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ScienceDirect

Energy Procedia 84 (2015) 204 – 213

Energy Procedia

E-MRS Spring Meeting 2015 Symposium C - Advanced inorganic materials and structures for photovoltaics

Realistic simulation of metal nanoparticles on solar cells

F.Cortés-Juan[a,b*], Alba Espinosa-Soria[a], J.P.Connolly[a], Guillermo Sánchez-Plaza[a], J.P.Hugonin[c], P.Sanchis[a]

[a] *Valencia Nanophotonics Technology Center, Ed 8F Camino de Vera s/n 46022 Valencia. Spain*
[b] *Laboratoire de Photonique et Nanostructures (LPN-CNRS), Route de Nozay, 91460 Marcoussis, France*
[c] *Institut d'Optique, CNRS, Université Paris-Sud 11, 2, Avenue Augustin Fresnel, 91127 Palaiseau Cedex, France*

Abstract

We present a strategy for simulating the scattering effect of an array of self-aggregated (SA) metal nanoparticles (NPs) on the light absorption in solar cells. We include size and shape effects of the NPs, the effect of a layered substrate and the effect of the interaction between NPs. The simulation relies on realistic characterization by SEM microscopy of the random NP arrays. Time and memory limitations of numerical approaches are overcome using semianalytical expressions. Size and shape considerations deal with truncated-sphere shapes by using a polarisability tensor. This is a development of other models leading to equivalent dipoles from the external source and the radiated fields from the rest of NPs. Once an equivalent array of 3-D dipoles is found, the total electromagnetic field and optical simulations are performed. The general trends show good agreement with experimental measurements. A critical analysis of the model is presented, and some improvement strategies are discussed for future studies.

Peer-review under responsibility of The European Materials Research Society (E-MRS)

Keywords: Plasmonics; Solar cells; Nanoparticles; Green Function; Simulation

1. Introduction

The majority of solar cell technologies are currently based on Si, as the industry is still focused on Si-based processes. However, as other minor technologies are increasing its efficiency most industrials look for a competitive

* Corresponding author. Tel.: +34-963-877-000 (Ext.88110); fax: +34-963-877-827.
E-mail address: frecorju@ntc.upv.es

Peer-review under responsibility of The European Materials Research Society (E-MRS)
doi:10.1016/j.egypro.2015.12.315

advantage by reducing costs while maintaining high efficiency. In Si photovoltaics, up to 51% of the cost is due to the silicon wafer, so a thickness reduction of the cells is therefore planned in the next years [1].

However, this thickness reduction leads to incomplete light absorption. Thinner solar cells therefore require light trapping strategies different from the traditional texturing, as textured thinner solar cells are expected to have a much greater breaking ratio during production.

A solution is possible with the use of nanostructures which provide scattering and therefore an enhancement in light absorption. Moreover some techniques, such the self-aggregation, have already been demonstrated to be economically feasible from the industrial point of view in the photovoltaic industry [2].

The self-aggregation method lead to nanoparticles that are not completely spherical or spheroidal [3], but rather truncated forms. This is intrinsic to the fabrication process and the wetting properties of the materials involved. Thus, traditional spherical models based on Mie seem not so appropriated to predict the behaviour of those systems, and the final application makes the multi-layered substrate too important to neglect its effect.

This work presents an approach to simulate the behaviour of metal nanoparticles over a stratified media assuming truncated spheres and a dipole-like radiation system solved using Green's function techniques. Thus, in Section 2 the details of a semianalytical model to obtain the polarisability of truncated spheres are presented, together with a critical analysis of its numerical particularities and the results. In section 3, the strategy in the use of Green functions to solve the induced dipoles is presented, taking as the exciting source not only the external exciting field but also the field radiated by the rest of the nanoparticles/dipoles. The model is tested in Section 4, where a critical comparison between experimental and simulated data is performed.

Nomenclature

NP	Nanoparticle
SA	Self-aggregated
α_H	Parallel or horizontal eigenpolarisability
α_V	Normal or vertical eigenpolarisability
$\boldsymbol{\alpha}$	Polarisability tensor
R	Radius of the spherical nanoparticle
a	Radius of the theoretical intersection between the spherical nanoparticle and the substrate
θ	Truncation angle
ε	Permittivity function of a material
V	Volume of a nanoparticle of radius R
$V_{a=1}$	Volume of a truncated nanoparticle in Jesper-Jung's model
$K_{H,V}$	Integral Kernels (Parallel and Vertical, respectively)
N	degree of the Laguerre polynomial / degree of Gauss-Laguerre quadrature
z_j	j^{th} zero of the Laguerre Polynomial of degree N
ω_j	j^{th} weighting factor for the Gauss-Laguerre quadrature

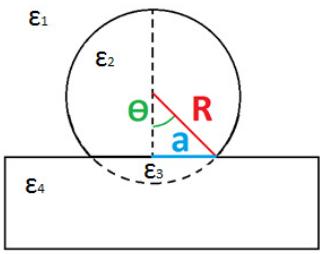

Figure 1 Schema of the structure studied by Jesper Jung. Three different materials can be considered in four different regions, corresponding to the substrate (4 or 3-4), the nanoparticle (2-3 or 2) and the surrounding upwards media (1, usually air). The truncation angle is defined from the bottom of the particle. All the solutions are calculated assuming that the parameter "a" is kept constant to 1.