Analytical study of enhanced optical absorption of molecules near silver nanoparticles

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The effective mode volume model is employed to study an enhanced light absorption of absorbing molecules in solar cells when they are positioned in close proximity to Ag nanospheres. Furthermore, a procedure for optimal design of Ag nanoparticles for a promising improvement of light absorption is presented. 2010 Optical Society of America

1. Introduction

Thin-film solar cells are promising candidates for highly efficiencent and cost effective photovoltaic devices. In particular, microcrystalline silicon (μc-Si:H) and InGaN-based solar cells have attracted significant attention in recent years [1]. One of the foremost challenges in designing those thin-film solar cells is to achieve efficient light-trapping in the absorption layers. For enhancing the absorption efficiency, we normally prefer to employ a thin i-layer or absorption layer for enhancing the build-in field such that it can effectively separate the generated electrons and holes. However, with the reduced i-layer thickness sunlight absorption may become ineffective leading to the decrease of the energy conversion efficiency of a solar cell. To overcome this problem one of the most commonly used method is to use metallic nanoparticles (NPs) embedded in the absorption layer to generate localized surface plasmon (LSP) modes. An LSP mode can effective absorb light around the resonance frequency.

In this work we investigate the influence of silver (Ag) NPs on the light absorption of absorption centres ("molecules") which are embedded in the absorption layers in thin-film solar cells using the effective mode volume theory. We show that an enhanced light absorption is obtained when they are positioned in close proximity to Ag nanospheres while the enhancement factor is strongly dependent on sphere size of the Ag NP, absorption cross section of the molecules and separation between the Ag sphere and the molecule. Furthermore, based on the analytical results of the enhancement factor we present a procedure for optimal design of Ag NPs for a promising improvement of light absorption of nanoscale objects.

2. Analytical model of enhancement of optical absorption

The analytical model used to predict an enhancement of light absorption in this work is the effective mode volume theory presented in [2]. When an incident light beam falls on a nanosphere, it can be coupled into the dipole mode (the lowest-order mode). This excited dipole mode has a resonant frequency and an effective mode volume. The optical absorption can be described as a two-step process. First, the energy from free-space modes contained in the beam gets coupled into the dipole mode with an in-coupling coefficient. The second step is that the energy in the dipole mode actually gets absorbed by molecules located at distance d away from the metal sphere. These molecules have an absorption cross section (σ_a). This results in an enhanced light absorption . The absorption enhancement factor (F_a) is defined as the ratio of the absorption rate of dipole energy to that of the incident wave at the focusing spot in the absence of the metal sphere.

3. Results

We study the influence of Ag NPs on the light absorption of molecules with different absorption cross section placed in a matrix of InGaN or Si . Figure 1 shows the absorption enhancement as a function of NP sphere radius *a* when absorbing molecules with different total absorption cross sections are placed at *d*=5 nm from the Ag NP. For Ag/InGaN the optimal radius of Ag NP is found at 41 nm with a resonance frequency 603.5 nm in combination with 100 nm^2 total absorption cross section while with $N_a\sigma_a$ = 300 nm^2 the optimal radius is found at 50 nm with a resonance frequency 604 nm. The same figure shows that for Ag/Si the optimal radius of Ag NP is found at 51 nm with a resonance frequency 730 nm in combination with $N_a\sigma_a$ =100 nm^2 while $N_a\sigma_a$ = 300 nm^2 the optimal radius is found at 63 nm with the same resonance frequency. From the figure it is seen that the enhancement factor is strongly dependent on the NP size and total absorption cross section. Indeed, the stronger the original absorption the less enhancement is attainable.

The enhanced light absorption as a function of Ag sphere radius *a* with respect to the separation *d* between the molecule (a total absorption cross section is fixed at 300 nm^2) and the NP is depicted in Figure 2. The dependence of the enhancement factor on distance *d* is clearly seen in the figure. Unsurprisingly, the larger the distance *d* the smaller the optimal radius *a* is observable.

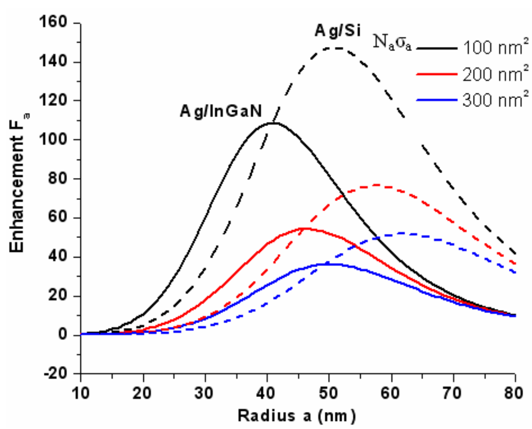

Fig. 1. Absorption enhancement as a function of sphere radius *a* with respect to a range of total absorption cross section.

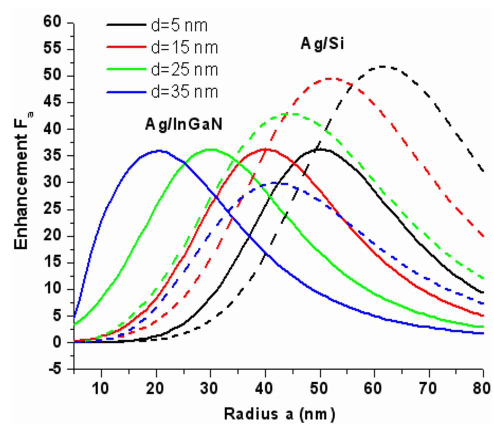

Fig. 2. Absorption enhancement as a function of sphere radius *a* with respect to a range of separation between molecule and Ag sphere.

References

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2. J. B. Khurgin and G. Sun, “Enhancement of optical properties of nanoscaled objects by metal nanoparticles,” J. Opt. Soc. Am. B **26,** B83–B95 (2009).