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Numerical Simulations of Optical Absorption and Spectral Selective of Ni Nanowire/AAO Composites

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Abstract. Spectral selectivity absorber is a key component in the solar collectors, which absorbs solar energy and converts it to thermal energy by heating liquid water. Metal nanowire arrays (NWAs) have potential to be used as solar collector because of good optical absorption in the visible region. In the paper, we use finite-difference time-domain (FDTD) solutions to calculate the optical absorption and spectral selectivity of nickel (Ni) NWA/AAO composites. By changing the length (L), fill-factor (FF), and surface roughness, we simulate the optical absorption and the spectral selectivity in terms of structural parameters of Ni NWA/AAO composites. Results demonstrate that Ni NWA/AAO composites with the length of 2 μm and the fill-factor of 0.13 (the diameter is 0.04 μm) have good optical absorption and spectral selectivity, and rough surfaces is better for higher conversion efficiency of Ni NWA/AAO composites.

Introduction

Solar selective absorbers are key component of solar thermal collectors to improve their photo-thermal conversion efficiently [1-6]. A good selective absorber should have good absorption in the visible-near IR region and little thermal emission in infrared region. In the last thirty years, cermets composed of metal and metallic oxide attracted lots of attention because of their good optical properties and excellent thermal stability [7]. Recently, with the development of nanotechnology, the solar absorption properties of nanowire arrays aroused researcher's interest. Hu et al. [8] simulated the absorptance of Si NWAs and found that NWAs have higher absorptance than their thin film counterparts in a high-frequency regime. Z-P Yang et al. [9] prepared low density CNT (carbon nanotube) arrays, created an extremely low reflectance material by controlling of tube diameter and tube-to-tube spacing in the 10-50 nm range. Rephaeli et al. [10] simulated the optical absorption of tungsten pyramid arrays; the result indicated that the tungsten pyramid arrays exhibited extremely high absorption for all solar wavelengths. Anodic aluminum oxide (AAO) template had been widely used as templates of synthesizing one-dimensional nanowires and nanotubes because it possessed many desirable characteristics, including tunable pore dimensions over a wide range of diameters and lengths, good mechanical strength and thermal stability. Zong et al. [11] prepared the composite of noble metallic nanowire arrays in the AAO membrane and exploited their optical properties. However, few results are available on optical selectivity of metal nanowire arrays.

In this paper, we simulate the optical absorptance, infrared radiance, and the conversion efficiency of Ni NWA/AAO composites by FDTD solutions. The effect of the length, fill-factor, and surface roughness on the optical absorption and conversion efficiency are investigated. These results indicate that Ni NWA/AAO composites have good solar spectral selectivity. Longer Ni nanowire with 0.13 fill factor and rough surface is better for higher conversion efficiency absorber. The results are instructive to manufacture high efficiency solar selective absorber.

Methods and Models

Fig. 1 is the schematic diagram of the NWA/AAO composites. The black arrows in Fig. 1a indicate the direction of incident light. The structure includes metal NWAs, anodic aluminum oxide (AAO) template, and aluminum (Al) basement. According to our experiment results [12], the pore distance *a* (Fig. 1b) is fixed on 0.105 μm. The red rectangle exhibits a simulation unit with periodic boundary conditions in simulations. The fill factor is defined as:

$$FF = \frac{\pi}{2\sqrt{3}}\left(\frac{d}{a}\right)^2. \tag{1}$$

where, *FF* stands for the fill factor, *d* is the diameter, and *a* is the pore distance of 0.105 μm. The effect wire length *L*, fill factor *FF*, and surface roughness of NWAs are considered in our simulation. For wires with such small diameters, we have to consider the wave effects by solving the full wave vector Maxwell's equations. To simulate the optical absorption of such ordered structures, the FDTD solutions had been proved to be effective tools [13]. The absorption of NWA/AAO composites could be expressed as $A(\lambda) = 1\text{-}R(\lambda)\text{-}T(\lambda)$, where λ is the wavelength of incident light, and $A(\lambda)$, $R(\lambda)$, and $T(\lambda)$ are the wavelength dependent absorption, reflection, and transmission, respectively. The transmission is neglected in our calculation, because the Al film is thick enough. So the absorption $A(\lambda) = 1\text{-}R(\lambda)$. The range of absorption wavelength in this simulation varies from 0.28 to 2.5 μm, according to Air Mass 1.5 (AM1.5) solar irradiance spectrum [14]. According to Kirchhoff's laws [15], the infrared irradiation of the composite at the thermal equilibrium conditions equals to their absorption. The range of the infrared wavelength in our simulation is between 1 and 9 μm. To get the absorptance α, conversion efficiency η, and emittance ε of NWA/AAO composites, we integrate the $A(\lambda)$ and $E(\lambda)$ with following equations:

