Optical properties and electronic structure of $V_2O_5$, $V_2O_3$ and $VO_2$

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Abstract
The electronic structure of the three main vanadium oxides—$V_2O_3$, $VO_2$ and $V_2O_5$—is reviewed. The optical properties of vanadium pentoxide thin films were determined. It was found that a direct allowed transition is the most probable one in the studied vanadium pentoxide thin films.

Abbreviations

| Acronym | Definition |
|---------|------------|
| APW     | Augmented-plane wave |
| CB      | Conduction band |
| DA      | Direct allowed |
| DF      | Direct forbidden |
| DFT     | Density function theory |
| $E_F$   | Fermi energy |
| $E_g$   | Energy gap |
| ELS     | Electron energy loss |
| IA      | Indirect allowed |
| IF      | Indirect forbidden |
| MIT     | Metal–insulator transmission |
| PES     | Photoemission spectroscopy |
| PL      | Photoluminescence |
| SXS     | Soft X-ray spectroscopy |
| T.F.    | Thin film |
| VB      | Valence band |
| XAS     | X-ray adsorption spectroscopy |
| XES     | X-ray emission spectroscopy |
| XPS     | X-ray photoelectron spectroscopy |
| XRF     | X-ray fluorescence |

1 Introduction

Correlated electrons in vanadium oxides are responsible for their unique structural, electrical, optical and magnetic properties. Their electronic band structures are affected by crystallographic structure, crystal field splitting and hybridization between $O_2p$ and $V_3d$ bands. There have been many experimental and theoretical studies of the band structure of the main vanadium oxides—$V_2O_3$, $VO_2$ and $V_2O_5$. The first experimental studies on band structure were based on optical spectroscopy that utilized absorption and reflection of light. Ceramic materials, single crystals and thin films were the subjects of these studies. Lately, new methods such as photoemission spectroscopy (PES), X-ray absorption or emission spectroscopy (XAS, XES) [1], X-ray reflectivity (XRR), X-ray fluorescence (XRF) [2], photoluminescence (PL) [3, 4], Raman scattering and scanning tunnelling microscopy (STM) [5] have been used.

Theoretical calculations used several quantum mechanics models such as the Hartree–Fock self-consistent field method based on one-electron approximation, the Hubbard–Mott model [6] introducing the effects of electron correlations on the Hamiltonian, Peierls mechanism [7, 8] involving electron–phonon interactions, or the density functional theory (DFT) [9].

One of the most important parameters with regard to the properties of materials is the bandgap energy ($E_g$). Generally, the $E_g$ of a semiconductor or an insulator has been found to decrease with increasing temperature. The variation of the fundamental $E_g$ with temperature is very important for both basic science and technological applications.

2 Electronic structure

The theoretical basis of optical properties results from Maxwell’s equations. From optical spectra, the complex dielectric function $\varepsilon(\omega)$ is derived [10]:

$$\varepsilon(\omega) = \varepsilon_1 - i\varepsilon_2 \quad (1)$$
where \( \omega \) is angular frequency of light (\( \omega = 2\pi \nu \)), \( \epsilon_1 \) and \( \epsilon_2 \) represent real and complex parts of \( \varepsilon \), and \( i \) is the imaginary unit.

\[
\epsilon_1 = n^2 - \kappa^2 \tag{2}
\]

and

\[
\epsilon_2 = 2n\kappa \tag{3}
\]

where \( n \) and \( \kappa \) are real and imaginary parts of the refractive index.

