

CORRELATION OF THE OPTICAL PROPERTIES AND INTRABAND TRANSITION OF VANADIUM THIN FILMS

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Abstract

The possibility of using the optical constant n and k of vanadium thin films, to calculate the free-electron optical effective masses, and relaxation time were calculated and discussed from the theoretical and experimental point of view. Throughout the optical constants, the optical conductivity $\sigma = \sigma_1 + \sigma_2$ as well as the volume and surface energy loss function are derived. The intraband contribution to the imaginary part of the dielectric constant is also obtained by subtracting the free electron contribution.

Introduction

Transition metal possess complicated electronic band structure. This is mainly due to the fact that band states are mainly of S and d-types in addition to traces of P states formed in the solid phase. 3d wave functions are localized and exhibit a narrow energy width of about 5 eV. This in turn, reduces the conductivity and increases the effective mass m^* [1,2].

The optical constants for a limited number of transition metals have been accurately determined throughout a continuous spectral range from the near infrared to the near ultraviolet. The determination of optical constants n and k of vanadium in thin film form of thickness varied from 50 to 100 nm, in the spectral range of 2.5 – 8.5 μm was previously discussed [3]. The previously obtained results revealed a relatively small discrepancy in the calculated values of n and k , in comparison with the mean value in the whole range of wavelength.

This leads us to the conclusion, that both parameters (n , k) are independent on the film thickness.

The purpose of this study is to use the obtained optical constants of thin vanadium films in the spectral range of 2.5 – 8.5 μm in the determination of optical conductivity in this spectral range as well as the lattice dielectric constant.

Results and Discussion

As mentioned before, the optical constants (n & k) of V films of different thicknesses in the thickness range between 50 and 100 nm do not depend on the film thickness, thus the absorption A was calculated according to [4],

$$A = \frac{4n}{(N + 1)^2 + K^2} \quad (1)$$

Fig. (1) illustrates A against $(h\nu)$. This relation has a peak at $h\nu = 0.415$ eV corresponding to wavelength $(\lambda) = 2.99$ μm .

The electronic transition in a solid is more directly related to the complex dielectric constant $\epsilon = \epsilon_1 + i\epsilon_2$, instead of the complex index of refraction $n = n + ik$. These are connected by $\epsilon = n^2$, so that $\epsilon_1 = n^2 - k^2$ and $\epsilon_2 = 2nk$. The real and imaginary parts of the dielectric constant can be rewritten [5] in terms of the physical parameters of the material as follows:

$$\epsilon_1 = n^2 - K^2 = \epsilon_L - \frac{N e^2}{m^* \epsilon_0} \frac{\tau^2}{1 + \omega^2 \tau^2} \quad (2)$$

$$\epsilon_2 = 2 n K = \frac{N e^2}{m^* \epsilon_0 \omega} \frac{\tau}{1 + \omega^2 \tau^2} \quad (3)$$

Where N is the carrier density, ϵ_0 is the dielectric constant of free space, ω is the angular frequency of the incident radiation, τ is the

