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Enhanced Light Trapping From Nanoparticle Arrays

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Abstract: The metal nanoparticles possess the unique properties of light interaction. Here we focus on incorporating these nanoparticles in thin film structures to determine their effect on light scattering and capturing in thin film devices. These particles can exhibit large optical field enhancements, resulting in large enhancements in the absorption or scattering of the incoming light. The interaction of light with a metal nanoparticle causes the conducting electrons in the metal to oscillate; the collective oscillation of these electrons is defined as a plasmon and results in large optical field enhancements. This phenomenon can result in either the conversion of the energy of the incident light into thermal energy via absorption or the acceleration of these electrons and subsequent radiation as scattering. Thin film solar cells can potentially benefit greatly from increased near-field enhancement associated with metal nanoparticles, and increased scattering can result in a greatly enhanced path length through the thin film by laterally redirecting incident light and increasing the fraction of light trapped in the film by total internal reflection.

Keywords: Thin-film, Plasmon, Scattering, Nano-particle, Absorption, Light-trapping.

1 Introduction

The major issue in organic solar cells is the poor mobility and recombination of the photo generated charge carriers. The active layer has to be kept thin to facilitate charge transport and minimize recombination losses. However, optical losses due to inefficient light absorption in the thin active layers can be considerable in organic solar cells. Therefore, light trapping schemes are critically important for efficient organic solar cells.

Light trapping in solar cells is achieved when the absorption of incident light is higher than the absorption of a single light pass through the absorber material. Thus for optically thin solar cells the light-trapping effect enhances the jsc, light trapping increases the solar cell efficiencies and reduces the cost of electricity generation with solar cells.

When the particles are placed at an interface between two materials, the light will be preferentially scattered into the materials with the higher optical density, so placing metal scattering particles on silicon will direct the scattered light into this underlying substrate due to the higher density of optical states available in the higher index material. If the

particles are small relative to the wavelength of light they can be described as point dipoles, and the interaction of these metal dipoles with incident light can be characterized by their relative scattering and absorption cross sections. The absorption cross section describes light absorbed by the particle and converted to thermal energy, while the scattering cross section accounts for the fraction of light scattered, with the total extinction cross section equal to the sum of these quantities, light scattering + light absorption.

2 Light Trapping Fundamentals and Limits

Essential for all research on light trapping is the understanding of the maximum achievable absorption enhancement in solar cells. Initially, the limits of light trapping were studied for optically thick solar cells, typically made of crystalline silicon where the absorber layer is many wavelengths thick. Light trapping in these solar cells is achieved by the scattering of incident light at a textured interface in combination with a highly reflective back contact. Due to internal reflection the average length of the light path and hence the absorption in the absorber material is enhanced.

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2.1 Nanoparticle Array Fabrication

Various methods for the synthesis of Ag arrays have been developed and utilized. One method is to evaporate and subsequently anneal a thin film of Ag on the substrate. The annealing causes an agglomeration of Ag clusters with moderately uniform distribution, but non-uniform shape and size.

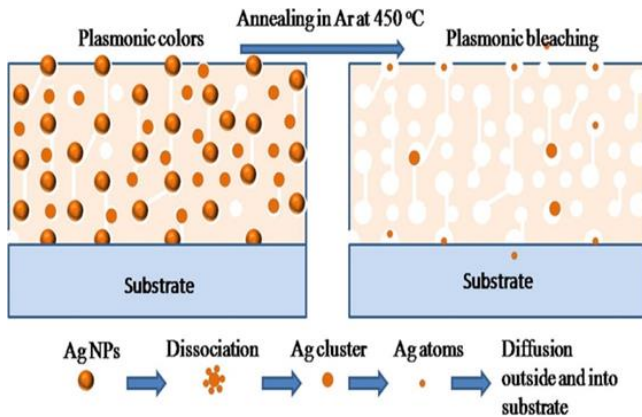


Fig.1: Distribution of Ag clusters after thermal annealing and Distribution of colloidal suspension of Ag particles.

Using this fabrication technique, Stuart and Hall demonstrated the use of Ag metal islands to couple into waveguide modes of a 165nm-thick silicon photodetector, with photocurrent enhancements of over 18 observed at the resonant wavelength and an overall enhancement over a large portion of the spectrum.

A second method for metal nanoparticle array fabrication is the deposition of a colloidal suspension of Ag nanoparticles in a monolayer on the substrate, resulting in an array with uniform diameters but non-uniform pitch. While both of these methods are easily scalable, annealing does not allow precise control over particle diameter, while the dispersion of a colloidal suspension does not permit accurate manipulation of interparticle spacing; to realize the full potential of light trapping with metal nanoparticles, precise control of array geometry is necessary.

