Development of Beyond 20% Efficiency Kesterite (CZTSSe) Solar Cells: win the PV race with sustainable low-cost, low-toxic and stable materials-2017/RND006

Public Dissemination Report

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Executive Summary

PV has been the most important renewable energy source combating escalating climate change. High-efficiency, low-cost, low-toxic, stable, and versatile PV technology is a long-sought goal. This goal is potentially to be achieved by next generation thin-film solar cells based on emerging earth-abundant and RoHS-compliant compound PV materials, which has become an intensified race of PV research world-wide.

This project aims to develop a new generation thin-film PV technology based on emerging low-toxic (RoHS-compliant) and earth-abundant kesterite copper-zinc-tin sulfuroselenide (CZTSSe) for a wider application than the conventional crystalline-Silicon PV technologies. The main challenges of realizing this promising technology include exploitation of the potential of CZTSSe thin-film materials and exploration of technologies to fabricate high efficiency solar cells.

During the execution of the project, two main connected strands are designed and implemented to tackle the research challenges. The first one is establishing a reproduceable, cost-effective, and scalable CZTSSe fabrication technology. This generated a series of intellectual property related to the frontier knowledge for thin film PV technology development, established close collaboration with international and domestic academic institutions and industry partners. The thin film solar cell research team at UNSW set 1 independently confirmed world record efficiency of CZTSe solar cells, consolidating the leadership position of UNSW and Australia in the thin film PV research community.

The second strand is to explore the key limiting loss mechanisms of CZTSSe solar cells in every step and to identify the feasible pathway toward higher power conversion efficiency. Advanced characterization technologies and analytical models have been developed to investigate the microscopic energy loss mechanism in different microscopic regions of CZTSSe thin-film solar cells. The dominant energy loss mechanisms have been identified by integrating multiple advanced characterization technologies and 3-dimensional device simulations. Key strategies and a pathway have been identified for >20% efficiency CZTSSe thin-film solar cells, providing fundamental technical knowledge for UNSW and Australian research teams focusing on thin-film technology.

Project Overview

Project summary

This project aimed to work with international collaborators to design and develop a new generation of thin-film PV technology based on less-toxic (RoHS-compliant) and earth-abundant CZTSSe compound semiconductor materials to give high power conversion efficiency. International recognized record efficiency has been achieved during the project progress, establishing Australia's leadership position in inorganic thin film solar cell research area. The exploration of stability, the cost analysis, and the identified road map toward 20% efficient solar cell also demonstrated the promising commercialization potential of this technology.

Project scope

The project scope is to explored the potential of CZTSSe materials as a next generation thin-film solar cells, which includes exploring the technologies for material synthesis, material optoelectronic quality tailoring, and the device structure and device fabrication techniques, the key loss mechanisms, and also included evaluating the long-term stability and the manufacturing cost, providing the pathways toward the commercialization of high efficiency CZTSSe solar cells.

Outcomes

During the investigation of exploiting high conversion efficiency CZTSSe solar cells, the material growth process, the control of the morphology, and the formation and engineering of the key defects in the material have been systematically studied. In addition, the device physics of the thin film solar cells and the interface engineering, architectural design of the device structure have also been investigated. 1 CZTSe world record efficiencies have been achieved which consolidated the leadership of Australia in thin film research area.

An analytical model of heterojunction interface recombination mechanisms and a dynamical device and material loss mechanism analysis model by integrating multiple advanced characterization technologies and 3 dimensional device simulations have been established, which are recognised as powerful tools for the analysis of thin-film solar cells. Using these tools, key strategies and pathways have been identified for >20% efficiency CZTSSe thin-film solar cells, providing fundamental technical knowledge for UNSW and Australian researcers focusing on thin-film technology.

The commercialization potential and possible scale-up pathway of CZTSSe thin film PV technology have been evaluated via cost analysis, stability analysis, and life cycle assessment. The practical potential, challenges and strategies towards the commercialization of CZTSSe cells have been identified based on the manufacturing cost, energy conversion efficiency, long term stability scalable manufacturing method studied during this project.

Transferability

The technical challenges that the project seeks to address are relatively specific to CZTSSe solar cell technology. However, the achievement and lessons learnt can be applied to other projects which involve other chalcogenide thin film technology, especially the high bandgap chalcogenide solar cells that can be used as the top cells for Silicon based tandem cells. Tandem solar cells are currently widely studied as they are the pathway to cost reduction through higher efficiencies.

