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Comparison between periodicity and randomness from an effective refractive index point of view; applicable to thin-film solar cells

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Abstract. In this paper, embedding plasmonic nanoparticles inside the solar cell's active layer, both in a periodic and in a random manner, is extensively investigated. The aim of this study is to investigate optical mechanisms inside the active layer as a consequence of nanoparticle inclusion as well as to compare periodicity and randomness in such structures, where the intended maximization of the ultra-broadband absorption renders the analysis complicated. To perform such study, an effective refractive index analysis is employed to simultaneously cover the influential parameters. The results show that although fully periodic structures are more desirable in narrow-band applications such as grating-assisted waveguide coupling, random inclusion of plasmonic nanoparticles in the solar cell's active layer yields a much higher optical absorption. Furthermore, random inclusion of nanoparticles is easier and much cheaper than periodic inclusion to implement in solar cell fabrication.

1. Introduction

Enhancing the optical absorption in thin-film solar cells is a key to improve solar cell technology and many research groups have proposed different techniques to extend the photon path length inside the active layer, leading to increase in optical absorption of the active layer [1-3]. One of the promising approaches relies on embedding plasmonic nanoparticles (p-NPs) inside the active layer, where the resulting plasmonic and scattering effects are adequate measures to improve performance of the solar cell's active layer [4,5]. However, there are still some important concerns regarding, e.g., size and material properties of the underlying NPs [6] as well as the distribution of such inclusions [7], which, when selected properly, can significantly raise the optical absorption of the active layer.

One important parameter is the NPs distribution, which determines the strength of light coupling with the active layer, as well as the excited modes inside the active layer. Fully periodic distribution excites few distinct well-defined modes that may be capable to enhance the optical absorption in the resulting narrow spectral range, whereas random structures excite a lot of weak modes over a wide spectral range, yielding less distinct enhancements in the optical absorption. Besides, the realization of stochastic NP distributions is both less expensive and easier to handle, which is an important aspect regarding the fabrication of

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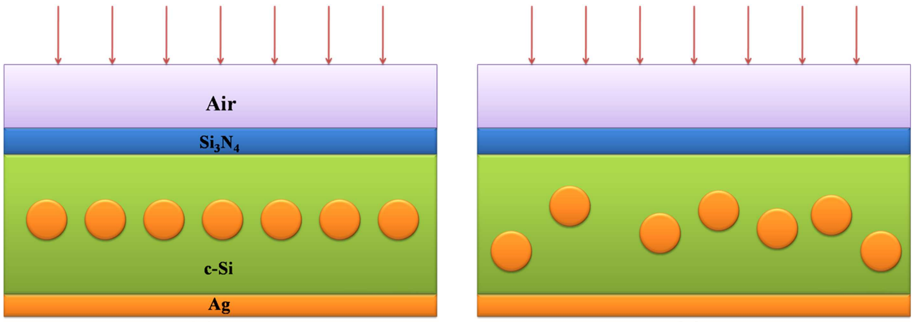

Figure 1. Cross-sections of the modeled solar cell topologies: (a) Periodic structure, and (b) randomized structure, both having Ag-NPs with 60 nm diameter as inclusions with a volume filling fraction of 11%.

solar cells. To study the effect of different NPs arrangements, a thin-film solar cell with both random and periodic NPs inclusions is modeled and numerically studied. A 400 nm crystalline silicon slab on top of a 40 nm Ag back-electrode is given as a starting layer combination. On top of the c-Si layer, a 55 nm thick Si_3N_4 anti-reflection coating is placed. Ag nanoparticles with 60 nm radius are introduced into the middle of the active layer having either a periodic or a random distribution as shown in Figure 1. An effective refractive index analysis [8-10] of the overall NPs settings is used to investigate the results as it turned out to be more effective than the proper analysis of optical field distributions with respect to different quantities such as the field localization in the active layer, the reflection and transmission properties, and the resulting absorption.

The rest of the paper is organized as follows. In Section 2, periodicity and randomness are compared, and in Section 3, the effective refractive index approach is discussed. Results are shown and discussed in Section 4, and in the last section, a brief conclusion is drawn.

2. Periodicity versus randomness

The comparison between periodic structures and random ones is not an easy task with clear results. This quest is highly context-dependent regarding the different structures within various specific applications. A remarkable technology based on nanoplasmonics that encompasses miniature structures with a high degree of accuracy has been reported in [11,12], where many miniaturized periodic devices have been designed based on periodicity in one, two, or three dimensions. However, random structures can beat periodic ones when it comes to optimized optical broadband devices, e.g. in thermal applications or in solar cells.

