A Simulation Tool for Ion Transport in Semiconductors: Applications to Thin-film Photovoltaics ANUJA PARIKH, MARCO NARDONE, Bowling Green State University — Thin-film photovoltaics (TFPV) such as cadmium telluride (CdTe) and copper indium gallium diselenide (CIGS) are leading candidates for cost-effective solar electricity. The impacts (positive or negative) of ion migration in these polycrystalline semiconductor devices is an area of ongoing research. Given the fact that grain boundaries exist in thin-film device components, diffusion mechanisms require special attention. In this work, we review the physics of ion transport in solids (crystalline and polycrystalline), develop a general numerical simulation tool for ion drift-diffusion, and validate it against literature data and analytical expressions for the technologically important cases of phosphorous and copper in CdTe, and sodium in CIGS. Calculations are conducted by the finite element method using COMSOL Multiphysics®software. After validation of this initial model, the simulation tool will be extended to predict the effects of ion migration on the performance of CdTe and CIGS devices by coupling it to a device simulator.

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