Abstract QUANTSOL 2026 Winter Workshop

Why grain boundaries are always detrimental for the device performance of solar cells and dislocations are not (in some material systems)

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In solar-cell devices, grain boundaries reduce the device performance mainly via enhanced nonradiative recombination, leading to losses in the open-circuit voltage (V_{oc}). As discussed in a recent report [1], the barriers for charge carriers at grain boundaries in all relevant photovoltaic materials - Si, CdTe, Cu(In,Ga)Se_2, $Cu_2ZnSn(S,Se)_4$, halide perovskites - do not exhibit values sufficiently large (only several ± 10 meV) to affect charge transport substantially and thus, to affect the current of the solar-cell device. After analyzing grain boundaries in more than 35 solar-cell absorbers based on various material systems (i.e., the ones mentioned above), it can be concluded that grain boundaries influence the conversion efficiency mainly via decreases in V_{oc} and the corresponding part of the fill factor linked to the V_{oc}. The V_{oc} losses due to recombination of charge carriers at grain boundaries can be estimated using a simple model [2,3], ranging from few mV to few 100 mV, depending on the absorber material. Thus, grain boundaries in solar-cell absorbers are always detrimental for the device performance.

At dislocations in Si and CdTe, enhanced nonradiative recombination occurs in a similar manner as at grain boundaries in the same material. However, this is not the case for Cu(In,Ga)Se_2, in which luminescence signals measured at dislocations do not differ from those acquired in the surrounding matrix [4]. I will discuss the reason for this behavior and give an overview of a microscopic study analyzing epitaxial Cu(In,Ga)Se_2 layers with various composition and with/without the addition of Na. It will be shown that dislocations in Cu(In,Ga)Se_2, independent of the composition, do not exhibit different luminescence emissions than the matrix and thus, cannot be expected to affect the V_{oc} values of the solar cells considerably, in contrast to grain boundaries in the same material. I will outline why a similar behavior can be expected for dislocations in $Cu_2ZnSn(S,Se)_4$ and halide perovskites.

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