

Characterization and modelling of the new structures of antimony chalcogenide solar cells

Summary

Lastly significant progress was achieved in the development of the Sb-chalcogenide based solar cells. Apart from the growing efficiency, new structure compositions and new manufacturing methods unique features were achieved. This includes semi-transparency and semiconductor junction engineering. Main goal of this project is to develop efficient methods for characterization of the new Sb₂S₃ based solar cells structures. Specific opto-electronic and material parameters shall be obtained for defined group of cell structures. Experimental and measurement work is aimed at the preparation of the adequate simulation models corresponding to the actual parameters and behavior of these devices. After the construction of fully functional model for SCAPS 1D program obtained results will be confronted with the parameters of cells obtained in Laboratory for Thin Film Energy Materials at TalTech and adjusted for precise illustration of the device behavior. After this final verification the numerical analysis will be conducted towards formulating of the future technology optimization steps.

Research field:	Chemical, materials and energy technology
Supervisors:	Dr. Atanas Katerski Maciej Sibiński
Availability:	This position is available.
Offered by:	School of Engineering Department of Materials and Environmental Technology
Application deadline:	Applications are accepted between October 02, 2023 00:00 and October 23, 2023 23:59 (Europe/Zurich)

Description

Supervisor: Prof. Maciej Sibiński

Co-supervisor: Dr. Atanas Katerski

Description

Sb₂S₃ as the potential photovoltaic material is characterized by several important advantages, including low toxicity, simple phase chemistry, low cost, high elemental abundance and high optical absorption to name just a few. Thus recent effort in the development Sb₂S₃ based PV devices is dynamically growing. The Laboratory for Thin Film Energy Materials at TalTech was the first to demonstrate semi-transparent Sb₂S₃ solar cell fabricated by chemical spray deposition methods. In the current stage of the development, Sb₂S₃ thin film solar cells by ultrasonic spray pyrolysis show efficiency of 6.0 % under AM1.5 condition. The average visible transparency of structure glass/TCO/TiO₂/Sb₂S₃/HTM is 32% fulfilling the semi-transparency requirement of solar windows.

The key for further increasing the efficiency of the solar cells relays on optimization of the optoelectronic properties of Sb₂S₃ absorber layer by post-deposition treatments and optimization of solar cell component layers and interfaces. The post-deposition heat treatment approach is planned in a sulfurizing or selenizing atmosphere. It has been demonstrated for chemical bath deposited Sb₂S₃ coatings, that implementing this type of post-deposition treatment increases the phase purity and decreases the concentration of deep level defects in the bulk of Sb₂S₃. Developing of the adequate simulation models corresponding to the actual parameters of produced devices and behavior of the designed cells will be conducted towards formulating of the future technology optimization steps.

The specific candidate challenges lays within proper multi-faceted characterization of these new devices towards elaboration of the complex functional model suitable for advance numerical simulation. Basing on the achieved results this PhD research topic focuses on development of systematic post-deposition strategies for the Sb₂S₃ thin films optimization. Precise results of various simulation variants will deliver valuable guidelines for further experiments, including post-deposition treatment effect on the Sb₂S₃ physicochemical properties, fabrication of the standard and semi-transparent solar devices and their best characterization strategies.

In this PhD thesis, antimony chalcogenide and metal oxide thin films will be fabricated by robust, resource saving, and easily scalable method such as ultrasonic spray pyrolysis. Spray deposition has great potential to become front-line technology for rapid, cost-effective, large-area and high yield mass production of solar cell. The project will involve cooperation in synthesis of materials, fabrication of solar cells, characterization of materials and devices. After

complex characterization of the device and separate layers the adequate and fully functional solar cells simulation model for SCAPS 1D program shall be constructed. Consequently precise adjustment of the constructed model to the actual parameters and behavior of the prepared solar cells will enable results generation, which will be the base for prediction of the future technology optimization steps.

The candidate should submit a research plan for the proposed topic, describing the understanding of current state of the art of Sb_2S_3 based solar cells and propose their testing methodology. Additionally candidate should describe his/her experience with the numerical modelling of solar cell parameters, including SCAPS program experience.

To the potential candidate **we offer:**

- 4 year position in one of the most internationalized and leading PV research group in Estonia.
- The chance of to do high-level research in one of the most rapidly growing photovoltaic sector.
- Additional supervision by ERA Chair Holder professor.
- Opportunities of conference visits, research stays and networking with leading universities in the field.
- Participation in EU COST action CA21148 – RENEW PV, Research and international Networking on Emerging Inorganic Chalcogenides for Photovoltaics (<https://renewpv.eu>), coordinated by the TatTech.

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