$$\alpha = \int_\lambda A(\lambda)\Phi(\lambda)d\lambda \Big/ \int_\lambda \Phi(\lambda)d\lambda. \tag{2}$$

$$\varepsilon = \int_\lambda E(\lambda)W(\lambda,T)d\lambda \Big/ \int_\lambda W(\lambda,T)d\lambda. \tag{3}$$

$$\eta = \left(\int_\lambda A(\lambda)\Phi(\lambda)d\lambda - \int_\lambda E(\lambda)W(\lambda,T)d\lambda\right) \Big/ \int_\lambda \Phi(\lambda)d\lambda. \tag{4}$$

where, $\Phi(\lambda)$ is the spectral solar intensity of AM1.5, $W(\lambda, T)$ is the blackbody radiation intensity at working temperature T. The optical constants of Ni, aluminum oxide (Al_2O_3), and Al are adopted from experimental results [16].

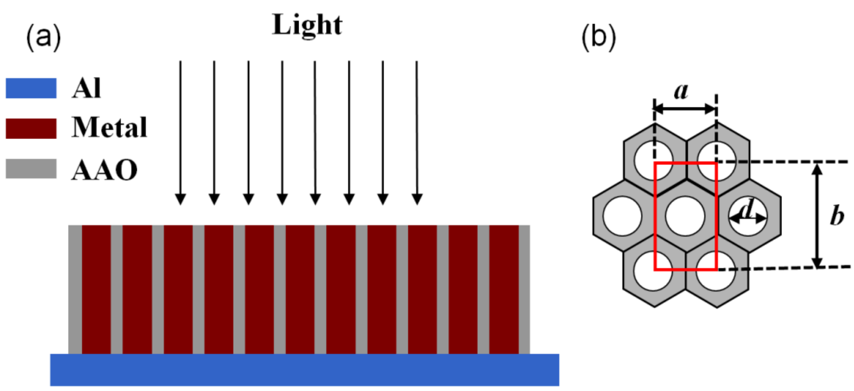

Fig. 1 The schematics of the ordered NWA/AAO composites in our simulations. (a) the model in FDTD solutions, the black arrows are incident light and colorful rectangles are metal NWAs (red), AAO template (grey), and Al basement (blue), respectively. (b) AAO template with pore distance *a*, the white circles are NWAs with diameter *d*, and the red rectangle (with width *a* and height *b*) is the simulation unit with periodic boundary conditions.

Results and Discussions

The influence of dimensions on the optical properties of metal NWA/AAO composites is studied based on Ni/AAO material system. The values of absorptance, conversion efficiency, and emittance are calculated according to equation (2) to (4). Fig. 2a gives the optical absorption of Ni NWA/AAO composites with a fixed fill factor of 0.13, the length of nanowires varying from 0.1 μm to 20 μm. It could be found that the optical absorption is poor in the entire spectrum for the Ni NWA/AAO composites with a length of 0.1 μm, which may ascribe to poor light-trapping effect and short light reflection paths of scattering light in thin Ni NWA/AAO composites. With the increase of nanowire length, the optical absorption enhances in all spectrum, which results from the surface plasmon polariton (SPP). SPP is constituted *via* the resonance interaction between the electromagnetic field of incident light and the surface charge oscillations at the interface of NWA/AAO [17]. The momentum of SPP enhances as the length increases, which prevents the spread energy escape out of NWA/AAO composites. The effect of momentum of SPP increasing is more obviously in short wavelength regime. Fig. 2b is the absorption curves of Ni NWA/AAO composites in visible-near IR region. It could be observed that the optical absorptions improve and oscillations reduce with the increase of nanowire length. To obtain the best spectral selective absorption for Ni NWA/AAO composites, we also need lower IR emission in region of 1 to 9 μm. Fig. 2c displays the absorptance, conversion efficiency, and emittance of Ni NWA/AAO composites at 400 K. The absorptance and conversion efficiency increase sharply before the length of Ni NWA/AAO composites reaches 2 μm. After that, they change a little. We conjecture that 2 μm is the propagation length of the SP mode for Ni nanowires [17]. The values of absorptance and conversion efficiency are 0.834 and 0.832 for 2 μm Ni NWA/AAO composites. But for 20 μm Ni NWA/AAO composites, the two values are 0.873 and 0.858, respectively. However, IR emittance is linear increase with length of NWA/AAO composites (red curve in Fig. 2c). To obtain high conversion efficiency, high absorptance is welcome, but high emittance must be avoided. Considering the conversion efficiency and the fabrication cost, the length of 2 μm is the balance choice for a good Ni NWA/AAO spectral selective absorber.

