

## Optical properties of a thin layer of the Vanadium dioxide at the metal state

Abderrahim Ben Chaib<sup>1</sup>, Abdesselam Mdaa<sup>2</sup>  
Izeddine Zorkani<sup>1</sup>, Anouar Jorio<sup>1</sup>.

<sup>1</sup> Physics laboratory of solid FSDM Fès, university Sidi Mohamed Ben Abdellah, Morocco.

<sup>2</sup> Laboratory of the thin layers and surface treatment by plasma ENS-Fès, Morocco.

Abderrahim Ben Chaib - [abderrahim-196@hotmail.com](mailto:abderrahim-196@hotmail.com)

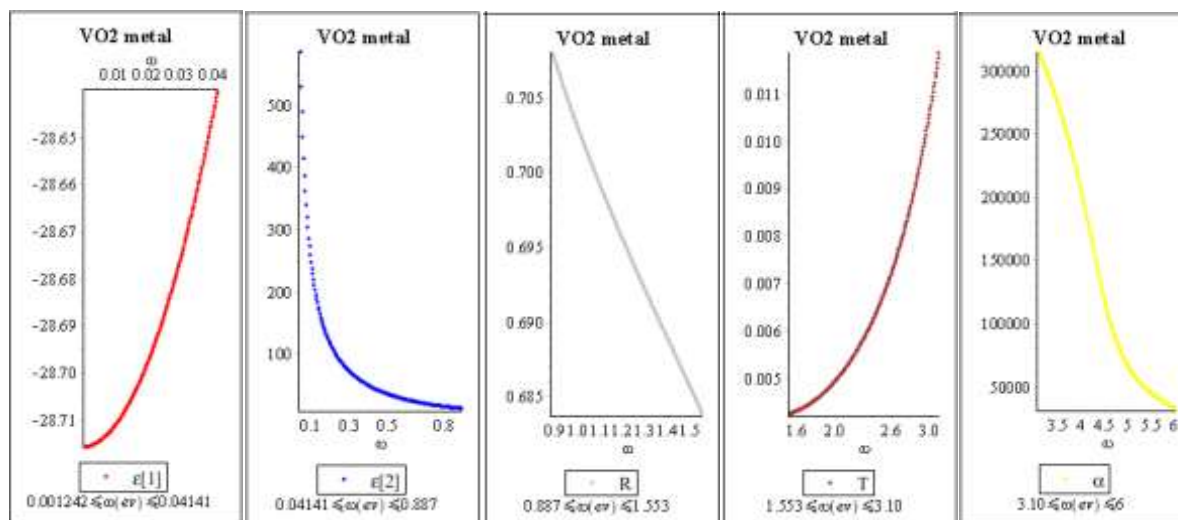
Abdesselam Mdaa- [abdou261175@gmail.fr](mailto:abdou261175@gmail.fr)

Izeddine Zorkani - [izorkani@hotmail.com](mailto:izorkani@hotmail.com)

Anouar Jorio - [a\\_jorio@hotmail.com](mailto:a_jorio@hotmail.com)

### ABSTRACT

The vanadium dioxide VO<sub>2</sub> currently became very motivating for the nanotechnologies' researchers. It makes party of the intelligent materials because these optical properties abruptly change semiconductor state with metal at a critical temperature  $\theta = 68^\circ\text{C}$ . This transition from reversible phase is carried out from a monoclinical structure characterizing its semiconductor state at low temperature towards the metal state of this material which becomes tétragonal rutile for  $\theta > 68^\circ\text{C}$ ; it is done during a few nanoseconds. Several studies were made on this material in a massive state and a thin layer. We will simulate by Maple the constant optics of a thin layer of VO<sub>2</sub> thickness  $z = 82\text{ nm}$  for the metal state according to the energy  $\omega$  of the incidental photons in the energy interval:  $0.001242 \leq \omega (\text{ev}) \leq 6$ , from the infra-red (I.R) to the ultra-violet (U.V) so as to be able to control the various technological nano applications, like the detectors I.R or the U.V, the intelligent windows to increase the energy efficiency in the buildings in order to save the cost of energy consumption by electric air-conditioning and the paintings containing nano crystals of this material. The constant optics, which we will simulate, is: the index of refraction, the reflectivity, the transmittivity, the coefficient of extinction, the dielectric functions  $\epsilon_1$  real part and  $\epsilon_2$  imaginary part of the permittivity complexes  $\epsilon$  of this material and the coefficient absorption.



Curves simulated of the different optical constants of a thin layer of VO<sub>2</sub> according to the model of the harmonic oscillator deadened in the photonic spectrum in the infra-red, the visible, and in the ultra-violet.

### Indexing terms/Keywords

Vanadium dioxide, thin layer, index of refraction, transmittivity, reflectivity, coefficient absorption, dielectric function, coefficient of extinction, ellipsometric spectroscopy, intelligent material.

