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

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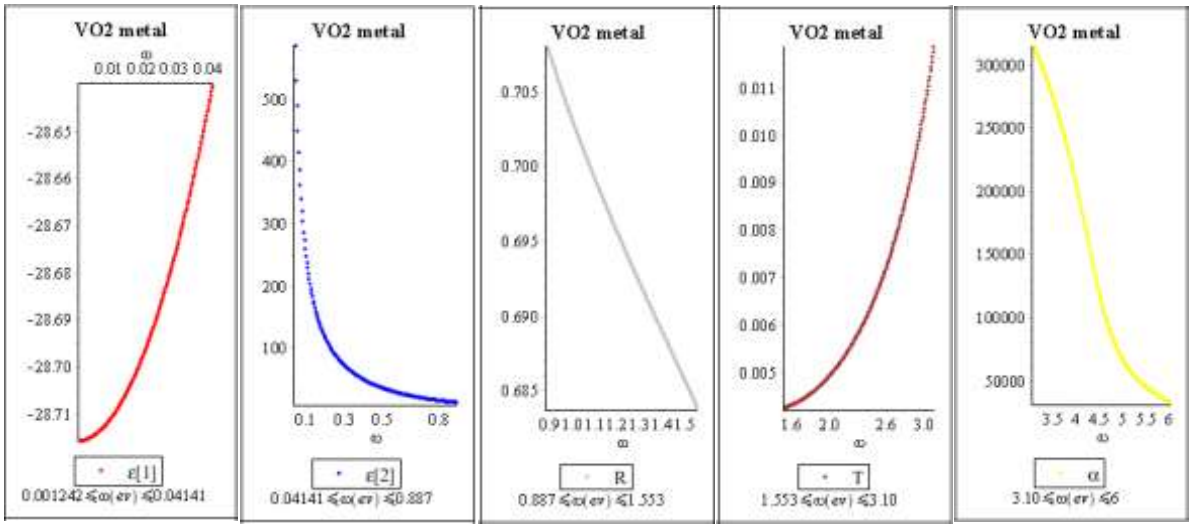
ABSTRACT

The vanadium dioxide VO_2 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 $\theta = 68\,℃$. 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 $\theta > 68°C$; 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_2 thickness $z = 82\,\mathrm{nm}$ for the metal state according to the energy ω of the incidental photons in the energy interval: $0.001242 \leq \omega\,(\mathrm{ev}) \leq 6$, 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 ε_1 real part and ε_2 imaginary part of the permittivity complexes ε of this material and the coefficient absorption.



Curves simulated of the different optical constants of a thin layer of VO_2 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.

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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 Mossanek **[7]** extracted the dielectric response from VO_2. Verlor et al. **[8]** studied the dielectric function of massive VO_2 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 :

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

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

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

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

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

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

$\varepsilon_\infty \to 1$, for the state metal

ε_∞ : the high frequency permittivity of the electronic transition.
Γ_d : the frequency of collision.

ω_p : the frequency plasma.

ω : the frequency of the incidental photon in (ev).

ε : the permittivity complexes material

ε_1 : the real part of the complex permittivity.

ε_2 : the imaginary part of the complex permittivity.

By using this model, we can make a simulation of the VO_2 constant optics according to the energy ω (ev) of the incidental photon, while being based on the film parameters of VO_2 according to the table [10,12], and by taking an oscillator for the temperature $\theta = 85°C$.

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Table. Drude-Lorenz parameter values of VO_2 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	**0,87**	1,76	2,35	-8
ω_{0j}	1,02	1,92	1,39	3,45	4,28	7,57	2,98	**2,87**	3,46	5,26	0,57
γ_j	0,54	3,02	0,88	1,34	2,24	2,02	0,65	**0,77**	1,34	2,81	3,7
ω_p								**4,47**			
Γ_j								**0,82**			

ω_{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.
γ_j : The widening of each oscillator j knowing damping.