In broadband optical devices like solar cells, the optical absorption covers a very broad spectral range, namely, 350-1100 nm, following a solar spectral profile according to AM1.5. Using a fully periodic structure, such as an array of p-NPs, a significant enhancement in optical absorption is expected; however, in specific spectral ranges in which a well-defined set of modes is excited inside the active layer, a regular interference pattern is formed that is commensurable to the periodic NP distribution. On the other hand, in an amorphous setting with a random distribution of p-NPs, no distinct mode can be excited and the resulting field distribution inside the active layer becomes a mixture of different mode fields interfering with various NPs. However, in such inclusion of NPs, the absorption enhancement becomes effective in much broader spectral range as many weak modes are excited, yielding a large aggregate absorption with respect to the overall spectral range. Hence, one can conclude that in broadband optical applications, randomness is apt to beat periodicity.

3. Effective refractive index

The refractive index of a material defines its optical wave propagation behavior inside the material. When pores (i.e., air particles) or particles are added to such material, its optical property and, therefore, the wave propagation will change accordingly. To study the effect of such inclusion, the wave propagation inside the material should be fully investigated, which may become challenging due to the morphology of the inclusions and many parameters that should be considered in this regard. Another point of view would encompass a macroscopic perspective by defining an (dispersive) effective refractive index for such a composite medium as the influence of pores and nano-particles would be added in an averaged sense to the refractive index of the host medium. The potential of such homogenization procedure is that it takes into account the influential parameter in a compact and comprehensive way that can be interpreted easily. For the computation of the effective material properties, a vast body of literature is already available addressing, e.g. spectral homogenization, volumetric mixing formulae, and scattering procedures with emphasis on effective impedances and effective permittivity as well as providing some critical account of effective refractive indices [13-15]. In our numerical analysis, we have calculated the effective refractive index for periodic and random inclusions of silver nanoparticles within a thin active layer using a canonical reflection and transmission analysis to retrieve the corresponding dispersive, complex-valued index data of the active layer.

4. Modeling and simulation scenario

A thin-film solar cell is modeled with a 400 nm crystalline Silicon (c-Si) layer as the active layer, under which there is a 40 nm Ag layer as back-electrode (as well as back reflector) that is on top of a 55 nm Si_3N_4 anti-reflection coating. Ag nanoparticles with 60 nm radius and 200 nm periods are embedded in the middle of the active layer in periodic and random arrangements. Figure 1 depicts the schematics of the simulated thin-film solar cell topologies for both the periodic and randomized arrangements. In randomized arrangement, the Ag NPs are embedded approximately in the middle region of active layer while no agglomerations are allowed. Defining the position of each NP in such randomized arrangement is quite challenging: the position of each particle is statistically defined using a random number. Afterwards, the geometry based on these numbers is modeled and reflection and transmission spectra are calculated. Such realization is unique and not reproducible; thus, each time the analyzed quantities would differ. However, the randomized structures may become representative in a statistical sense; after producing 100 various randomized structures, the results are normally dispersed around the mean values with relatively low variances confirming that the study gets reliable insights into the inclusion of randomly distributed nanoparticles.

A perpendicular plane wave with mixed polarization (50% TE and 50% TM) and AM 1.5 spectrum is used as top illumination of the solar cell material stack. Numerical simulations are performed using the Finite-Element-Method (FEM) provided by the well-known simulation platform COMSOL Multiphysics^{TM}. For the randomized morphology, the geometry is set up by MATLAB and then exported to COMSOL Multiphysics^{TM} for further analysis, where reflection and transmission data are imported back to MATLAB for future processing, yielding the (dispersive) effective refractive indices of the corresponding composite structures.

5. Results and discussion

The embedded nanoparticles scatter light inside the active layer, which is even more pronounced by the excitation of plasmonic modes, creating strong near fields in the vicinity of the nano-particles and, hence, a strong intensity pattern in the absorbing material. These mechanisms enhance the spectral response of the optical absorption in the active layer and become key to the improvement of the solar cell's performance. The spectral responses of the optical absorption of the two arrangements together with the absorption spectrum of a bare reference cell without NP inclusions are shown in Figure 2. As can be seen, the periodic structure has shown some narrow peaks compared to the reference case, resulting in 21.1% enhancement of the spectrally integrated absorption relative to the reference cell. However, the optical absorption in the randomized structure does not include sharp spectral peaks showing a rather broadband enhancement compared to the reference case, resulting in an impressive 85.4% increase in the spectrally integrated absorption. A distinct enhancement happens prominently in the long wavelength range, where c-Si is known to be an intrinsically poor absorber yielding a sort of spectral rectification in this spectral range.

