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# Local Surface Plasmon Resonance of metallic nanoparticles embedded in amorphous silicon

A. Fantoni<sup>a,b,\*</sup>, M. Fernandes<sup>a,b</sup>, Y. Vigranenko<sup>a,b</sup>, M. Vieira<sup>a,b,c</sup>

<sup>a</sup>ISEL-ADEETC, R. Conselheiro Emídio Navarro, 1949-014 Lisboa, Portugal

<sup>b</sup>CTS-UNINOVA, Quinta da Torre, Monte da Caparica, 2829-516 Caparica, Portugal

<sup>c</sup>DEE-FCT-UNL, Quinta da Torre, Monte da Caparica, 2829-516 Caparica, Portugal

## Abstract

This work reports a theoretical study aimed to identify the plasmonic resonance condition for a system formed by metallic nanoparticles embedded in an a-Si:H matrix. The study is based on a Tauc-Lorentz model for the electrical permittivity of a-Si:H and a Drude model for the metallic nanoparticles and the polarizability of an aluminium sphere-shaped particle with radius of 10–20 nm. We also performed FDTD simulations of light propagation inside this structure reporting about the effects caused by a single nanosphere of aluminium, silver and, as a comparison, an ideally perfectly conductor. The simulation results show that it is possible to obtain a plasmonic resonance in the red part of the spectrum (600–650 nm) when 10–20 nm radius aluminium spheres are embedded into a-Si:H.

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## 1. Introduction

The optical path length of an optoelectronic device like a solar cell or a photodiode can be defined as the distance that an (unabsorbed) photon can successfully travel within the device before escaping out. This feature is usually described in terms of device thickness.

Light entering a device engineered with good light trapping features may get to be reflected back and forth many times, presenting an optical path many times higher than its physical thickness. This effect may enhance light absorption and, generally speaking, device performance. An attractive approach to improve the light trapping involves the introduction of plasmonic nanostructures coupled to absorbing

semiconductors [1]. Amorphous silicon (a-Si:H) has an optical gap of about 1.75 eV and it presents good absorption properties under visible light irradiation. This characteristic, together with an attractive low cost of production, has gathered the attention of scientific community during the last two decades of the last century. Today, arrived to its maturity, a-Si:H is one of the most used semiconductors in the photovoltaic industry for production of thin film solar cells. However, the poor transport properties and the high defect density of this material limit the thickness of the absorbing layers to about 500 nm. Also the degradation induced by the Staebler-Wronsky effect can in some measure be minimized by the use of a thin intrinsic layer [1]. Such thickness limitation forces the absorption of wavelengths longer than 550 nm to low values and suggested the use of a-Si:H in tandem junction configuration [1].

\* Corresponding author.

E-mail address: [afantoni@deetc.isel.ipl.pt](mailto:afantoni@deetc.isel.ipl.pt) (A. Fantoni)

In recent years, much attention has been recently given to the use of metal nanoparticles (NPs) embedded in semiconductor materials due to the possibility of enhancing light absorption in the semiconductor through the plasmonic near-field enhancement. Such an enhancement is expected at photon energies in the vicinity of the localized surface plasmon resonance condition (LSPR) of the metal nanoparticle. The LSPR condition depends on the metal/interface properties, on the particle size and shape, and finally on the average distance in the particle distribution [1,2]. Light trapping for improving solar cell efficiency based on plasmonic effects is reported in literature mainly for silver nanoparticles embedded in silicon solar cells [1,2] and in thin film amorphous silicon solar cells [1-3]. Reports on aluminium nanoparticles embedded in a-Si:H solar cells have also been recently published [1-3]. In this work we report about a theoretical study aimed to identify the plasmonic resonance condition for a system formed by metallic nanoparticles embedded in an a-Si:H matrix. The study is based on a Tauc-Lorentz model for the electrical permittivity of a-Si:H, a Drude model for the metallic nanoparticles and the polarizability of an aluminium sphere-shaped particle with radius of 10-20 nm. a-SiC:H has also been considered in our simulations, as it is used as a standard material for deposition of p-layers in a-Si:H solar cells. We also performed FDTD simulations of light propagation inside this structure reporting a comparison among the effects caused by a single nanosphere of aluminium, silver and, as a comparison, an ideally perfectly conductor. We considered a perfect conductor as an idealized material with infinite conductivity acting as a perfect reflector at optical frequencies. Such a comparison in the simulations permits the outlining and understanding of the plasmonic effects in opposition to standard optical reflections.

## 2. Theory

Optical properties of metal nanoparticles present unique characteristics, which, depending on size and shape, could get to be very different from the characteristics of bulk material. Coupling of light with the NPs surface produces a localized surface plasmon resonance resulting in an enhanced optical scattering and an enhanced optical field around the particle and thus enhancing the fraction of total power absorbed in the embedding semiconductor. The coupling strength of the NP and the embedding medium can be

measured by the nanoparticles polarizability which, in its turn, defines the nanoparticles scattering cross section. If we assume the size of the nanoparticles to be much smaller than the wavelength of the incident radiation, the field intensity can be considered constant all over the nanoparticle region. This approximation will lead to a simplified expression for the particle (complex) polarizability ( $\alpha$ ) that, for a simple spherical geometry, is quantified by the following expression:

$$\alpha = 4\pi r^3 \frac{\epsilon_m - \epsilon_s}{\epsilon_m + 2\epsilon_s} \quad (1)$$

where  $r$  is the radius of the nanosphere,  $\epsilon_m$  and  $\epsilon_s$  the permittivity of the metal and of the embedding semiconductor, respectively.

Once known the value of the polarizability, the nanoparticles scattering cross section for a determined wavelength  $\lambda$  can be calculated as:

$$\sigma_{\text{scat}} = \frac{1}{6\pi} \left( \frac{2\pi}{\lambda} \right)^4 |\alpha|^2 \quad (2)$$

Both the permittivities  $\epsilon_m$  and  $\epsilon_s$  are function of the light wavelength ( $\lambda$ ). It can be easily deduced by Eqs. (1) and (2) that the satisfaction of the condition  $\epsilon_m \approx -2\epsilon_s$  leads to a maximization of the polarizability and the scattering cross section. Under this condition, a surface plasmon resonance can be then expected.

The analysis we present is based on the Urbach-Tauc-Lorentz model [1] for the electrical permittivity  $\epsilon$  of a-Si:H and its Lorentz reduction for application in Finite Difference Time Domain (FDTD) simulation [1]. The permittivities of all the metals considered in this study are taken from experimental results published in literature [1,2]. The FDTD simulations were executed with the 32-bit version of the OptiFDTD software [1].

## 3. Discussion

Aiming to identify the LSPR condition for a system of metal nanoparticles embedded in a matrix of a-Si:H, the polarizability of a single metal nanosphere has been analysed. In Fig. 1 it is reported the absolute value of the polarizability of a metal nanosphere, with a 10 nm radius, embedded in a-Si:H and a-SiC:H. In this case, the analysis is performed on copper, gold and silver, which are the mostly utilized metals in plasmonic applications. This plots are obtained combining, through Eq. (1), the experimental results for the metal permittivity and the UTL model for

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