Let us note:

T: transmittivity of a thin layer of VO_2.
R : reflectivity of a thin layer of VO_2 for the normal incidence.
α : the absorption coefficient of a thin layer of VO_2.
n: the index of refraction of material.
k: the coefficient of extinction of material.

$$\varepsilon_1(\omega) = 1 - \frac{19{,}9809}{\omega^2 + 0.82^2} \quad (6)$$

$$\varepsilon_2(\omega) = \frac{16{,}384338}{\omega \cdot (\omega^2 + 0.82^2)} \quad (7)$$

$$n = \frac{1}{\sqrt{2}}\left(\varepsilon_1 + (\varepsilon_1{}^2 + \varepsilon_2{}^2)^{\frac{1}{2}}\right)^{\frac{1}{2}} \quad ; \quad k = \frac{1}{\sqrt{2}}\left(-\varepsilon_1 + (\varepsilon_1{}^2 + \varepsilon_2{}^2)^{\frac{1}{2}}\right)^{\frac{1}{2}} \quad (8)$$

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

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 ≤ ω(ev) ≤ 0.04141
Average I.R : 0.04141 ≤ ω(ev) ≤ 0.887
The close I.R : 0.887 ≤ ω(ev) ≤ 1.553
The visible spectrum : 1.553 ≤ ω(ev) ≤ 3.10
The ultra-violet : 3.10 ≤ ω(ev) ≤ 6

Results

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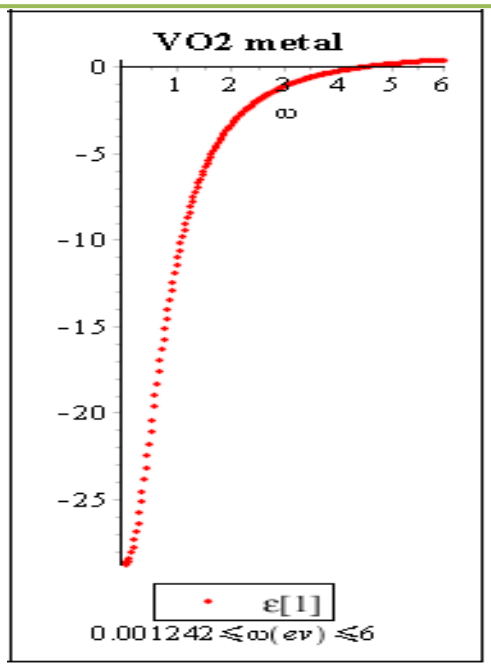

Figure 1. Variation of the real permittivity part ε_1 according to energy of the incidental photon.

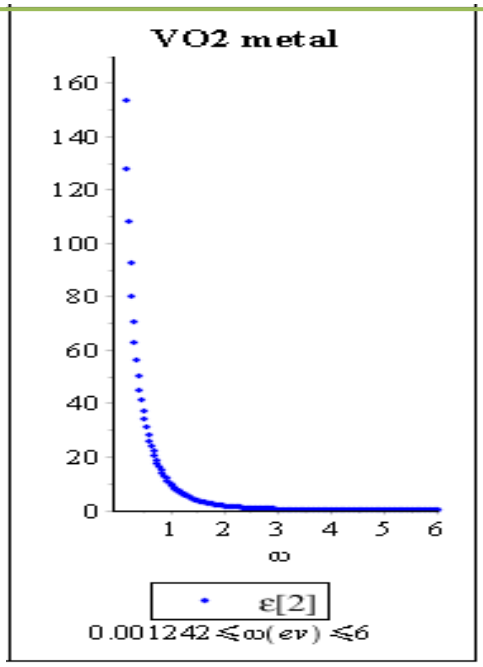

Figure 2. Variation of the imaginary permittivity part ε_2 according to the energy of the incidental photon.

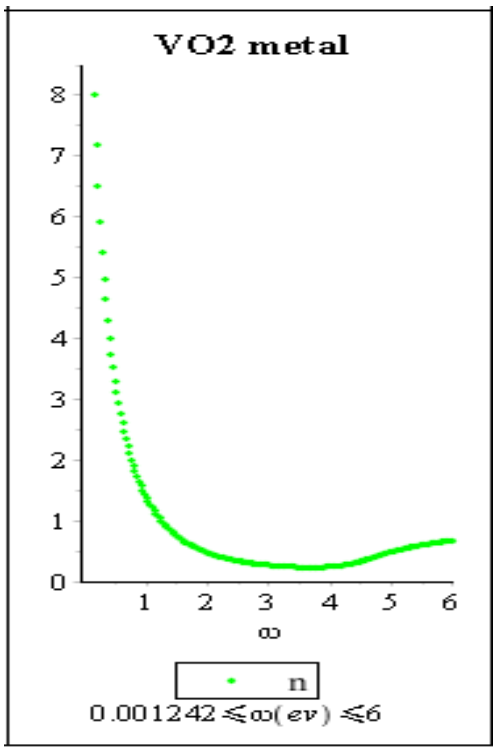

Figure 3. Variation of the index of refraction n according to energy of the incidental photon.

