BACK TO BASICS: STUDY OF DEFECTS IN SINGLE CRYSTAL $CuInS_2$ SOLAR CELL ABSORBER MATERIAL

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To improve the efficiency of a solar cell, a good understanding of the defect chemistry of the absorber material is needed. For the fabrication of high efficiency solar cells the ternary chalcopyrite semiconductor $CuInS_2$ is considered to be a promising material. This is due to its optimum band gap of 1,5 eV, its direct type transition structure and its large absorption coefficient above the band gap energy. $CuInS_2$ belongs to the I-III-VI_2 family of compounds and is derived from the sphalerite lattice by doubling the unit cell of II_2-VI_2. The two group-II atoms are replaced by one group-I atom and one group-III atom. The deviation in stoichiometry is reflected in the electrical properties and affects the level and sign of doping. The material is p-type for Cu or S rich and n-type for In rich or S poor compositions. Up to now, efficiencies of around 12, 5 % have been achieved (1) for these types of solar cells.

To allow a detailed characterization and identification of the defects in the absorber material, $CuInS_2$ single crystals are needed. We use the vertical Bridgman growth method. The complex phase diagram of $CuInS_2$ shows that single phase material can only be formed in a small compositional region. Stoichiometric amounts of high purity Cu, In and S are mixed in a carbon crucible with conical tip that is vacuum sealed in a quartz ampoules. The elements are prereacted at 600°C for 7 h and then the ampoule is placed in the hot part of a two-zone oven and kept at a temperature (1150°C) above the melting point of all individual components to obtain a homogeneous melt. It is then slowly lowered into the oven region below the $CuInS_2$ melting temperature. The temperature gradient, the growth rate and the dimensions of the crucible are varied in order to optimize the crystal growth. The crystal quality will be crucial for a correct interpretation of the results of defect analyses.

X-ray diffraction (XRD) is used for assessing the phase composition; scanning electron microscopy is used for surface and particle morphology. To investigate defect states in the band gap of $CuInS_2$ photoluminescence measurements are performed. The results allow understanding the recombination paths which are a key issue for the solar cell performance.

(1) J. Klaer, J. Bruns, R. Henninger, K. Siemer, R. Klenk, K. Ellmer, “ Efficient CuInS2 thin-film solar cells prepared by a sequential process”, Semicond. Sci. Technol. 13 (1998) 1456–1458.