

# Abstract

The demand for a source of renewable energy has been the driving force to achieve significant advancements in the field of photovoltaic energy generation during the past decades. To reach the goal of solar cell efficiency enhancement, the development of novel materials is a strategy of paramount importance. Research towards multijunction solar cells has resulted in record-breaking efficiencies, at the expense of structural complexity and high cost. A promising concept to overcome this is the use of quantum dots embedded within the cell active region to absorb lower energy photons in the near infrared region that would otherwise not be absorbed by the main cell. The resulting quantum dot solar cells (QDSCs) therefore enable an increase in the short-circuit current while theoretically maintaining a high open-circuit voltage, assuming perfect material growth. However, QDSCs suffer from limitations such as the low absorption of the QD layer stack and the difficulty in growing a large number of layers to compensate for the low absorption. In fact, increasing the number of layers in the stack results in an increasingly large reduction of the open circuit voltage.

Light trapping is a photon management technique used to enhance the effective optical path length of the solar cell in order to increase the photogeneration in thin or low absorbing QD layers. The potential optical path length enhancement is dependent on the refractive index of the active region material, and for III-V solar cells it turns into an enhancement of approximately fifty times. Owing to the fact that light trapping enables the use of thin-film cells by reducing the active region thickness keeping the same short-circuit current density, it allows for reduced volume recombination loss and can result in higher open-circuit voltage. Finally, light trapping-enhanced thin-film cells exhibit a high power-to-weight ratio, which is a desirable feature for space power sources.

The research presented in this dissertation was undertaken as part of the European H2020 project Thin-Film Quantum Dot (TFQD) photovoltaic cells. The project aimed to develop light-trapping enhanced TFQD cells as an enabling technology for lightweight, flexible, high-efficiency space solar arrays. The project involved multiple academic as well as industrial partners, and allowed the candidate to undertake two mobility periods at the Tampere University in order to participate in experimental characterization activities.

The scope of the studies in this dissertation covers the investigation of different photon management techniques to enhance the photoabsorption of thin-film QDSCs. Additionally, an approach to the self-consistent electro-optical modelling of light-trapping enhanced solar cells is investigated as an enabling tool for the optimization of such cells.

The introduction (Chapter 1) provides a brief overview about thin-film solar cells. The theory behind light trapping is described, where the enhancement limits are derived. An introduction to QDSCs is also provided to contextualize the requirement for light trapping methods.

The first study investigates light trapping-enhanced III-V QDSCs incorporating back-side diffraction gratings. The gratings are redesigned and optimized to efficiently diffract the light towards high-order modes using full-wave electromagnetic simulations implementing the rigorous coupled wave analysis method. The optimization is performed with the target of enhancing interband photoabsorption in the near infrared region. Nanostructured anti-reflection coatings are also studied with the aim of increasing the fraction of light injected into the cell and reducing front-side surface reflectance. It is then demonstrated using simulations that light trapping effectiveness can be improved in double-sided nanostructured cells, owing to the interplay between the diffraction grating and antireflection coating. Prototype diffraction gratings were fabricated by nanoimprint lithography on GaAs wafer. Efficient diffraction of light was observed in both simulated and experimental results using periodic gratings, allowing for the validation of the modelling approach and the proof of concept of the designed structures.

The following study aims to improve the absorption of low-energy photons for QDSCs working in the intermediate band regime, where mid-far infrared photoabsorption is low. Guided-mode resonance effects may enable large enhancement of QD intraband optical transitions. Ultra thin-film QDSCs are designed to have significant field waveguiding in the QD stack region and patterned at the rear-side with a sub-wavelength diffraction grating. Remarkable increase of the optical path length at mid-infrared wavelengths is shown owing to guided-mode resonances. Design guidelines are presented for typical energy and strength of the second-photon absorption of III-V QDs, such as InAs/GaAs and GaSb/GaAs.

The design of the aforementioned periodic photonic structures generally requires 2D or 3D full-wave approaches that are difficult to combine in a self-consistent fashion with electronic transport models to fully account for carrier collection and carrier-photon interactions. A novel and computationally efficient multiphysics approach is presented for coupled electrical-optical simulations, based on the multimodal scattering matrix formalism, wherein the grating is modelled by a scattering matrix that can be derived from simulations performed by the rigorous coupled wave analysis method.