## Council for Innovative Research

Peer Review Research Publishing System

Journal: JOURNAL OF ADVANCES IN PHYSICS

Vol.9, No.1

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## Academic Discipline And Sub-Disciplines

Science; Physics

## SUBJECT CLASSIFICATION

Materials Physics; Thin Film Physics

## TYPE (METHOD/APPROACH)

Model of Drude, based simulation and modeling

## INTRODUCTION

The vanadium dioxide is a relevant thermochrome material because of these enormous technological nano applications in photonic, with an energy gap of 0.7 eV [1,2], detecting ultra-violet [3,4], optical memory whose principle is based on the hysteresis loop at the time of this transition from the reversible phase [5,13,14,15,16] and the intelligent panes [6,18]. A dramatic change of these thin layers' optical properties is clearly observed. Several theoretical studies were made to explain the answer of the dielectric function for these two phases: metal and semiconductor. Abbate and Mossaneq [7] extracted the dielectric response from VO<sub>2</sub>. Verlor et al. [8] studied the dielectric function of massive VO<sub>2</sub> by using the method of the reflectivity and transmittivity. Currently, Kakiuchida et al. [9] used the ellipsometric spectroscopy (SE) for the determination of the constant optics of the vanadium dioxide's thin layers.

## Methods

We use the Drude model [11] for the dielectric function :

$$\varepsilon(\omega) = \varepsilon_{\infty} + \frac{\omega_p^2}{-\omega^2 + i\Gamma_d \cdot \omega} \quad (1)$$

$$\varepsilon(\omega) = \varepsilon_{\infty} - \frac{\omega_p^2}{\omega \cdot (\omega - i\Gamma_d)} \quad (2)$$

$$\varepsilon(\omega) = \varepsilon_1(\omega) - i\varepsilon_2(\omega) \quad (3)$$

$$\varepsilon_1(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + \Gamma_d^2} \quad (4)$$

$$\varepsilon_1(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + \Gamma_d^2} \quad (4)$$

$$\varepsilon_2(\omega) = \frac{\omega_p^2 \cdot \Gamma_d}{\omega \cdot (\omega^2 + \Gamma_d^2)} \quad (5)$$

$\varepsilon_{\infty} \rightarrow 1$ , for the state metal

$\varepsilon_{\infty}$  : the high frequency permittivity of the electronic transition.

$\Gamma_d$  : the frequency of collision.

$\omega_p$  : the frequency plasma.

$\omega$  : the frequency of the incidental photon in (eV).

$\varepsilon$  : the permittivity complexes material

$\varepsilon_1$  : the real part of the complex permittivity.

$\varepsilon_2$  : the imaginary part of the complex permittivity.

By using this model, we can make a simulation of the VO<sub>2</sub> constant optics according to the energy  $\omega$  (eV) of the incidental photon, while being based on the film parameters of VO<sub>2</sub> according to the table [10,12], and by taking an oscillator for the temperature  $\theta = 85^\circ\text{C}$ .



**Table. Drude-Lorenz parameter values of VO<sub>2</sub> thin films determined from the simulation of ellipsometric spectra.**

	T=30°C							T=85°C			
$f_j$	0,67	-0,46	1,11	2,38	1,6	3,4	0,54	<b>0,87</b>	1,76	2,35	-8
$\omega_{0j}$	1,02	1,92	1,39	3,45	4,28	7,57	2,98	<b>2,87</b>	3,46	5,26	0,57
$\gamma_j$	0,54	3,02	0,88	1,34	2,24	2,02	0,65	<b>0,77</b>	1,34	2,81	3,7
$\omega_p$								<b>4,47</b>			
$\Gamma_j$								<b>0,82</b>			

- $\omega_{0j}$  : Frequency of resonance for the oscillator of energy corresponding to the peak of absorption in electronvolt.
- $f_j$  : The oscillator strength j of Lorentz.
- $\gamma_j$  : The widening of each oscillator j knowing damping.

**Let us note:**

- T: transmittivity of a thin layer of VO<sub>2</sub>.
- R : reflectivity of a thin layer of VO<sub>2</sub> for the normal incidence.
- $\alpha$  : the absorption coefficient of a thin layer of VO<sub>2</sub>.
- n: the index of refraction of material.
- k: the coefficient of extinction of material.

$$\epsilon_1(\omega) = 1 - \frac{19,9809}{\omega^2 + 0.82^2} \tag{6}$$

$$\epsilon_2(\omega) = \frac{16,384338}{\omega \cdot (\omega^2 + 0.82^2)} \tag{7}$$