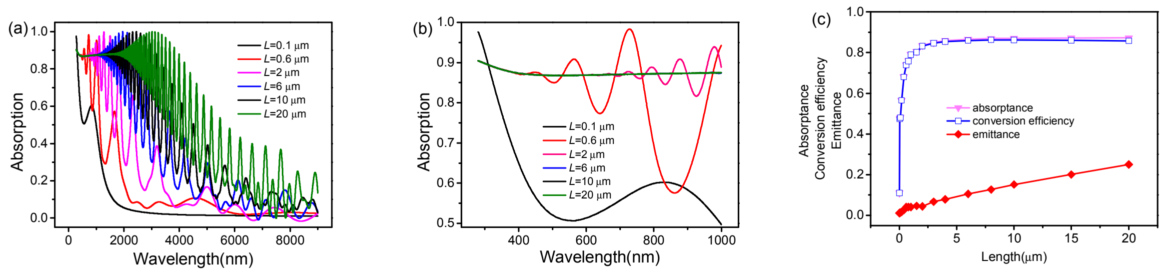

Fig. 2 Spectral selective absorption of Ni NWA/AAO composites with different lengths from 0.1 μm to 20 μm. (a) the optical absorption in the entire spectrum, (b) the magnified curves in short wavelength regime, and (c) the absorptance, conversion efficiency, and emittance of Ni NWA/AAO composites at 400 K.

We also consider the influence of another structure parameter: the fill factor. The optical absorptions of the Ni NWA/AAO composites with various fill factors (from 0.0020 to 0.40), and a fixed length of 2 μm are presented in Fig. 3a. It is observed that absorption peaks of Ni NWA/AAO composites exhibit red shift with the increase of fill factor. The red shift could be explained by the small size effect. The intervals between the nanowires decline when the fill factor enhances, the overlap of SPP resonance field narrows the energy gap and results in the red shift of absorption peak. Fig. 3b provides more detailed information of the optical absorption in visible-near IR band, and it indicates that the Ni NWA/AAO composites with fill factors of 0.074 and 0.13 have better absorption in short wavelength range, but the absorption spectrum of FF 0.13 shows less oscillation. The absorptance (Fig. 3c) shows parabola-like waves as a function of fill factor, and the maximum absorptance is obtained at the fill factor of 0.13, which may because that the absorption spectrum of

FF 0.13 matches well with the AM1.5 solar irradiance spectrum. The emittance (red curve in Fig. 3c) enhances as the fill factor increase. High emittance could reduce the spectral conversion efficiency in service. For the best solar conversion efficiency, i.e. higher absorptance and lower emittance, 0.13 is the best choice for fill factor in our simulations.

