Intrinsic defects and passivation mechanisms of Al_2O_3-ALD films deposited on $CH_3NH_3PbI_3$ at room temperature

Małgorzata Kot[1,2], Klaus Müller[1,2], Karsten Henkel[*1,2], and Dieter Schmeißer[2]

[1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Konrad-Zuse-Straße 1, 03046 Cottbus, Germany

[2]Applied Physics and Sensor Technology, Brandenburg University of Technology Cottbus-Senftenberg, Konrad-Wachsmann-Allee 17, 03046 Cottbus, Germany

[*]henkel@b-tu.de

$CH_3NH_3PbI_3$ (MAPI) based photovoltaic devices showed recently increased long-term stability upon the growth of Al_2O_3 films prepared by atomic layer deposition at room temperature.

Synchrotron radiation based photoelectron spectroscopy is applied to study the initial interaction of these Al_2O_3 layers on MAPI. We focus on the electronic properties of MAPI and its interface and identify a delicate charge balance between polaronic and excitonic states in MAPI and Al_2O_3. The polaronic states up-take a charge from the MAPI substrate which is transferred to and stabilized in the excitonic state of Al_2O_3. The initial Al_2O_3 film at the MAPI interface shows a high abundance of excitonic states which are assigned to predominately tetrahedral coordinated Al sites. The aforementioned charge transfer further stabilizes a covalent bonding at the interface which is confirmed by Cooper minima found for both, the Pb5d and the O2p states.

The presence of Iodine and MA vacancies at the interface is deduced from changes in the core level intensities. Vacancies provide charges to ensure the covalent bonding described above. In addition, they lead to the formation of grain boundaries and a roughening of the interface. Such initial grain boundaries are sealed again by the growth of 2D clusters of Al_2O_3 and the vacancy concentration is stabilized against interdiffusion (long term instabilities). Further Al_2O_3 growth causes a self-healing of the structural defects and causes a long-term passivation.