Structural and phase analysis of polycrystalline thin films by grazing incidence X-ray diffraction

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Surface sensitive X-ray diffraction can be realized using small incidence angles and a multilayer mirror to produce a parallel incoming beam. Because wave penetration is limited, grazing incidence X-ray diffraction (GIXRD) is a powerful method to study surfaces and layers. We applied this method to study polycrystalline thin films with regard to a depth-profiled structural as well as qualitative phase analysis. The experiment consists of a number of detector scans performed at fixed incident angle, the latter is varied between 0.5° and 5°.

Three examples will be discussed in the presented work. Two of them deal with the structure and phase content of polycrystalline thin films within a thin film solar cell. Highly efficient thin film solar cells are based on the quaternary compound semiconductor Cu(In,Ga)Se_2, which crystallizes in the tetragonal chalcopyrite type structure (space group). Such absorbers are characterized by a varying Ga content from top to bottom of the layer, resulting in a variation of the structural and electronic properties. To investigate this Ga gradient, GIXRD is applied. Analysing the shift of the Bragg peaks of the chalcopyrite type phase, the Ga content in dependence of the depth can be determined. Analysing the intensity ratios between the main Bragg reflections, informations about preferred orientations of the layer can be obtained. It should be noticed, that the Ga gradient determined by GIXRD is in very good agreement with values resulting from an EDX (energy dispersive X-ray) analysis of the absorber profiles.

To realize the p-n junction of the thin film solar cell, a buffer layer (e. g.) is deposited on top of the absorber layer. This more complex layer structure will be discussed in the second example. In dependence of the deposition temperature of the In_xS_x a number of different ternary and quaternary phases growth on the Cu(In.Ga)Se_2 layer. Amongst them is $CuIn_5S_8$, which crystallizes in the spinel type structure, and Cu(In,Ga)$_3Se_5$, which crystallizes in the stannite type structure and belongs to the group of so-called ordered vacancy compounds.

The third example steps over to geological materials in discussing the GIXRD investigation of a polycrystalline forsterite thin film deposited on quartz.

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