

ANALYSIS OF OPTICAL SPECTRA OF Ni_{1-x}Zn_xFe₂O₄ NANOFERRITES

Sh.N. ALIYEVA

aliyeva.shahla2020@gmail.com

Institute of Physics, Ministry of Science and Education of Azerbaijan Republic,

Baku, AZ-1073, Azerbaijan

Azerbaijan State Oil and Industry University, Baku, AZ-1010, Azerbaijan

The Kramers-Kronig relations [1–5] are extensively employed in various areas of theoretical physics to retrieve one component of the complex dielectric constant from the known second part. One component of the dielectric constant is derived from calculations of a material's optical properties based on measurements, such as the reflection coefficient across a broad spectrum, as well as in other issues closely connected to optics and solid-state physics.

Keywords: Kramers-Kronig relations, optical spectra, permittivity.

DOI:10.70784/azip.1.2024436

The Kramers-Kronig relations [1-5], or dispersion relations, are an integral relationship between the real and imaginary parts of any complex function that is analytic in the upper half-plane. They are often used in physics to describe the relationship between the real and imaginary parts of the response function of a physical system, since the analyticity of the response function implies that the system satisfies the causality principle, and vice versa [6]. In particular, the Kramers-Kronig relations express the relationship between the real and imaginary parts of the permittivity in classical electrodynamics and the transition probability amplitude (matrix element) between two states in quantum field theory.

To calculate the Van der Waals equations, information about the frequency dependence of the permittivity is required. These experimental dependences are usually determined in a very limited region, which introduces a significant error in calculations using the Kramers-Kronig relations, since in these relations, the range of determination of the permittivity extends from 0 to ∞.

$\epsilon(\omega)$ is a complex value ($\epsilon = \epsilon'(\omega) + i\epsilon''(\omega)$), and its imaginary part is always positive and determines the dissipation of the energy of an electromagnetic wave propagating in a given medium. By formally considering $\epsilon(\omega)$ as a function of the complex variable ω , the Kramers-Kronig relations equation

By formally considering $\epsilon(\omega)$ as a function of the complex variable ω , the Kramers-Kronig relations equation

$$\epsilon''(i\xi) = 1 + \frac{2}{\pi} \int_0^\infty \frac{\omega \epsilon''(\omega)}{\omega^2 + \xi^2} d\omega \tag{1}$$

determine the values of the function ϵ of the complex argument $\omega = i\xi$.

The frequency dependence of the dielectric constant of semiconductors is determined experimentally, most often, in studies of the reflection spectrum and is then analyzed using the Kramers-Kronig relations, which have the form:

$$\left. \begin{aligned} \epsilon_1(\omega) = (n^2 - k^2)_{\omega_0} &= 1 + \frac{2}{\pi} \int_0^\infty \frac{\omega \epsilon_2(\omega)}{\omega^2 - \omega_0^2} d\omega \\ \epsilon_2(\omega) = (2nk)_{\omega_0} &= -\frac{2\omega_0}{\pi} \int_0^\infty \frac{\epsilon_1(\omega)}{\omega^2 - \omega_0^2} d\omega \end{aligned} \right\} \tag{2}$$

The relationship between the refractive index and absorption coefficient with reflection is established through the complex amplitude of the electromagnetic radiation beam reflected from the surface of the semiconductor in the form:

$$r = R^{\frac{1}{2}} e^{i\theta}; \ln r = \ln R^{\frac{1}{2}} + i\theta \tag{3}$$

where R is the reflection coefficient; θ is the phase angle of reflection. It is obvious that the real and imaginary parts of this expression are related to each other, according to the Kramers-Kronig relations, by the equation

$$\int_0^\infty \ln \left(\frac{R(\omega)}{R(\omega_0)} \right) \cdot \frac{d\omega}{\omega^2 - \omega_0^2} \tag{4}$$

Because

$$R^{\frac{1}{2}} e^{i\theta} = \frac{n-ik-1}{n-ik+1} \tag{5}$$

that

$$k = \frac{2\sqrt{R} \sin\theta}{1+R-2\sqrt{R} \cos\theta}; n = \frac{1-R}{1+R-2\sqrt{R} \cos\theta} \tag{6}$$

