VO2-polymer nanostructured coatings for smart windows: a numerical study

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Abstract: Thermochromic vanadium dioxide loaded into a polymer opal photonic crystal is studied through optical simulations. The possibility of using this material as flexible transparent energy efficient smart material is explored.
OCIS codes: (160.5298) Photonic crystals, (160.4760) Optical properties, (160.5470) Polymers

1. Introduction

Vanadium dioxide (VO_2) undergoes a phase transition with temperature that switches its behavior from semiconducting to metallic and thus modifies its optical properties. Its thermo-active characteristics have been studied for coating applications related to solar-irradiation on substrates that can be either transparent or absorbent materials (fluid absorber, smart windows, smart tiles). Among the various processes that have been explored to produce VO_2 glazings, a promising approach relies on the mixing of VO_2 nanoparticles with a glass or a polymer matrix [1].

This work is a numerical study of a model smart glazing made of a VO_2 nanoparticles mixed with a polymer latex that could enable to form a VO_2-polymer composites with an opal-like nanostructure [2]. The performances of such model glazing in terms of visible and IR transmittance are evaluated using Maxwell-Garnett [3] (MG) approximation and Fourier Modal Method [4] (FMM). Considering these two complementary modelling approaches enables to highlight the impact of introducing photonic affects related to highly ordered nanostructured (opals) compared to more disordered nanostructured.

2. Materials and process

2.1. Nanostructure of the model material

Our model material is a closed-packed opal made of hard polystyrene (PS) spheres (refractive index n=1.58) in a soft polyethylacrylate (PEA) matrix (n=1.47). The spacing between each PS sphere is set to a = 500nm. VO_2 nanoparticles have been loaded into the matrix. VO_2 refractive indices used in these calculations are extracted from [5] Four different VO_2 concentrations have been considered: 0.1vol%, 0.5vol%, 1vol% and 1.3vol%. Low concentrations are required for the material to stay transparent to visible light.

2.2. Homogeneous equivalent material: Abeles Matrices Model

A first approach consists in using the MG approximation to model the coating as an average material having an effective permittivity ε_{eff} depending on f the volumic fraction of the nanoparticles, ε_p and ε_m the dielectric permittivity of the nanoparticles and surrounding material here, the model material is a monolayer, and the transmittance characteristics are computed through an Abeles Matrices Model (AMM). [6]

2.3. Nanostructured material: Fourier modal method

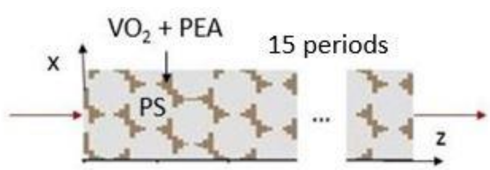

Fig. 1: Numerical representation of a close packed polymer opal made of PS spheres in PEA filled with VO_2 nanoparticles, and light incident over the (111) crystallographic direction

Light is injected along the (111) crystallographic direction of the considered polymer opal photonic crystal (Fig 1). In this direction, the structure is modelled by 15 periods, each of them are 866nm thick. The material total thickness is then 12.99µm. The interstices containing VO_2 nanoparticles and PEA have been modelled using the Maxwell-Garnett approximation. The material is surrounded by air. FMM is usually limited to 1D or 2D photonic crystals. In order to extend to 3D crystals, we approximated each sphere by a superposition of cylinders of constant heights. The spatial resolution is set so that each period is modelled by 24 layers.

2.3. Criteria used to evaluate the materials performances

Optimizing such smart glazings for smart windows applications relies on maximizing the visible transmittance T_{vis} in both warm and cold conditions and maximizing the infrared (IR) transmittance modulation ΔT_{IR} as defined herafter.

$$T_{vis} = \frac{\int_{400nm}^{800nm} E_\lambda\, T(\lambda)\, d\lambda}{\int_{400nm}^{800nm} E_\lambda\, d\lambda} \quad \text{and} \quad T_{IR} = \frac{\int_{800nm}^{2500nm} E_\lambda\, T(\lambda)\, d\lambda}{\int_{800nm}^{2500nm} E_\lambda\, d\lambda} \qquad (1)$$

E_λ is the weight coefficient for solar direct normal irradiance extracted from ASTM G173-03 and $T(\lambda)$ is the material spectral transmittance. The transmittance modulation in IR is then defined as the difference in the infrared transmittance between both states of the thermochromic VO_2.

$$\Delta T_{vis} = |\, T_{vis}(cold) - T_{vis}(warm)\, | \quad \text{and} \quad \Delta T_{IR} = |\, T_{IR}(cold) - T_{IR}(warm)\, | \qquad (2)$$

