MS122.O02

Solar cell structure at micro- and nanoscale through TEM

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The expensive vacuum based synthesis used for the synthesis of thin film photovoltaics based on Cu2ZnSn(S,Se)4 (CZTSSe) and CuInxGa1-x(S,Se)2 (CIGSSe) typically results in pore-free layers with large densely packed grains. However, the control over the composition and microstructure thin film photovoltaics with cheaper non-vacuum methods is challenging.

The non vacuum methods often result in various undesirable secondary phases (crystalline as well as amorphous), limited control over the compositional homogeneity, a high density of voids at the back contact/absorber interface and nanosize grains that can hinder the electrical performances of the solar cells. The grain boundaries for example can act as recombination centres, reducing the efficiency of charge transfer and increasing series resistance, while the pores can lead to a decreased shunt resistance value by the formation of shunt paths between the n- and p-type electrodes. Chemical cleaning can reduce secondary phases, but defects, vacancies and dangling bonds formed during their presence and subsequent removal can remain. On the other hand, nanosized extra layers can also be introduced intentionally in order to function for example as passivation layers.

To be able to control all these micro- and nanostructural influences, intentional and non-intentional both, it is important to be able to study them at the appropriate scale. During our research, transmission electron microscopy (TEM) proved to be the optimal tool for detecting the micro- and nanoscale effects missed by other techniques, but important for understanding the properties.

In this lecture, different cases will be shown where the micro- and nanostructure as characterized by TEM was crucial for understanding the photovoltaic properties of the cells. Regular imaging (bright field and dark field TEM) still gives the most clear view of the different layers and grains, however, energy dispersive X-ray analysis mapping allows to detect easily all secondary phases or thin extra layers of even just a few nm between these grains and inhomogeneities or gradients in the composition, high resolution techniques (imaging and spectroscopic) allow to study the interfaces between the layers in detail and automated electron diffraction scans allow to map the relative orientations between the grains, the different phases and small changes in cell parameters and strain.

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Keywords: transmssion electron microscopy, thin film photovoltaics, CZTS