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UNSW SYDNEY

Efficient Adamantine Thin-Film on Silicon Tandem Cells: The Next Step in Commercial Cell Evolution -2017/RND011

Public Dissemination Report

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Lead organisation:	University of New South Wales (UNSW)		
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Contact name:	Martin Green; Xiaojing Hao		
Title:	Scientia Professor; Professor		
Email:	m.green@unsw.edu.au; xj.hao@unsw.edu.au	**Phone:**	+61 2 9385 4018 +61 2 9385 4381
Website:			

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Executive Summary

This project targets reduced solar cell cost, achieved by improving the efficiency with which they convert sunlight into electricity. Improved efficiency reduces cost by reducing the area required for a given power output, reducing the cost of encapsulation, transport and installation for a given power. This is why the whole industry is presently employing an earlier generation of UNSW cell technology known as the PERC cell, which allows high efficiency up to 25%. To further boost the efficiency of Silicon (Si) solar cells, the most viable approach is to stack thin-film cells made from another a higher bandgap material onto the top surface of a silicon cell. One overlying cell will eventually allow 25% efficiency to be increased to 35% and two overlying cells to 40%.

To achieve this goal, an exhaustive theoretical and experimental exploration of suitable materials for the overlying cells has been undertaken. The search has focused on absorber materials that are stable, non-toxic, and abundant, with the same crystal structure as silicon and diamond (adamantine semiconductors) as this increases the prospects for success. The project has made excellent progress on materials simulation, new adamantine materials synthesis, solar cell device fabrication, and performance optimisation.

A new semiconductor bandgap simulation method has been developed and subsequently used to assess bandgaps for candidate novel adamantine compounds. Various chemical and physical synthesis methods have been investigated to synthesise new materials such as $NiZnIn_2S_4$, $CoZnIn_2S_4$, and $NiSi_3P_4$. Different types of solar cell devices have been successfully demonstrated, including the notable first working $Ni(Co)ZnIn_2S_4$ device. Moreover, a novel tandem cell interconnecting layer and a new top cell fabrication method have also been developed and patented to fabricate Si tandem cells using new adamantine materials. In addition, stability testing and cost analysis have been conducted for the Si-tandem cell processing sequences, providing guidance for the commercialisation of this technology. These new findings in this project benefit the development of next-generation Si tandem solar cells technology which will accelerate the PV deployment to provide clean energy and reduce carbon emissions.

Project Overview

Project summary

This project targets photovoltaics (PV) cost reductions, leveraged by improved cell efficiency. Recent auctions demonstrate PV costs are now the lowest for bulk electricity generation, although further reductions are essential to offset integration overheads. Improved cell efficiency contributed significantly to reduced costs, particularly system costs. Developing thin films deposited onto silicon to form tandem cells is a promising approach to achieve further efficiency gains. One overlying cell ultimately boosts 25% efficiency of Si single junction cell efficiency to 35%, and two overlying cells can improve to above 40% efficiency. This project involves finding suitable materials for these overlying cells that are stable, non-toxic and abundant with the search to focus on materials that have the same crystal structure as silicon and diamond (i.e. adamantine semiconductors), since this increases prospects for success.

Project scope

The project involves an exhaustive, combined theoretical & experimental exploration of closed-shell, adamantine compounds as the top cell for silicon tandem cells, involving five strands: (1) Top cell material identification and evaluation; (2) Top cell fabrication and performance optimisation; (3) Integration of top cells with silicon bottom cells; (4) Accelerated testing of candidate materials and devices; and (5) Development of practical manufacturing candidate sequences and their costing analysis.

Outcomes

Great progress has been made in this project, with significant advancements in material properties simulation, new adamantine materials synthesis, solar cell device fabrication and performance optimisations. To overcome the issues of conventional semiconductor bandgap simulation methods, an approximation has been implemented to provide increased accuracy with minimal additional computational overhead. We have effectively calibrated this technique for the first time and subsequently used it to assess bandgaps for candidate novel adamantine compounds. Based on the simulation-screened adamantine compound semiconductor materials showing favourable bandgap, various chemical and physical synthesis methods have been used to experimentally develop new materials. Several new adamantine materials have been successfully synthesised, such as $NiZnIn_2S_4$, $CoZnIn_2S_4$, and $NiSi_3P_4$. With the synthesised PV materials, various thin film solar cell devices have been successfully demonstrated, including the notable first working $Ni(Co)ZnIn_2S_4$ device. A novel tandem cell interconnecting layer and a new top cell fabrication method have also been developed to fabricate Si-based tandem cells using new adamantine materials. In addition, stability testing and cost analysis are conducted for the Si-tandem cell processing sequences, providing guidance for the commercialisation of this technology.