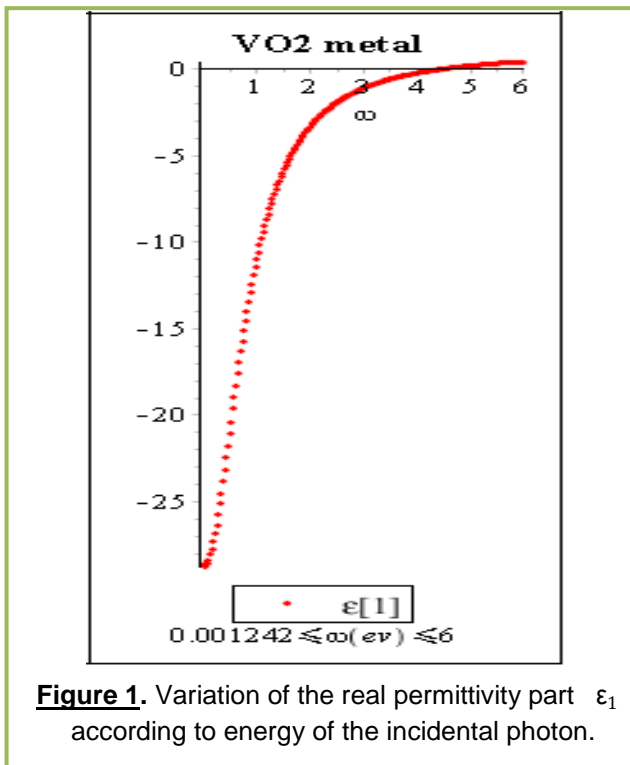
$$n = \frac{1}{\sqrt{2}} \left( \epsilon_1 + (\epsilon_1^2 + \epsilon_2^2)^{\frac{1}{2}} \right)^{\frac{1}{2}} ; \quad k = \frac{1}{\sqrt{2}} \left( -\epsilon_1 + (\epsilon_1^2 + \epsilon_2^2)^{\frac{1}{2}} \right)^{\frac{1}{2}} \tag{8}$$

$$R = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2} ; \quad \alpha = \frac{4\pi \cdot k \cdot \omega \cdot 10^5}{12.424125} ; \quad T = \frac{(1-R)^2 \cdot e^{-\alpha z}}{1-R^2 \cdot e^{-2\alpha z}} ; \quad z = 82 \cdot 10^{-7} \text{ cm} \tag{9}$$

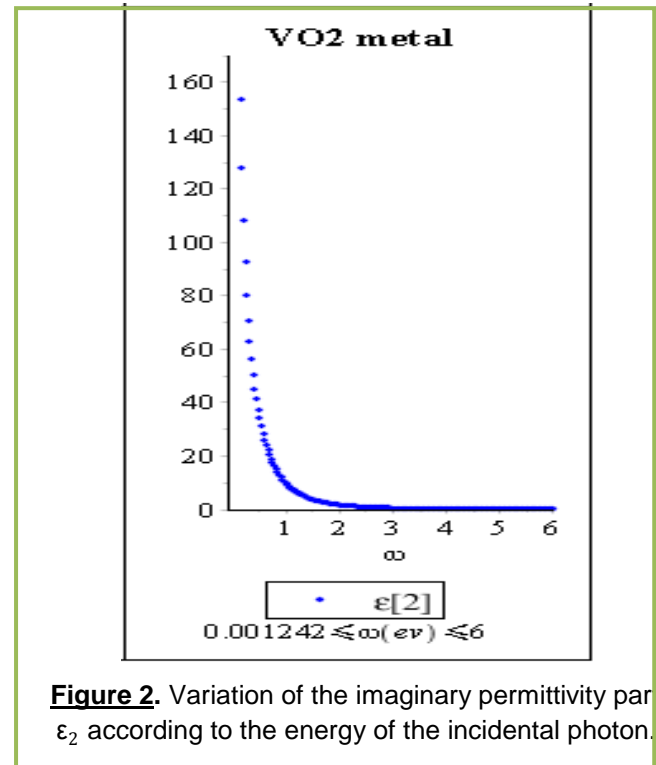
We will simulate by Maple this constant optics in the incidental photon's energy intervals to be able to exploit the optical response of this material in each field of the energy spectrum :

- The remote I.R :  $0.001242 \leq \omega(\text{ev}) \leq 0.04141$
- Average I.R :  $0.04141 \leq \omega(\text{ev}) \leq 0.887$
- The close I.R :  $0.887 \leq \omega(\text{ev}) \leq 1.553$
- The visible spectrum :  $1.553 \leq \omega(\text{ev}) \leq 3.10$
- The ultra-violet :  $3.10 \leq \omega(\text{ev}) \leq 6$

