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

LESSONS LEARNT REPORT 1

Project Details

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Lessons Learnt

Lessons Learnt Report: “intrinsic defect control of CZTSSe by engineering of local chemical environment”

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 formation of intrinsic defects and defect clusters in CZTSSe are fund to be governed by the local chemical environment at the time when the synthesis of CZTSSe initiates. By engineering the local chemical environment (including the oxidation states of precursor elements and the local chemical composition), the formation of detrimental defects such as Sn_{Zn} antisites can be effectively suppressed, and the desired shallow acceptors V_{Cu} can be created, thus significantly improving the optoelectronic properties of CZTSSe absorber and corresponding power conversion efficiencies.

Implications for future projects

The intrinsic defect formation mechanism under practical non-equilibrium condition is governed by the local chemical environment during the synthesis of compound semiconductor materials. This new strategy enabling the control of intrinsic defects could be generalized to other compound semiconductors to improve their intrinsic qualities by engineering local optoelectronic properties such as surface type inversion or passivation.

Background

Objectives or project requirements

The current challenge in the field of CZTSSe is to obtain high quality absorber with suppressed intrinsic defects. The common strategy intensively researched is extrinsic doping and alloying. But no substantial breaking through has been made as the large V_{OC} loss is still prevailing and the record efficiency is pinned by devices nominally without extrinsic doping nor alloying. Therefore, more robust strategy to control the intrinsic defects is urgently needed.

Process undertaken

Using metallic precursor, a soft-selenization process between alloying treatment and high temperature selenization is introduced into the growth process. This effectively modified the oxidation states and local chemical composition, i.e. modified the local chemical environment.

Lessons Learnt Report: “improved p-type doping via solution-processed alkali-PDT treatment”

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Key learning

The effective p-type doping density of CZTSSe absorber could be improved by solution processed alkali-PDT treatment. For CZTSSe absorber, the efficient alkali dopant is Li and K. The solution processed alkali-PDT is a new PDT method with more feasibility.

Implications for future projects

The significant interdiffusion of alkali element during the solution soaking under a relatively low temperature provides a new strategy for surface treatment. Using this method, the surface or subsurface properties could be effectively changed in a feasible way without changing the bulk.

Background

Objectives or project requirements

Controlling the effective doping density is important to reduce non-radiative recombination and thereby improve the device performance. Alkali PDT treatment at relatively high temperature in alkali flux and chalcogenide atmosphere is employed in CIGS solar cells to improve the effective p-type doping and surface quality. For CZTSSe, this method may cause Sn loss during the annealing. More feasible method is required for the alkali PDT of CZTSSe.

Process undertaken

Alkali chloride is added in the solution for PDT process. The recipe including solution concentration, solution temperature, and process duration are optimized. Li and K have been tested and provided positive results.

Lessons Learnt Report: “controllable work function of MoS_x back contact interfacial layer by incorporation of Cu”

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Key learning

The fill factor of CZTSSe solar cells is partly limited by the back-contact barrier due to the insufficiently large work function of back contact materials. The work function of MoS_x can be effectively improved by the incorporation of Cu. Very little Cu incorporation could lead to significant change in work function.

Implications for future projects

For future work to remove the back-contact blocking barrier and reduce back contact resistance, a Cu doped Mo(S,S)x interfacial layer with tunable work function could be developed.

Background

Objectives or project requirements

The blocking barrier at the back contact of CZTSSe solar cells (especially high bandgap CZTSSe) is an important issue responsible for the unfavourable fill factor. This reverse barrier also reduces the voltage of devices. Chemical stable back contact materials with sufficiently high work function is important for high efficiency CZTSSe solar cells.

Process undertaken

CZT precursor with relatively high Cu content ($Cu/Sn \approx 1.95$) is found to effectively introduce Cu into the MoS_x interfacial layer. No Cu incorporation was observed with low Cu content ($Cu/Sn \approx 1.85$).