**Asymmetrical resonant cavity thin film devices designed for vanadium dioxide applications**

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**Abstract**:Vanadium dioxide (VO2) is a volatile phase change material (PCM) that will rapidly change its structure when heated above the transition temperature and revert back when cooled below. This will also cause its optical property to change significantly compared to normal materials. Researchers can use this property to design various thin film devices. In this paper, VO2 thin film devices have been redesigned to introduce an asymmetrical resonant cavity structure. The structure is designed with the goal of enhancing the optical performance of the central VO2 layer and have an antireflection property in the cold state. The advantages, and limitations of such a design are discussed.

**Keywords:** optical thin film, thin film design, vanadium dioxide

1. Introduction

Phase change materials (PSMs) are materials that change their crystal structure when sufficient energy (e.g. thermal) is applied, and the material’s temperature is increased above the transition temperature. This significantly alters some of their physical, chemical and optical properties. In this paper, we will only focus on the real and imaginary refractive index. This change can be reverted by decreasing the temperature below the transition temperature for volatile PSM or increasing the temperature further to the melting point and then rapidly quenching for non-volatile PSM.

Vanadium dioxide (VO2) is a volatile PSM with phase transition type of Metal-insulator-transition (MIT), that is, it’s an insulator in at the ‘cold’ state and change to a metal at ‘hot’ state. The optical difference between cold and hot states are pronounced, particularly in the IR spectrum and above. It has one of the lowest transition temperatures at ~68 °C. And the MIT hysteresis for each loop has low variant, which cause it to be reusable multiple times. These properties cause it to become popular among researchers for designing thin film devices, for example, a thermochromic window coating that change its reflectivity in the infrared spectrum based on temperature [1,7]. An optical diode/limiter that while in the ‘on state’, allows light to travel freely but will ‘turn off’ and acts like an opaque filter to protect the sensitive light source when heated to sufficient temperatur [2,6,8,9]. A tunable filter for various applications [10]. Or a gas sensor based on VO2 nanowire thermistor [11]. As for this paper, we will only be focusing on the first two use cases. It should be noted that the difference in both refractive indices is more pronounced in the longer wavelength, hence it’s mainly used in the IR spectrum.

Resonant cavity design allows lights (photons) to cycle through the central cavity layer multiple times. This cause the optical property of VO2 to be enhanced many folds. The structure generally consists of a cavity layer sandwiched between two identical reflector layers. By changing the phase thickness of the central layer, the device can be tuned for various applications. It’s mainly used for line-pass or band-pass filters. But a problem will occur when we use PSMs as a central cavity layer. This is because, compared to dielectric layer(s) normally used, PSMs have a much higher imaginary refractive index which will result in the loss of resonant when substituting the central layer that’s made of dielectric with PSM, even if the real refractive index is comparable. Previously, the solution was to use a genetic algorithm [3] or use numerical optimization to get an approximation [4] both of which can’t give a solution when given a desired resonant wavelength and materials index. To solve this, Saragan, A. introduced a new design approach, by modifying resonant cavity DBR structure with asymmetrical reflector layers [5]. This allows us to get a solution for any given resonant wavelength or materials index.

In this paper, various Vanadium dioxide (VO2) devices are computationally recreated using refractive index data from the original references otherwise we pick the data from [12] with the closest conditions. And then we redesigned to introduced the asymmetrical resonant cavity structure. The redesigned results are compared to the original’s, mainly the transmission, reflection, absorption properties and the thickness of VO2 used. The purpose of which is to weigh the pros and cons of asymmetrical resonant cavity designs, so that we can discover the real world use cases.

2. Theory

Traditional resonant cavity DBR structures are composed of a dielectric central cavity layer placed between two reflector layers that will help lights cycle through the central layer multiple times. Because lights pass through the central cavity layer multiple times the devices optical properties will be enhanced significantly. For both the thermochromic window coating and the optical diode, we will only focus on the transmission and the absorption properties of the devices. High absorption will lower the time it take for VO2 to reaches the transition temperature, but this may cause the transmission to be too low for the intended purpose. Hence, we want the design to be antireflection, so that we can use the reflected light to transmitted or absorbed instead. To archive this, we need to design a high reflective reflector comprised of a unit cell(s) with quarter-wave thick films of high (H) and low (L) real refractive index [13]. In this paper, we pick TiO2 and SiO2 because of the difference in the real refractive indices in broad wavelength and both have no imaginary refractive index in most wavelength. Each unit cell has a notation of [H/2 L H/2], where H/2 denote a half quarter-wave thick film, and L denote quarter-wave thick film. The number of unit cells used on each side is symmetrical normally. Consider the symmetrical structure with central layer H of [U]2 H [U]2 where U denote a unit cell:

(1)

This can be rewritten as:

(2)

When two layers with the same refractive index is placed side by side. The total phase thickness is half-wave thick, which will result in an absentee layer. Following this, the two H layers in the middle can be rewrite as:

(3)

The same goes for the two L layers:

(4)

Most of the structure will became absentee, leaving only two H/2 layers from each reflector:

(5)

