Suppressing Deep-Level Trap and Energy Band Alignment Enable Air-Solution-Processed Cu_2ZnSnS_4 Thin Film Solar Cell with Certified Record Efficiency

Tong WU[1-2], Michel Cathelinaud[1], Shuo Chen[2], Hongli Ma[1], Xianghua Zhang[1], Guangxing Liang[2]

1 CNRS, ISCR (Institut des Sciences Chimiques de Rennes), UMR 6226, Université de Rennes, Rennes F-35000, France

2 Shenzhen Key Laboratory of Advanced Thin films and Applications Shenzhen, Guandong 518060 PR. China

The sulfide kesterite Cu_2ZnSnS_4 (CZTS) is widely recognized as a highly competitive photovoltaic material, especially for use in multi-junction solar cells, due to its excellent photoelectric properties. However, the power conversion efficiency (PCE) of CZTS/CdS solar cells has remained stagnant for years. The presence of deep level defects, such as V_S (sulfur vacancies), has been demonstrated to provide a kind of effective nonradiative recombination pathway, leading to serious open-circuit voltage (V_{OC}) deficit and reduced efficiency in carrier migration and separation. Herein, we propose a novel directional passivation strategy for V_S through an easily operable heterojunction heat treatment. By introducing O_2 during this process, sulfur vacancies can be readily occupied by oxygen atoms in an oxygen-rich environment, thus contributing to eliminating the already-existing V_S defects. In addition, the thermal movement of ions during this process induces Cd diffusion to the absorption layer to occupy the Cu or Zn lattice sites, these collective effects lead to reduced charge recombination and more favorable band alignment. As a result, CZTS thin film solar cells with a PCE of 11.89% and a certified record efficiency of 11.51% was achieved. The present study offers valuable insights into defect passivation mechanism of kesterite thin-film solar cells.

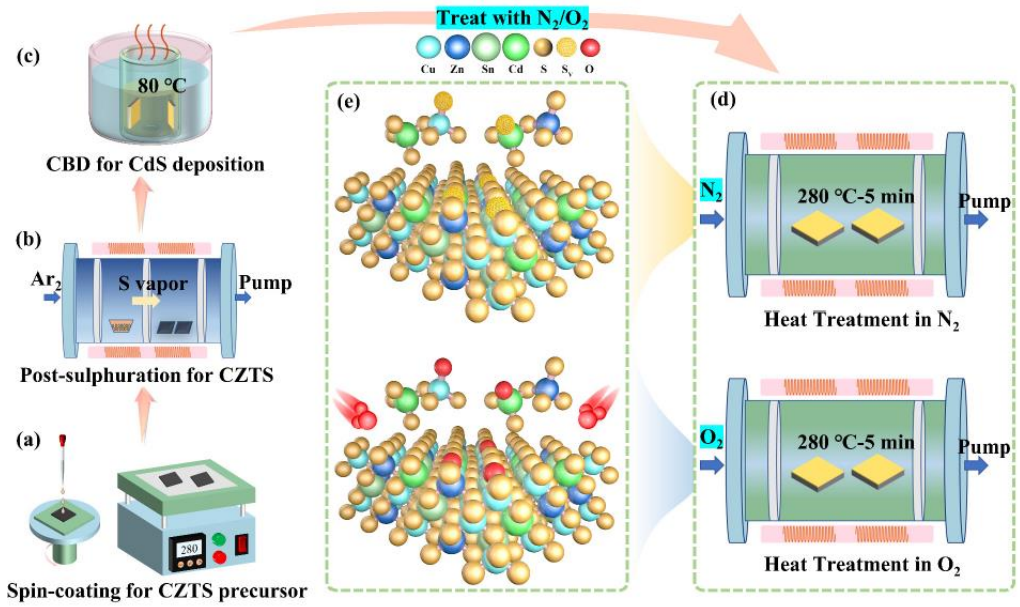

Fig. 1. Schematic diagram of production procedure

[1] Green, M. A.; Dunlop, E. D.; Yoshita, M.; Kopidakis, N.; Bothe, K.; Siefer, G.; Hao, X., Solar cell efficiency tables (Version 63). *Prog. Photovoltaics Res. Appl.* **2023,** *32* (1), 3-13.