Measurement of light absorption is one of the most important techniques used to determine the optical properties of solids. In absorption measurements, the intensity of light \( I(d) \) after it has travelled through a certain thickness of a material is compared with the incident intensity \( I_o \), thereby defining the absorption coefficient \( \alpha \):

\[
I(d) = I_o \exp[-\alpha(\omega)d] \tag{4}
\]

The dependence of the absorption coefficient on frequency is shown in Fig. 1. Since \( I(d) \) depends on the square of the field variables, it immediately follows that

\[
\alpha(\omega) = \frac{2\omega\kappa}{c} = 4\frac{\pi\kappa}{\lambda} \tag{5}
\]

where the factor of 2 results from the definition of \( \alpha(\omega) \) in terms of light intensity, which is proportional to the square of the optical fields. This expression entails that the absorption coefficient is proportional to \( \sim \kappa(\omega) \), the imaginary part of the complex index of refraction (extinction coefficient), so that \( \kappa \) is usually associated with power loss.

It can be concluded from Eqs. (2), (3) and (5) that either set—\( (\epsilon_1, \epsilon_2) \) or \( (n, \alpha) \)—represents the wavelength-dependent constants characterizing the optical properties of a studied solid. Many efforts have been devoted to the determination of the refractive index \( (n) \), but there is so far no universal approach. Several methods of calculating the refractive index of vanadium oxide \([11–18]\) and other materials \([19–23]\) have been proposed. Various assumptions were used in these methods, and the results are often subjective/debatable and ambiguous.

## 2.1 Optical properties \( \text{V}_2\text{O}_5 \)-literature survey

The electronic structure of vanadium pentoxide has been the subject of intensive studies \([24–34]\). Various theoretical calculations of \( \text{V}_2\text{O}_5 \) band structure include both semi-empirical and ab initio techniques.

Lambrecht et al. \([24, 25]\) presented a calculation of the energy band structure using a tight-binding model in which the oxygen \( p \)-bands and vanadium \( d \)-bands were decoupled. They applied a perturbation approximation in order to obtain an effective Hamiltonian for the valence and conduction bands separately. The theoretically determined dispersion of the energy bands was verified by applying electrical transport properties. The valence band density of states was compared with XPS (X-ray photoelectron spectroscopy) and SXS (soft X-ray spectroscopy) data. The valence-conduction band transitions were compared with optical and electron energy loss (ELS) data. A satisfactory agreement between theoretical and experimental data was found \([25]\).

Kempf et al. \([26]\) reported on pseudo potential periodic Hartree–Fock calculations on a \( \text{V}_2\text{O}_5 \) crystal. The determined V-O bond lengths and stretching force constants were found to be in good agreement with experimental data. The estimated band structure and density of states remain in contrast with tight-binding calculations. There is no gap between the conductor and valence bands. According to the authors, vanadium pentoxide is partially ionic.

Bullett \([27]\) determined the electronic structure of vanadium pentoxide using direct and non-empirical atomic orbital techniques. He postulated an indirect semiconducting energy gap of 2.6 eV.

Eyert and Höck \([28]\) computed the band structure of bulk vanadium pentoxide using the density-functional theory (DFT) and local-density approximations (LDA). Its electronic properties were modified via strong hybridization between O 2p and crystal-field-split V3d orbitals. A strong deviation of VO_6 octahedra from the cubic coordination led to a narrow split-off conduction band.

The electronic structure of vanadium pentoxide is strongly connected with its anisotropy, which in turn is associated with its crystal structure. The atoms form double chains within planes that are separated by a van der Waals gap.

Kenny et al. \([29]\) studied the optical absorption coefficients of \( \text{V}_2\text{O}_5 \) single crystals using incident polarized light with wavelengths in the range of 0.47–1.8 \( \mu \)m and unpolarized light with wavelengths from 1.5 to 7.5 \( \mu \)m. Fundamental absorption was observed at incident photon energies of
2.15, 2.22 and 2.17 eV for $E_{\parallel a}$, $E_{\parallel b}$ and $E_{\parallel c}$, respectively. Some evidence for a direct forbidden transition mechanism with bandgaps of 2.36 and 2.34 eV was observed for $E_{\parallel a}$ and $E_{\parallel c}$, respectively. The most notable property of V$_2$O$_5$ is its ability to produce monolayers (or materials only several layers thick) [30]. Vanadium pentoxide is the second material known to exhibit such a property. The first one was graphite forming a single monolayer, known as graphene. Chakarbarti al. [31] determined the V$_2$O$_5$ monolayer band structure using ab initio density-functional theory (DFT). The obtained results are in excellent agreement with experimental crystallographic data as well as with other experimentally determined surface properties [32, 33].