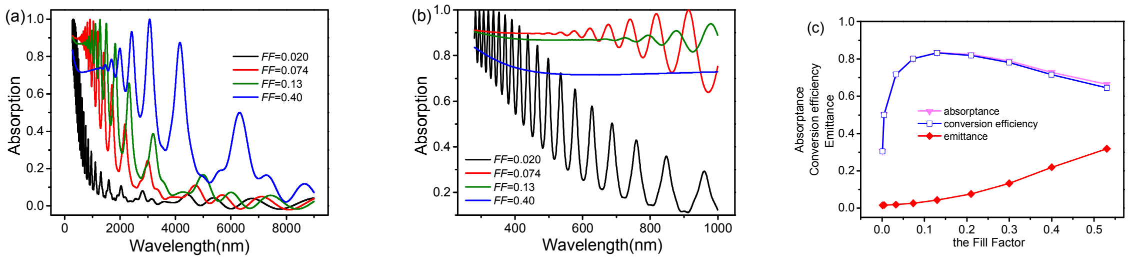

Fig. 3 Shows spectral selective absorption of Ni NWA/AAO composites with varying fill factor from 0.0020 to 0.40. (a) the optical absorption in the entire spectrum, (b) the magnified curves in short wavelength regime, and (c) the absorptance, conversion efficiency, and emittance of Ni NWA/AAO composites at 400 K.

The absorptances of Ni NWA/AAO composites are all less than 90% in this simulation. However, the absorptance of Ni NWA/AAO composites reaches 98.4 % in our previous experiments [12], and it shows stable absorption in the wavelength from 0.25 μm to 2.5 μm (Fig. 4a). We speculate that the difference in surface roughness between experiments and simulations may be the key point. Because the surface of nanowire in our simulations is smooth, but the SEM image (inset picture in Fig. 4a) shows that the surfaces of Ni nanowires fabricated through two-step anodization is rough. Then we simulate the optical absorption (Fig.4b) of Ni NWA/AAO composites with rough surface (the structure parameters are length of 2 μm and fill factor of 0.13). The inset in Fig. 4b exhibits the schematic of Ni NWAs with rough surface (on the left) and smooth surface (on the right) in our simulations. The raised and invagination areas on the surface of nanowires result in surface rough and the amplitude is 0.0015. It could be observed from Fig. 4b that the NWAs with rough surface achieve higher absorption (higher than 90%) in visible region, which attribute to local surface plasmon resonance of the bumps on the interface between NWAs and AAO. Furthermore, the reflected paths of incident light are also enhanced. While in the long-wavelength range, the tiny roughness does not induce the obvious change in absorption. The absorptance and conversion efficiency of Ni NWA/AAO composite with rough surface are 0.863 and 0.860, higher than that (0.834 and 0.832) of composite with smooth surface. The Ni NWA/AAO composite with rough surface has higher conversion efficiency, which is beneficial for the spectral selective absorber.

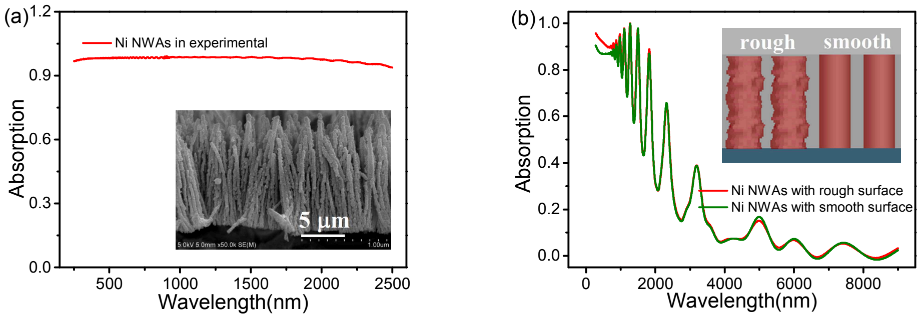

Fig. 4 The effect of surface roughness. (a) the hemispherical absorptance of Ni NWA/AAO composite in the UV-VIS-NIR region. The inset picture is the SEM image of Ni NWAs, and rough surface of Ni NWA/AAO composite could be observed. (b) the absorption of Ni NWA/AAO composite with rough or smooth surface, and the insets are schematic of Ni NWA/AAO composite with rough surface (on the left) and smooth surface (on the right) in simulations.

Conclusions

We investigate the optical properties in ordered Ni NWA/AAO composite by the FDTD solutions. Our simulations exhibit that the SPP resonance and light-trapping effect play an important role in optical absorption. The best structure parameters of Ni NWA/AAO composite are length of 2 μm and fill factor of 0.13 (diameter of 0.04 μm) at the operating temperature of 400 K. Meanwhile, Ni NWA/AAO composite with rough surface have the beneficial effect for higher absorptance and conversion efficiency, which is useful for photothermal utilization.

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