

Determining the Mobility of Ions in Perovskite Solar Cells – Measurement and Simulation

Evelyne Knapp^a, Martin Neukom^{a,b}, b, Stéphane Altazin^b, Simon Züfle^{a,b}, Beat Ruhstaller^{a,b}

a Institute of Computational Physics, ZHAW, 8401 Winterthur, Switzerland

b Fluxim AG, 8406 Winterthur, Switzerland

The evidence is compelling that mobile ions are responsible for the IV-curve hysteresis observed in perovskite solar cells. Calculations show that iodine and methylammonium (MA) vacancies are indeed mobile within the perovskite crystal. The calculations predict a diffusion coefficient for both types of vacancies [1, 2]. Cell simulations incorporating mobile ions confirm the scan-rate dependent occurrence of an IV-curve hysteresis [3, 4, 5]. In order to elucidate the dynamics of electronic and ionic charges in the perovskite cells we acquire current responses to a voltage-step in the dark in a large range of time scales from microseconds to seconds. The measurement results are compared with simulations that employ a fully-coupled drift-diffusion solver incorporating mobile ions. We explain distinct features of the current-rise and how they are attributed to motion of mobile ions within the bulk. The delay time between voltage step and current-rise is used to estimate the ion mobility. We furthermore show evidence that a second ion type is mobile with a much lower mobility, presumably MA vacancies. Moreover, it is observed that the extracted ion mobilities depend on the fabrication type (evaporated versus solution-processed). Shao and co-workers presented evidence that ion migration is dominant in grain boundaries [6]. Thus, different grain-size and grain-boundaries might be the origin of the variation in ion mobility of the perovskite devices produced with different processing conditions. We conclude that transient currents acquired over a broad range of time scales combined with numerical device simulation represent a powerful method to study electronic and ionic charge transport properties.

References:

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