

Experience of Germany shows that significant portion of the energy needs of the society might be supplied by utilizing sunlight - even in our climate zone it is possible and profitable in the long run. Second generation solar cells based on thin films of semiconductor compounds strongly absorbing light it is cheaper and less energy-consuming in production alternative to the currently dominating silicon solar cells. Structures based on Cu(In,Ga)Se₂ (CIGS) feature the highest efficiency of the second-generation cells (22.6%) combined with long-term stability and might be a serious alternative to the Si-based PV, e.g. for building integrated photovoltaics (BIPV), mobile applications (flexible panels) or powering the Internet of Things (IoT). Record laboratory cell efficiency above 20% have been largely achieved thanks to the intuition of the technologists, rather than supported by a deeper understanding of the properties of this material. To very interesting problems that have not yet obtained satisfactory explanation belong the effects of sodium and other alkali metals on the properties of the material and CIGS solar cells. For more than 20 years already it is known that the presence of sodium diffusing from the glass substrate has a beneficial effect on the efficiency of these devices. The spectacular increase in the efficiency of CIGS cells made over the last 2-3 years has been achieved through the use of both sodium and heavier alkali metals - potassium, and quite recently also rubidium and cesium - in the processing of CIGS absorbers. It has also been found that supplying alkalis into CIGS layer after deposition (post-deposition treatment PDT) leads to desired effects. The goal of the project AlkaCIGS is to clarify what are the fundamental causes of the beneficial influence of sodium and other alkali metals on the opto-electronic properties of the CIGS cells. In particular following issues being a subject of long-going discussions and controversy are to be addressed:

- are alkali elements active only at the surfaces (at grain boundaries and at front/rear interface of the cell) or do they diffuse into the material and change spectrum of defects responsible for conductivity and for recombination losses?
- are such interesting phenomena as metastabilities in the electrical characteristics of CIGS cells leading to the persistent increase of the efficiency under the influence of sunlight linked to the presence of sodium?
- is the effect of alkalis at the front and rear surface of CIGS layer in the photovoltaic structure due to surface defects passivation or do they facilitate the formation of thin layers of compounds modifying the electrical activity of the front and back surfaces (MoSe₂ at the back contact and K-In-Se phases at the front heterointerface)?
- are the effects due to alkali elements, including those responsible for conductivity, influenced by the ratio of copper to group III elements in CIGS?
- what are the interactions between lighter and heavier alkali metals during PDT

The answer to these questions will be possible only if especially designed samples will be prepared and characterized by a wide selection of experimental and theoretical tools. In this project, we focused on the removal of the causes that hindered previously a clear interpretation of the above mentioned problems. First, the samples will be prepared using post-deposition treatment which does not change the defect structure and morphology of the material. In many previous studies samples in which sodium was supplied during deposition of the CIGS layer were used. In this case the effect of sodium on the material formation and its defect structure could not be separated from the influence of Na on the opto-electronic properties. Using samples with controlled and varying amount of alkalis provided after material growth will remove many interpretational ambiguities. Secondly, the experiments will be conducted in parallel on solar cells and on CIGS thin films using a set of complementary electrical and optical methods. This approach will make possible to a distinction between the phenomena which occur in the volume of material from those associated with the surfaces and grain boundaries. Thirdly, experiments will be accompanied and conclusions constantly verified by supporting numerical simulations and first principles calculations.

The activities planned in the project can only be successful in close cooperation between the team of engineers with experience in CIGS technology and researchers with expertise in experimental and theoretical analysis of semiconductors and photovoltaic structures. In the project collaboration of two groups with adequate expertise is proposed: the best group in CIGS technology in Europe - ZSW Stuttgart's holding world record in efficiency of CIGS cells in recent years and the team from the Faculty of Physics, with many years of experience in optoelectronic characterization of CIGS cells and photovoltaic materials and experimental and simulation facilities necessary for the realization of the planned tasks.