ISSN 2181-8622

Manufacturing technology problems

Scientific and Technical Journal Namangan Institute of Engineering and Technology

INDEX COPERNICUS INTERNATIONAL

Volume 10
Issue 3
2025

Google Scholar Crossref doi SLIB.UZ Scientific library of Uzbekistan

CALCULATION OF ABSORPTION COEFFICIENT OF ORGANIC DYE N719 FOR DYE-SENSITIVE SOLAR CELL (DSSC)

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Abstract: The paper presents a review of literature articles devoted to the study of the effect of dye on the operation of solar cells based on titanium oxide. The absorption coefficient of the organic dye based on rhytinium N719 for dye-sensitive solar cells (DSSC) was calculated, and the light path on TiO_2 was calculated based on the Bouguer–Lambert–Beer equation, taking into account the porous structure of the anode layer. It is shown that the effective layer thickness in the porous structure exceeds the physical thickness by 5–10 times, which ensures a high absorption rate of photons in the visible range.

Keywords: absorption coefficient, N719 dye, dye-sensitive solar cell (DSSC), light absorption, Beer–Lambert–Bouguer equations, light collection efficiency (LHE), spectral absorption coefficient, optical density, molar absorption coefficient, effective path length, photon, current density.

Introduction. For the first time, photons were converted into electricity by injecting electrons of excited dye molecules into the wide band gap of a semiconductor [1]. Many studies have been done on ZnO single crystals [2], but the efficiency of these dye-sensitized solar cells was very low because a monolayer of dye molecules could absorb only 1% of the incident light. Therefore, the efficiency was improved by optimizing the porosity of the electrode made of fine oxide powder so that the absorption of the dye by the electrode could be improved and as a result, the light harvesting efficiency (LHE) could also be improved. As a result, nanoporous titanium dioxide (TiO2) electrodes with a roughness factor of about 1000 were discovered and DSSCs with an efficiency of 7% were invented in 1991 [3]. Dye-Sensitized Solar Cells (DSSCs) have attracted increasing attention due to their ease of fabrication and high efficiency under diffuse light. In DSSC solar cells, the main process determining the short-circuit photocurrent (Jsc) is the absorption of photons by dye molecules adsorbed on the surface of nanostructured TiO_2. The Bouguer–Lambert–Beer law, modified to account for porosity and multiple light scattering, is used to quantitatively describe the light absorption.

To predict the characteristics of DSSC, it is necessary to accurately estimate the spectral absorption coefficient ($\alpha(\lambda)$) and the integrated absorption of the photon flux in the operating wavelength range. The aim of this work is to develop a calculation method for determining the absorption coefficient of the dye in the porous TiO_2 layer and to plot the dependence of $\alpha(\lambda)$ on the wavelength, taking into account scattering and the effective layer thickness.

In the work by Mohsen et al., the absorption spectra of some dyes (N719, N3, N749 and SQ2) were measured as sensorized materials for dye-sensitized solar cells (DSSCs). Commercially available dyes namely N719, N3, N749 and SQ2 were used. All the samples were prepared as solutions at different concentrations (10^{-4}, 10^{-5}, 10^{-6} M) using ethanol as solvent except SQ2 which used methanol as solvent. The samples were evaluated

spectrometrically; the results of UV-Vis spectra showed that for (N719, N749 and N3), there were two peaks at (390 and 530 nm), (430 and 626 nm) and (390 and 540 nm), respectively [4].

Examples from established organic dye sensitizer structures, such as TA-St-CA, Carbz-PAHTDDT (S9), and metalloporphyrin (PZn-EDOT), are used as reference structures for an examination of this concept applied to generate systematically modified structural derivatives and hence new photosensitizers (i.e., dyes). Using computer-aided rational design (CARD), the in silico design of new chromophores targeted an improvement in spectral properties via the tuning of electronic structures by substitution of molecular fragments, as evaluated by the calculation of absorption profiles [5]. In [6] specifically, 17 different structures were investigated, and classified into four categories based on the shape of the dye molecule, namely L-shaped (linear), V-shaped, X-shaped and Y-shaped, and into two different categories based on the donor moiety. The five of studied structures contained a triphenylamine (TPA) donor moiety, and twelve structures contained carbazole (CAR) donor moiety. Parameters related to the performance of DSSCs such as absorption spectra, intramolecular charge transfer indices, frontier molecular orbitals, light harvesting efficiency, excited-state lifetime, exciton binding energy, electrostatic potential, charge transfer and electron injection ability were studied using results obtained from electronic structure calculations.