Tolhurst et al. [34] studied a double-layered polymorph of V$_2$O$_5$ (named ε'-V$_2$O$_5$) using soft X-ray spectroscopic measurements and density-functional theory calculations. This polymorph has increased interlayer separation, which leads to a dramatic increase in the bandgap. Table 1 summarizes the representative literature data [28, 34–37] of the band gap and its temperature dependence.

Figure 2 shows the refractive index for vanadium pentoxide thin films as a function of wavelength [13, 38]. Parameter $n$ decreases with wavelength. This dependence may be verified using the theoretical equation proposed by Cauchy [39]:

$$n(\lambda) = A + \frac{B}{\lambda^2}$$

(6)

where $A$ and $B$ are independent of $\lambda$. According to Fig. 3, the experimental points are consistent with the theory postulated by Cauchy.

The analysis of the dependence of the absorption coefficient on light frequency is very significant from the viewpoint of the semiconducting properties of vanadium oxide and its subsequent areas of application. Generally, the frequency dependence of the absorption coefficient ($\alpha(\omega)$) is rather different for various physical processes which occur during the interaction of light with the solid. In particular, the following cases can be observed [10]:

1. Free carrier absorption
   (a) typical semiconductor
      $$\alpha(\omega) \sim \omega^{-2}$$
      (7)
   (b) metals at low frequencies
      $$\alpha(\omega) \sim \omega^{1/2}$$
      (8)

| $E_g$ (eV) | $dE_g/dT$ (eV/K) | Orientation | References |
|-----------|-----------------|-------------|------------|
| 2.17      | $-6.1 \times 10^{-4}$ | $E_{\parallel c}$ | [29], [35] |
| 2.34      |                 |             |            |
| 2.25      |                 |             |            |
| 2.49 ($T \rightarrow 0$) |                 |             | [37] |
| 2.19      |                 | $E_{\parallel b}$ | [35] |
| 2.363     |                 | $E_{\parallel b}$ | [29] |
| 2.22      |                 | $E_{\parallel a}$ | [29] |
| 2.23      | 7.3             | $E_{\parallel a}$ | [36] |
| 2.15      |                 |             | [29] |
| 2.54 ($T \rightarrow 0$) | $-6.1 \times 10^{-4}$ | $E_{\perp c}$ | [37] |

Table 1 Bandgap ($E_g$) of V$_2$O$_5$ and its temperature dependence—$dE_g/dT$

Fig. 2 Refractive index ($n$) determined for V$_2$O$_5$ thin films [13, 38]

Fig. 3 Cauchy’s plot of the refractive index ($n$) for V$_2$O$_5$ thin films [13, 16, 38]
2. Direct interband transition (conservation of crystal momentum)
   (a) allowed transition
   \[ a(\omega) \sim \frac{(\hbar \omega - E_g)^2}{\hbar \omega} \]  
   (9)

   (b) forbidden transition
   \[ a(\omega) \sim \frac{(\hbar \omega - E_g)^2}{\hbar \omega} \]  
   (10)

3. Indirect interband transition (change in crystal momentum)
   (a) allowed transition
   \[ a(\omega) \sim \frac{((\hbar \omega - E_g) \pm \hbar \omega_{\text{phonon}})^2}{\hbar \omega} \]  
   (11)

   (b) forbidden transition
   \[ a(\omega) \sim \frac{((\hbar \omega - E_g) \pm \hbar \omega_{\text{phonon}})^3}{\hbar \omega} \]  
   (12)

The \( \hbar \omega_{\text{phonon}} \) factor is generally omitted in Eqs. (11) and (12) because of the fact that phonon energy is several times lower than the energy of electron transition.