The phase angle can be calculated in different ways. Without going into details of limitations, errors, etc., a mathematical apparatus that has not been used by anyone, but gives good results with a low error, was used to calculate the phase angle. As usual, the frequency ranges from 0 to ∞ is divided into three areas:

1. from 0 to ω_1 , in which it is assumed that $R(\omega) = R_1$, i.e., constant (more precisely, equal to the first experimental value;

2. from ω_1 to ω_N - the area of experimental data
 3. from ω_N to ∞ , which uses the $c\omega^{-4}$, extrapolation inherent in the far ultraviolet region of the spectrum.

In the frequency range from ω_1 to ω_N , it becomes necessary to further define the integrand at the point $\omega = \omega_0$. Revealing the uncertainty according to L'Hôpital's rule, let us consider the limit to which the integrand tends at the point $\omega = \omega_0$:

$$\varphi = \lim_{\omega \rightarrow \omega_0} \frac{\ln R(\omega) - \ln R(\omega_0)}{\omega^2 - \omega_0^2} = \frac{1}{2\omega^2} \lim_{\omega \rightarrow \omega_0} \frac{R'(\omega)}{R(\omega)} \quad (7)$$

To find this limit, we must remember that we represent the experimental spectrum as a broken line. Smoothing the experimental curves by using cubic or other splines, however, does not solve the main problem, namely: the equation of the j-link of the broken line has the form:

$$R(\omega) = \frac{R_{j+1} - R_j}{(\omega_{j+1} - \omega_j)} (\omega - \omega_j) + R_j \quad (8)$$

and, therefore, near the singular point it is necessary to consider three cases:

1. the special point is located inside the broken line link, that is: $\omega_j < \omega_0 < \omega_{j+1}$. When

$$\varphi = \frac{1}{2\omega_0 R(\omega_0)} \cdot \frac{R_{j+1} - R_j}{\omega_{j+1} - \omega_j} = \frac{1}{2\omega_0} \cdot \frac{R_{j+1} - R_j}{(\omega_{j+1} - \omega_j)} \cdot \frac{\omega_{j+1} - \omega_j}{(R_{j+1} - R_j)(\omega_{j+1} - \omega_j) + R_j(\omega_{j+1} - \omega_j)} \quad (9)$$

and after transformations, we get that the limits on the right and left coincide.

2. At $\omega_j = \omega_0$
 a. when $\omega \rightarrow \omega_0 + 0$
 b.

$$\varphi = \frac{1}{2\omega_0} \cdot \frac{R_{j+1} - R(\omega_0)}{\omega_{j+1} - \omega_0} \quad (10)$$

c. when $\omega \rightarrow \omega_0 - 0$

$$\varphi = \frac{1}{2\omega_0} \cdot \frac{R_j - R_{j-1}}{\omega_j - \omega_{j-1}} \cdot \frac{1}{(R_j - R_{j-1})(\omega_0 - \omega_{j-1}) + R_{j-1}(\omega_j - \omega_{j-1})} = \frac{1}{2\omega_0 R(\omega_0)} \cdot \frac{R(\omega_0) - R_{j-1}}{\omega_0 - \omega_{j-1}} \quad (11)$$

3. At $\omega_0 = \omega_{j+1}$

Obviously, cases 2 and 3 are identical up to the number j. Thus, by defining the value of the integrand at the point $\omega = \omega_0$, we can calculate the phase angle in the entire frequency range under study, considering that:

1. in the frequency range from ω_N to ∞ during measurements in the region of residual rays

$$\frac{\omega_0}{\pi} \int_0^{\infty} \ln \left(\frac{R(\omega)}{R(\omega_0)} \right) \cdot \frac{d\omega}{\omega^2 - \omega_0^2} = \frac{1}{2\pi} \ln \left(\frac{R_{\infty}}{R(\omega_0)} \right) \ln \left| \frac{\omega_N + \omega_0}{\omega_N - \omega_0} \right| \quad (12)$$

