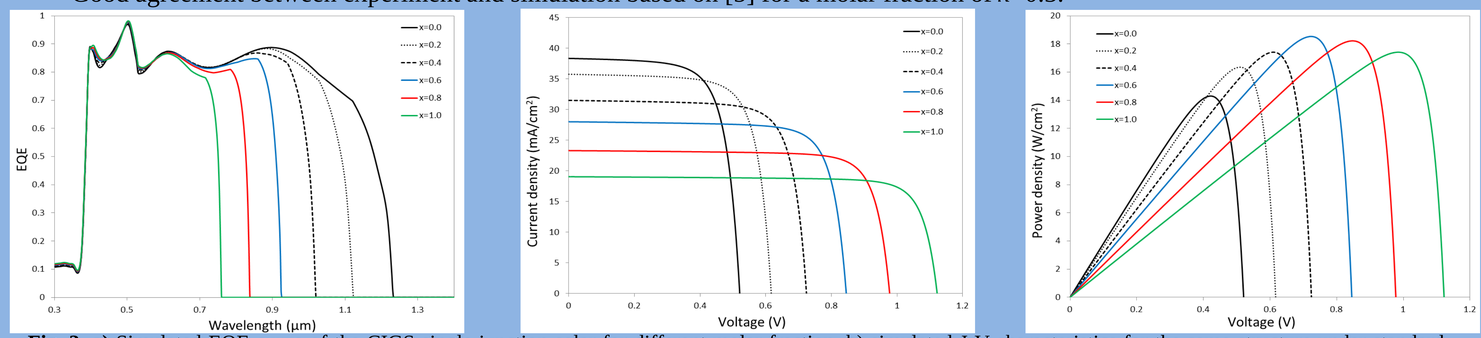

Fig. 3. a) Simulated EQE curve of the CIGS single junction solar for different molar fraction, b) simulated J-V characteristics for the same structure under standard testing conditions (room temperature, 1 sun illumination at 1 kW/m2) for different molar fraction, and c) simulated P-V characteristics for different molar fraction.

B. CIGS multi-junction solar cell simulation

- Propose a novel MJSC structure based on a Cu(In,Ga)Se_2 bottom sub-cell.
- Realistic growth considerations are taken into account by TDD and surface recombination at the relevant heterointerfaces.
- Figures 5a and 5b outline the effect of TDD on the EQE and J-V characteristics respectively.
  - Below a TDD concentration of 1e6 cm-2, the performance degrades by 5% absolute and falls below the standard MJSC performance.

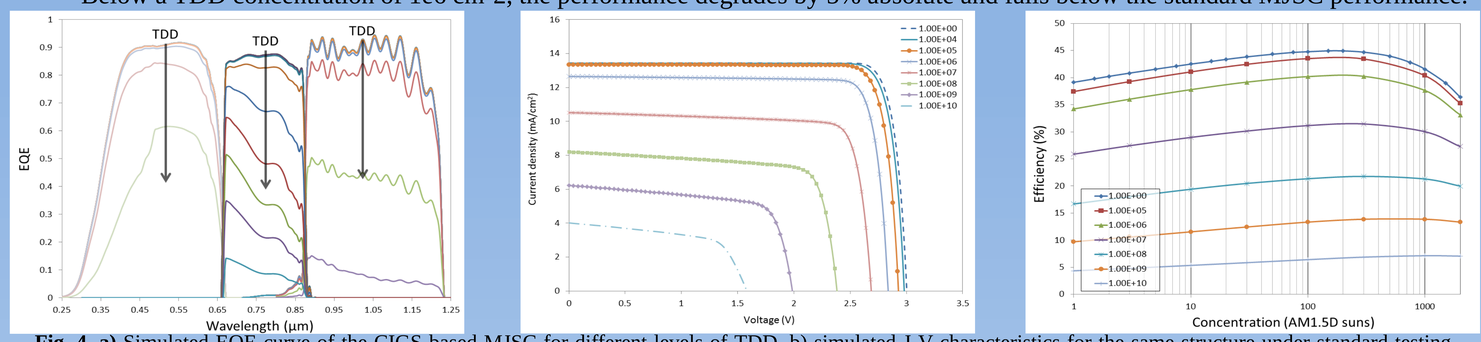

Fig. 4. a) Simulated EQE curve of the CIGS-based MJSC for different levels of TDD, b) simulated J-V characteristics for the same structure under standard testing conditions (room temperature, 1 sun illumination at 1 kW/m2), and c) simulated efficiency as a function of concentration.

C. Concentrated illumination

- MJSC's targeted for high concentrated illumination conditions to enable high efficiency coupled to reduced levelised cost of energy.
- Peak efficiency reached for X=200 at TDD=0

Concentration	TDD (cm^{-2})	J_{sc} (mA/cm^2)	V_{oc} (V)	*FF* (%)	η (%)
300 suns (3×10^5 W/m^2)	1e0	4210	3.49	85.5	**44.7**
	1e6	4010	3.34	85.4	**40.2**
	1e7	3340	3.23	82.7	**31.4**
364(WR [2])	N/A	5340	3.19	88.7	**41.6**

Fig. 5. Simulated performances of CIGS-based MJSC at 300 suns compare to WR.

Conclusions

- A Cu(In,Ga)Se2 based MJSC demonstrates potentially higher efficiencies under concentrated illumination than the standard III-V based MJSC when modeled in TCAD Sentaurus using threading dislocation densities and surface recombination to model the lattice mismatched gradient layers at the GaAs/Cu(In,Ga)Se_2 interface.
  - The growth of such a structure must emphasize a TDD less than 1×10^6 cm^{-2} in order to realize a better performing MJSC.

References

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