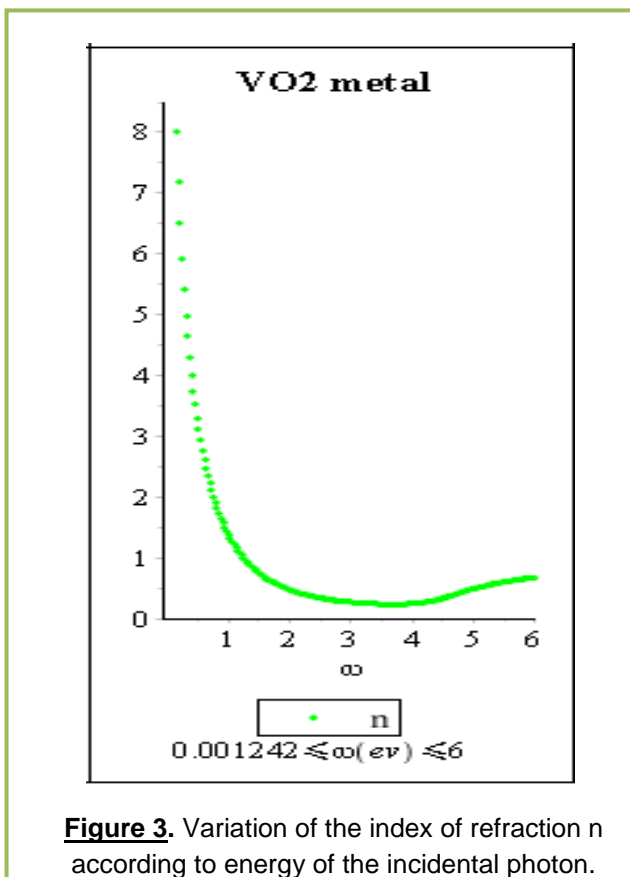
**Results**



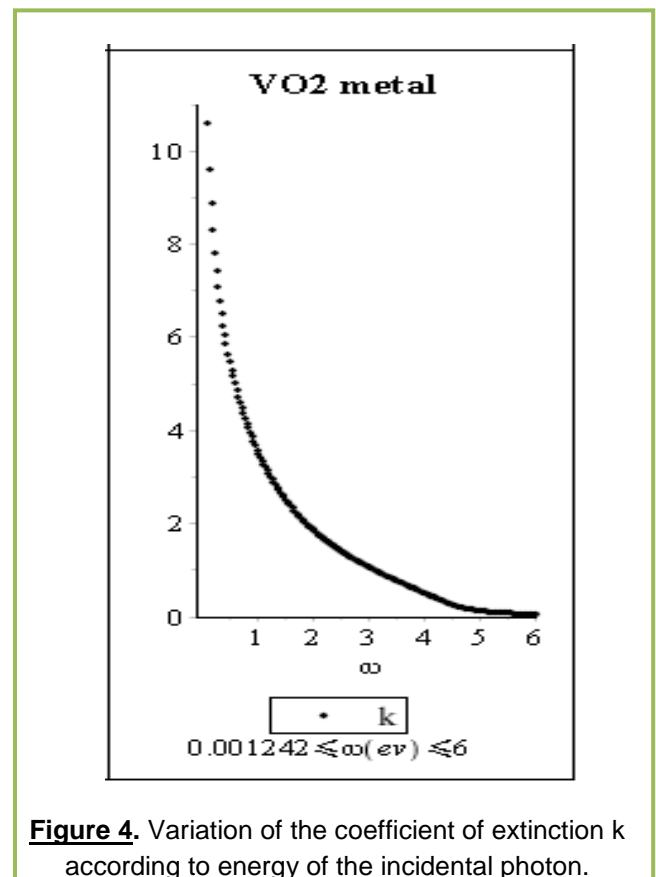
**Figure 1.** Variation of the real permittivity part  $\epsilon_1$  according to energy of the incidental photon.