Equations (9)–(12), known as Tauc equations, are applied to determine the bandgap \( (E_g) \) of semiconductors.

Figure 4 shows the mechanisms of electron interband transition for direct and indirect semiconductors. A direct transition corresponds to the photon–electron interaction process in which the \( k \)-vector does not change. The crystal momentum of electrons and holes is the same in both the conduction band and the valence band. In an indirect transition photon, electron and phonon of the lattice take part. This process is accompanied by a change in the \( k \)-vector. The allowed transitions remain in agreement with particular selection rules, assuming a dipole model. On the other hand, if this model is not valid, the transition is called forbidden. More complex models can then be taken into account (involving, for instance, a magnetic dipole, electric quadrupole, etc.).

According to [29, 37], the edge is direct and forbidden. Diffuse reflectance spectra [40] give an \( E_g \) of 2.31 eV at room temperature, but the band edge has been determined to be direct and Mousavi et al. [41] observed that for \( \text{V}_2\text{O}_5 \) films prepared by means of spray pyrolysis \( E_g \) changes with the substrate temperature \( (T_{\text{sub}}) \). When \( T_{\text{sub}} \) increases, the \( E_g \) decreases gradually from 2.46 to 2.22 eV.

Kang et al. [5] studied the interband transition in a \( \text{V}_2\text{O}_5 \) film deposited via RF magnetron sputtering using absorption and photoluminescence spectral measurements. Transmission measurements indicate two distinct interband transitions, implying indirect and direct transitions.

![Fig. 4](image-url)

**Fig. 4** Direct and indirect mechanisms of electron interband transition
2.2 Optical properties of V$_2$O$_5$ thin films: experimental results

Vanadium pentoxide thin films were deposited by means of reactive radio frequency sputtering. Deposition conditions of the thin films and their properties such as structure, morphology were described in detail elsewhere [42]. Table 2 summarizes characterization of the films used in the studies.

Optical transmittance and reflectance spectra were measured over a wide wavelength range from 180 to 3200 nm with a Lambda 19 Perkin-Elmer double beam spectrophotometer equipped with a 150 mm integrating sphere. Thin films from Series 1, 2 and 3 were the subject of spectrophotometric studies. Each of Figs. 5, 6 and 7 shows the reflectance ($R$), transmittance ($T$) and absorbance ($A$) spectra recorded for one of the thin films. The transparency region of vanadium pentoxide is limited by the fundamental absorption edge at ca. 500 nm. The reflectance values vary in the

![Fig. 5 Reflectance ($R$), transmittance ($T$) and absorbance ($A$) spectra recorded for a Series 1 V$_2$O$_5$ thin film](image)

![Fig. 6 Reflectance ($R$), transmittance ($T$) and absorbance ($A$) spectra recorded for a Series 2 V$_2$O$_5$ thin film](image)

![Fig. 7 Reflectance ($R$), transmittance ($T$) and absorbance ($A$) spectra recorded for a Series 3 V$_2$O$_5$ thin film](image)

| Deposition conditions                     | Series |
|-------------------------------------------|--------|
| Ar flow [cm$^3$/s]                        | 1      |
| O$_2$ flow [cm$^3$/s]                     | 2      |
| Input power (W)                           | 3      |
| RF voltage ($U_{rf}$) (V)                 | 4      |
| Ar/O$_2$ gas atmosphere pressure (Pa)     |        |
| Deposition time (min)                     |        |
| Thickness (nm)                            |        |
| Substrate                                 |        |
| Substrate temperature (K)                 |        |

![Table 2 Deposition conditions for a series of vanadium oxide thin films and their properties](image)
range of 10–20% for the Series 1 sample (mostly amorphous), in the range of ca. 0–10% for the Series 2 and 3 samples (crystalline). The observed non-monotonic plots of $R$, $T$ and $A$ may result from additional absorption bands due to the departure from stoichiometry [11, 12].

