CYBERNETICS AND PHYSICS, VOL. 5, NO. 4, 2016 , 116–122

SOME CYBERNETIC ASPECTS OF DIELECTRIC SYSTEMS DESCRIPTION

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Abstract
The article describes possibility of increasing the effectiveness of dielectric systems research through systematization of causal relationships between electric fields according to the Lorentz model. The research also shows the objective reason for causing negative qualities of the dielectric constant of the Clausius-Mossotti formula. Authors propose proper way of identifying the low-frequency of polarization process.

Key words
Mathematical model, effective electric field, feedback, transmission function, structural scheme.

1 Introduction

Forced electric polarization of dielectric charged particles, discovered by Faraday, is one of the fundamental characteristics of matter. The theory of electron polarization, developed by Lorentz, is the conceptual basis of most of the existing electromagnetic nature representations. An example is the so-called Lorentz local field correction, which is the part of traditional wide description of polarization processes. Lorentz local field correction is also considered to be the classical equation of the relative permittivity (theory of Clausius-Mossotti).

However, despite the well-deserved popularity of this formula, current researches revealed the number of significant computational drawbacks, which, as a rule, are connected with the drawbacks of the original interpretation of the intensity model of Lorentz field concept [Böttche and Bordewijk, 1992; Bonin and Kresin, 1997; Raju, 2003; Potapov, 2004]. The traditional way out of this situation is seen as the need to generate subjective corrections, introduced into the basic formula, to account the polarized state of the particles filling local microscopic Lorentz's sphere [Bernardo et al., 1994; Kootstra, Baci and Snijders, 2000; Jensen, 2002; Van Duijnen et al., 2002].

In turn, the alternative solutions of this problem can be obtained by integrating the classic theory of the dielectrics polarization with mathematical methods of technical cybernetics, carried out with the purpose of the system describing the properties of a physical system, identified by allocating existing feedbacks [Ott, Grebogi and York, 1990; Fradkov, 1999; Fradkov and Jakubowsky, 2003; Fradkov, 2003; Fradkov, 2005].

2 The Inductive Model of Dielectric Permittivity

Historically, the first theoretical premise, used to express the strength of the electric field effectively acting in a polarized dielectric, called E, was a theoretical model of middle macroscopic field, proposed by Faraday. At the same time the essence of the formal description of magnitude E_m was the implementation of composition (superposition) of external field strength E_0 and a common set of micro field intensity, induced by polarized particles in the sample [Hippel, 1960; Decker, 1962]:

$$E_m = E_0 - \frac{1}{\varepsilon_0} \sum_{i=1}^{K} \mu_i N_i, \qquad (1)$$

where ϵ_0 – free space permittivity; K – the total number of particles' variety; $\mu_i$and N_i – induced dipole moments and their concentrations.

Therefore, as part of hypothesis that secondary macroscopic field is equivalent to the effective field E (if $E_0 = \varepsilon E_m$), the average macroscopic field strength is calculated as:

$$E_m = \frac{1}{(\varepsilon - 1)\varepsilon_0} \sum_{i=1}^{K} \mu_i N_i, \qquad (2)$$

where ε – relative dielectric constant of the sample.

However, the subsequent theoretical analyses of polarized micro field interaction induced in the metaphysical sample, necessitated entering a certain number of adjustments into the description of effectiveness of electric field tension. As a result, we managed to formulate some new formula of its quantity, based on the continuum model of the Lorentz's sphere:

$$E = E_m + E_1 + E_2, \tag{3}$$

where E_1 – tension of macroscopic field, formed by exiting of dipole chains on the surface of an imaginary sphere of containment; E_2 – tension of microscopic fields, generated inside the sphere.

The quantity of the macroscopic field E_1 is traditionally defined by integrating the charge density, induced on the outer surface in local microscopic Lorentz's sphere, as follows:

$$E_1 = \frac{1}{3\varepsilon_0}\sum_{i=1}^{K}\mu_i N_i. \tag{4}$$

In turn, the microscopic field strength E_2, determined by particle polarization inside the sphere, is regarded as equal to zero, with the account of symmetrical dipole charges' mutual compensation, noted by Mossotti.

Consequently, the formal unification of the formulas (2) and (4) provides a classical formula of relative transmittivity by Clausius-Mossotti:

$$\frac{\varepsilon - 1}{\varepsilon + 2} = \frac{1}{3\varepsilon_0}\sum_{i=1}^{K}\alpha_i N_i, \tag{5}$$

where α_i – electric polarizability of the particles. In addition, when considering the dynamic properties of the dielectric medium, such as the processes of elastic electron polarization in the framework of the classical theory, researches often use the formula of equation of forced oscillations of the electromagnetic liners, set by the harmonic oscillator:

$$\frac{d^2\mu_k(t)}{dt^2} + 2\beta_k\frac{d\mu_k(t)}{dt} + \omega_{0k}^2\mu_k(t) = \frac{q_k^2}{m_k}E_0(t), \tag{6}$$
$$k = \overline{1,K},$$

where β_k and ω_{0k} – damping factors and natural frequencies of specific particles; q_k and m_k – their charge and mass. It is obvious enough that the general solution of this equation in the complex domain enables to denote the complex polarizability of particle as $\alpha(j\omega)$:

$$\alpha_k(j\omega) = \frac{q_k^2/m_k}{\omega_{0k}^2 - \omega^2 + 2\beta_k j\omega}, \quad k = \overline{1,K}. \tag{7}$$

