Fundamental Light Trapping Limits in Plasmonic Solar Cells

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Abstract: We analytically investigate the light trapping performance in plasmonic solar cells with Si/metallic structures. We consider absorption enhancements for surface plasmon polaritons (SPPs) at planar Si/metal interfaces and localized surface plasmon resonances (LSPRs) for metallic spheres in a Si matrix. We discover that the enhancement factors at Si/metal interfaces are not bound to the conventional Lambertian limit, and strong absorption can be achieved around plasmonic resonant frequencies. In addition, those enhancements are greatly reduced as the fields decay away from the Si/metal interfaces. Therefore, localized plasmonic resonances can be used as efficient light trapping schemes for ultrathin Si solar cells (< 50 nm), while photonic guided mode enhancement is more appropriate for thicker films.

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1. Introduction

In this paper, we analytically explore the fundamental light trapping limits for solar cells with various plasmonic structures. Research in thin-film silicon solar cells has been actively pursued in order to further reduce the module cost of the conventional Si wafer-based technology [1]. Current thin-film Si technology, however, still show inferior performance compared to its wafer-based counterpart, mainly because of the low near-bandgap absorption for Si. Recently, solar cells based on plasmonic structures have been widely studied and considered to be a promising candidate for achieving high performance [2]. In such dielectric/metallic structures, the induced plasmonic modes cause significant absorption enhancement and therefore can possibly improve the cell efficiency. However, metallic structures also suffer from parasitic loss and should be carefully designed enhance absorption in the active device layer while suppressing loss in metals.

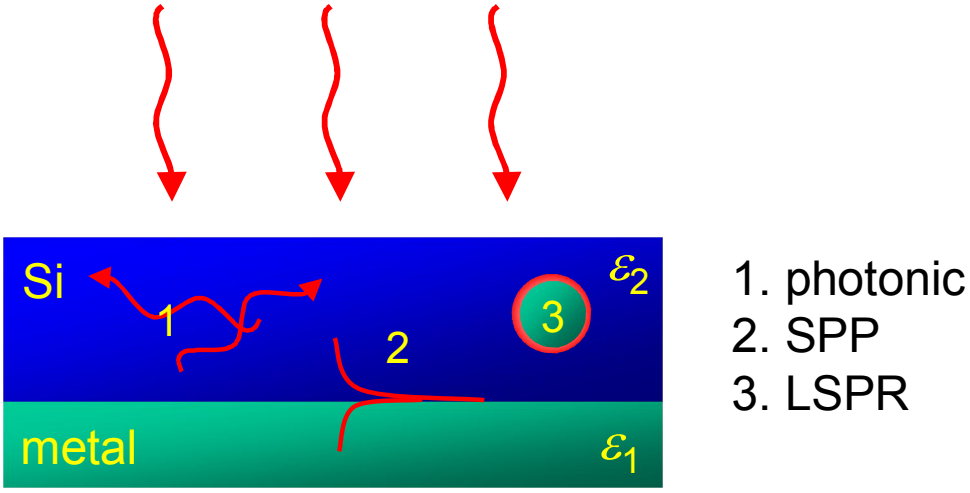

Fig. 1. Different light trapping mechanisms existing in a Si/metal composite solar cell structure. (1) Photonic guided modes induced by various optical scattering due to spatial inhomogeneity. (2) Propagating surface plasmon polaritons (SPPs) at planar Si/metal interface. (3) Localized surface plasmon resonances (LSPRs) induced by metal particles in the dielectric medium.

The schematic solar cell structure we investigate is illustrated in Fig. 1. When sunlight is incident upon a Si/metal solar cell structure, various processes can be induced to cause light trapping in the active Si layer, improving photon absorption: (1) Photonic guided modes propagate in the Si layer. These modes can be obtained by various scattering schemes like random textures [3], periodic gratings [4] and metal particles [5]; (2) Surface plasmon polaritons (SPPs) propagate at the planar Si/metal interface, which can be accomplished by coupling through corrugated films [6] or prisms [7]; (3) Localized surface plasmon resonances (LSPRs) are induced by metallic nanoparticles or gratings [8], which increase the effective photon absorption cross-section. Therefore, we can assume the incident light intensity is splitted into those three different ports that can be analyzed independently. The fundamental limits for photonic guided modes inside a weakly absorptive material have been extensively studied. The well-known results are classical $4n^2$ Lambertian limit [9], which concludes that the single pass absorption (αd) can be optimally enhanced by a factor $F_{ph} = 4n^2$ (F_{ph} is about 50 for crystalline Si). Modified Lambertian theories in thin film regime have also been