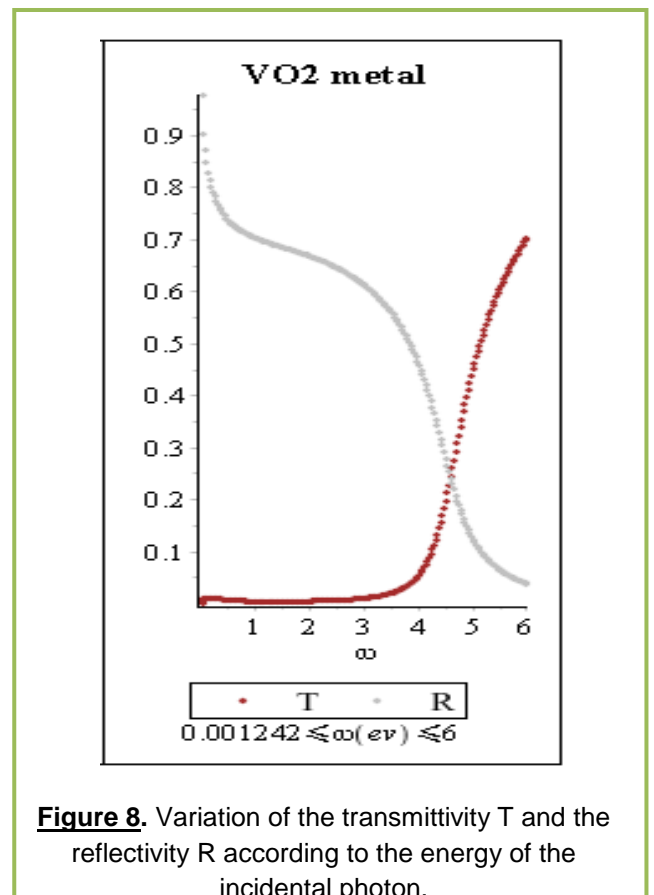
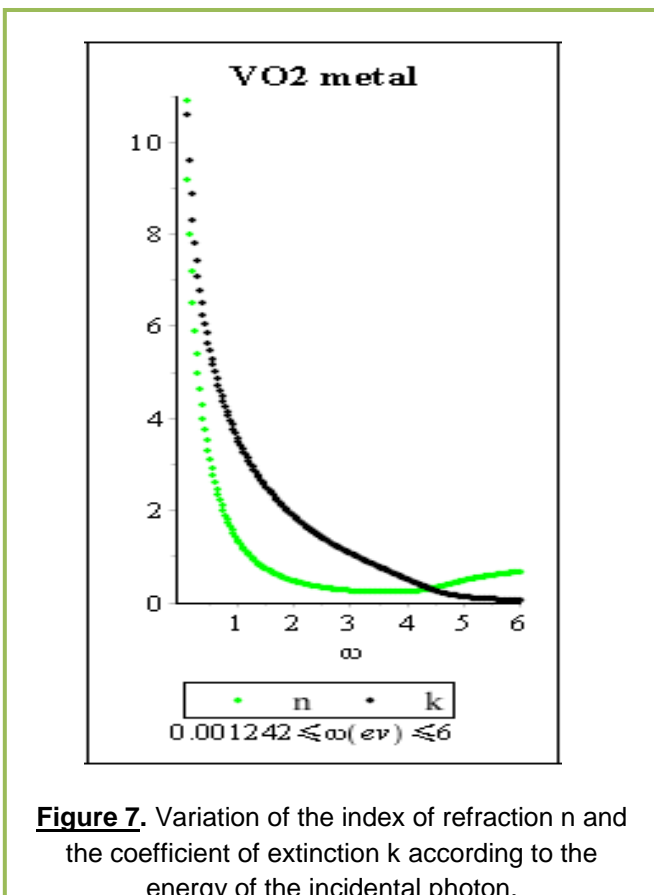
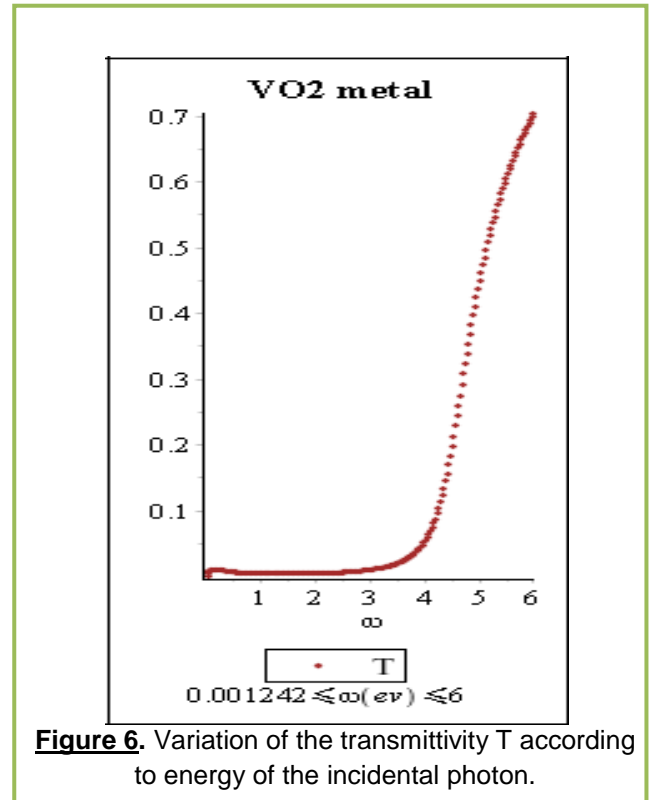
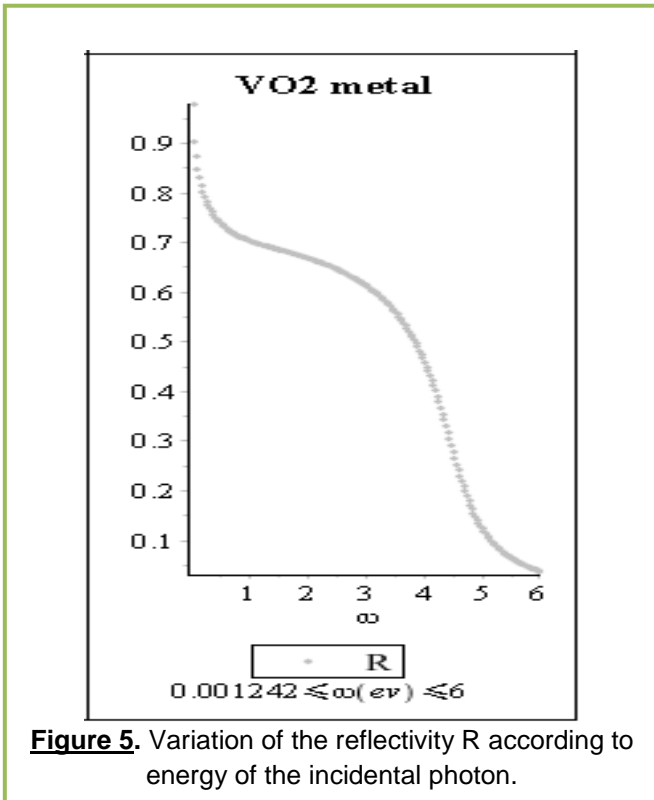
**Figure 2.** Variation of the imaginary permittivity part  $\epsilon_2$  according to the energy of the incidental photon.

