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UV-blocking ZnO nanostructure anti-reflective coatings

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ABSTRACT

In this paper, we apply finite difference time domain simulation to determine the absorptance and reflectance of ZnO nanowire and nanohole array structures for an efficient UV-blocking anti-reflective coating. Comparing to ZnO thin films, both nanowires and nanoholes have much improved performance. ZnO nanowires and nanoholes have similar absorptions in the UV range. However, ZnO nanowires have lower absorptance than nanoholes in the visible range. Influences of different parameters including lattice constant a, ZnO filling ratio f and nanowire heights h are analyzed. The optical properties of the nanostructures are less dependent on the incident angle of light, which enables them to be used as wide angle anti-reflective coatings with UV blocking.

Anti-reflective coatings (ARCs) have become indispensable to modern optical and electro-optical systems. Most of the ARCs are needed to be transparent in the visible range with UV blocking to protect the devices. For example, the ARCs are essential parts for high efficiency and low cost solar cell devices especially for thin film solar cell devices. The commonly used ARCs are plate ones [1–6] including single layer and multi-layer ARCs. Obviously, single layer ARCs are designed for one single wavelength or a narrow wavelength range and the multi-layer ones are used for broad band anti-reflective applications. However, multi-layer ARCs have some problems such as material selection, thermal mismatch, sensitivity to thickness variation and large thickness. On the other hand, front surface texturing [7–9] is a promising way to achieve efficient ARCs. With front surface texturing, the reflectance has been reduced tremendously owing to the gradual change of refractive index of the textured surface. The scale of front surface texturing is normally in the range of tens of micrometers which is not suitable for thin film ARCs. With the development of nanotechnology, more efforts have been put on the fabrication of nanostructure ARCs, including random textured nanostructures [10–13], nanowire and nanohole structures [14–17]. With these nanostructures, the light reflection can be largely reduced due to the multiple scattering of the incident light.

ZnO has high transparency in the visible range and high absorptance in the UV range, so it is widely used in ARCs [11–13,16,18,19]. With the rapid growth of research interests in solar cell area, ZnO nanostructure ARCs have been successfully applied for solar cells [11–13,16]. For some organic solar cells, most of the absorption of the active layer occurs at visible range, the UV absorption of ZnO can protect the active layer from damage by the unused UV light. Element (Al, Ga and so on) doped ZnO results in high conductivity property which makes the ZnO a good candidate to substitute the expensive ITO as the transparent conducting layer for solar energy applications. According to these two properties, ZnO nanostructures can be used as conductive layer and UV-blocking anti-reflective layer simultaneously. However, the influences of nanostructure parameters such as lattice constant and filling ratio on optical properties have not been studied systematically and the UV-blocking property has never been considered.

In this manuscript, we apply ZnO nanostructures to design UV-blocking ARCs. The nanostructures considered here are ZnO nanowires and ZnO nanoholes. The finite difference time domain (FDTD) [20] method is used for the absorptance and reflectance calculation. Commercial software package FDTD Solution was used for absorptance and reflectance calculations.

The inset of Fig. 1(a) shows the schematic of the nanowire and nanohole structures. The nanowires and nanoholes are both arranged in a square lattice in x–y plane with the same lattice constant a and height h. The filling ratio f is defined as the ratio of ZnO area over one unit cell area. Light is normally incident on the x–y plane.

In the simulation, we use Forouhi–Bloomer (F–B) dispersion formula [21,22] to determine the refractive index of ZnO. The real (n) and imaginary (k) parts of the refractive index calculated according to the F–B model are shown in Fig. 1(a). The solid line and the short-dashed line represent the real and imaginary parts of the refractive index of ZnO respectively. It is clearly shown that the imaginary part of the refractive index of ZnO is almost equal to zero for wavelength exceeding 400 nm which is in agreement with measured data [23].