We can then make the structure exhibit an antireflection property by introducing two H/2 films on the outside of each reflector. These will combine with the two H/2 left from the reflector. The final structure will become absentee. For clarity’s sake, we will write these as {H/2}:

(6)

The redesigned structures have a notation of H/2 [U]N [D] [U]N H/2, N denote the number of unit cells, and D denote the dielectric material. If we choose to use another dielectric material, D, instead of H in the central cavity layer. The resonant will remain near the designed wavelength with similar antireflection property if D has similar refractive indices to H. Problems will occur if we replace the central materials with metals or PSMs because both have a significantly large imaginary index in most wavelength. This is problematic for PSMs devices that reach transition temperature using optical stimuli, e.g. laser or sunlight, since the absorption is directly correlated to imaginary index.

Problems with the difference in imaginary index can be compensated by using asymmetrical number of unit cells for each reflector [3]. As for the methods mentioned in the introduction, neither method can give the solutions for an exact phase thickness of each layer when given a targeted wavelength and the materials refractive index. This will be a problem for cases like an optical diode [2] mentioned above or a similar, self-activating optical limiter device [6,8,9] since both intend use cases are for a targeted wavelength. The new modified-structure will have a notation of H/2 [U]N [C] [U]M H/2, where C denote the central cavity complex layer (VO2), N denote the number of unit cells in the transmission (back) side, and M represent incident (front) side. The central cavity layer can be modified with additional D(s) or C(s) or metal(s), M(s), layers depending on the use cases.

3. Result and Discussion

Table 1. Comparison of the originals and the redesigned devices. The redesigned layouts shown are the central cavity layer. N and M represent the number of [H/2 L H/2] unit cells in the back and front side respectively.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Reference | Wavelength (nm) | Layout | Transmission | | | Absorption | | Reflection | | VO2 used (nm) |
| **on** | **off** | **ratio** | **on** | **off** | **on** | **off** |
| **[2]** | **1320** | **C Au(10nm)** | **0.22** | **0.03** | **7.7** | **0.14** | **0.18** | **0.64** | **0.80** | **100.0** |
|  |  | [C D C] N=5, M=4 | 0.41 | 0.08 | 5.3 | 0.59 | 0.39 | 0.00 | 0.53 | 2.8 |
|  |  | [C D C] N=4, M=3 | 0.41 | 0.08 | 5.1 | 0.59 | 0.39 | 0.00 | 0.53 | 7.0 |
|  |  | [C D C] N=3, M=2 | 0.41 | 0.09 | 4.5 | 0.59 | 0.40 | 0.00 | 0.51 | 18.6 |
|  |  | [C D] N=4, M=3 | 0.38 | 0.06 | 6.0 | 0.62 | 0.38 | 0.00 | 0.55 | 8.5 |
|  |  | [D C] N=4, M=2 | 0.22 | 0.02 | 9.2 | 0.78 | 0.02 | 0.00 | 0.63 | 36.5 |
| **[6, 8]** | **1550** | **Au(6nm) C** | **0.49** | **0.13** | **3.7** | **0.17** | **0.21** | **0.34** | **0.66** | **52.0** |
|  |  | [C D C] N=5, M=4 | 0.41 | 0.04 | 10.4 | 0.59 | 0.29 | 0.00 | 0.67 | 5.2 |
|  |  | [C D C] N=4, M=3 | 0.41 | 0.04 | 9.5 | 0.59 | 0.29 | 0.00 | 0.66 | 13.2 |
|  |  | [D C] N=5, M=4 | 0.42 | 0.04 | 10.7 | 0.58 | 0.30 | 0.00 | 0.66 | 5.3 |
|  |  | [D C] N=4, M=3 | 0.44 | 0.04 | 10.3 | 0.56 | 0.30 | 0.00 | 0.66 | 13.6 |

For the optical limiting devices. The best redesigns of ref [2] and [6] are shown in Table 1. Because of the antireflection design, each redesign has a better or comparable transmission and absorption value in the ‘on’ state. The increased transmission value will make the device more efficient, and the increase in absorption value will decrease switching time. And because of the two reflector layers, the redesign use significantly less VO2. To note, the ratio between the transmission and absorption, which will affect the amount of time and thermal energy it took for the devices to undergo phase change, wasn’t considered.

As for the thermochromic windows coating (not shown here). The largest challenge for real-world adoption is in the high phase change temperature, not the device design [2, 9]. And because of the large surface area and the commercial intent, it’s in the author’s opinion that the complexity of the redesign device outweighs any benefit it gave. There have been a review of the effect of elemental doping on the optical properties of VO2 [7], which is better suited to solve this challenge.

The main advantage of this design method is less VO2 used, while having equal or better transmission. The limitation is the narrow operating bandwidth, which limited the use case to narrow wavelength e.g. laser. The disadvantages are the complexity of fabricating multiple reflector layers, which will also cause the overall device to be thicker than the originals, and the sensitivity to the PSMs phase thickness. For a large N and M values, a few nanometers difference from the design could cause the resonant wavelength to be shifted significantly.

4. Conclusion

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