The absorption coefficient ($\alpha$) and photon energy were determined from Figs. 5, 6 and 7 using the following equations:

$$a = \frac{1}{d} \ln \frac{1 - R}{T}$$

$$E_{\text{photon}} [eV] = h\omega = \frac{1240}{\lambda [nm]}$$

where $d$ represents film thickness.

One of the crucial parameters used to evaluate a semiconductor’s properties is the bandgap ($E_g$). The bandgap of a semiconductor can be determined from experimentally measured transmittance $T$ and reflectance $R$ within the range of fundamental absorption using the following Tauc equation:

$$(h\omega a)^{1/n} = A(h\omega - E_g)$$

where the $A$ coefficient is constant and $n$, according to Eqs. (9)–(12), assumes values $1/2$, $3/2$, 2 and 3 for direct allowed (DA), direct forbidden, indirect allowed and indirect forbidden transitions, respectively.

Figures 8, 9, 10 and 11 illustrate the absorption coefficient data experimentally determined for the Series 2 thin film in the coordinate system of $(h\omega a)^{1/n}$ versus $h\omega$ for $n = 1/2$, $3/2$, 2 and 3, respectively.

The bandgap was determined by extrapolating the linear part of the best fit of $(h\omega a)^{1/n}$ vs. $h\omega$ to $h\omega = 0$. The values of $E_g$ were obtained from the $h\omega$ axis intercepts. Similar plots were computed for the other two $\text{V}_2\text{O}_5$ samples: Series 1 and Series 3. The results are presented in Table 3.

The analysis of spectrometric results presented in Figs. 8, 9, 10 and 11 as well as in Table 3 suggests that $\text{V}_2\text{O}_5$ thin films undergo both direct and indirect transitions. However, it is not possible to decide which type of the electron interband transition is predominant in this case. Based on the following evidence,

- agreement with theoretical band calculations [24–26, 30],
- agreement with recent reports on single crystals [26, 43],
- agreement with recent experimental studies based not only on

\[ E_{\text{photon}} = \frac{1240}{\lambda [nm]} \]

\[ E_g = 2.307\pm0.043 \text{ eV} \]

\[ E_g = 2.893\pm0.039 \text{ eV} \]

\[ E_g = 2.209\pm0.021 \text{ eV} \]
spectrophotometric measurements such as photoluminescence
and ellipsometry [17],

the direct allowed (DA) transition can be considered the
most probable. The available literature on the bandgap of
V₂O₅ thin film is vast. The impact of the following factors
affecting the bandgap of films based on vanadium pentoxide
has been studied:

- thin film deposition technique [44–46] (Table 3),
- anisotropy [28, 29, 31, 47]
- film thickness [34]
- substrate type [47]
- non-stoichiometry [13, 48, 49]
- UV irradiation [48]

The results are presented in Table 4.

Figure 12 illustrates the Tauc plots corresponding to
hω energy between 2.97 and 3.23 eV. The best agreement
with the theoretically predicted dependence is observed for
the direct allowed (DA) transition. The results obtained by
applying the least squares method are listed in Table 5.

### 2.3 Optical properties of V₂O₃

Based on papers [52–55], the most significant calculations
were reported [56, 57]. The main controversy has been over
the ordering of the components of the trigonally split t₂g
band. Several band schemes have been suggested [58–60].
The V³⁺ ions in V₂O₃ have a 3d² electronic configuration.
These vanadium ions in the metallic phase (corundum)
occupy two-thirds of the octahedral sites formed by oxygen
anions. A trigonal distortion causes the splitting of the t₂g
orbital into a non-degenerate a₁g and a doubly degenerate
e_{II}g orbital [61]. Castellani et al. [57] suggested the forma-
tion of a molecular bond between the a₁g orbitals of V–V
pairs spread into a band. This model is consistent with many
experimental results [62–65]. However, taking into account
the fact that the c/a lattice parameter ratio is too high for
a₁g to couple between two V cations, Ivanov [66] and Ezhov
et al. [58] contradicted the postulated model of the molecular
orbital. Shinna et al. [67] assumed a strong hybridization of
the V pair.