In order to provide a coherent reasoning behind the observed enhancements, we have computed the effective refractive index using corresponding reflection and transmission spectra of the thin active layer, where both the real (**n**) and imaginary (**k**) parts of the effective refractive index are plotted in Figures 3 and 4, respectively. An efficient active layer should have low (**n**) to poorly reflect the incoming light and high (**k**) to highly absorb the in-coupled light. As shown in Figure 3, both absorber structures have lowered **n** substantially.

In Figure 4, the corresponding imaginary part (**k**) of the effective refractive index is plotted, which implies that both randomized (i.e., amorphous) and periodic structures are capable to enhance **k** at wavelengths

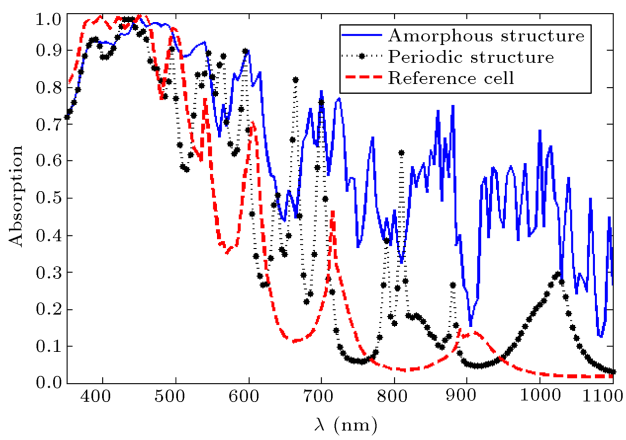

Figure 2. Simulated spectral response of the optical absorption in the active layer for the randomized (i.e., amorphous) structure (solid blue line), the periodic structure (marked dotted black line), and the bare unstructured c-Si reference cell (dashed red line).

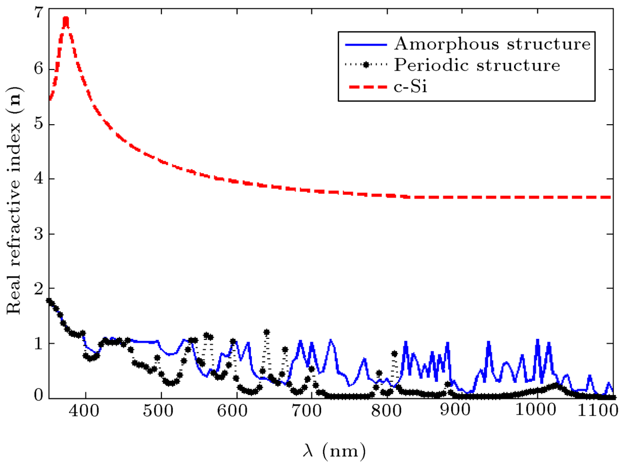

Figure 3. Simulated spectral response of the real part of the effective refractive index (**n**) for the randomized (i.e., amorphous) structure (solid blue line), the periodic structure (marked dotted black line), and the bare c-Si reference structure without NPs (dashed red line).

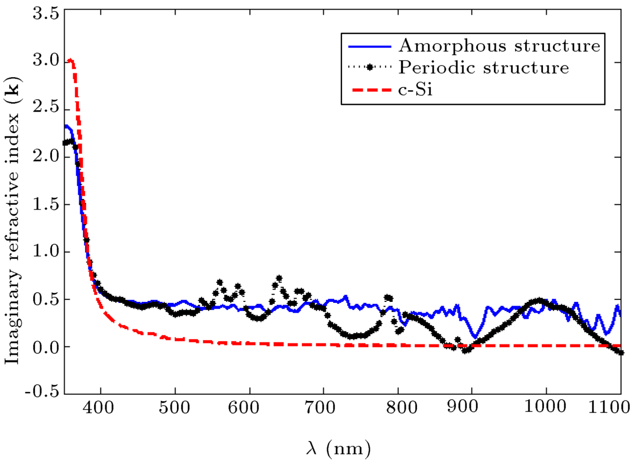

Figure 4. Simulated spectral response of imaginary part of the effective refractive index (**k**) for the randomized (i.e., amorphous) structure (solid blue line), the periodic structure (marked dotted black line), and the bare c-Si reference structure without NPs (dashed red line).

above 400 nm. However, below 400 nm, the **k** values of the bare cell exceed the corresponding values of both structured cells. As expected, the periodic structure creates peaks in the **k** spectrum whereas the randomized structure shows a broadband enhancement, which is highly preferable within any efficient thin-film solar cell design. From 350 to 400 nm, c-Si is a good absorber. Hence, the smaller imaginary part (**k**) of both structured cells may be partly rooted in the smaller c-Si volume due to p-NPs inclusion. On the other hand, beyond 400 nm, c-Si tends to be a poor absorber and, therefore, the emergent field localizations inside the active layer due to presence of plasmonic NPs become effective to improve the c-Si absorption properties.

