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Simulation of smart windows in the $ZnO/VO_2/ZnS$ sandwiched structure with improved thermochromic properties

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ABSTRACT

We modeled a sandwiched structure $ZnO/VO_2/ZnS$ potentially as a VO_2-based smart window with a goal to increase both luminous transmittance (T_{lum}) and solar modulation ability (ΔT_{sol}). Compared to the previously used single-layer antireflection coating, the new sandwiched structure broadens the reflectance minimum in the visible light range and enlarges the transmission gap in the near-infrared (NIR) region, when switching between the semiconducting and the metallic states and when utilizing an intermediate index ZnS layer imbedded between the VO_2 film and substrate. The 3/4-1/4-3/4 wavelength–thickness model exhibited a high solar modulation ability (ΔT_{sol} = 13.01%), and maintained a high T_{lum} at 63.24% and 57.39% both in semiconducting and metallic phases, respectively.

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1. Introduction

Excessive energy consumption in buildings, transportations, and other industries have led to growing concerns on using renewable energy and energy saving, which are two increasing important aspects of the economy sustainable development [1,2]. Particular attention on energy saving in buildings and man-made constructions should be paid, since it consumes as much as 30–40% of the primary energy in the world [1,3].

One efficient way to make an effective use of solar energy in buildings is to modulate sunlight transmission through glass windows by solar-controlling coatings, also called "smart windows" [4,5]. Chromogenic materials based smart windows can modulate the amount of solar irradiation in response to the external stimulus intelligently [5,6]. Common chromogenic materials include electrochromic thin films varying their optical properties by electrical voltage or discharging [7–11], photochromic ones coloring under ultraviolet irradiation or bleaching in the dark [12,13] and thermochromic ones changing solar light transmission depending on the temperature [14–23]. Among them, the thermochromic smart windows, typically based on vanadium dioxide (VO_2), have been attracting particular research interests roughly due to the below three aspects. Firstly, VO_2 has a rapid response to the environmental temperature, switching between a near-infrared (NIR) transparent semiconducting state and an opaque metallic state [14,22]. Secondly, during the phase transition, ultraviolet light is almost fully absorbed while the transmission of visible light remains almost unaffected [16,24]. Thirdly, the semiconducting-metallic phase transition temperature (T_c) could be reduced almost to room temperature by doping [25,26], or by reducing crystal sizes [27], from its normal phase–transition temperature of ~68 °C [28].

However, due to VO_2's high reflectance and strong absorption resulting from its high refractive index (RI) and large absorption coefficient, low luminous transmittance (T_{lum}) and insufficient solar modulation ability (ΔT_{sol}) retard the practical application of VO_2-based smart windows [14,16]. The main fabrication methods for VO_2 films include chemical vapor deposition [29], sputtering deposition [15], pulsed laser deposition [30], polymer-assisted deposition [22,24], and so on.

In order to improve T_{lum} and ΔT_{sol}, people have reported that involving an additional antireflection layer could improve the transmittance in set wavelength [22,31,32]. Unfortunately, concurrent improvement on both T_{lum} and ΔT_{sol} is still a challenge.

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For example, a TiO_2 antireflection layer was employed in the VO_2-based smart window [22], by using the destructive interference and reducing the interface reflectance. However, the improvement in T_{lum} is weak as it produced a narrow transmittance dip in the visible light region. It only improved the transmittance in a narrow wavelength range. In fact, enlarging the transmittance gap in the NIR region for two states is needed in order to further explore an improvement on ΔT_{sol}.

In this work, we introduced a sandwiched structure $ZnO/VO_2/ZnS$ to the common VO_2-based smart windows. The structure consists of a layer of intermediate index ZnS next to the substrate, followed by a high-index VO_2 layer and finally by a low-index ZnO layer on the most outside. This special structural design considers both broadening reflectance minimum in the visible light region to improve T_{lum} and enlarging transmittance gap in the NIR region for the two states' transition to improve ΔT_{sol}. Very importantly, the added ZnO and ZnS materials are common to window coatings or as conductive coatings and semiconductive coatings in electronics, respectively, [33,34]. Our simulation indicates that this special antireflection design with the optimized optical thicknesses concurrently improves the visible transmittance and the solar modulation efficiency to a great extent. The 3/4-1/4-3/4-wavelength thickness multilayer films exhibit a high solar modulation ability (ΔT_{sol} = 13.01%), while maintaining a high T_{lum} at 63.24% and 57.39% both in semiconducting and metallic phases. For practical purposes, we also explored a range of low RI, which could be selected as a top layer in VO_2-based smart windows. The concurrent improvement on visible transmittance and switching efficiency with the use of our sandwiched structure provides an attractive prototype development for new smart windows.