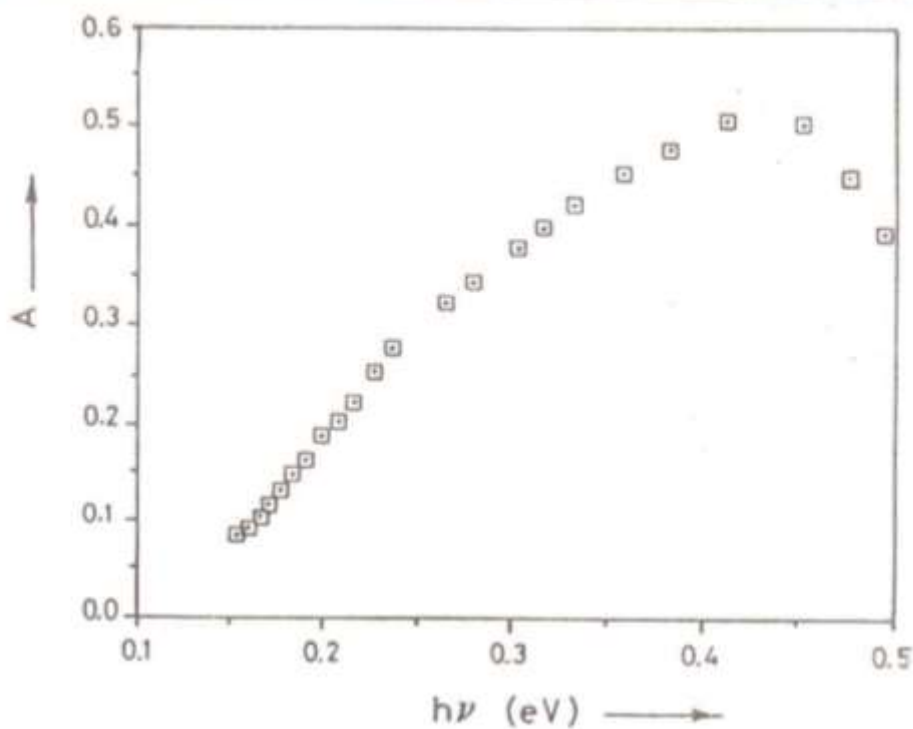


Fig. 1 Variation of the absorption (A) with the photon energy ($h\nu$)

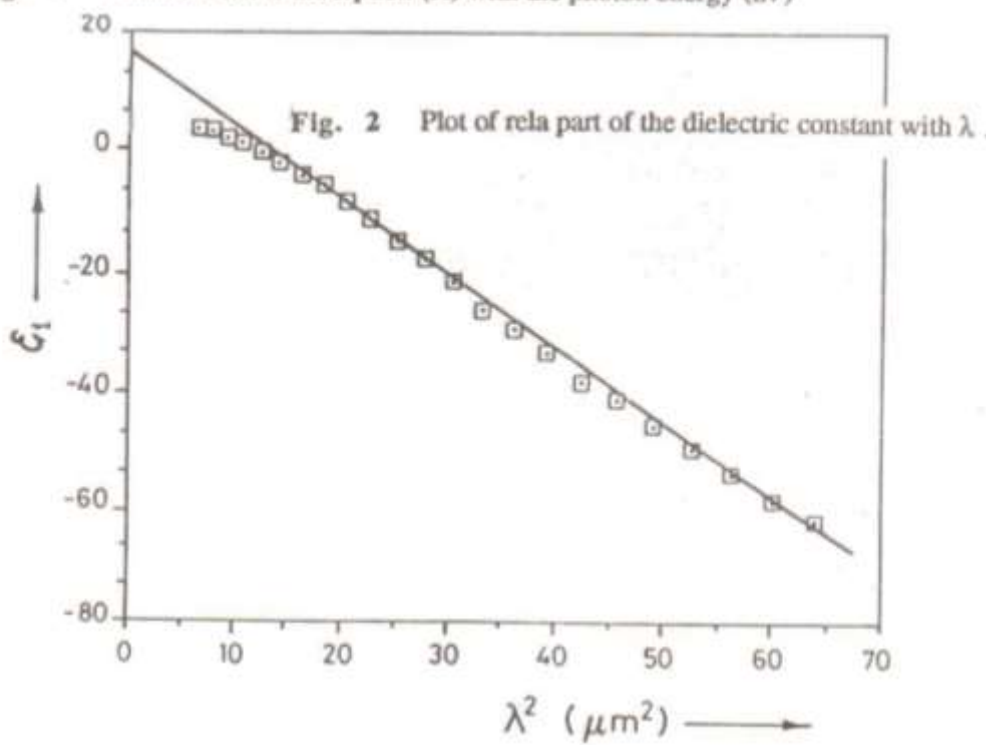


Fig. 2 Plot of real part of the dielectric constant with λ

relaxation time and m^* is the conductivity effective mass of the carriers.