The comparison of ZnO nanowire structure and thin film is shown in Fig. 1(b). Both of them have the same thickness of 1 μm. The nanowire structure has parameters of $a = 200$ nm and $f = 0.3$. Comparing

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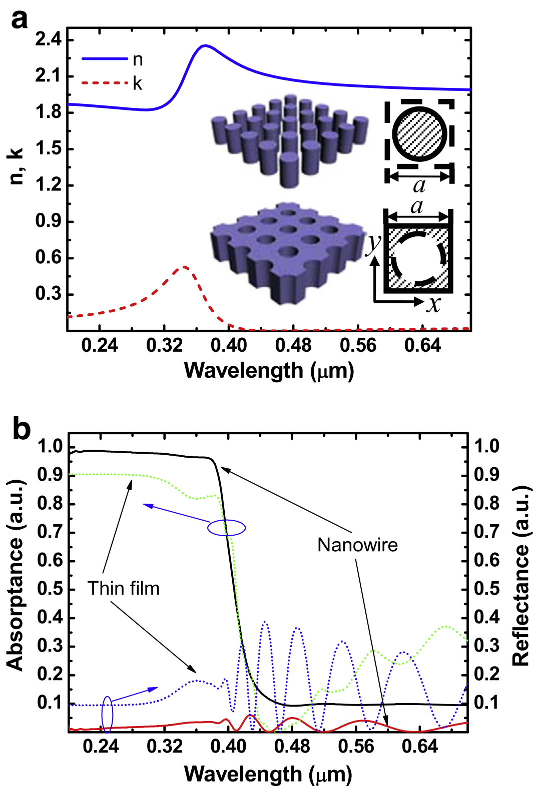

Fig. 1. (a) Real (n) and imaginary (k) parts of the ZnO refractive index calculated with F–B dispersion relationship. Inset is the schematic of ZnO nanowire and nanohole structures arranged in square lattice and their corresponding unit cell with lattice constant a. (b) Absorptance and reflectance of ZnO nanowire and thin film with the same thickness (1 μm). For nanowire structures, $a = 200$ nm, $f = 0.3$.

with ZnO thin film, the ZnO nanowire has lower reflectance in the entire simulated range owing to the surface texturing of the nanowire. In the visible range, the ZnO nanowire has lower absorptance than the ZnO thin film which means that the ZnO nanowire has better transmittance in the visible range. In the UV range, almost 100% of the absorptance is achieved for the ZnO nanowire which is also much better than the ZnO thin film layer. The filling ratio of ZnO is 0.3 which means better performance can be achieved with only 30% materials.

Fig. 2(a), (b), (c) and (d) shows the absorptance and reflectance spectra of ZnO nanowire for various of a, f and h respectively. In Fig. 2(a), (b) and (c), the absorptance and reflectance are calculated with $a = 100$ nm, 200 nm and 400 nm respectively. The height h of the nanowire is fixed at 1 μm. In Fig. 2(a), the absorptance and reflectance of different fs are compared for $a = 100$ nm. With the decrease of f, reflectance decreases simultaneously for the entire simulated wavelength range which means that the less ZnO material is used, the lower the reflectance of the nanowire structures. The absorptance in the visible range also decreases with the decrease of f. The absorptance in the UV range increases when f decreases from 0.7 to 0.5 and then increases when f reaches 0.3. In Fig. 2(b), lattice constant a is increased to 200 nm, the reflectance is still very low for different fs and has a similar trend as in Fig. 2(a). The enhancement of absorptance of nanowire structures in the UV range can easily be seen from this figure. When f decreases from 0.7 to 0.3, the absorptance increases accordingly and almost all UV light is absorbed by the nanowire. In the visible range, the absorptance trend is similar to that of Fig. 2(a). Additionally, we can see that when $f = 0.3$, the absorptance drops faster from UV to visible range compared to the other two filling ratios which means that UV absorption has lower influence on active layer absorptance. In Fig. 2(c), the absorptance and reflectance are plotted for $a = 400$ nm. Clearly, when lattice constant is large (400 nm in our case), the reflectance and absorptance in the visible range are large which makes it not suitable for ARCs. From Fig. 2(a), (b) and (c), $a = 200$ nm and $f = 0.3$ are