2. when measuring in the visible and far ultraviolet spectral range

$$\frac{\omega_0}{\pi} \int_0^{\infty} \ln \left(\frac{R(\omega)}{R(\omega_0)} \right) \cdot \frac{d\omega}{\omega^2 - \omega_0^2} = \frac{1}{2\pi} \ln \left(\frac{R_{\infty}}{R(\omega_0)} \right) \ln \left| \frac{\omega_N + \omega_0}{\omega_N - \omega_0} \right| - \frac{4\omega_0}{\pi} \int_0^{\infty} \frac{\ln \omega d\omega}{\omega^2 - \omega_0^2} \quad (13)$$

The constructed algorithm was implemented in a program for analyzing optical reflection spectra, for example, of Ni_{1-x}Zn_xFe₂O₄ (x=0, 0.25, 0.5, 0.75) nanoferrites, the loss functions of which are presented in Fig. 1. As other tests, materials of III-V compounds were used: GaAs, InAs, etc., the experimental data of which are given in [6].

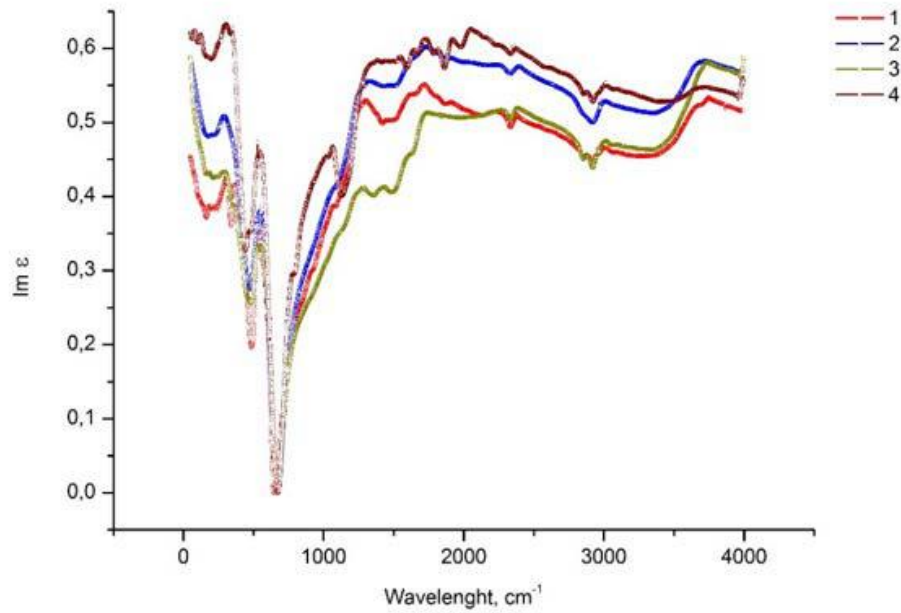


Fig.1 Loss functions of $Ni_{1-x}Zn_xFe_2O_4$ ($x=0, 0.25, 0.5, 0.75$) nanoferrites.

- | | |
|---|--|
| <p>[1] В.Б. Тимофеев. Оптическая спектроскопия объемных полупроводников и наноструктур.СП.:Лань. 2014. 512 с.</p> <p>[2] V. Lucarini, J.J. Saarinen, K. Peiponen, and E. Vartiainen. Kramers-Kronig Relations in Optical Materials Research. В.: Springer. 2005.162 p.</p> <p>[3] P. Martin. Physical. Review. - 1967,- vol. 161, p. 143.</p> | <p>[4] Л.И. Альперович, Н. Г. Бахшиев, Ю.Е. Забиякин, В.С. Либов. Оптика и спектроскопия. -1968, - т. 24, с. 60-63.</p> <p>[5] J.S. Toll. Physical Review. - 1956, - vol.104, p.1760-1770.</p> <p>[6] Р. Уиллардсон, А. Бир. Оптические свойства полупроводников.М.: МИР.1970.483 с.</p> |
|---|--|

Received: 25.11.2024