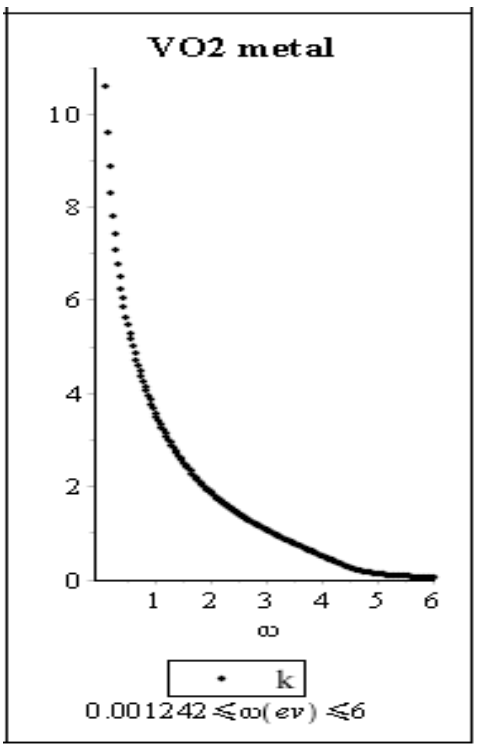

Figure 4. Variation of the coefficient of extinction k according to energy of the incidental photon.

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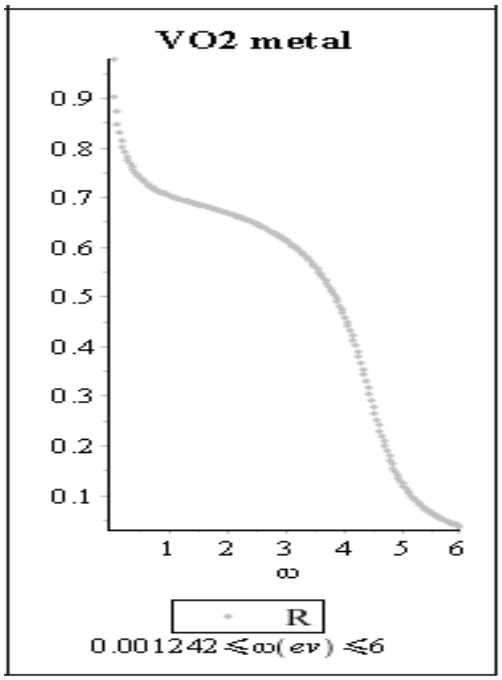

Figure 5. Variation of the reflectivity R according to energy of the incidental photon.

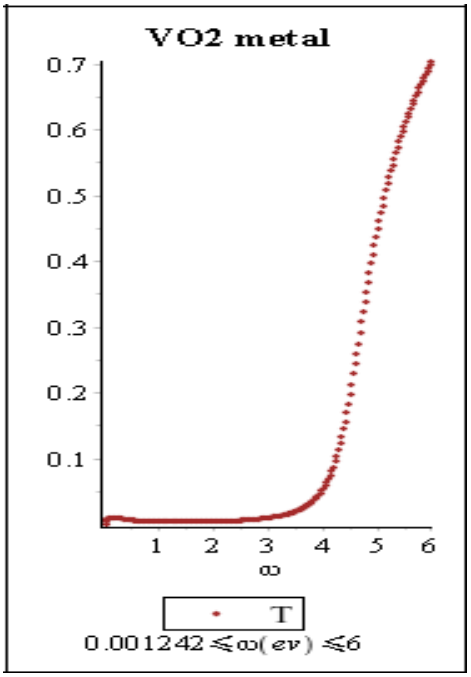

Figure 6. Variation of the transmittivity T according to energy of the incidental photon.

