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Simulation of Current Transport in Polycrystalline CdTe Solar Cells

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Polycrystalline thin-film CdTe solar cells have demonstrated laboratory efficiency exceeding 17% and are nowadays a commercial technology (albeit with somewhat lower efficiencies). The standard process features a poorly understood recrystallization step, obtained by annealing with a source of chlorine. This study uses two-dimensional numerical modeling to investigate current transport inside the polycrystalline CdTe absorber with and without recrystallization effects [increase of grain size and donor Cl_{Te} states at grain boundaries (GBs)]. Solving the Poisson equation and the drift–diffusion model for transport with Fermi statistics, while treating the optical problem by the one-dimensional transfer matrix method and complex refractive indexes, this study shows that: (i) in a columnar absorber (i.e., one where only vertical GBs exist), the presence of Cl_{Te} donor traps at GBs results in a dip in the band profiles that effectively serves as an electron collector, significantly increasing the short-circuit current and efficiency compared with nondecorated GBs; (ii) while the same dip acts as a hole barrier and thus can be expected to block holes from flowing when horizontal GBs are present, under illuminated conditions electron collection at GBs reduces the dip enough to allow substantial hole flow, and the cell performance is only moderately affected.

Key words: Photovoltaic, thin-film solar cells, CdTe, grain boundaries, numerical modeling

INTRODUCTION

Thin-film solar cells based on copper indium gallium selenide (CIGS) or CdTe absorbers have been studied in research laboratories for at least 20 years, but only recently entered the phase of industrial production. While still lagging behind their Si-based competitors in terms of efficiency and dollars/watt, these technologies are poised to conquer increasing market share, and perhaps even reach market dominance, with forecast production costs approaching 0.4 US$/W.[1] However, for the time being, CdTe solar cells still underperform compared with theoretical limits and even with CIGS cells,[2] and in spite of a relatively long history of research and development, there is still room and need for better understanding of the physics underpinning the photovoltaic performance of CdTe cells and modules.

One difficulty lies in the fact that, while single-crystal materials used in traditional (silicon) and high-efficiency tandem (GaAs-based) solar cells are well known and fully characterized, polycrystalline materials used in thin-film solar cells show widely varying characteristics depending on the growth/deposition process and conditions; the polycrystalline nature of the absorber is itself an obstacle to full understanding of the cell behavior, and often the device is studied by simulating an "equivalent" single-crystal solar cell where the material parameters, such as carrier lifetimes, are modified to give a reasonable match to experiments. This approach has the major advantage of allowing a one-dimensional

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