3. Results and discussion

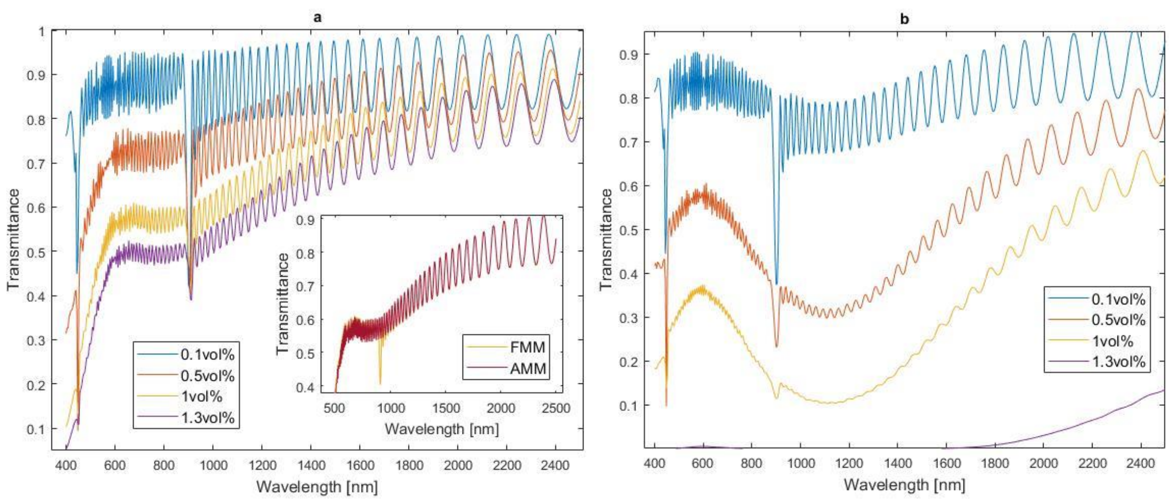

Fig. 2: Transmission spectra of the polymer opal loaded with different VO_2 concentrations computed with FMM (a) in cold state (inset: comparison with an equivalent homogeneous material computed with AMM, in the case of 1vol% VO_2) and (b) hot state

Using MG and FMM, transmission spectra of the nanostructured material are calculated over the 400-2500nm wavelength range for different VO_2 concentrations in both VO_2 phases (fig. 2). The oscillations observed at high wavelengths are due to thin film interferences, incident light reflected at the sample surface interfering with the light reflected at the bottom of the sample. Note that for the VO_2 hot state at higher concentration (fig. 2b), the incident light is absorbed before reaching the substrate, leading to the oscillations disappearance.

The transmission minimum observed in all transmittance spectra around 900 nm is due to the photonic bandgap (PBG), characteristic of ordered photonic crystals which is consistent with Bragg's law at normal incidence. As the VO_2 concentration increases, the material transmittance significantly decreases due to the absorption by the VO_2 nanoparticles. In fig. 2b, the transmission decrease around 1100 nm is due to the plasmonic absorption in metallic VO_2 nanoparticles. To confirm these assumptions, we compared the transmission spectra computed with FMM with those obtained for the equivalent homogeneous material using AMM, as presented in the inset of Figure 2a in the case of 1vol%. As expected the oscillations observed for the equivalent homogeneous thin film perfectly fit those in our opal photonic crystal, confirming their origin as the thin film interference. We also observe the disappearance of the minimum around 900 nm for the homogeneous thin film, confirming that its origin comes from the material ordering.

The corresponding solar visible and infrared transmittances in both cold and warm conditions as a function of VO_2 concentration are presented in fig. 3a and 3b. In order to use this coating for smart energy efficient material, we are looking for a high visible transmittance in both states of the material with no or little differences between both states (low ΔT_{vis}), and a large difference in infrared transmittance between both states (high ΔT_{IR}). Fig. 3c gives these transmission modulations as a function of the VO_2 concentration. The optimized VO_2 concentration is obtained for the highest difference between the infrared and visible transmission modulations, shown in fig. 3d. A high infrared transmission modulation ($\Delta T_{IR} = 0.42$) and low visible modulation ($\Delta T_{vis} = 0.26$) is obtained for a 1vol% VO_2 concentration.

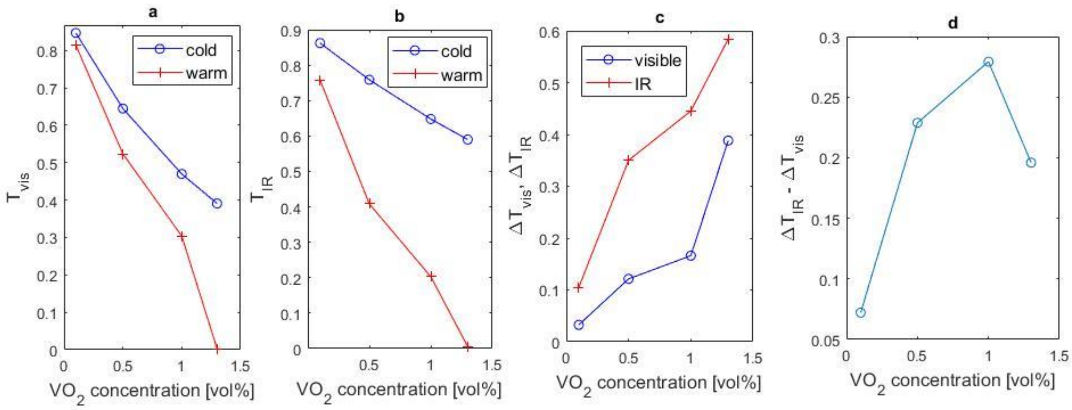

Figure 3: Impact of the VO2 concentration in solar transmittances for both cold and warm states of the material, in the visible (a) and infrared region (b), their modulations between both states of the material (c) and difference between infrared and visible transmission modulations (d)

4. Conclusions and prospects

Optical numerical simulations have been performed on a polymer opal photonic crystal loaded with VO_2 nanoparticles. As expected, the transmittance in both visible and IR regions decreases as the VO_2 concentration increases in both cold and warm conditions. The transmittance modulation increases as the VO_2 concentration increases. Thus an optimal value that maximizes the transmittance modulations is found at 1vol% VO_2 concentration, in the case of a light injection along the (111) crystallographic direction. In order to conclude on the coating global performance as a smart transparent energy efficient material, further studies considering all incidence angles would be required. Also, the influence of the coating thickness and possibility of a multilayer are still open questions.

Acknowledgements

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