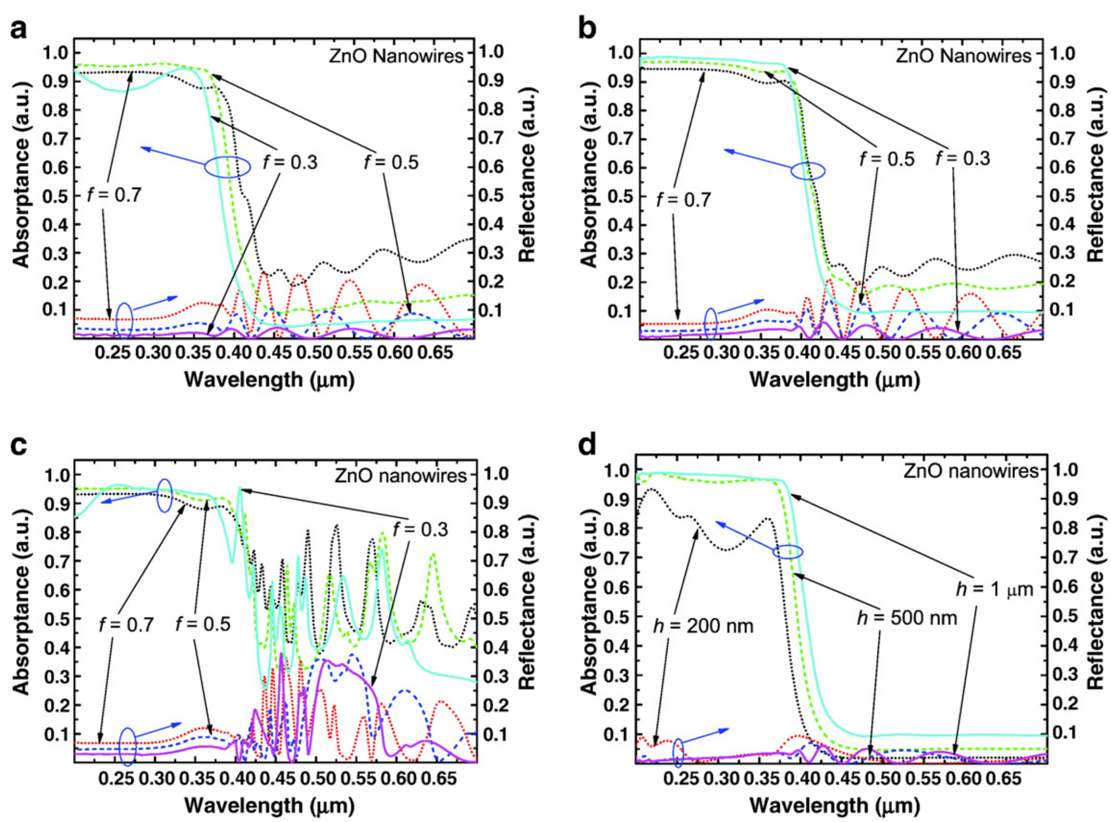

Fig. 2. Absorptance and reflectance of different filling ratio f at fixed nanowire height $h = 1$ μm with lattice constant (a) $a = 100$ nm, (b) $a = 200$ nm, (c) $a = 400$ nm. (d) Absorptance and reflectance of different heights of nanowire with lattice constant $a = 200$ nm and $f = 0.3$.

optimized parameters. In Fig. 2(d), we also show the influence of different heights ($h = 200$ nm, 500 nm, and 1 μm) of nanowire structures with $a = 200$ nm and $f = 0.3$. Obviously, the reflectance does not have large changes with various heights. A thinner nanowire has lower absorptance both in the visible range and UV range. When $h = 1$ μm, we can get an efficient nanowire ARC with excellent UV blocking.

For many applications, the ARCs are needed to have lower reflectance in the visible range and large absorptance in the UV range even when the light is lunched with a large incident angle. The absorptance of different incident angles for wavelength range from 0.2 μm to 0.7 μm of TE mode is shown in Fig. 3(a). The absorptance in the UV range is very high even for large incident angles up to 70° and the absorptance in the visible range is quite small for the incident angles examined. The reflectance of different incident angles is shown in Fig. 3(b). It is clear that the reflectance is also very low for both broad wavelength range and large incident angles. The absorptance and reflectance in a broad wavelength range and for different incident angles of TM mode are shown in Fig. 3(c) and (d) respectively. Similar results are also obtained for TM mode. From the above discussion, large light incident angle only has slightly influence on absorption and reflection properties of ZnO nanowires.