To simultaneously control both the size of the particles and pitch of the array, e-beam lithography has been employed to fabricate regular nanoparticles arrays of various

metals. This method permits a large degree control, but is impractical to use over large areas; to address these challenges in array fabrication, a templating method has been developed that achieves both uniform diameter and pitch over large areas; these parameters can be controllably varied over a large parameter space for optimization of array geometry to maximize light scattering and trapping.

3 FDTD Simulations

To optimize the metal nanoparticle array geometry, full-field electromagnetic simulations of SOI structures decorated by metal nanoparticle arrays were employed to predict and optimize the field enhancement and light trapping attributable to the Ag nanoparticle arrays on the surface of 220nm-thick Si. Using commercially available Lumerical software, a finite-difference time domain (FDTD) algorithm was utilized to determine the electromagnetic field characteristics resulting from light interaction with these arrays on thin film structures. This method uses Maxwell's equations, specifically the derivative expressions, to solve for the EM field at discrete space and time intervals to determine the field profile in the simulated structure.

The FDTD algorithm alternately solves each of these equations at discrete time steps and uses the resulting solution as input for the other equation, thus proceeding through the requisite number of time steps in a leap frog fashion. The advantage of this simulation method is that it is a numerical algo

rithm that can be applied to a wide variety of geometries and can be used to describe behavior of non-linear and dispersive materials, while the primary limitations include numerical dispersion and instability resulting from the finite nature of the calculated solutions to Maxwell's equations

3.1 Results of Simulations in 200 NM Pitch Varying Diameter

Simulations with a constant 200nm pitch and a changing diameter reveal the influence of particle proximity on the location of field enhancement in the silicon film. For particles separated by a distance greater than 10s of nanometers, the influence they have on each other will be dictated by the interference of the scattered waves from each particle. However, for particles impinging on one another, the near-field enhancement of each particle resulting from the plasmon excitation will interact with the near-field of the adjacent particle. As the particle diameter is increased while maintaining a constant pitch, the distance between the circumference of the hemispheres decreases and near-field effects are expected. A mapping of the optical generation rate from these simulations reveals enhancement peaks centered at wavelengths of 505nm, 590nm, and 690nm

The location of these peaks is constant across the simulated spectrum and can therefore be attributed to the periodic modes of a 200nm pitch array. The intensity and width of these peaks varies across the spectrum, however. The peaks are broad with lower amplitudes for smaller diameters, but gain in intensity and narrow in bandwidth as the diameter increases. The spectral location of the enhancement remains constant with sharply increasing amplitude due to this near-field interaction between the particles. An increase in diameter with constant pitch corresponds to increased

proximity between metal particles; this increased proximity increases the interaction between the Ag hemispheres and intensifies the effect of the resonance from the periodic Bloch modes. In addition, the increased diameter corresponds to a larger effective scattering cross section with less parasitic absorption in the metal.

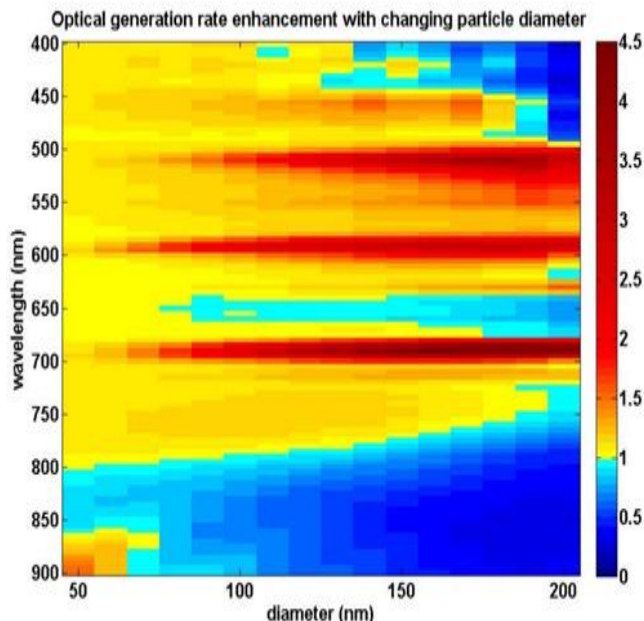


Fig. 2: Simulated optical generation rate enhancement with changing particle diameter.

These optical generation rate calculations show that smaller particles with smaller pitch demonstrate a decrease in performance over much of the spectrum range, but remarkably the largest enhancement is exhibited by dense arrays where the Ag particles are impinging on each other, despite the large fraction of metal coverage with this array geometry. At longer wavelengths, greater enhancement is exhibited with

Smaller diameters, with only 50nm diameter particles exceeding the performance of bare silicon; at these longer wavelengths there is little coupling into metal, and consequently less scattering. In this wavelength range the increase in reflection from the metal coverage dominates and decreases absorption for increased particle size.