In [7], a thorough study of four triphenylamine-based organic sensitizers with D–π–A configurations is presented and their photoelectric performance is compared with that of a conventional ruthenium-based sensitizer N719. In [8], the effect of chemical modifications on the electronic structure of N719 derivatives for their application in dye-sensitized solar cells (DSSCs) is analyzed using density functional theory (DFT). The UV-visible spectra indicate that the electronic configurations are necessary for studying the solar radiation absorption and analyzing the charge transfer mechanism between the electron transport layer (ETL), electrolyte, and dye [9].

Methodology & empirical analysis.

The absorption of light in DSSC is described by the Beer–Lambert–Bouguer law. [10]:

$$I(x,\lambda) = I_0(\lambda) \cdot e^{-\alpha(\lambda)x} \qquad (1)$$

Where the optical density of the layer is determined by expression:

$$\alpha(\lambda) = \varepsilon(\lambda) \cdot c \cdot l \qquad (2)$$

Where: $\alpha(\lambda)$ – optical density, $\varepsilon(\lambda)$ – molar absorption coefficient ($l \cdot mol^{-1} \cdot sm^{-1}$), c – dye concentration ($mol \cdot l^{-1}$), l – layer thickness (sm).

In solutions, this law describes the linear dependence of the optical density on the cuvette thickness and the concentration of the substance. For DSSC, the ccc parameter is defined as the effective concentration calculated from the density of adsorbed molecules on the TiO_2 surface, and l is replaced by teff, reflecting the increase in the path due to the porous structure[11].

Absorption coefficient $\alpha(\lambda)$ is expressed through optical density:

$$\alpha(\lambda) = 2{,}303 \cdot \varepsilon(\lambda) \cdot c \qquad (3)$$

For a porous layer of TiO2 nanoparticles, the actual optical path length of light significantly exceeds the physical thickness of the layer t due to multiple scattering. To account for this effect, an effective thickness is introduced:

$$t_{eff} = \beta \cdot t \qquad (4)$$

Where: $\beta \approx 10$ – coefficient of increase in the light path length from the porosity and particle size of TiO_2.

Current research shows that the effective path length in DSSC can be 5–10 times greater than the physical thickness of the nanoporous TiO_2 layer structure. Developing models that take into account the angular distribution of light, multiple scattering, and spectral dependence of the extinction coefficient is an important direction for accurately predicting the efficiency of solar cells [12].

The fraction of absorbed photons at wavelength λ is calculated using the formula:

$$P_{abs}(\lambda) = 1 - e^{-a(\lambda)t_{eff}}. \qquad (5)$$

The short-circuit current is determined by integration over the solar radiation spectrum.

$$J_{sc} = q \int_{\lambda} \phi_{in}(\lambda) \cdot P_{abs}(\lambda) d\lambda \qquad (6)$$

Where: q – electron charge, $\phi_{in}(\lambda)$ – photon flux per unit area.

The calculation of the dependence of the short-circuit current of the DSSC solar cell on the wavelength of solar radiation is shown in Figure 2. [13].