Transferability

This project has significantly contributed to our understanding of the suitability of different semiconductors for stacking onto silicon, as well as identifying new materials that are viable. This knowledge can be transferred into manufacturing sequences for the development of high-efficiency Si tandem solar cells, and ultimately enable large-scale deployment.

The novel interconnecting layer integrating top and bottom cells developed in this project has several advantages, such as being fabricated using low-cost materials and a simple process, and minimum requirements and impacts on the subcells (both top and bottom cells). As a result, this interconnecting layer technology has the potential to be widely applied to the fabrication of tandem cells consisting of various types of sub cells, and provide a new solution for optoelectronic devices integration.

Furthermore, the new adamantine materials that were discovered as part of this project have good optoelectronic properties and can be utilised for the development of hydrogen production devices. This highlights the potential for this project to contribute to advancements in other areas beyond solar cells.

Conclusion and next steps

This project has successfully developed multiple new technologies that have the potential to advance the next-generation Si tandem solar cells. These include a new simulation method of screening PV materials, the synthesis of new materials, a novel approach to fabricating thin film solar cells, and a new interconnecting method for tandem solar cells. All of the project milestones have been met utilising the developed new technologies.

Moving forward, the novel interconnecting approach will be further investigated in the new ARENA TRAC program-funded project to fabricate chalcogenide/Si tandem solar cells. Future work will also include the development of large-area fabrication technologies for the top cells and Si tandem cells, which will be crucial for next-stage upscaling and commercialisation. The cost analysis of the fabricating sequences in this project provides valuable guidance on how to reduce the cost of production and design the commercialisation roadmap of the Si tandem solar cell production. In summary, this project has made significant progress and paved the way for developing next-generation Si tandem solar cells, which will accelerate PV deployment to provide clean energy and reduce carbon emissions.

Lessons Learnt

Lessons Learnt Report: The density functional theory (DFT) calculations of $ZnIn_2S_4$ nanosheets metamaterial

Project Name: Efficient Adamantine Thin Film on Silicon Tandem Solar Cells

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

Key learning

Density functional theory (DFT) calculation is employed to correlate the special $ZnIn_2S_4$ nanosheets metamaterial structures to their unique optoelectronic properties. The partial density of states charts of stacks of four $ZnIn_2S_4$ layers are firstly calculated, which indicates that the dangling metal atoms on the outer layer of nanosheets will provide extra surface states and thus reduce the band gap. Furthermore, accurate electronic band structure dispersions for $ZnIn_2S_4$ bulk and slab are calculated, using the projector-augmented wave (PAW) method. Thus, the unique ~750 nm photoluminescence (PL) peak can be directly correlated to the allowed optical transition occurring between bands for $ZnIn_2S_4$ slab (nanosheets).

Implications for future projects

Using DFT method to calculate the morphology-dependent electronic band structure of semiconductor material provides a new idea in the theoretical understanding of metamaterial structures. The discovery of effectively reduced band gap and enhanced photon absorption in $ZnIn_2S_4$ nanosheets metamaterial is proved to result from the introduced surface states and dangling atoms, which can be used as an effective method for tuning band gap of semiconductor materials.

Background

Objectives or project requirements

Morphology-dependent optoelectronic properties have been discovered in $ZnIn_2S_4$, it is of great scientific significance to understand the underlying mechanism of the connection between the unique properties and the morphologies. Thus, this new type of semiconductor metamaterial can be further expanded and employed in the optoelectronic fields.

Process undertaken

The density functional theory calculations were performed to optimise the crystal structure of $ZnIn_2S_4$ using the projector-augmented wave method.

Lessons Learnt Report: Remarkably enhanced performance in Co-$ZnIn_2S_4$ micro flowers compared to $ZnIn_2S_4$ material system

Project Name: Efficient Adamantine Thin Film on Silicon Tandem Solar Cells

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

Key learning

Co atoms can be inserted into the ternary $ZnIn_2S_4$ and form a quaternary compound, $Co_{0.5}Zn_{0.5}In_2S_4$ via a 2-step autoclave reaction. The as-obtained $Co_{0.5}Zn_{0.5}In_2S_4$ powders showed greatly-enhanced device performance compared with the ones of pure Zn-In-S material of different morphologies. PL spectra further confirms that this enhancement in device performance likely results from broadened light absorption range and faster carrier transport.