proposed [10, 11]. For example, for ultrathin films (in the single mode regime) the upper limit of photonic enhancement factor is $F_{ph} = \frac{2n_{wg}\alpha_{wg}\lambda}{\alpha d}$, where n_{wg} and α_{wg} are the group index and absorption coefficient of the waveguide mode, respectively [11]. All of these results are based on the analysis of photonic density of states, which scales with the volume of the active bulk material. However, plasmonic structures (SPPs and LSPRs) can provide unusually high local photonic density of states due to high field concentration at the dielectric/metal interfaces. These plasmonic modes significantly enhance the local photon absorption, and their optical enhancement cannot be evaluated by the conventional Lambertian models. In order to fully understand the light trapping for SPP and LSPR modes, we must resort to rigorous electromagnetic analysis.

2. Light trapping by surface plasmon polaritons (SPPs) at Si/metal interface

We consider a device geometry shown Fig. 2(a), which is a planar interface between semi-infinite Si and metal. We assume the refractive index for Si is $n_2 = 3.6$ ($\varepsilon_2 = 3.6*3.6$), with an absorption coefficient $\alpha = 12.56$ cm^{-1}. Metals are chosen to be Ag, Au or Cu, of which the optical constants (ε_1) are referred to [12]. By rigorously solving the Maxwell Equations and the corresponding boundary conditions [13], we can derive the field components for the surface plasmon polariton (SPP) propagating mode:

$$\text{for} \quad z > 0, \qquad \begin{cases} H_y = Ae^{i\beta x}e^{-k_2 z} \\ E_x = iA\dfrac{k_2}{\omega\varepsilon_0\varepsilon_2}e^{i\beta x}e^{-k_2 z} \\ E_z = -A\dfrac{\beta}{\omega\varepsilon_0\varepsilon_2}e^{i\beta x}e^{-k_2 z} \end{cases} \qquad (1)$$

$$\text{for} \quad z < 0, \qquad \begin{cases} H_y = Ae^{i\beta x}e^{k_1 z} \\ E_x = -iA\dfrac{k_1}{\omega\varepsilon_0\varepsilon_1}e^{i\beta x}e^{k_1 z} \\ E_z = -A\dfrac{\beta}{\omega\varepsilon_0\varepsilon_1}e^{i\beta x}e^{k_1 z} \end{cases} \qquad (2)$$

The SPP propagation constant is:

$$\beta = k_0\sqrt{\frac{\varepsilon_1\varepsilon_2}{\varepsilon_1+\varepsilon_2}} \qquad (3)$$

and

$$\begin{cases} k_1^2 = \beta^2 - k_0^2\varepsilon_1 \\ k_2^2 = \beta^2 - k_0^2\varepsilon_2 \end{cases} \qquad (4)$$

Here we consider a thin region with a thickness d in the Si side of the interface, where the field of SPP is mostly concentrated. Outside this region, the absorption enhancement is mainly

induced by scattering and can be analyzed using Lambertian models. The ratio of absorption in this thin Si active layer to the total absorption in the SPP mode is:

$$A_{SPP} = \frac{\mathrm{Im}(\varepsilon_2)\int_0^d \left|\vec{E}\right|^2 dz}{\mathrm{Im}(\varepsilon_1)\int_{-\infty}^0 \left|\vec{E}\right|^2 dz + \mathrm{Im}(\varepsilon_2)\int_0^{+\infty} \left|\vec{E}\right|^2 dz} \qquad (5)$$

A_{SPP} can be compared with the single pass absorption in the thin region, and the enhancement factor for SPP light trapping can be obtained:

$$F_{SPP} = \frac{A_{SPP}}{\alpha d} \qquad (6)$$

Fig. 2(b) plots F_{SPP} as a function of wavelength for different metals when d approaches zero. All the curves peak at the corresponding plasma frequencies of the metals (when $\varepsilon_1 + \varepsilon_2 = 0$), of which the corresponding wavelengths are 0.582 μm, 0.679 μm and 0.652 μm for Ag, Au and Cu, respectively. As the electric fields evanescently decay away from the Si/metal interface, those peak values of F_{SPP} are greatly decreased in thicker films, as illustrated in Fig. 2(c).

