Optimization of Sb_2Se_3 Thin-Film Solar Cells Grown by Selenization of Sb Layer

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Low-dimensional antimony-chalcogenide materials have received an outstanding interest for PV devices in the last years. They show high stability, low environmental impact, low cost, low carbon footprint and high technological flexibility. In particular, $Sb_2(S,Se)_3$ shows a high absorption coefficient > 10^5 cm^{-1}, allowing to reduce the film thickness to 50-500 nm, band gap energy Eg tuneable between 1.2 to 1.8 eV, and, a much lower melting point than that of CIGSe, CdTe and CZTSSe, requiring lower processing temperatures. Currently, efficiencies above 10% have already been achieved for $Sb_2(S,Se)_3$-based solar cells [1]. The versatility of this material makes it very promising for different PV applications. In this work, Sb_2Se_3 thin films have been grown by selenization of evaporated Sb layer on Mo/SLG and SLG substrates. Different growth parameters such as the thickness of the precursor Sb layer, the maximum selenization temperature and Se added during the thermal treatment have been investigated on the device performance. XRD, XRF, AFM, SEM, EDX, TEM and ellipsometry techniques have been used to investigate the compositional, structural, morphological and optical properties of the active layer. Independently from the used growth parameters, all absorbers show an orthorhombic structure with [hk1] preferred orientation, and a compact structure free of pinholes. However, the band gap energy E_g of Sb_2Se_3 is modified by the variation of the absorber thickness, the thinner the active layer, the higher the E_g. The best solar cells with ITO/ZnO/CdS/Sb_2Se_3/Mo/SLG substrate configuration correspond to the Sb layer selenized at 340 C, and, when [Se]/[Sb] ratio is not much higher than 1.6. It is also found that the device performance enhances when the absorber thickness is reduced from 1300 nm to 400 nm. A maximum efficiency of 4.9% (active area) is achieved. An increase in the device performance is expected by optimal combination of all the growth parameters, absorber thickness and a fine control of the Se content. The limitation of the efficiency is not only given by the absorber quality, but also by other layers that build the photovoltaic solar cells. Here, we investigate the effect of the variation of the CdS buffer layer on the performance of the solar cells. For that, TEM investigation of the interface in completed devices has been carried out. The variation of the chemical bath deposition of CdS has an important impact on the short circuit current density J_{SC} that resulted in an improved efficiency from 3.6% to 5.4%. This enhanced performance is very well correlated with the decreased defect concentration from 3.4×10^{17} cm^{-3} to 7.8×10^{16} cm^{-3}, as determined from DLCP and CV measurements. Further investigation is being performed to define the optimal active layer and heterojunction to enhance the devices performance.

[1] X. Chen et al., Adv. Energy Mater. 13 (2023) 2300391.