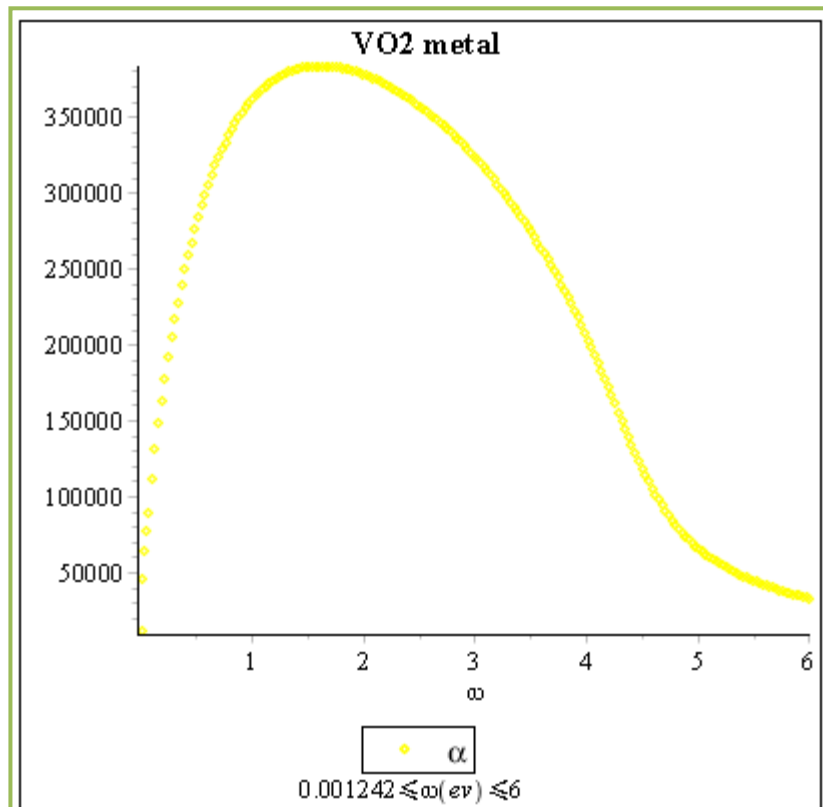


**Figure 3.** Variation of the index of refraction  $n$  according to energy of the incidental photon.

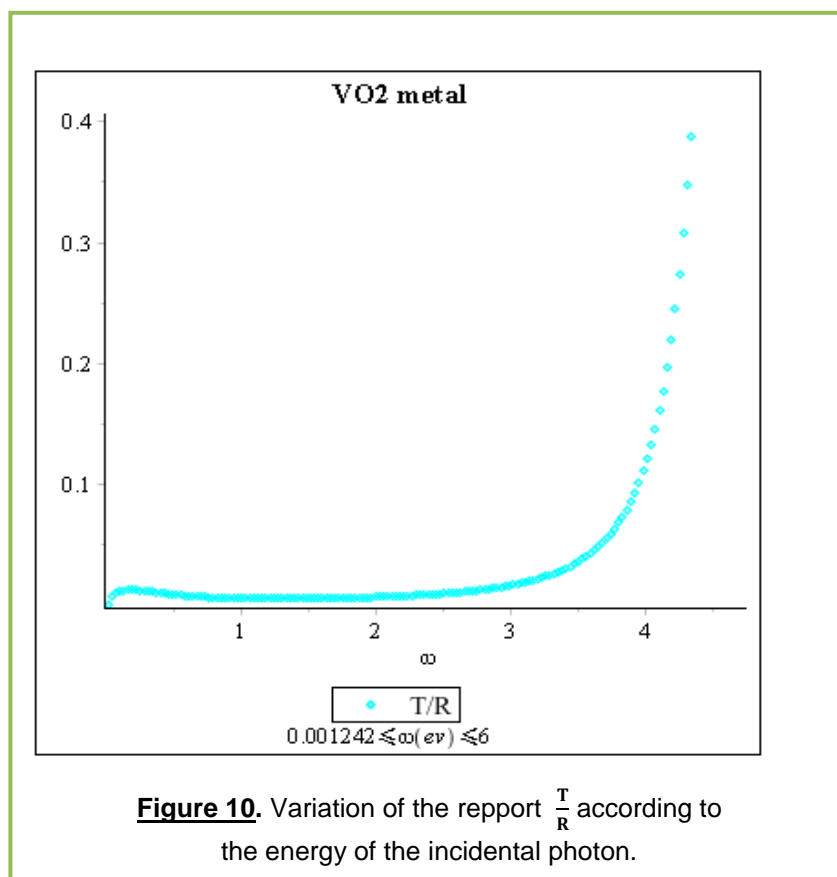


**Figure 4.** Variation of the coefficient of extinction  $k$  according to energy of the incidental photon.





**Figure 9.** Variation of the absorption's coefficient  $\alpha$  according to the energy of the incidental photon.



**Figure 10.** Variation of the repport  $\frac{T}{R}$  according to the energy of the incidental photon.



## Discussion :

For the permittivity real part  $\epsilon_1$ , we see that it is negative in the energy interval  $0 < \omega < \omega_p$ , grows if the energy  $\omega$  photon, increases in this interval and is cancelled for  $\omega = \omega_p$ ; the material is, thus, reflective of the infra-red until the visible spectrum.

For  $\omega > \omega_p$ , we notice that  $\epsilon_1$  becomes positive; the material in this case is transmissive, in the ultra-violet where  $\epsilon_1$  grows slowly. If  $0.001242 < \omega(\text{ev}) < 6$ , we then note that the imaginary permittivity part  $\epsilon_2$  is positive and decreases when  $\omega$  increases.

Concerning the index of refraction  $n$ , we also see a decrease in the infra-red if  $\omega$  increases in the interval  $0.001242 < \omega(\text{ev}) < 1.533$ , in the visible spectrum for  $1.553 < \omega(\text{ev}) < 3.10$ ; it reaches a minimum of 0.231 for  $\omega = 3.668 \text{ ev}$ , then it increases up to 0.676 for  $\omega = 6 \text{ ev}$ ; it takes a value of 0.326 for  $\omega = \omega_p = 4.47 \text{ ev}$ .