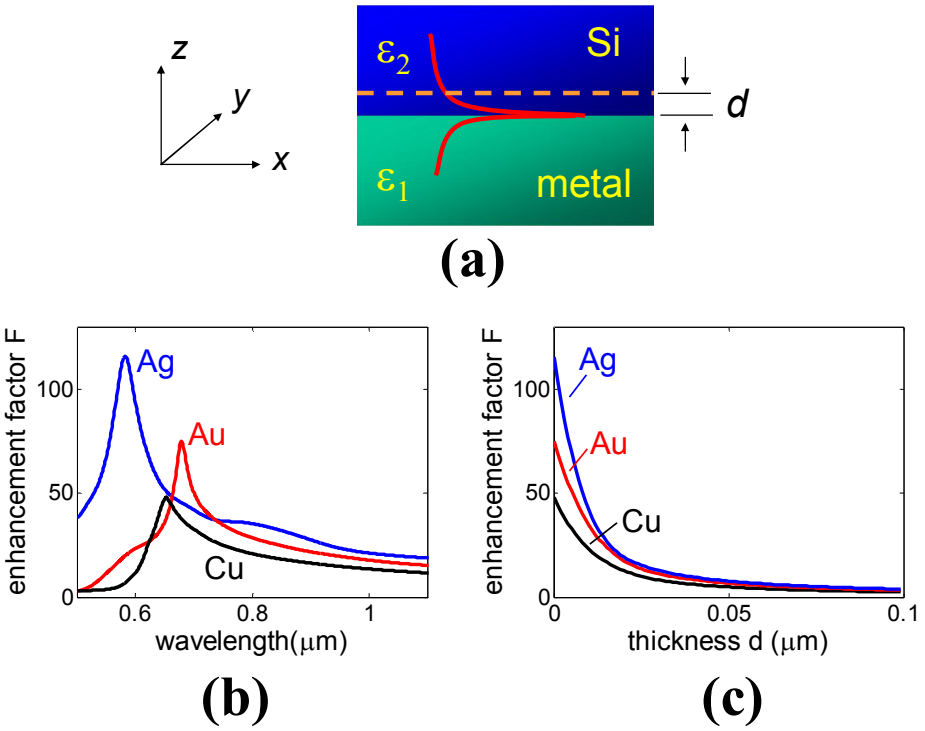

Fig. 2. (a) Schematic device geometry illustrating the SPP mode at the Si/metal interface; (b) Absorption enhancement F_{SPP} as a function of wavelength in the thin Si region ($d \approx 0$); (c) Peak value of F_{SPP} as a function of the layer thickness d.

3. Light trapping by localized surface plasmon resonances (LSPRs) in metal spheres

Another light trapping design is to use the localized surface plasmons excited by metal nano/micro particles embedded in semiconductors. In Fig. 3(a), we consider a metal sphere (with a radius a) inside the dielectric Si medium. The absorption cross-section for this sphere

can be described as the difference of the extinction cross-section and scattering cross-section [14]:

$$C_{abs} = C_{ext} - C_{sca} = \frac{2\pi}{k_0^2}\sum_{n=1}^{+\infty}(2n+1)\left[\mathrm{Re}(a_n + b_n) - \left|a_n\right|^2 - \left|b_n\right|^2\right] \quad (7)$$

In addition, the internal field E_1, the scattered field E_s, and the incident field E_i can be described by [14],

$$\vec{E}_1 = \sum_{n=1}^{+\infty}\frac{2n+1}{n(n+1)}\left(c_n\vec{M}_{o1n}^{(1)} - id_n\vec{N}_{e1n}^{(1)}\right) \quad (8)$$

$$\vec{E}_s = \sum_{n=1}^{+\infty}\frac{2n+1}{n(n+1)}\left(ia_n\vec{N}_{e1n}^{(3)} - b_n\vec{M}_{o1n}^{(3)}\right) \quad (9)$$

and

$$\vec{E}_i = \sum_{n=1}^{+\infty}\frac{2n+1}{n(n+1)}\left(\vec{M}_{o1n}^{(1)} - i\vec{N}_{e1n}^{(1)}\right) \quad (10)$$

where a_n, b_n, c_n, and d_n are Mie coefficiencts. We consider a thin region (with a thickness d) in the Si material surrounding the metal sphere. The portion of absorption by the active Si shell can be estimated as:

$$A_{LSPR} = \frac{\mathrm{Im}(\varepsilon_2)\int_a^{a+d}\left|\vec{E}_s + \vec{E}_i\right|^2 r^2 dr}{\mathrm{Im}(\varepsilon_1)\int_0^a\left|\vec{E}_1\right|^2 r^2 dr} \quad (11)$$

This can be compared with the single pass absorption (if we assume the absorbing Si shell is a planar film with the same volume), and the enhancement factor F_{LSPR} can be obtained

$$F_{LSPR} = \frac{A_{LSPR}}{\alpha\dfrac{\frac{4}{3}\pi(a+d)^3 - \frac{4}{3}\pi a^3}{C_{abs}}} \quad (12)$$