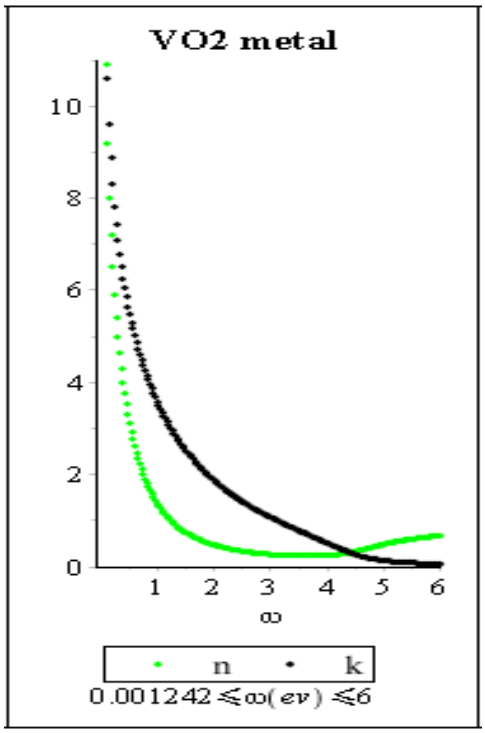

Figure 7. Variation of the index of refraction n and the coefficient of extinction k according to the energy of the incidental photon.

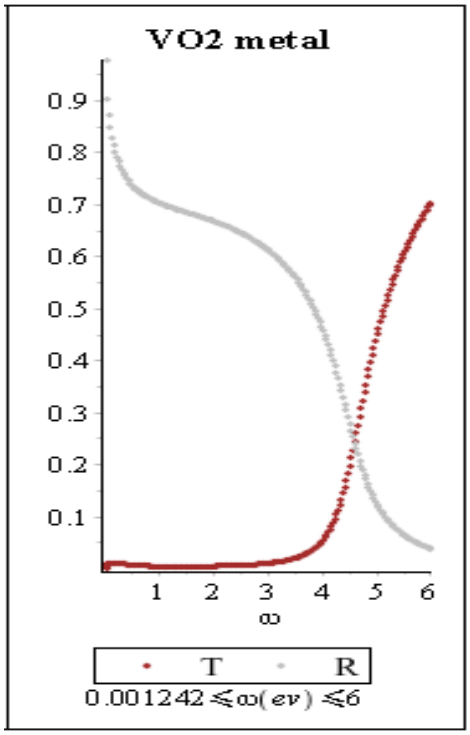

Figure 8. Variation of the transmittivity T and the reflectivity R according to the energy of the incidental photon.

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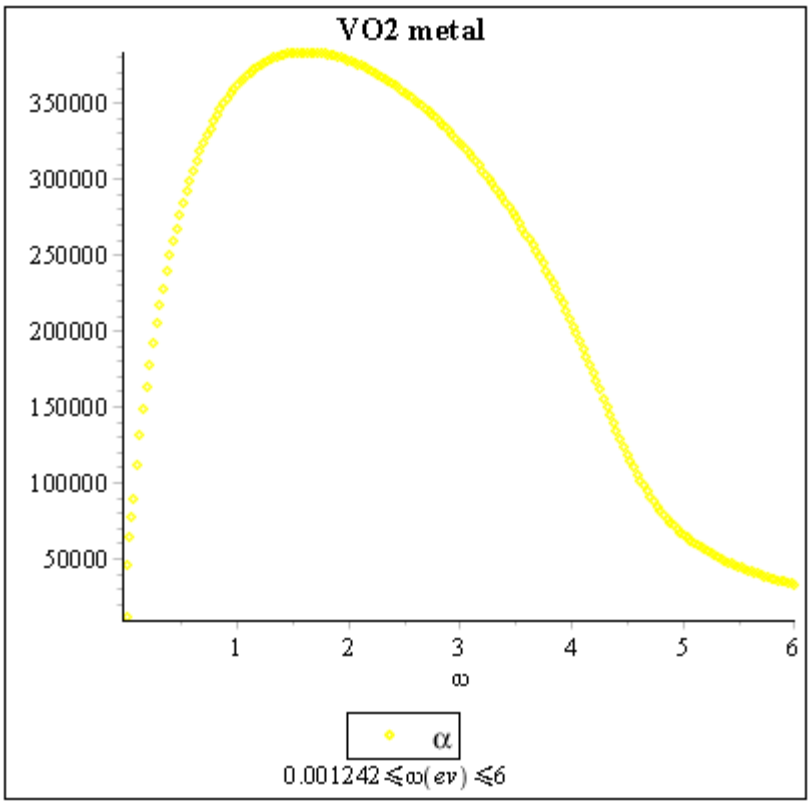

Figure 9. Variation of the absorption's coefficient α according to the energy of the incidental photon.

