Improving the absorption rate of thin-film solar cells by composite structures

Liang Xiao1*, Qunzhi Zhu1
1Shanghai University of Electric Power, Shanghai 200090, China
*Corresponding author’s e-mail: xiaoliang_light@163.com

Abstract. In order to improve the absorption rate of polycrystalline silicon thin film cells, an inverted pyramid structure was constructed and the metal nanoparticles were dispersed in the inverted pyramid structure. The absorption rate of the designed composite structure was improved by utilizing the LSPR effect generated by the metal particles, and the change of the absorption rate under different conditions was studied by changing the type, volume fraction and H/P ratio of the periodic structure in the composite structure. By using FDTD software to simulate, this paper finds that the designed inverted pyramid structure has a maximum absorption rate of 20% in the 0.4~0.55um band. In the composite structure, the dispersed Ag nanoparticles have the best absorption rate in the 0.55~0.8um band; The volume fraction of the particles in the inverted pyramid structure is found to increase slowly with the increase of volume fraction in a certain band. By changing the ratio of the depth of the inverted pyramid structure to the length of the period, it is found that as the ratio increases, the whole absorption rate will increase to some extent.

1. Introduction
Solar energy resources are inexhaustible, pollution-free, safe, and have the potential to become future energy sources [1]. Solar cells are an effective way to use solar energy to convert solar energy into electricity directly. In the development of solar cells, it is subject to the price of raw materials and photoelectric conversion efficiency [2]. Thin film solar cells are relatively low in cost due to the use of small amounts of raw materials. However, the absorption rate of light by the absorption layer is small; the photoelectric efficiency is relatively low. It is one of the ways to research high-efficiency photovoltaic systems to solve future human energy problems [3]. Scholars have done a lot of research to improve the absorption rate of solar cells. Applying metal nanoparticles to solar cells, using the local surface plasmon resonance effect generated by metal particles to improve the absorption rate of incident light is one of the means to improve the photoelectric efficiency of solar cells [4-6].

The metal particles are randomly distributed in the matrix, and the diffusion properties of the specific properties can be made by the principle of metal Mie resonance [7]. Composite materials with different properties can be obtained by regulating the morphology, content and other related parameters of the metal particles. There are also previous studies on the absorption of incident light by a metal particle reinforced structure deposited on the surface of a solar cell [7-11]. In this paper, by designing a certain micro-nano structure on the surface of polycrystalline silicon thin film solar cells, the metal particles are dispersed in the micro-nano structure of the thin film solar cell, and the local surface plasmon resonance effect excited by the metal nano particles is used to improve the absorption rate of the solar cells. What’s more, we control the surface structure of the thin film and the parameters of the metal nanoparticles to study their influence on the optical characteristics of the solar cell.
2. Structural design and research method

2.1. Structural design
In this paper, a polycrystalline silicon thin film battery is used as the substrate, an inverted pyramid structure is constructed on the surface of the substrate, and an inverted pyramid structure of the substrate is filled with an ITO composite material randomly dispersed by the metal nanoparticles, and then above the overall structure. A layer of ITO material is applied. The overall structure is shown in Figure 1. The incident light is perpendicular to the model. The overall thickness of the silicon layer in the model is the sum of the depth H and h₁ of the inverted pyramid structure.

![Figure 1](image)

2.2. Research method
The time-domain finite difference method is a method for solving the electromagnetic field Maxwell's equation. The core idea is to convert the Maxwell's curl equation with time variable into a differential form to simulate the time-domain response of the electronic pulse and the ideal conductor. This method can directly and accurately simulate the distribution of electromagnetic fields. The Lorentz-Drude model is a commonly used dielectric constant model that expresses the complex permittivity of a material as the sum of the in-band effect of free electrons and the effect of the banding effect of bound electrons.

\[ \varepsilon(\omega) = \varepsilon_{\infty} + \sum_{m=0}^{M} \frac{\omega_{mp}^2}{\omega_{m}^2 - \omega^2 + i\gamma_{m}\omega} \]  

where:
- \( \varepsilon(\omega) \) —Complex permittivity of materials;
- \( \omega_{m} \) —The resonant frequency of the m harmonic oscillator;
- \( \omega_{mp} \) —Plasma frequency of the m harmonic oscillator;
- \( \gamma_{m} \) —Damping coefficient of the mth harmonic oscillator.

By far-field extrapolation of the calculated near-field information around the particle, the far-field scattering or absorption information of the object can be obtained, so that the absorption rate of the material can be obtained.

In this paper, the time domain finite difference (FDTD) is used to numerically simulate the established three-dimensional structure model. In order to simulate the periodic structure, periodic boundary conditions will be set on the x-axis and y-axis, and a perfect matching layer (PML) will be set above and below the z-direction completely matches the wave impedance of the layer medium with the wave impedance of the adjacent medium, so that the incident wave can pass through the PML interface without reflection, thereby preventing the non-physical reflection from interfering with the simulation result. The composite film structure is vertically irradiated by a plane wave having a wavelength of 400 nm to 800 nm. A reflected light monitor \( R(\lambda) \) and a transmitted light monitor \( T(\lambda) \) are respectively disposed at the top and bottom ends of the composite film structure and the incident light energy absorbed by the composite structure can be calculated by the two monitors. In FDTD, the software calculates the energy of \( R(\lambda) \) and \( T(\lambda) \) monitors as follows:

\[ R(\lambda), T(\lambda) = 0.5 \int \text{real} \{ p(\lambda) \}_{\text{monitor}} dS/P_{\text{in}}(\lambda) \]
3. Results and discussions