2. Computational method

For antireflection coatings neglecting their absorption, the condition of the reflectance at wavelength λ_0 to achieve the minimum is that the optical thickness should satisfy the following equation [35]:

$$nd = \frac{j\lambda_0}{4} \quad (j = 1, 2, 3\ldots) \tag{1}$$

where n and d denote the RI and the thickness of the antireflection films, respectively. The antireflection principle is based on the destructive interference of light reflected from interfaces of the respective coating layers [36].

Values of T_{lum} and T_{sol} evaluating the performance of smart windows were obtained from the following equation [17,22]:

$$T_{lum} = \frac{\int \phi_{lum}(\lambda)T(\lambda)d\lambda}{\int \phi_{lum}(\lambda)d\lambda} \tag{2}$$

$$T_{sol} = \frac{\int \phi_{sol}(\lambda)T(\lambda)d\lambda}{\int \phi_{sol}(\lambda)d\lambda} \tag{3}$$

where ϕ_{lum} is the spectral sensitivity of the light-adapted eye and ϕ_{sol} is the solar irradiance spectrum for an air mass of 1.5 (corresponding to the sun standing 37° above the horizon) [37]. Additionally, we calculated the value of $T_{NIR,sol}$ in the following study using the equation:

$$T_{NIR,sol} = \frac{\int \phi_{NIR,sol}(\lambda)T(\lambda)d\lambda}{\int \phi_{NIR,sol}(\lambda)d\lambda} \tag{4}$$

where, $\phi_{NIR,sol}$ is the NIR solar irradiance spectrum (780–2000 nm) for an air mass of 1.5. ΔT_{sol} and $\Delta T_{NIR,sol}$ are obtained from the equations [24]:

$$\Delta T_{sol} = T_{sol,s} - T_{sol,m} \tag{5}$$

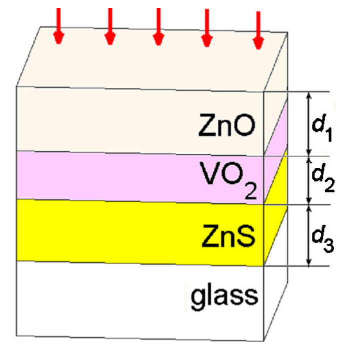

Fig. 1. A 3D conceptual schematic of the $ZnO/VO_2/ZnS$ sandwiched structure.

$$\Delta T_{NIR,sol} = T_{NIR,sol,s} - T_{NIR,sol,m} \tag{6}$$

where s and m denote the semiconducting and metallic state, respectively.

To improve T_{lum}, one efficient way is to broaden the reflectance dip in the visible light range, which in turn enlarges the transmittance in the visible region as far as possible. However, to improve ΔT_{sol}, we have to increase the transmission gap in the NIR region between the semiconducting and metallic state. In our design, we adopted a sandwiched structure with RI of n_f, n_s and n_t, where n_f, n_s and n_t represent the RI of the first, second and third layer from the top, respectively, which can both improve the performance of smart windows highly and utilize relatively simple fabrication technology [16]. Among the three layers, usually n_f has the lowest value, n_s has the highest value, and the value of n_t is in the middle. Thus, the structure with low-high-middle RI can generate broad reflection dip on the two sides of wavelength λ_0 set in the beginning, resulting in relatively wide spectral optimization [38].

Fig. 1 shows the schematic of the sandwiched structure, using those common window or electronics coating materials. Technically, the multilayers could be deposited by RF magnetron sputtering, which has been widely used in the low-emissivity window coating production lines [39]. According to the literatures and in more details to elaborate, the ZnS film could be firstly deposited onto the pre-cleaned glass substrate using ZnS target with proper sputtering conditions [40]; then the VO_2 film could be deposited by sputtering a vanadium target in argon and oxygen gas flow with a proper pressure, power, and temperature [17]; lastly, the ZnO film could be deposited by sputtering a Zn target in argon and oxygen gas flow with proper conditions [41]. The thickness of different films can be modulated by coordinating the sputtering conditions, time, et al. [17,40,41]. Furthermore, the VO_2 film could be prepared by other techniques such as the polymer-assisted deposition method [24], ZnO and ZnS films could be spin-coated using presynthesized sols [22]. In this way, the thickness of different films can be regulated by modulating sol concentration and spinning speed [22].

In our simulations, all material property parameters were taken from previous literatures and they reflect the practical situations to be simulated. For examples, dielectric constants of VO_2 were taken from the interpolation of the experimental spectroscopic data reported by others [42,43]. Optical constants of ZnO and ZnS were taken from the Refs. [44,45], respectively. Compared with those of VO_2, ZnO and ZnS, the RI of glass substrate's dispersion is much smaller in the wavelength range involved in the study, which was neglected in our simulation. A constant RI of 1.51 was used for the glass substrate.

To improve T_{lum}, position and value of the reflection minima are two key factors. This is because solar energy distributes unequally across entire spectra range and the response of human eyes to different wavelength light is different [3,46–48]. Position of the

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