Bulk and interfacial defects in structures based on ZnO and ZnO semiconducting alloys

Materials with radically enhanced properties are essential for devices with improved performances and novel applications. Among the currently investigated new semiconductors, ZnO as well as its alloys ZnMgO and ZnSnO represent very promising candidates for photovoltaic utilization, since novel structures extremely appealing in terms of efficiency and/or costs based on ZnO have been recently proposed. In these devices the ZnO layer is acting not only as transparent front contact, as in already commercially available thin films solar cells, but also as n-type counterpart of the p-type absorber. This approach significantly reduces the fabrication complexity, while it maintains theoretically predicted efficiencies above 20%, for example when combined with p-Si or Cu_2O. Hence, it has the potential to revolutionize the present solar cells market. Due the large bandgap of ZnO (~3.4 eV) a different semiconductor has to be used as absorber in such structures. This implies that the final device rely on the formation of an heterojunction, where the interfacial electrical active defects plays a major role in reducing the theoretically maximum efficiency achievable. In addition, also the presence and possible impact of bulk defects on the final electrical and photovoltaic properties of the junction have to be considered. However, so far very limited information is present in the scientific literature concerning the bulk and interfacial defects in ZnO based structures and the physical nature of most of them is still under debate. Furthermore, most of the studies were focused on single crystal hydrothermally grown material, even though, polycrystalline layers deposited on specific substrates and with electrically tuned properties are necessary for applications. Therefore, the present knowledge is clearly not sufficient in assigning an electrically detected defect present in ZnO layers of possible practical use to a chemical impurity, to misplaced or missing atoms as well as to defects of larger dimensionality introduced during growth. Such fundamental knowledge is essential to exploit the potential of the above mentioned proposed structures, since it paves the way to new possible routes to reduce or to passivate bulk and interfacial detrimental defects. Furthermore, as it has been shown by theoretical calculations in the case of p-Si/n-ZnO heterostructures, band tuning, i.e. reduction of the impact of interfacial recombination by enlarging the energetic distance between the free carrier and the defect, represents an alternative to defect engineering. In the case of ZnO such effect can be achieved by Mg/Sn alloying, even though growth conditions and especially substrate surface pretreatments can also have an impact on it.

Goal of the present project is to achieve a better fundamental understanding of the chemical and physical nature of electrically active bulk and interfacial defects present in ZnO, ZnMgO and ZnSnO based structures and to study the dependence of band alignment on the Mg/Sn content, growth conditions and substrate pretreatments. For this purpose, the layers with application potential will be grown and studied by using advanced electrical measurements techniques to establish the presence of commonly electrically active defects. These results will be combined with the information extracted from structural and chemical characterization to determine their nature. In addition, the overall fundamental effects of band alignment, bulk and interfacial defects on the macroscopic electrical performances of selected structures, that are exhibiting promising performances as solar cells, will be studied by performing a complete optoelectronic characterization. These measurements will be combined with numerical simulations to establish the weight of the different contributions, i.e. bulk, interfacial defect and band alignment on the macroscopic electrical properties.

The achievements of the present project will verify the feasibility of realizing high quality n-ZnO, n-ZnMgO and n-ZnSnO films to unlock the potential of these materials in photovoltaic applications. Further, a laboratory dedicated to the advanced electrical measurements with novel characterization techniques and a team able to tackle complex numerical simulations of heterostructures based on thin films will be created with the aim to compete with world renowned research teams.