The electronic properties of V₂O₃ are strongly dependent
on oxygen stoichiometry.

A slight variation in oxygen concentration changes the
effective mass [68, 69].

### Table 3 Tauc plot results

| Transition          | Results | Series 1 T.F. | Series 2 T.F. | Series 3 T.F. |
|---------------------|---------|---------------|---------------|---------------|
| Direct allowed      | E_g (eV)| 2.811 ± 0.065 | 2.893 ± 0.039 | 2.739 ± 0.089 |
|                     | Linear regression | 29   | 36   | 31   |
|                     | Pearson correlation | 0.9983 | 0.9978 | 0.9958 |
| Direct forbidden    | E_g (eV)| 2.575 ± 0.105 | 2.307 ± 0.042 | 2.207 ± 0.051 |
|                     | Linear regression | 20   | 36   | 99   |
|                     | Pearson correlation | 0.9968 | 0.9988 | 0.9948 |
| Indirect allowed    | E_g (eV)| 2.579 ± 0.064 | 2.209 ± 0.021 | 2.072 ± 0.030 |
|                     | Linear regression | 32   | 37   | 120  |
|                     | Pearson correlation | 0.9981 | 0.9997 | 0.9976 |
| Indirect forbidden  | E_g (eV)| 1.969 ± 0.046 | 1.974 ± 0.012 | 1.782 ± 0.024 |
|                     | Linear regression | 30   | 52   | 107  |
|                     | Pearson correlation | 0.9988 | 0.9998 | 0.9985 |
V$_2$O$_3$ is treated as the model system used to study the MIT in a correlated electron system ($T_{\text{MIT}} = 160$ K).

### 2.4 Optical properties of VO$_2$

The calculation of the electronic structure of VO$_2$ has been the subject of intensive research involving many models such as the cluster type [70, 71], tight-binding type [72–74], or augmented-plane-wave (APW) [75, 76], as well as energy band studies using Bloch functions in a linear combination of atomic orbitals [77].

Gavini et al. [78] determined the real ($n$) and imaginary ($\kappa$) parts of the refractive index. Studies of the absorption coefficient performed by Gavini et al. and Merenda et al. [79] revealed that the electronic structure at $E < 1.8$ eV can be attributed to d-d transitions with a threshold of 0.6 eV. At 1.82 eV, and the threshold for O2p–V3d transitions is observed, with peaks at 2.64 eV and 3.56 eV.

The temperature of MIT for bulk single-crystal VO$_2$ is 541 K [80]. Below $T_{\text{MIT}}$, VO$_2$ exhibits a monoclinic structure.
with the P2$_1$/c space group in which the partially filled d-band is split into an unoccupied part pushed past the π$^*$ band and the filled part of the d-band. Above the $T_{\text{MIT}}$, VO$_2$ transforms to a tetragonal (rutile) phase with the partially filled d-band located at the Fermi level and the material is metallic [81]. Jiang et al. [82] studied the optical properties of vanadium dioxide thin films deposited under different oxygen partial pressures via reactive magnetron sputtering. The bandgap decreased from 339.6 to 319.4 K. The near-infrared extinction coefficient (k) and optical conductivity increased with decreasing oxygen partial pressure.

### 3 Conclusions

The electronic structure of the three main vanadium oxides (V$_2$O$_3$, VO$_2$, and V$_2$O$_5$) was reviewed. The optical properties of vanadium pentoxide thin films were determined. It was found that the direct allowed (DA) transition is the most probable type observed in the case of the studied films.

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