In this case, we assume d is small so that F_{LSPR} is a function of material permittivity and sphere radius a. When the radius is small (a = 10 nm in Fig. 3(b)), only dipole resonances are excited. Therefore, the calculated enhancement factors F_{LSPR} peak at the corresponding resonant frequencies ($\varepsilon_1 + 2\varepsilon_2 = 0$) [15]. Around these resonance frequencies, significant absorption enhancement can be obtained, which are about 400, 250 and 120 for Ag, Au and Cu respectively. When the sphere radius becomes larger, higher order resonances can be observed, as shown in Fig. 3(c) for a = 200 nm. However, the enhancement is greatly reduced, because larger spheres generally provide greater scattering (instead of absorption) [5], which can in turn be analyzed by classical or modified Lambertian light trapping [9–11].

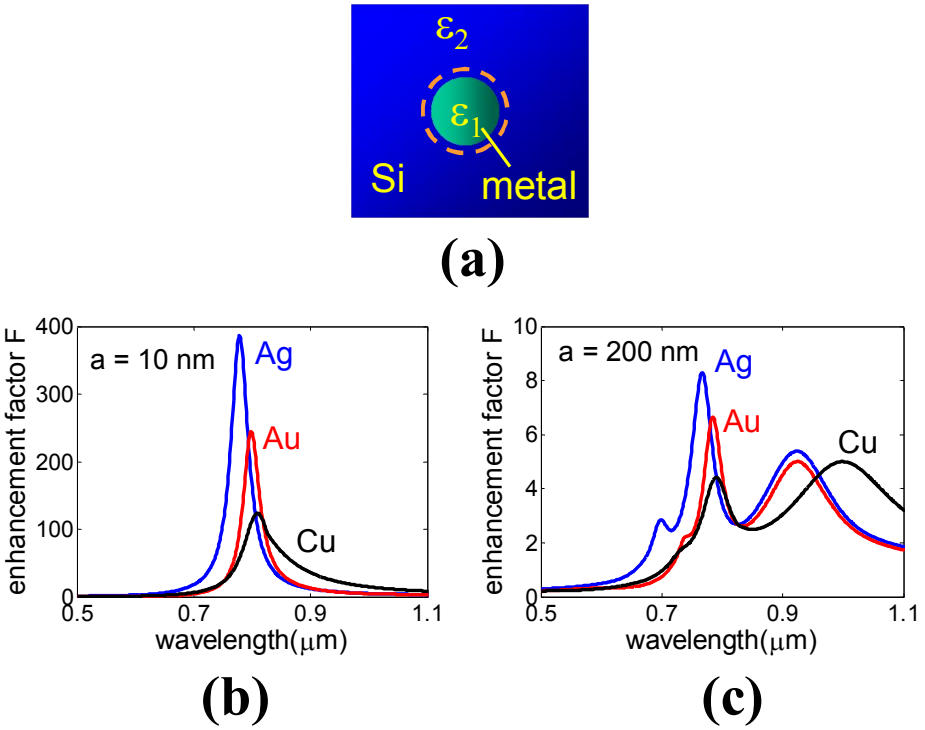

Fig. 3. (a) Schematic device geometry illustrating a metal sphere in Si matrix, which can induce LSPR modes. Here we assume a thin Si shell (with a thickness d) is weakly absorbing. Plot the absorption enhancement factor F_{LSPR} as a function of wavelength for different Si/metal systems, sphere radius (b) a = 10 nm and (c) a = 200 nm.

4. Conclusion

To summarize, we use theoretical approaches to analyze the fundamental light trapping limits for plasmonic solar cells, especially for SPPs at planar Si/metal interfaces and LSPRs in spherical metal particles. We show that the absorption enhancement due to highly concentrated field in plasmonic structures is not bound to conventional $4n^2$ light trapping limit. However, it should be noted that these calculations only provide upper limits for enhancements induced by SPPs and LSPRs in the ultrathin region closed to the Si/metal interfaces. Photonic modes in the dielectric body should still be explained by classical Lambertian models [9–11]. Therefore, scattered photonic modes rather than plasmonic induced local resonances dominate the absorption enhancement in a film with a considerable thickness (for example, larger than 50 nm), consistent with literature reports [16]. For a real device, other issues like surface recombinations are also to be taken into account. For SPP modes, practical coupling methods should be introduced, which are not discussed in this paper. Angular sensitivity will be another issue for SPPs. LSPRs may have no coupling issues and less sensitive angular responses, but the metal particle size and shape should be carefully designed, depending on whether absorption or scattering is preferred. LSPRs induced by particle interactions can also enhance field concentration and should be explored in the future.

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