3.2 Theoretical Potential for Light Absorption in Thin-Film Structures

Arrays of metal nanoparticles have demonstrated enhanced photocurrent generation due to their plasmonic properties and increased effective scattering cross section. However, the performance of these types of devices is restricted by the losses due to light absorption in the metal and increased reflection at the surface from metal coverage. An alternate

technique for engineering structures that maximize light trapping in sub-micron silicon films is to exploit the scattering mechanisms of dielectric arrays on the surface of the absorbing material. The scattering properties of these arrays are determined by the geometry and material properties of the surface features,

and by changing the size, pitch, and shape of these arrays, the light scattered into the film and absorbed can be maximized.

4 Shape of Scattering Structures

The influence of the shape of the scattering object on the reflectivity at the surface was next examined. The textured portion of the silicon layer has an effective refractive index between that of air and the underlying solid layer of silicon due to its modulation between the refractive indices of the two materials, and consequently could be described as a graded index of refraction. Since such a graded index of refraction will suppress reflectivity at an interface, the surface geometry was examined in terms of the effective refractive indices gradient through the dielectric surface features. Both a pyramidal and cylindrical geometry were simulated in this study; since the pyramidal structure will provide a more gradual graded index, this geometry may be expected to exhibit a larger suppression of reflectivity compared with the cylindrical structure, especially at short wavelengths where reflective scattering is most pronounced. To determine the reflectivity, three varying scattering geometries were constructed in the FDTD simulation environment representing a close-packed pyramid surface with a pitch of 400nm and a height of 75nm, a pyramid structure with a pitch of 400nm, a 200nm base, and 75nm height, and a cylindrical structure with a 400nm pitch, 175nm diameter, and 75nm height. The close packed pyramid represents the most gradual change of refractive index from air to

that of silicon, while the second pyramid geometry represents a more abrupt change in index. The cylinder represents the least gradual of the structures since it allows only one intermediate index between air and silicon for the entire thickness of the structured layer. A decrease in reflectivity at shorter wavelengths is observed for the 200nm pitch pyramid structure compared with the 400nm, close-packed pyramids, indicating that the observed anti-reflective properties cannot solely be attributed to a graded index effect. Most notably, however, a significant decrease in reflectivity at smaller wavelengths is seen for the cylindrical structure, despite its discrete changes in index at the interfaces between the surface texture and both the air and the underlying substrate. This phenomenon clearly demonstrates the significant role of the periodicity of surface arrays in the collection of incident light in these structures. A

reflectivity map over varying pitches reveals peaks in reflectivity for a 400nm pitch array of silicon cylinders are most pronounced at $\lambda=675\text{nm}$, 750nm , and 775nm and increase linearly with wavelength as the pitch increases.

This corresponds to the three highest peaks seen for cylinder arrays in the reflectivity versus wavelength plot, and moreover confirms that this modulation of peaks is a result of periodic modes in the surface structure

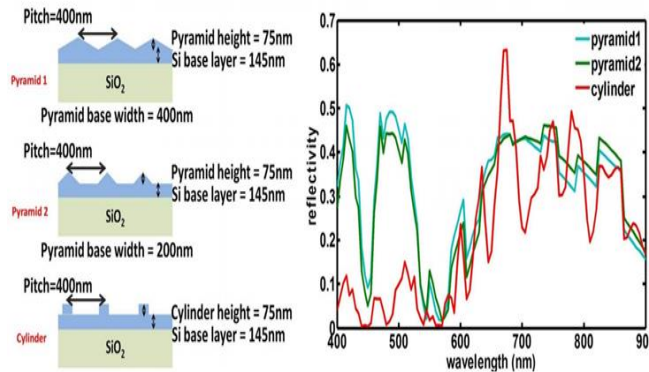


Fig. 3: Calculated Reflectivity Spectrum with Varying Surface Feature Geometry.

5 Conclusions

Organic solar cells have been attracting considerable attention owing to their potential merit of low cost energy conversion. By employing FDTD simulations to determine the optimal expected optical characteristics of the thinfilm device structure and to examine the potential of surface structures for increasing light absorption in these films. the incorporation of sub-micron surface structures on thin-film silicon has resulted in a dramatic increase in light absorption due to decreased reflectivity and increased light trapping enabled by the scattering characteristics of these surface structures. While both metal and dielectric arrays demonstrate this result, the use of periodic dielectric cylinders yielded significantly more enhancements in light absorption in the silicon film. With these observations we postulate a promising method for achieving inexpensive and highly efficient solar cells.

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