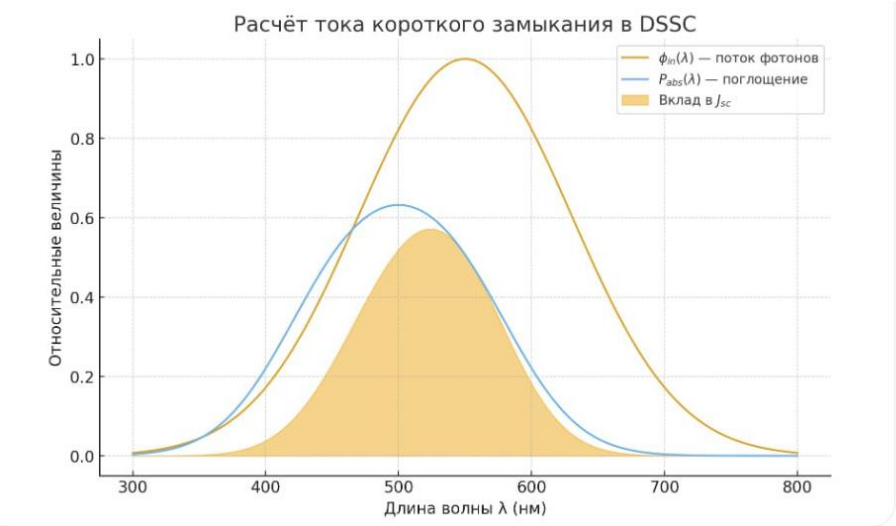

Figure 2. Dependence of the short-circuit current of the DSSC solar cell on the wavelength of solar radiation.

Results. To demonstrate the approach, a numerical calculation of the spectral absorption coefficient and the integrated absorbance of the dye in the DSSC was performed. The following parameters were used as initial data:

Table 1.

Parameter	Value
Spectral range	400-700 nm, step 50 nm.
Molar absorption coefficient	1000–30000 $l \cdot mol^{-1} \cdot sm^{-1}$
Dye concentration	$1.0 \cdot 10{-}3$ $mol \cdot l^{-1}$
TiO_2 layer thickness	$t=20\mu m=2.0 \cdot 10^{-3}$ sm
Effective layer thickness	$t_{eff}=100\mu m=10 \cdot 10^{-3}$ sm
Light path magnification factor	$\beta=10$

We accept for calculation λ, $\varepsilon(\lambda)$ (for organic dye N719), $c=10^{-3}$ mol/l. We substitute into (3) and find α for each wavelength:

Table 2.

λ (nm)	$\varepsilon(\lambda)$, $l \cdot mol^{-1} \cdot sm^{-1}$	$\alpha(\lambda)$, sm^{-1}
400 nm	12000	27.64
450 nm	18000	41.45
500 nm	25000	57.28
550 nm	22000	50.67
600 nm	15000	34.55
650 nm	8000	18.42
700 nm	3000	6.91

Average value $\alpha=33.03$ sm^{-1}

Based on the data in Table 2, we will plot a graph of the dependence of the absorption coefficient of the N719 dye on the radiation wavelength.

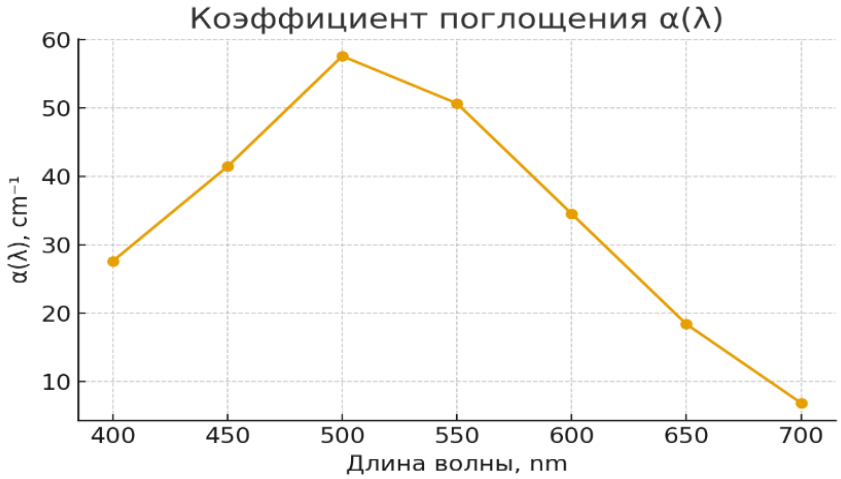

Figure 2. Dependence of the absorption coefficient of the N719 dye on the radiation wavelength.

Conclusions. The fraction of absorbed photons can be determined by expression 5 by substituting the values of $\alpha(\lambda)$, sm^{-1} from table 2. For visible light 400-700 nm it has a value of 0.23. Therefore, using expression 6 we calculate the current density (photocurrent) of 5.7 mA/sm-1. Since our calculations cover the visible range of sunlight, it has a slightly lower value than the experimental data. In [14], the current density values for the DSSC panel with N719 dye obtained experimentally are presented. The difference arises because the experimental data takes into account ultraviolet and infrared waves in addition to the visible spectrum.

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