In infrared region, different interactions can take place, such as intraband transition and plasma reflection. For I.R. frequencies two approximations hold

$$\omega \gg 1/\tau \text{ and } n^2 \gg K^2$$

consequently

$$\epsilon_1 = n^2 - K^2 = \frac{e^2}{4\pi c^2 \epsilon_0} \frac{N}{m^*} \lambda^2 \quad (4)$$

$$\epsilon_2 = \frac{N e^2}{m^* \epsilon_0 \omega \tau} \quad (5)$$

Therefore, a plot representing ϵ_1 against λ^2 will yield a straight line, the point of intercept on the y-axis yields the required value of ϵ_L , while the optical mass is determined from the slope [6]. Fig. (2) illustrates $\epsilon_1 = f(\lambda^2)$. It is seen that the lattice dielectric constant ϵ_L and the optical mass are found to be 17 and $1.4 m^*$ respectively. These values agree with the behavior three-d functions (narrow band and strong interaction). On the other hand Fig. (3) shows the relation between ϵ_2/λ and λ^2 , from which τ is found to be 10×10^{-15} S. These results are in good agreement with those reported by other workers [3, 7].

The volume and surface energy-loss functions $-\text{Im}(1-\epsilon)$ and $\text{Im}(1/\epsilon+1)$ describe the probability that fast electrons will lose energy when traversing the bulk and surface of the material respectively. They are related to the real and the imaginary parts of the complex dielectric constant (ϵ) by the following relation [8]:

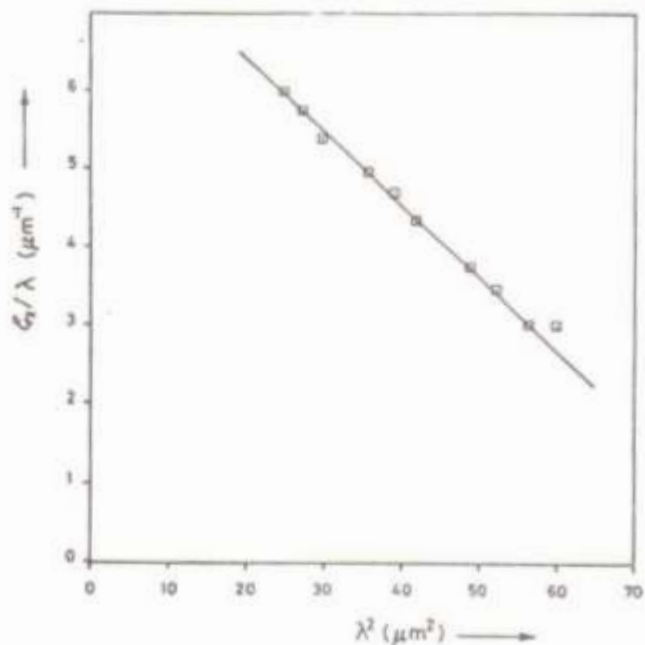


Fig. 3 Plot of (ϵ_2/λ) vs. (λ^2) .