Similar analyses of nanohole structures are shown in Fig. 4(a), (b), and (c). In Fig. 4(a), the influences of different *f*s on absorptance and reflectance are studied with $a = 200$ nm and $h = 1$ μm. From Fig. 4(a), when $f = 0.3$, the nanohole structures show better anti-reflectance with better UV blocking. The absorptance and reflectance of different *a*s with $f = 0.3$ and $h = 1$ μm are obtained in Fig. 4(b). It is clear that the nanohole structures show better UV-blocking anti-reflectance when $a = 200$ nm. For different *h*s with $a = 200$ nm and $f = 0.3$, the absorptance and reflectance are plotted in Fig. 4(c). Better UV-blocking anti-reflective performance are obtained when $h = 1$ μm. The absorptance and reflectance of nanohole and nanowire structures are compared in Fig. 4(d). These two structures have the same behavior in the reflectance. Both of them have good reflectance in the entire simulation wavelength range. For the absorptance, the two nanostructures are also similar to each other in the UV range. The only difference is that the nanowire structure has lower absorptance in the visible range compared to the nanohole structure, which indicates that ZnO nanowire structure is slightly better compared to ZnO nanohole structure.

In conclusion, an efficient UV-blocking ARCs is demonstrated using the FDTD method. Different lattice constant (a varying from 100 nm to 400 nm), filling ratio ($f = 0.3$, 0.5, 0.7) and height ($h = 200$ nm, 500 nm, 1 μm) are considered in the simulation. According to our simulation, the best parameters for an efficient UV-blocking ARCs are $a = 200$ nm, $f = 0.3$, $h = 1$ μm. The optical properties of nanostructures are less dependent on the incident angle of the

