Identification of secondary phases in thin film solar cells by 3DXRD and multigrain crystallography

M. Mar Lucas(1), C. Rein(1), H.F. Poulsen(2), J. W. Andreasen(1)

(1) DTU Energy, Technical University of Denmark, Frederiksborgvej 399, 4000 Roskilde, Denmark.
(2) DTU Physics, Technical University of Denmark, Fysikvej, 2800 Kgs. Lyngby, Denmark.
mmarlu@dtu.dk

Here, we present advances in Three-Dimensional X-ray Diffraction (3DXRD)\(^1\) for the analysis of submicron size quaternary polycrystalline thin film solar cells.

3DXRD was used to identify crystallographic phases in photovoltaic thin films. One target system used for these investigations is Cu\(_2\)ZnSnS\(_4\) (CZTS)\(^2\), a promising material for 3rd generation solar cells. CZTS is a polycrystalline material and through its formation process, secondary phases arise. These phases cannot be identified with conventional methods such as powder diffraction. Hence, the motivation to apply 3DXRD to reveal the structural properties, texture and their effect on the solar cell efficiency.

We have performed 3DXRD experiments at APS beamline 1-ID and at beamline BL20XU at Spring-8. We first demonstrate that we can index the grains that constitute the absorber layer and thereby identify the crystallographic phases and orientations. Next, we map the crystal growth dynamics of the annealing process of CZTS. Finally, we present the status on reconstructing a 3D grain map of a CZTS thin film solar cell through scanning 3DXRD, providing the size, location, and orientation of each individual grain and allowing a grain boundary study of such system. We discuss the potential use for other materials and the limitations of the method.

![Fig. 1.](image)

Fig. 1. (a) SEM image of a silver-doped CZTS thin film accompanied by its (b) harvested diffraction spots from 3DXRD represented in 2D. (c) Scattering vectors in 3D in the reciprocal space. Each colour label represents the powder rings associated to the crystal lattices of CZTS.