If  $\omega > \omega_p$ , the index of refraction of this thin layer increases.

The coefficient of extinction  $k$  decreases in the interval  $0.001242 < \omega(\text{ev}) < 6$  when the energy  $\omega$  of the incidental photon increases. If  $\omega = \omega_p = 4.47 \text{ ev}$ , we have  $k \cong 0.272$ , and for  $\omega = 6 \text{ ev}$ ,  $k \cong 0.056$  characterizes a slightly absorbent state of this thin layer which becomes transmissive for  $\omega > \omega_p$ .

This material becomes absorbent for  $0 < \omega(\text{ev}) < 0.002854$  and reflective in the interval  $0.002854 < \omega(\text{ev}) < 4.47$ . This result is confirmed in literature by the Drude model for metal during the variation of the index of refraction  $n$  and the coefficient of extinction  $k$ .

For the metal state of this  $\text{VO}_2$  thin layer, the reflectivity  $R$  decreases in the infra-red and the visible spectrum for our simulation, of the value:

0.98 if  $\omega = 0.001242 \text{ ev}$ ; 0.892 if  $\omega = 0.04141 \text{ ev}$ ; 0.708 if  $\omega = 0.887 \text{ ev}$ ; 0.683 if  $\omega = 1.553 \text{ ev}$ ; and 0.604 if  $\omega = 3.10 \text{ ev}$ .

In the ultra-violet, the reflectivity  $R$  decreases towards the value 0.288 if  $\omega = \omega_p = 4.47 \text{ ev}$ ; it continues to decrease towards 0.038 for  $\omega = 6 \text{ ev}$ .