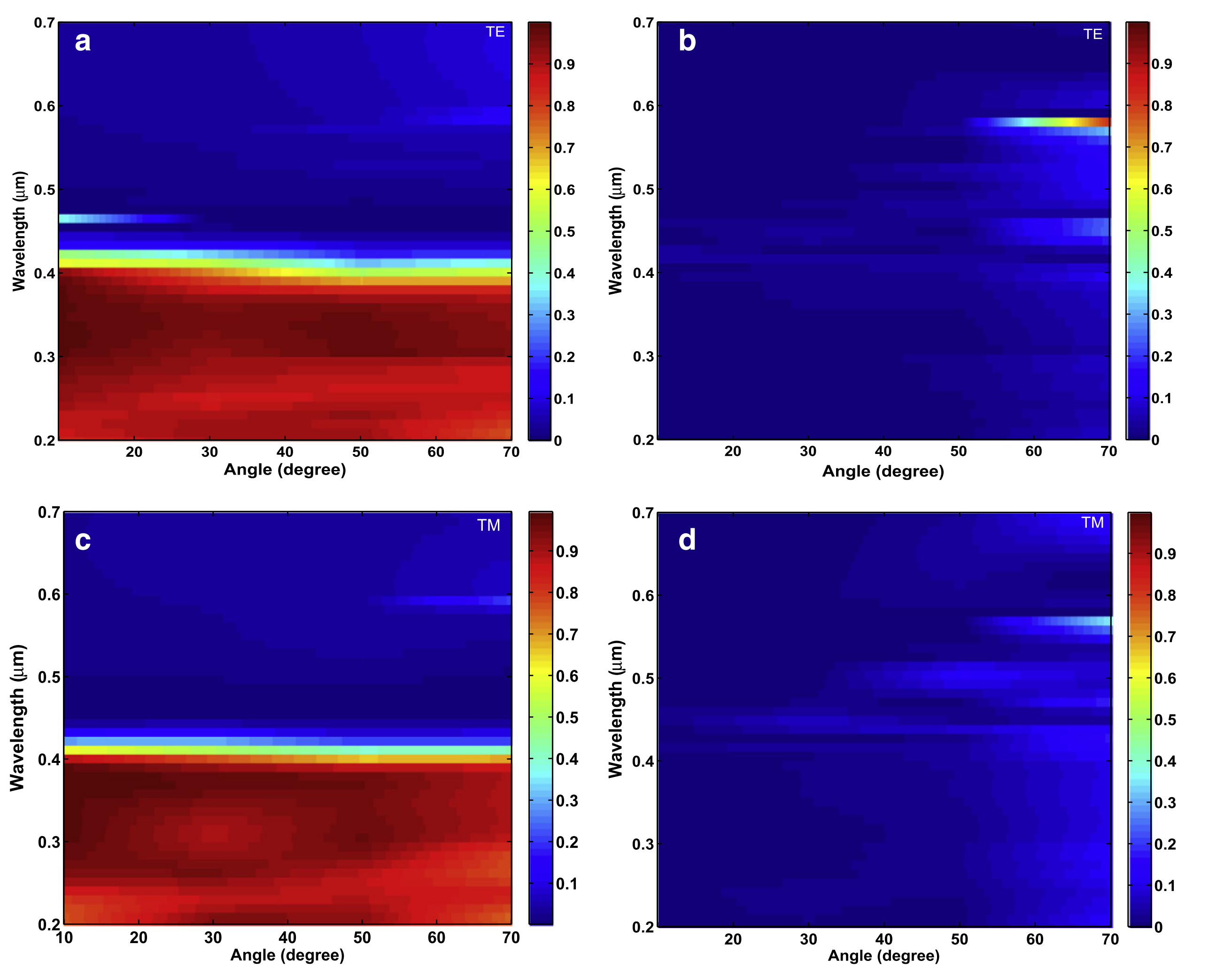

Fig. 3. Influence of different incident angle on absorptance and reflectance of ZnO nanowire. (a) The absorptance of TE, (b) the reflectance of TE, (c) the absorptance of TM, and (d) the reflectance of TM.

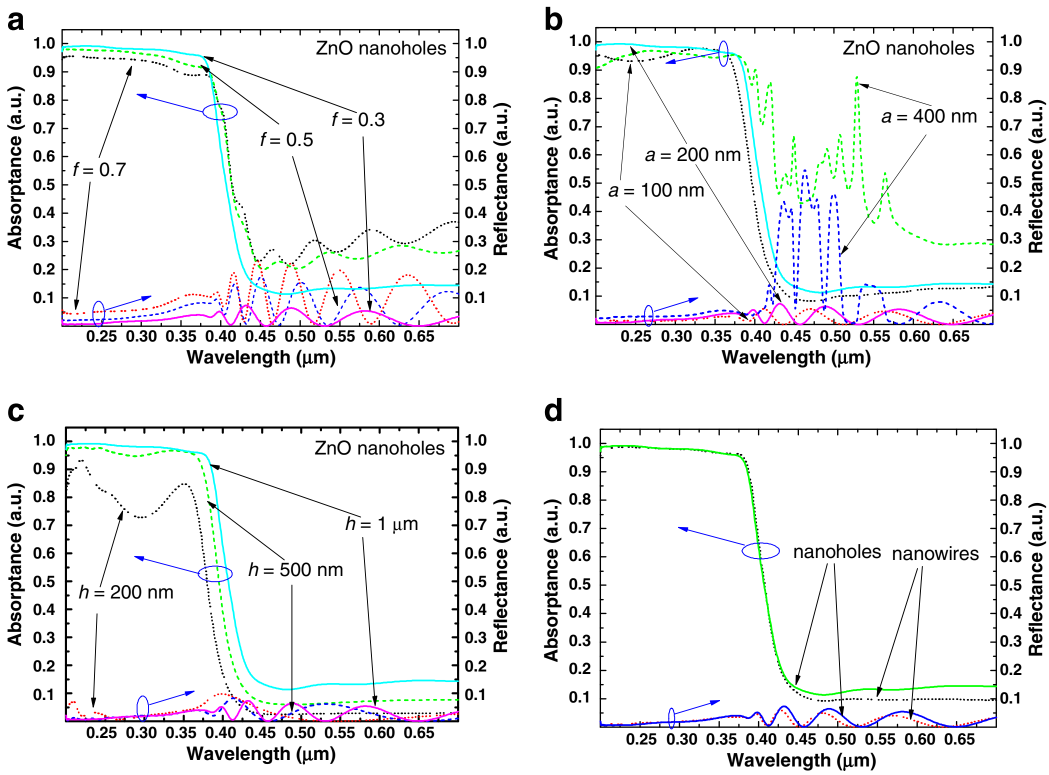

Fig. 4. Absorptance and reflectance of nanoholes of (a) different f with $a = 200$ nm, and $h = 1$ μm, (b) different a with $f = 0.3$, and $h = 1$ μm, (c) different h with a = 200 nm, and $f = 0.3$. (d) Absorptance and reflectance of ZnO nanowires and nanoholes with the same parameters.

light. The comparison of ZnO nanowire and nanohole structures is also presented in this work, the ZnO nanowires are slightly better than nanoholes.

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