Abstract for the Quantsol Winter Workshop, March 2025

Grain boundaries in various absorber materials for solar cells

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For polycrystalline absorber materials used in high-efficiency solar cells, the role of grain boundaries on the device performance has always been a matter of concern. Basically, it can be expected that the enhanced, nonradiative Shockley-Read-Hall recombination at the grain-boundary plane leads to a corresponding decrease in the effective lifetime of the minority-charge carriers and thus, to a decrease in the open-circuit voltage of the corresponding solar cells. The present contribution will give an overview of this concept, including a grain-boundary model describing the recombination velocities in various photovoltaic absorber materials (microcrystalline Si, CdTe, $(Ag,Cu)(In,Ga)(S,Se)_2$, kesterites, halide perovskites). The validity of this model will be demonstrated by discussing case studies for all these material systems. At each grain boundary, the recombination velocity is determined by the effective, charged defect density and by its capture cross-section, in addition to the corresponding excess charge, which can be positive or negative. For a $Cu(In,Ga)Se_2$ layer in a high-efficiency solar cell, two-dimensional device simulations using results from microscopic analyses demonstrate losses in open-circuit voltage of about 10-20 mV by enhanced, nonradiative recombination at grain boundaries.