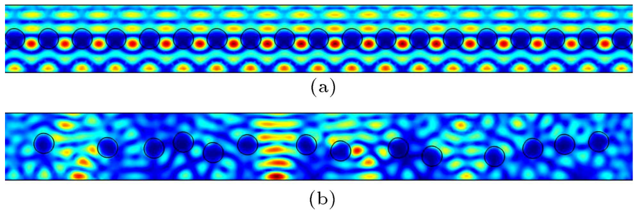

Figure 5. Simulated electric field distributions within the structured active layer of the thin-film solar cell at an operating wavelength of 600 nm for (a) periodic structure and (b) randomized (i.e., amorphous) structure.

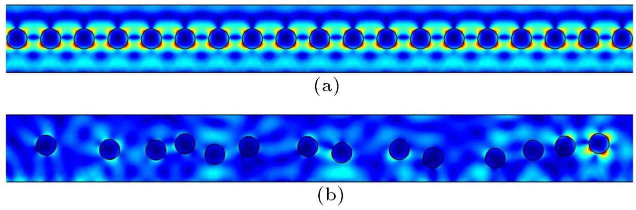

Figure 6. Simulated electric field distributions within the structured active layer of the thin-film solar cell at an operating wavelength of 1025 nm for (a) periodic structure and (b) randomized (i.e., amorphous) structure.

Periodic inclusions of p-NPs have created narrow peaks in both spectra, namely, the active layer absorption spectra, and their effective refractive indices. These peaks are transformed into broadband enhancement in the absorption spectra of randomized arrangement. Inclusion of periodically arranged NPs excites modes and mode groups inside the active layer, which are responsible for the spectral peaks in the absorption spectra. Destroying this periodic order lowers the spectral selectivity of the excited modes, yielding weak, but, on average, spectrally extended mode sets, which are intrinsically broadband and thus more likely to contribute to a broadband enhancement of the optical absorption.

In Figure 5, the electric field distributions in both periodic and random structures are illustrated at an operating wavelength of 600 nm. A narrow spectral peak is observed at this wavelength in optical absorption of the active layer of the periodic structure case, which is then broadened as a result of an emerging non-periodicity in the p-NPs order. It is shown in the figure that the well-defined field patterns in the periodic structure are transformed into dispersed pattern of localization peaks, which extends through the whole active layer aiming at a larger overall absorption.

Another interesting feature happens at an operating wavelength of 1025 nm. Here, a coupled plasmonic mode is excited within the periodic p-NPs structure as depicted in Figure 6. In the randomized (i.e., amorphous) structure, such strong coupling is absent. However, an overall increase in the optical absorption spectra is achieved due to the dispersed field localizations throughout the active layer.

6. Conclusion

Periodic and random distributions of plasmonic NPs in the active layer of a c-Si thin-film solar cell were compared, showing that randomness could beat periodicity with respect to an enhanced overall absorption of the broad solar spectrum. Our investigations illustrated that as periodic structures created some narrow peaks in the absorption spectrum, they showed poor overall enhancement in the spectrally integrated absorption, and hence were less suitable for such true broadband applications. Random structures were capable of providing overall light coupling with a broad range of multiple modes and were therefore good candidates for the broadband management of the optical absorption in thin-film solar cells. In our analysis, we relied on an effective refractive index point of view, which allowed for a comprehensive and simple explanation of the underlying mechanism governing the observed broadband absorption enhancement.

Our NP-based thin-film solar cells yield significant enhancements in the spectrally integrated optical absorption relative to the bare reference cell. In case of periodic NP arrangement, the enhancement amounts to 21.1%, while for the randomized NP arrangement (i.e., the amorphous structure), an impressive 85.4% enhancement was achieved. It should be noted that any randomized structure yields its own broadband absorption spectrum as the NP arrangement is unique. Nevertheless, the presented results provided a valuable estimation of the expectation value regarding the broadband absorption efficiency of such thin film solar cells.

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Biographies

Mandana Jalali was born in 1985 in Shiraz. She received her BS degree in Solid State Physics from Shahid Chamran University in 2007 and MS degree in Particle Physics from Shiraz University in 2010. Her MSc thesis was focused on light matter interaction, entitled "Computation of the Quantum Efficiency and the Decay Rate for an Emitter in the Vicinity of Nanostructures". She started her PhD in Optics and Laser in 2011 at Shiraz University in collaboration with University of Duisburg-Essen.

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