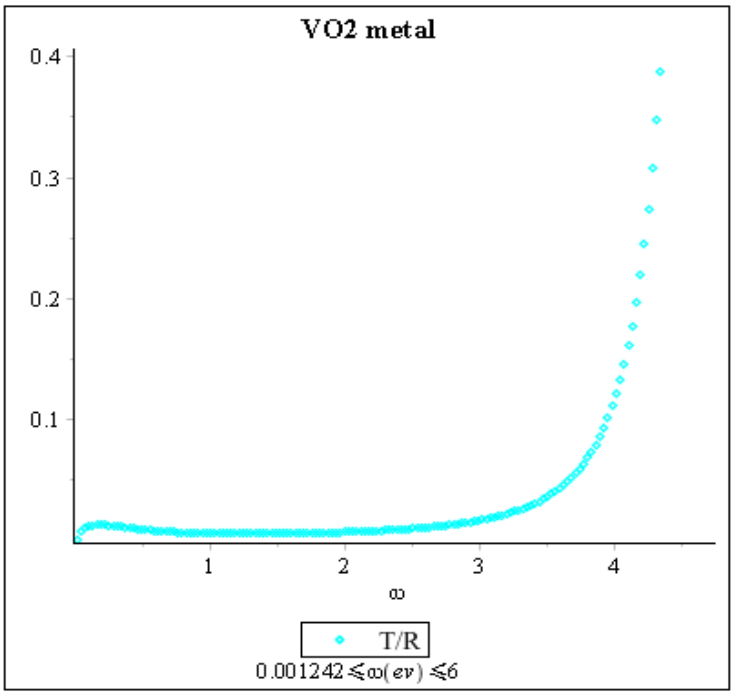

Figure 10. Variation of the repport $\frac{T}{R}$ according to the energy of the incidental photon.

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Discussion :

For the permittivity real part ε_1, we see that it is negative in the energy interval $0 < \omega < \omega_p$, grows if the energy ω 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 ε_1 becomes positive; the material in this case is transmitive, in the ultra-violet where ε_1 grows slowly. If $0.001242 < \omega(ev) < 6$, we then note that the imaginary permittivity part ε_2 is positive and decreases when ω increases.

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

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

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

This material becomes absorbent for $0 < \omega\,(ev) < 0.002854$ and reflective in the interval $0.002854 < \omega\,(ev) < 4.47$. 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 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 $\omega = 0.001242$ ev ; 0.892 if $\omega = 0.04141$ ev ; 0.708 if $\omega = 0.887$ ev ; 0.683 if $\omega = 1.553$ ev ; and 0.604 if $\omega = 3.10$ ev.

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

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

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

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

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

Finally, there is a weak absorption in the ultra-violet for the 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 VO_2 is characterized by the free electron model's features which are $\varepsilon(\omega_p) = 0$, the frequency plasma **[17]** $\omega_p = \sqrt{\frac{4\pi n e^2}{m}}$ in the unit C.G.S and $\varepsilon(\infty) \to 1$.

Where: n is the density of the electrons,

e is the elementary charge,

m is the mass of an electron,

If ε (ω) <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.

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Conclusion

By using the Drude model, we extractes the evolution from the constant optics of the thin layer of the vanadium dioxide VO_2 thickness 82 nm at a temperature of 85 °C; that is to say, with the metal state according to the energy ω of the incidental photons in the interval $0.001242 < \omega\,(\mathrm{ev}) < 6$.

In the interval 0.001242 < ω (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 refectivity 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_2 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_2 are due to the free electrons in the metal state and to the energy of the incidental photons if compared with the plasma frequency ω_p which characterizes the material.

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