3.1. Influence of inverted pyramid structure on absorption rate
This paper first compares the two cases that have inverted pyramids or not. Among them, the inverted pyramid is a regular pyramid, the bottom length is \( p = 0.1 \mu m \), the height is \( H = 0.1 \mu m \), and the thickness of the silicon layer is in the flat structure without pyramid. 0.4 \mu m, ITO thickness is 0.1 \mu m, the simulation results are shown in Figure 2. It can be seen that in the wavelength range of 0.4 \mu m~0.5 \mu m, the construction of inverted pyramid structure can increase the overall absorption rate by up to about 20%. The absorption rate of the two decreases gradually with the increase of the wavelength. When the wavelength is greater than 0.5 \mu m, the absorption rates of the two are comparable. This is because the shorter wavelength is affected by the trapping structure, increasing the optical path and making it more absorbed. As the wavelength gradually increases, the incident wave having a longer wavelength easily passes through the film, and the absorption rate decreases.

![Figure 2. Comparison of inverted pyramid and flat structure.](image)

3.2. Effect of dispersion media type on absorption rate
In order to explore the influence of the existence of diffused medium on the composite structure, this paper discusses the influence of the existence of different kinds of diffusing medium on the absorption rate of the composite structure.

![Figure 3. Absorption rate of composite structures with different types of dispersed media particles.](image)

Figure 3 is a graph of the absorptivity of different kinds of dispersing media, which the particle size of the control medium particles is 20 nm, and the volume fraction of the medium particles in the void of the inverted pyramid structure is 10%. It can be seen from the figure that the composite material to which the dielectric particles are added has a certain influence on the absorption of light, because the LSPR effect excited by the composite structure doped with the metal nanoparticles causes the incident
light to be absorbed to some extent. In the 0.4um~0.55um band, the absorption rate of the composite structure with different dispersed media particles is basically equal to that of the inverted pyramid structure. With the increase of the wavelength, when the wavelength is in the 0.55~0.8um band, there is a diffuse medium. The overall absorption rate of the structure is significantly higher than that of the composite structure without the medium particles. And in different diffuse media particles, Ag nanoparticles show better performance, and the absorption rate increases by more than 10% on average in the range of more than 0.55um.

3.3. Effect of volume fraction of dispersed media on absorption rate of composite structure

Since Ag nanoparticles are dispersed in the inverted pyramid structure, the overall absorption of incident light is better. Ag nanoparticles with particle size r=10nm are dispersed in the structure, and the volume fraction of Ag nanoparticles is controlled to five cases, i.e., 5%, 10%, 15%, 20%, and 30%. The absorption curves of the composite structures with different volume fractions are shown in Fig. 4.

As can be seen from the figure, the absorption rates of different volume fractions in the 0.4~0.5um band have small difference, and the absorption rate decreases with the increase of volume fraction; in the range of 0.5~0.8um, the absorption rate of composites with different volume fractions is quite different. With the increase of volume content, absorption rate have a certain increase; the absorption rate shows a downward trend throughout the entire band. The reason for this phenomenon is that light is more easily absorbed by the material in the overall structure in the smaller wavelength range, and in the larger wavelength range, the long-wavelength light is multiple refracted in the dispersion structure due to the increase of the metal particles, increasing the overall absorption rate.

Figure 4. Absorption rate curve of volume fraction composite structure of different metal particles.

3.4. Effect of different P/H on absorption rate of composite structure

This paper discusses the overall absorption rate of the composite structure under the condition that the depth H of the periodic structure inverted pyramid is different from the period length P ratio. The volume fraction of Ag nanoparticles in the inverted pyramid structure is controlled to be 10%, and remains unchanged. The length of the periodic structure is P=0.1um. By adjusting the size of H, three ratios H/P=0.5, H/P= 1, H / P = 2 are obtained. The simulation yields an absorbance curve as shown in Fig.4. It can be seen from the figure that in the whole visible light spectrum range, as the H/P ratio increases, the absorption rate increases, and the absorption rate decreases as a whole. This is because when H gradually increases, more particles are dispersed in the inverted pyramid structure, and more gold particles are in contact with the polysilicon surface, localized surface plasmon resonance effects occur under the action of incident light which promoting absorption of light.
Figure 5. Absorption rate curve of composite structure under different H/P conditions.

4. Conclusions
In order to improve the absorption rate of polycrystalline silicon thin film cells, this paper constructs an inverted pyramid structure on the surface of polycrystalline silicon thin film cells, and diffuses the metal nanoparticles in the inverted pyramid structure, and uses the local surface plasmon resonance effect generated by the metal nanoparticles to improve the absorption of composite film. The absorption of solar energy by the structured thin film cells is as follows:

1. Constructing an inverted pyramid structure on the surface of polysilicon, which can increase the overall absorption rate maximum by 20% in the 0.4–0.5 μm band;
2. The dispersion of metal nanoparticles with a particle size of 20 nm in the inverted pyramid structure has a certain increase in the absorption rate in the 0.55–0.8 μm band, and the dispersion of silver particles is best in the same case;
3. Under the condition that the Ag nanoparticles have a particle size of 20 nm and diffuse different volume fractions of Ag particles, the overall absorption rate increases with the increase of the volume fraction after 0.55 μm wavelength;
4. In the case of different ratios of H/P, as the ratio of H/P increases, the absorption rate of the overall structure gradually increases.

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