Modelling investigations of surface photovoltage including surface defects

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Abstract: Kelvin Force Probe Microscopy (KPFM) is a local scale advanced characterisation technique. It maps surface work function on an atomic scale with nanometric resolution. This can reveal information on band structure and electronic properties of semiconductor materials and is invaluable for the study of nanostructures. The difference between signals in the light and in the dark yields surface photovoltage spectroscopy which provides contactless information on the performance of devices and in particular solar cells. These techniques being dominated by the surface, and therefore by surface defects, the analysis of measurements is particularly challenging.

In this contribution we describe analysis of KPFM measurements by solving semiconductor transport and continuity equations numerically for the KPFM measurement geometry including the nanometric atomic probe and its position on the cross section of multilayer samples. The numerical methods allow a description of surface defect properties in terms of distributions in the gap, as well as descriptions of defect species in terms of their energy distributions and capture cross sections. We investigate the physical modification of band profiles across this section by distributions of donor and acceptor surface defects in the bandgap of the materials. We discuss the modification of net charge densities as a result of charged and neutral donor and acceptor populations, and the resulting band bending affecting the KPFM and SPV signals.

Applications of these methods are considered with a focus on photovoltaic applications, for the dominant materials in the field including group IV, III-V and concluding with considerations for emerging materials such as perovskites.