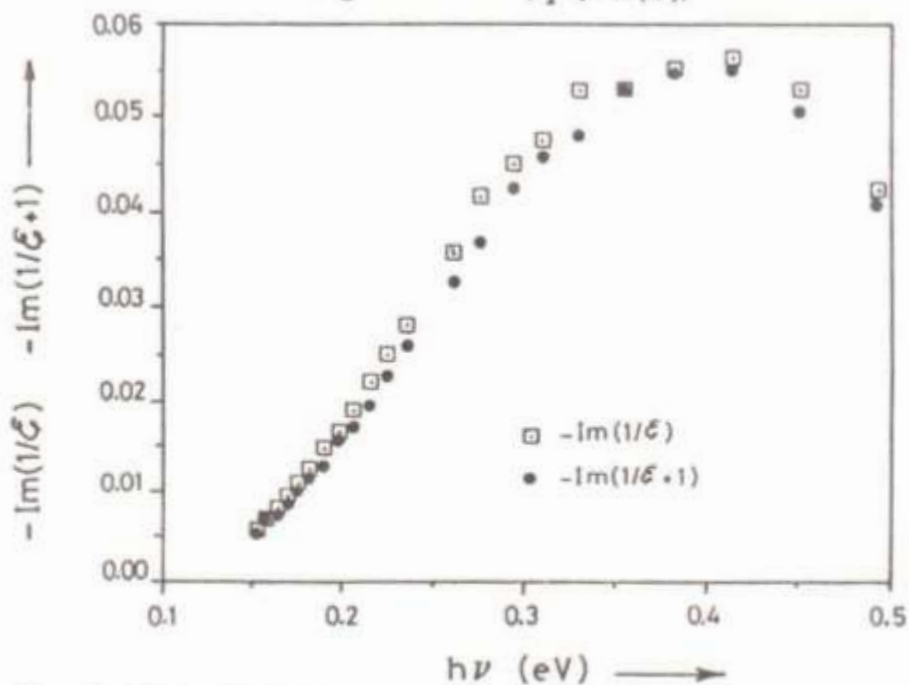


Fig. 4 The spectral behaviour of the volume energy loss function $-\text{Im}(1/\epsilon)$ and the surface energy loss function $-\text{Im}(1/\epsilon + 1)$ vs. $(h\nu)$.

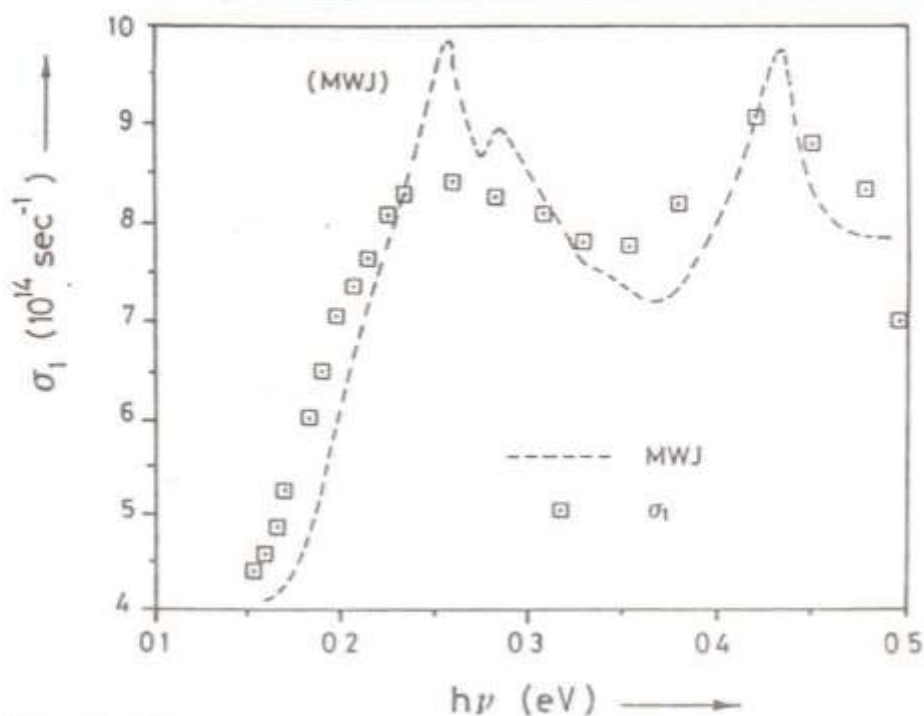


Fig. 5 The real part of the optical conductivity (σ_1) as a function of $(h\nu)$, compared with the theoretical use of Moruzzi, Williams and Janak (MWJ).

