Crystallization Study of the Cu2ZnSnS4 Chalcogenide Material for Solar Applications

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Second generation thin-film chalcogenide materials, in particular CuInGa(S,Se)2 (CIGS) and CdTe, have been among the most promising and quickly became commercial candidates for large-scale PV manufacturing. These materials offer stable and efficient (above 10%) photovoltaic modules fabricated by scalable thin-film technologies and cell efficiencies above 20 % (CIGS). Indium-free kesterite-related materials such as Cu2ZnSnS4 have attracted significant research interest due to their similar properties to CIGS. In these materials, indium is replaced with earth-abundant zinc and tin metals. The quaternary semiconductor Cu2ZnSnS4 (CZTS) is a relatively new photovoltaic material and is expected to be interesting for environmentally amenable solar cells, as its constituents are nontoxic and abundant in the Earth's crust. The CZTS thin films show p-type conductivity, a band gap of 1.44–1.51 eV that is ideal to achieve the highest solar-cell conversion efficiency, and relatively high optical absorption in the visible light range.

Various techniques have been developed in synthesizing CZTS but to meet the long term cost goal of cost effective fabrication of compound semiconductors, suitable thin film in-line coating and processing techniques have to be realized. For deposition, sputtering can provide good control on film composition at a relatively low cost and is suitable for large-area, continuous and multi-component deposition. This method is already an established technique for the preparation for thin films for magnetic, optical and contact applications. And for annealing, rapid thermal processing is a method that significantly reduces the thermal budget of the sample as compared to conventional furnace annealing. In addition to production related issues, some principal advantages of low thermal budget processing is the minimization of interdiffusion and impurity diffusion from the substrate as well as better control of the process kinetics.

In this Work, Cu2ZnSnS4 thin films were first deposited by RF magnetron sputtering at room temperature from a single quaternary target (Cu2Zn1Sn1S4 target 99.999% from Testbourne Ltd.) on molybdenum coated substrates using a Kurt Lesker NANO-38 thin film deposition system. The films were annealed in a Jipelec JetFirst 100 bench top Rapid Thermal Processor at 480, 500 and 520 degrees Celsius and for annealing times ranging from 2 min to 40 min. The Annealing was done without any toxic gases or reactive sulfur. The compositional and structural properties of the films were analyzed using EDX and XRD respectively and certain recipes were identified which produce films with good adhesion, good crystallinity and that show the ideal stoichiometry before and after annealing. Furthermore an in depth analysis of the phases formed was realized during the experiment.

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