Implications for future projects

The excellent charge-separating and charge-transfer properties of $ZnIn_2S_4$ make it a promising material that can be applied in photocatalysts and possible solar cell devices. By inserting transition metal element, Co, into the $ZnIn_2S_4$ base matrix, better photocatalyst performance is achieved, which can open the possibility of using similar methods in other semiconductor materials for improving light absorption and carrier transport.

Background

Objectives or project requirements

Due to the large band gap and poor charge-transfer properties in previously reported spinel (a form of adamantine) $ZnIn_2S_4$ material, extra processing or formation of hybrid structures are required to apply this kind of material in water splitting or PV devices. Herein we found the band gap and charge transfer properties can be effectively tuned by inserting the Co atoms into the $ZnIn_2S_4$ matrix.

Process undertaken

$Co_{0.5}Zn_{0.5}In_2S_4$ was synthesised via an autoclave reaction using previously prepared $ZnIn_2S_4$ as the precursor. As-obtained powders were directly employed in water splitting tests. Different electrolyte systems were used to realise optimal device performances.

Lessons Learnt Report: Bifacial and semitransparent $Sb_2(S,Se)_3$ solar cells

Project Name: Efficient Adamantine Thin Film on Silicon Tandem Solar Cells

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

Key learning

A bifacial and semitransparent $Sb_2(S,Se)_3$ solar cell was fabricated by employing indium tin oxide (ITO) as the electrode on top of MnS hole transporting layer (HTL) based on the state-of-art efficient $Sb_2(S,Se)_3$ opaque solar cell to broaden the application of this emerging quasi-1D light harvesting material. Then the bifaciality, capability of handling tilt incident light, and performance enhancement by exploiting albedo were further investigated.

Implications for future projects

By better regulating the band position of ITO, higher efficiency and bifaciality are expected. In addition, this innovative semitransparent $Sb_2(S,Se)_3$ solar cell can be further applied as the top cell in tandem solar cells with an appropriate bottom silicon solar cell.

Background

Objectives or project requirements

$Sb_2(S,Se)_3$ solar cells have gained remarkable increase in power conversion efficiency recently. However, all of them are opaque and mono-facial regardless of the configuration. Tracing the development of all other main-stream thin-film solar cells, either bifacial or assembled tandem solar cell is a feasible and promising way to potentially break the Shockley-Quisser limit of a single-junction cell. Therefore, modification towards high transparency and performance is supposed to be investigated.

Process undertaken

An appropriate transparent conducting oxide material (tentative candidate-ITO) was employed as the back electrode to enable incident light coming from both sides to be absorbed by $Sb_2(S,Se)_3$. Optimisation of the deposition parameters, including air pressure, time and power, contributed to improved performance.

Lessons Learnt Report: Inverted superstrate Sb_2Se_3 solar cells

Project Name: Efficient Adamantine Thin Film on Silicon Tandem Solar Cells

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

Key learning

Sb_2Se_3 was deposited on a p-type material for the first time. Substrate temperature varied to explore its influence on the subsequently growing Sb_2Se_3 thin film. Moderate heating was validated to be optimum from the perspective of orientation, morphology and element distribution, revealed by material property characterisations. The underlying reasons were indicated by further investigation of the defects and capacitance.

Implications for future projects

The inverted p-i-n structure reverses the direction of carrier transport in a superstrate Sb_2Se_3 solar cell, compared with the conventional n-i-p structure. This heterojunction is applicable to assembling a monolithic tandem solar cell by direct growth on top of Si bottom cell with a p-type top surface.

Background

Objectives or project requirements

The power conversion efficiencies of Sb_2Se_3 solar cells have achieved 10.57% and 10.12% for superstrate and substrate configuration, respectively. But Sb_2Se_3 grows either on opaque Mo layer in substrate configuration, or on n-type material (CdS, ZnO, TiO_2) in superstrate configuration, limiting the applicability in monolithic 2-terminal tandem solar cells. A novel heterojunction by depositing Sb_2Se_3 on p-type material is thereby desired to be realised.

Process undertaken

The selection of a proper p-type material took a series of experiments. Then the thickness and micro-structure were optimised. The substrate temperature was studied in order to grow a high-quality Sb_2Se_3 thin film with preferable orientation, large grain size and low concentration of deep-level defects.