Knowledge sharing within UNSW is through regular meetings and seminars, as well as internally produced documents that detail specific processes. We have a fortnightly kesterite meeting as well where all researchers present and discuss their results. We also have regular seminars which go into more detail about specific research topics. All group members regularly attend international and domestic conferences, visit research institutions and give talks at a variety of fora to both specialist and lay audiences to promote our research achievements. Conference and journal publications as well as patents have been published by the research team relating to the innovations developed over the course of this project. In addition, significant results like breaking word record efficiency also feature in media releases.

Conclusion and next steps

In conclusion, this project has been able to achieve all of its technical milestones. The importance of these milestones is that achieving them indicates the feasibility of the approaches being undertaken. The project has been successful in consolidating the leading position of Australia in thin film PV technology. However, there are still many remaining challenges for CZTSSe technology become commercially available. The next-step is to integrate the identified efficiency step-change strategies in an effective way to further the efficiency beyond 20%. Given the promise of itself as a bottom cell for all thin film tandem cells and the equal promise of its close cousins (high bandgap kesterite and chalcopyrite) as a top cell of tandem cells, we will continue to work with present project partners and leverage the knowledge established during this project to promote the chalcogenide thin film technology (not only CZTSSe, but also high bandgap CZTS and CIGS) as well as their application for tandem concept (e.g. all thin film tandem cells and Si-based tandem cells).

Ultimately, the benefit of the project will be to facilitate and accelerate the development of CZTSSe thin film PV technology toward commercialization, which not only provides another low-cost and ecofriendly “green” thin film PV technology but also forms valuable knowledge base for chalcogenide-based tandem cells that can be deployed in wider application scenarios with short energy payback times

, yet with everywhere PV deployment potential. This will contribute significantly to Australia’s shift-away from coal and gas and toward renewable energy sources, thus will translate to a significant economic and environmental benefit.

Lessons Learnt

Lessons Learnt Report: High performance kesterite Copper-Zinc-Tin-Sulfuro-selenide (CZTSSe) solar cell development

Project Name: Development of Beyond 20% Efficiency Kesterite (CZTSSe) Solar Cells: win the PV race with sustainable low-cost, low-toxic and stable materials

Knowledge Category:	Technical
Knowledge Type:	Technology
Technology Type:	Solar PV
State/Territory:	NSW

Key learning

Reproduceable, recognizable, and upscalable high-performance CZTSSe thin-film technologies have been developed. These technologies include low-cost synthesis of light absorber and the morphology and optoelectronic properties control, heterojunction interface and back interface engineering and device architecture design, as well as the dynamic loss mechanism analysis, which have been proved effective for kesterite CZTS top cell performance improvement. The techniques developed and learnt enable a rapid and steady progress of the project.

Implications for future projects

All compound heterojunction polycrystalline thin-film solar cells face the same challenges coped with in this project, including high quality absorber material synthesis, morphology and defect control, heterojunction interface device physics and device architecture design, as well as the materials and device performance loss analysis. The strategies and the techniques learnt in this project can be widely applied to future thin film PV technology projects like perovskite and other emerging new PV materials.

Background

Objectives or project requirements

The first objective and challenge in this project is developing industrial-scale and high performance kesterite CZTSSe solar cells. CZTSSe is an emerging thin film PV material with earth-abundant and low-toxic (RoHS compliant) constituents, sharing similar crystal structure with the commercialized $CuIn_xGa_{1-x}Se_2$ (CIGS) thus similar excellent optoelectronic properties for solar cells. However, the synthesis of CZTSSe and the defect control is much more challenging because of the more complicated phase evolution involving intermediate secondary phases system and the more intricate defect chemistry. This requires new techniques and strategies to be developed to realize a high performance CZTSSe solar cells.

Process undertaken

CZTSSe light absorber material growth and optimization have been studied to realize a stable, high reproduceable and less defective light harvesting absorber. These include absorber growth condition baseline establishing and optimization, critical material growth equipment design, secondary phase and optoelectronic properties control, defects formation mechanism and evolution study as well as doping and alloying strategy development. Interface engineering has been carried out including establishing analytical recombination model, band alignment measurement and adjustment, interface defects passivation. The device structure study and design have been realized through integrated device loss mechanism simulation and state-of-art characterisations.

Lessons Learnt Report: Defect engineering and optoelectronic property engineering for CZTSSe materials

Project Name: Development of Beyond 20% Efficiency Kesterite (CZTSSe) Solar Cells: win the PV race with sustainable low-cost, low-toxic and stable materials

Knowledge Category:	Technical
Knowledge Type:	Technology
Technology Type:	Solar PV
State/Territory:	NSW

Key learning

The performance of CZTSSe solar cells is mainly governed by the defects within the CZTSSe light absorber. The deep-level defects dominate the recombination process whilst the shallows defects dominant the carrier transport processes. It has been demonstrated in this project that the formation of deep defects and shallow defects in CZTSSe could be greatly modulated and suppressed by engineering the local chemical environment during the formation of CZTSSe phase and the shallow defects could also be tailored by Lithium post-deposition treatment. These strategies have led to the record efficiency pure-selenide CZTSe solar cells.

