Cu2ZnSnS4 Nanoparticle Absorber Layers for Thin-Film Solar Cells

In the search for a new material for solar cells, the quaternary chalcogenide copper zinc tin sulfide (Cu2ZnSnS4 or CZTS) is one potential candidate. It is abundant, environmentally-friendly, inexpensive, and presently it has a mediocre record efficiency of around 10% with potential to reach above 15%. This thesis is a part of the work done in making the prospects of solution-processed CZTS more fruitful. In addition to an inexpensive material, a cheap production pathway is also required for the material to be suitable for solar cells of the future. Solution-processing comprises either a nanoparticle ink or a precursor ink that can be printed, sprayed, or in another way coated on a substrate appropriate for mass production.

For CZTS, the power conversion efficiency of these device are lagging behind the vacuum processed CZTS thin films, as certain challenges arise with solution-processing. The conversion of the as-deposited amorphous or nanocrystalline thin films into an almost "monocrystalline" material is not effective under the current sulfurization conditions. In this work, means have been taken to improve the properties of the nanoparticles in order to make them easier to handle and better for the succeeding sulfurization step. For this objective, two main routes have been pursued. The first route was related to synthesizing larger nanoparticles than the typical outcome of the synthesis route used, as these could be a better starting material for grain growth. This was achieved by utilizing a two-step hot-injection method for synthesizing nanoparticles; it adds an extra step, but the desired particle sizes and particle size distributions were obtained. The second track concerned developing a type of nanoparticles without any hydrocarbon surface coatings, as these organic ligands have been challenging to remove in the succeeding annealing steps. By choosing suitable solvents and precursors, organic ligand-free nanoparticles were successfully synthesized in a facile one-step process. These particles further introduced the advantage that they could be dispersed in simple solvents such as water and ethanol. To understand what happens to the as-synthesized material when it is heated, a range of analyses were carried out with some slightly uncommon techniques for the field of CZTS: thermogravimetric analysis coupled with mass spectrometry. This characterization resulted in knowledge of how solvents and ligands evaporate or decompose as a function of temperature. The nal part of the work has been related to fabricating a thin-film absorber layer from the CZTS nanoparticles. It is a common obstacle that grain growth in these CZTS nanoparticle thin films is severely restricted, as the absorber layer remains very porous or an organic layer is present at the back interface, which was also seen here. Sodium in the form of NaCl salt was for the first time dissolved directly in the nanoparticle ink - again with focus on environmental friendliness and a low cost. The addition of sodium had a signicant impact, and it greatly enhanced both structural and optoelectronic properties of the films.

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