Absorption enhancement in organic solar cells by metallic nanoparticles

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Organic solar cells are promising devices in the search for green and cheap energy sources. However, their efficiency remains low. Recent research in plasmonics has shown the potential to significantly enhance light harvesting in solar cells by embedding metallic nanoparticles (MNPs). Here, based on numerical calculations, we investigate the effect of different geometrical parameters of MNPs on absorption enhancement and its mechanism. With optimized parameters an enhancement factor of around 1.56 is observed, bringing it on par to the absorption of much thicker active layers without particles.

Introduction

Organic solar cells (OSCs) have been the focus of attention in the last decade due to their strong potential to reduce the cost of photovoltaics and their other attractive properties like flexibility, feather-weight, easy to produce and so on. However, OSCs are still in the research phase and have low efficiency. This is because the exciton diffusion length is shorter (~10nm) than the absorption length (~100nm). Therefore, the advanced bulk heterojunction (BHJ) [1] concept was introduced to solve the diffusion length problem and to keep the required thickness of the active layer for sufficient light absorption. With the BHJ the efficiency of OSCs has been enhanced to 5-6% [2]. However, it is still much smaller than the commercial silicon-based solar cells.

The localized plasmon resonance arising from the interaction between light and metallic nanoparticles has drawn lots of attention from researchers. It is known that the localized plasmon resonance in MNPs can cause near-field enhancement and an enhanced scattering cross section, and both of them can be used to increase the absorption in a solar cell. Several experiments [3, 4] and numerical investigations [5] on the influence of MNPs in organic solar cells have been performed. By introducing MNPs into OSCs it is possible to enhance the light harvesting in the active material without increasing its thickness.

In this paper, we present our recent study [6] on absorption enhancement by embedding a MNP array in the active layer of OSCs based on a 2D numerical model. We discuss how different parameters of the MNP array affect the enhancement. In addition we investigate the enhancement mechanism.

Numerical model

Figure 1 shows the schematic picture of OSCs under investigations. The anode is a highly conductive polymer, poly (3, 4-ethylenedioxythiophene):poly (styrenesulfonate) (PEDOT: PSS) which is a polymer with good thermal and chemical stability and good flexibility. For the active layer, the commonly used polymer, poly(3-ethylthiophene):(6,6)-phenyl-C61-butyric-acid-methyl ester (P3HT:PCBM) with 1:1 weight ratio is used. The material of the cathode is aluminium and the MNPs are silver. In simulations, the thickness of the active layer is 33nm [6].
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![Schematic diagram](image)

Fig. 1. Schematic picture of OSCs under investigations

We use a 2D model instead of 3D, which means the MNPs are a periodic array of cylindrical nanowires that are embedded in the middle of the active layer. Simulations were performed using the commercial fully vectorial COMSOL software package. Light with electric field perpendicular to the nanowires is normally incident from the air into the solar cell (see Figure 1), passing the PEDOT:PSS, the active layer and then reaching the cathode. Some light is absorbed in the anode, the active layer and the cathode, and the rest of it is reflected away from the solar cell.

**Results**

In order to reveal the mechanism of absorption enhancement for a representative case the diameter of the MNPs is fixed at 10nm. Figure 2 shows the spacing (distance between neighboring MNPs, see Figure 1) dependence of absorption enhancement. Absorption enhancement (AE) is defined as a ratio of absorption with MNPs to that without MNPs. This figure shows that there exists an optimum spacing of 8nm that maximizes the AE with a factor of around 1.48.

![Graph](image)

Fig. 2. (a) Spacing dependence of Absorption enhancement. Depictions of the electric field enhancement with spacings (b) 2nm and (c) 16nm.

As the spacing increases, the electric field enhancement near MNPs gets smaller. However, the field enhancement begins to spread out. This is due to the decoupling between neighboring MNPs as illustrated by Fig. 2 (b) and (c). When MNPs are far away from each other, the structure converges to the case with no MNPs (no absorption enhancer spacing a configuration).

![Graph](image)

Fig. 3. Schematic showing the spacing dependence of absorption enhancement.

![Graph](image)

Fig. 4. Schematic showing the spacing dependence of absorption enhancement.

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enhancement). As a consequence of these competing effects, there exists an optimum spacing as shown in Fig. 2 (a).
From Fig. 2 (b) and (c), we can also see that the enhanced field is mainly localized in the spacing between MNPs, which implies that the absorption enhancement is mainly due to near field enhancement, not the enhanced scattering. In order to further reveal which mechanism is more prominent, near field enhancement or enhanced scattering, the active layer is divided into three sub-layers: front, middle and back sub-layers, as shown in the inset in Fig. 3. From Fig. 3 one observes that the enhanced absorption is obvious only in the middle sub-layer where the MNPs are. The black dotted line has a broadband enhancement in the range between around 385nm and 650nm. For the other two sub-layers enhanced absorption is only observed in small wavelength ranges while in other ranges the absorption is decreased. These phenomena imply that the absorption enhancement is mainly attributed to the near field enhancement, and not to the enhanced scattering effects.

![Figure 3](image1.png)

Fig. 3. Absorption spectra with MNPs (w) and without MNPs (wo) in front (F), middle (M) and back (B) layers when MNPs are embedded in the middle layer with 8nm spacing.

![Figure 4](image2.png)

Fig. 4. (a) Absorption enhancement as a function of MNP diameter and spacing between neighboring MNPs. (b) Absorption spectra for a solar cell (33nm) with (w) and without (wo) 24nm diameter MNPs and for a solar cell (61nm) without MNPs.

Figure 4 shows the dependence of absorption enhancement on the diameter of MNPs and spacing between neighboring MNPs. From this figure we can see the optimum
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absorption enhancement is around 1.56 with a diameter of 24nm and a spacing of 40nm. With this diameter and spacing, the solar cell can absorb 47%, which is close to the absorption of 50% with a 61nm active layer without MNPs.

Figure 4 (b) shows the absorption spectrum for solar cells with 24nm diameter MNPs and 40nm spacing. For comparison, we also plot the absorption spectra for solar cells without MNPs with 33nm and 61nm active layer thickness. We remark that the absorption spectrum of 33nm active layer with MNPs fits the spectrum of 61nm active layer without MNPs quite well. As a result the absorptions of these cells with (47%) and without (50%) MNPs are similar.

Conclusion

We performed a numerical study on the influence of metallic nanoparticles for light absorption in organic solar cells. We analyzed the influence of particle spacing on the absorption. We found that the near field enhancement is the main reason for the absorption enhancement in the active layer. For a thin active layer, such as 33nm, we noticed that a reasonable particle diameter of about 24nm is necessary for optimum absorption enhancement. With this diameter we find the best enhancement with a factor of around 1.56, bringing the structure close to the performance of a much thicker cell without MNPs.

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