Implications for future projects

Intrinsic defect engineering and understanding the defects evolution are the key challenge for most of the compound semiconductor materials and devices. The defect engineering strategies developed in this project could be widely applicable to other compound semiconductor materials and devices in general.

Background

Objectives or project requirements

Effective defect engineering is one of the keys to achieve high efficiency CZTSSe solar cells and is also one of the major challenges in this project. To address this issue, strategies to engineer the deep intrinsic defects and shallow defects respectively are required.

Process undertaken

The formation of deep defects like Sn_{Zn} antisites is suppressed by introducing a soft-selenization process which enables a favourable local chemical environment during the synthesis of CZTSSe. This process also promotes the formation of desired shallow defects copper vacancy (V_{Cu}). We have demonstrated that the dominant shallow acceptor in CZTSSe can be changed from Cu_{Zn} antisites to shallower Li_{Zn} antisites by introducing a solution-based lithium post-deposition treatment.

Lessons Learnt Report: Microscopic carrier loss mechanisms of CZTSSe thin-film solar cells

Project Name: Development of Beyond 20% Efficiency Kesterite (CZTSSe) Solar Cells: win the PV race with sustainable low-cost, low-toxic and stable materials

Knowledge Category:	Technical
Knowledge Type:	Technology
Technology Type:	Solar PV
State/Territory:	NSW

Key learning

Carrier loss mechanism analysis is one of the key challenges to develop high efficiency solar cells, especially for CZTSSe thin-film solar cells which have multiple microscopic structures. We have developed a dynamic microscopic carrier loss mechanism analysis platform by integrating multiple advanced characterization technologies and the 3-demensional device simulations. This platform is a powerful tool to dynamically diagnose the dominant loss mechanisms in thin-film solar cells and to identify the feasible pathway toward higher efficiency.

Implications for future projects

Loss mechanism analysis is critical for all kinds of solar cells. The carrier loss mechanism analysis platform developed in this project could be widely used for many types of solar cells. The strategies used to develop this platform are also valuable intellectual property for the development of other analysis platforms.

Background

Objectives or project requirements

To develop high efficiency solar cells, carrier loss mechanism analysis is imperative to give critical know-how feedback for any processing condition changes. For heterojunction solar cells based on polycrystalline thin-film absorber like CZTSSe, the carrier loss mechanism analysis is a big challenge which is an important objective of this project.

Process undertaken

An analytical heterojunction interface recombination model is developed to better understand the complicated interfacial recombination processes under different conditions. A dynamic microscopic carrier loss mechanism analysis platform is established by integrating multiple advanced characterization technologies and the 3-demensional device simulations, which has been used to identify the dominant carrier loss mechanisms in CZTSSe solar cells and the pathway towards >20% efficiency solar cells.

Lessons Learnt Report: Evaluation of the commercialization potential and pathway of CZTSSe solar cells

Project Name: Development of Beyond 20% Efficiency Kesterite (CZTSSe) Solar Cells: win the PV race with sustainable low-cost, low-toxic and stable materials

Knowledge Category:	Technical
Knowledge Type:	Technology
Technology Type:	Solar PV
State/Territory:	NSW

Key learning

The commercialization potential of CZTSSe solar cell is evaluated based on the cost analysis, long-term stability analysis and life cycle assessment. Further improvement of the conversion efficiency of CZTSSe solar cell and replacement of the Cd-containing buffer layer with non-toxic and more transparent material are identified as the key barriers and/or strategies for its industrial-scale fabrication.

Implications for future projects

The methods for evaluation of commercialization potential of CZTSSe solar cell and identification of key barriers and strategies for its commercialization can be applied to other PV technologies projects when considering it is in high Technology Readiness Level (TRL).

Background

Objectives or project requirements

CZTSSe thin film solar cell is an emerging PV technology, still in R&D stage without a market or business validation. The commercialization potential of new technology needs to be evaluated along with its development which can provide design advice and research direction for its future development.

Process undertaken

A bottom-up cost analysis model was built up to compare the CZTSSe technology with other commercialized thin film technologies like $Cu(In,Ga)(S,Se)_2$ thin film solar cells. The long-term stability of CZTSSe thin film solar cells is estimated. The benchmark efficiency of CZTSSe thin-film solar cells to be commercially competitive is identified.