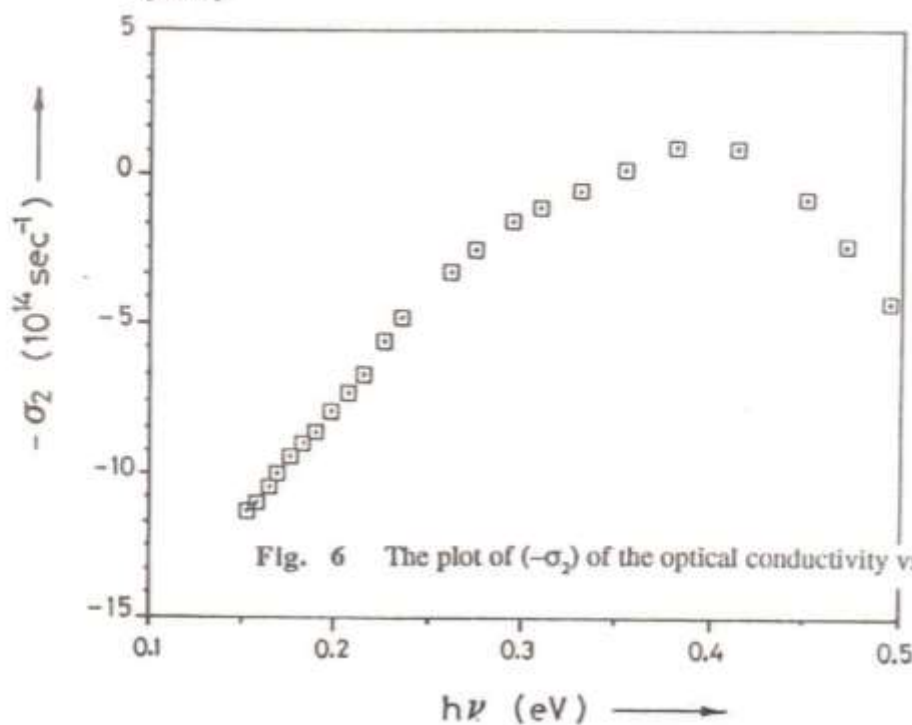


Fig. 6 The plot of $(-\sigma_2)$ of the optical conductivity vs. $(h\nu)$.

$$-\operatorname{Im}\left(\frac{1}{\epsilon}\right) = \frac{\epsilon_2}{\epsilon_1^2 + \epsilon_2^2} \quad (6)$$

$$-\operatorname{Im}\left(\frac{1}{\epsilon + 1}\right) = \frac{\epsilon_2}{[(\epsilon_1 + 1)^2 + \epsilon_2^2]} \quad (7)$$

Fig. (4) illustrates the spectral behaviour of both volume and surface energy loss functions against the photon energy of the incident radiation ($h\nu$). It is clear that, the photon energy lost on traversing the bulk is nearly equal to that lost on traversing the surface. Both functions show a peak at 0.415 eV. However, in the case of transition metals, the optical conductivity $\sigma_1 + i\sigma_2$ is more convenient. The optical conductivity (σ_1 & σ_2) are related to the components of the complex dielectric constant by $\sigma_1 = \epsilon_2 \omega/4\pi$ and $\sigma_2 = (1 - \epsilon_1) \omega/4\pi$ where $\omega (=2\pi\nu)$ the angular frequency of the incident radiation, σ_1 and σ_2 calculated from the optical constants are illustrated as a function of $h\nu$ (eV) in Figs. (5 and 6). It is seen that $\sigma_1 = f(h\nu)$ shows two distinct maxima, the sharp one at 0.416 eV and the broad one at 0.25 eV. The peak existing at 0.416 eV is in harmony with those peaks observed throughout the $A = f(h\nu)$ represented at 0.415 eV, and that given through the volume and surface energy loss function represents at 0.415 eV. This peak may be attributed to spin-orbit splitting, which is in good agreement with [9,1]. Several attempts have been made previously to determine the free-electron contribution by extending reflection measurements further into the infrared region. Lenham and Treherne [10] made measurements up to 15 μm for most of the metals including the vanadium. At these long wavelengths, the determined values for the optical mass and the relaxation time, but even their plots clearly showed contributions of intraband transitions. In this intraband region of the spectrum. The optical conductivity calculated theoretically by Moruzzi et al. [11] agrees with experimental data in the present work.

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