In the interval  $0.001242 < \omega(\text{ev}) < 0.04141$ , the transmittivity  $T$  slowly increases if  $\omega$  grows; it is very weak in the infra-red. In fact,  $T = 0.008$  if  $\omega = 0.04141 \text{ ev}$ ;  $T_{\text{max}} = 0.01$  if  $\omega = 0.143 \text{ ev}$ , then it decreases up to the value 0.0048 for  $\omega = 0.887 \text{ ev}$ . In the interval  $0.887 < \omega(\text{ev}) < 1.553$ , we note a decrease of the transmittivity  $T$ , reaching a minimum  $T_{\text{min}} = 0.042$ , if  $\omega = 1.3588 \text{ ev}$ , then it grows slowly in the visible spectrum up to the value 0.0118 for  $\omega = 3.1 \text{ ev}$ . But it becomes important in the ultra-violet. It grows from the value 0.018 for  $\omega = \omega_p = 4.47 \text{ ev}$ , up to 0.704 if  $\omega = 6 \text{ ev}$ .

We notice that for  $\omega = 4.553 \text{ ev}$ ,  $T = R = 0.2287$  in the ultra-violet where the coefficient of absorbance  $\text{coeff}A \cong 0.518$  is maximal. The report,  $\frac{T}{R} \cong 0.12$  for  $\omega = 4 \text{ ev}$ , grows towards the value 0.39 if  $\omega \cong 4.34 \text{ ev}$ .

In the infra-red, the absorption coefficient  $\alpha$  increases up to the maximum value  $383751.88 \text{ cm}^{-1}$  for  $\omega = 1.553 \text{ ev}$ , starting from the value  $12451.10 \text{ cm}^{-1}$  if  $\omega = 0.001242 \text{ ev}$ ; it decreases in the visible spectrum up to the value  $314909.61 \text{ cm}^{-1}$  for  $\omega = 3.10 \text{ ev}$ , and it continues its decrease in the ultra-violet.

When  $\omega = \omega_p = 4.47 \text{ ev}$ , the absorption coefficient takes the value  $\alpha \cong 122929.74 \text{ cm}^{-1}$ ; whereas,  $\alpha \cong 33380.05 \text{ cm}^{-1}$  if  $\omega = 6 \text{ ev}$ .

Finally, there is a weak absorption in the ultra-violet for the  $\text{VO}_2$  metal state. These results are in conformity with those of the literature, because these optical properties are managed by the free electrons which are less absorbents, and the reflection is dominant if compared to the transmittivity.

Thus, the metal state of this thin layer of  $\text{VO}_2$  is characterized by the free electron model's features which are  $\epsilon(\omega_p) = 0$ ,

the frequency plasma [17]  $\omega_p = \sqrt{\frac{4\pi n e^2}{m}}$  in the unit C.G.S and  $\epsilon(\infty) \rightarrow 1$ .

Where:  $n$  is the density of the electrons,

$e$  is the elementary charge,

$m$  is the mass of an electron,

If  $\epsilon(\omega) < 0$ , then the electromagnetic waves is completely reflected by the material; it is the damping field.

In the case where  $\omega > \omega_p$ , the waves propagates and the material transmits. These two results are checked by our Maple simulation. In our study, we did not take into account the influence of the optical phonons.



## Conclusion

By using the Drude model, we extract the evolution from the constant optics of the thin layer of the vanadium dioxide VO<sub>2</sub> thickness 82 nm at a temperature of 85 °C; that is to say, with the metal state according to the energy  $\omega$  of the incidental photons in the interval  $0.001242 < \omega \text{ (eV)} < 6$ .

In the interval  $0.001242 < \omega \text{ (eV)} < 4.47$ , we note that the reflectivity  $R$  is high if compared to the transmittivity  $T$  of this thin layer; whereas for  $\omega > \omega_p$  the transmittivity  $T$  becomes important in growth and the reflectivity  $R$  strongly decreases because of the influence of the optical phonons in the field of energy of the incidental photons.

Therefore, this thin layer of VO<sub>2</sub> becomes an important nanotechnologic means of effective detection of the ultraviolet radiation. In the infra-red, we notice that the reflectivity  $R$  is important :  $0.7 < R < 0.97$ ; this is of a great practical interest for the operation of the intelligent panes or the solar air-conditioners. From  $\omega > \omega_p$  the transmittivity  $T$  grows because the incidental light wave propagates in the material; but for  $\omega < \omega_p$ , we have a damping of these electromagnetic waves; the reflectivity  $R$  dominates and becomes important. These optical properties of the thin layers of VO<sub>2</sub> are due to the free electrons in the metal state and to the energy of the incidental photons if compared with the plasma frequency  $\omega_p$  which characterizes the material.

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