Thus, the direct substitution of formula (7) into formula (5) leads to inductive generation of traditional complex formula of dielectric constant by Lorenz-Lorentz-Clausius-Mossotti, that takes the following form with function $\varepsilon(j\omega)$:

$$\varepsilon(j\omega) = 1 + \frac{\frac{1}{\varepsilon_0}\sum\limits_{i=1}^{K}\alpha_i(j\omega)N_i}{1 - \frac{1}{3\varepsilon_0}\sum\limits_{i=1}^{K}\alpha_i(j\omega)N_i}. \tag{8}$$

It should be noted, that all the above presented formulas are the most common for dielectric processes in practical calculations. However, their ultimate effectiveness is more acceptable in consideration of crystals and liquids with mild polarization properties. The use of mentioned formulas in the study of active dielectrics can demonstrates awkward results. This well-known fact is named as "Mossotti disaster", as it is usually associated with inadequate approximation $E_2 = 0$.

On the one hand, the possibility of expanding the scope of mentioned formulas is implemented by entering some subjective corrections to characterize the real quantity of micro field voltage, induced within the scope of the continuum Lorentz's sphere. However, their numerical values are calculated theoretically or empirically for individual material, which is regarded as quite difficult and time-consuming computational task.

On the other hand, the "Mossotti disaster" can be directly related to the mathematical structure of the static formula of permittivity. Indeed, considering the Clausius-Mossotti formula (5) in the form of a functional dependence $\varepsilon(P)$, similar to the general type of formula (8), which takes into account the total polarization of particles of the sample (P), it can be seen that this function suffers the inevita-ble gap of the second kind under asymptotic condition $P = 3\varepsilon_0$ (Figure 1).

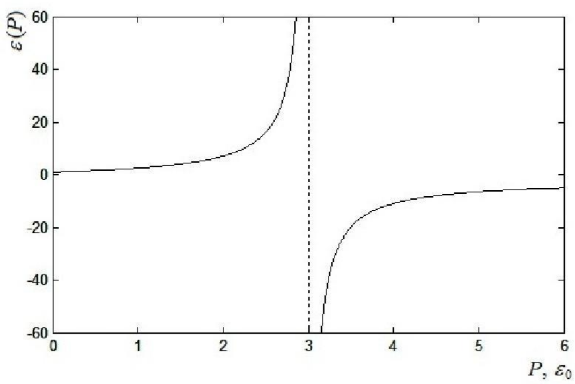

Figure 1. The dependence of the permittivity according to formula (5).

This circumstance leads to the generation of negative quantities of the dielectric transmittivity of actively polarized fused environments, calculated by means of Clausius-Mossotti formula.

3 Cybernetic Model of Effective Field Strength

As shown above, the general conclusion of complex dielectric permittivity formula by Lorenz-Lorentz-Clausius-Mossotti can be constructed only within the direct substitution of complex formula $\alpha(j\omega)$ in a static formula ε, i.e., by means of classical (inductive) approach to the description of the polarization characteristics of dielectric permittivity systems. In attempt to implement more current methods, namely systemic (deductive) approach, we will have to face such a situation: when considering the basic interpretation of polarization in dynamic pattern, we can get some not extend system of formulas, consisting of K linear-differential equations, using $K+1$ variable, which objectively determines the fundamental impossibility of finding a comprehensive solution with the help of function $\varepsilon(t)$:

$$\frac{d^2\mu_k(t)}{dt^2} + 2\beta_k\frac{d\mu_k(t)}{dt} + \omega_{0k}^2\mu_k(t) = \frac{q_k^2}{m_k}E(t), \quad (9)$$
$$k = \overline{1,K};$$
$$E(t) = \left(\frac{1}{(\varepsilon(t)-1)\varepsilon_0} + \frac{1}{3\varepsilon_0}\right)\sum_{i=1}^{K}\mu_i(t)N_i.$$

In order to eliminate this drawback and to represent the quantity of the average intensity of the macroscopic field as a part of the overall structure of function (3), it is proposed to adopt its basic expression (1) instead of the traditional formula (2).

In this case, the original system of formulas describing the dynamics of the total polarization of particles within the sample, using the model Lorentz-Mossotti approach, takes the following form [Kostyukov and Eremin, 2004; Eremin I., Eremin E. and Overchuk, 2005]:

$$\frac{d^2\mu_k(t)}{dt^2} + 2\beta_k\frac{d\mu_k(t)}{dt} + \omega_{0k}^2\mu_k(t) = \quad (10)$$
$$= \frac{q_k^2}{m_k}E(t), \quad k = \overline{1,K};$$
$$E(t) = E_0(t) - \frac{1}{\varepsilon_0}\sum_{i=1}^{K}\mu_i(t)N_i +$$
$$+ \frac{1}{3\varepsilon_0}\sum_{i=1}^{K}\mu_i(t)N_i.$$

Analyzing the formulas (10) from the point of Technical Cybernetics, we can conclude that they represent a mathematical model of some closed linear control system with negative feedback, therefore, simply converted to a second typical form of writing through the transfer functions:

$$\mu_k(s) = W_k(s)E(s), \; E(s) = W_\varepsilon(s)E_0(s), \quad (11)$$
$$W_k(s) = \frac{q_k^2/m_k}{s^2 + 2\beta_k s + \omega_{0k}^2}, k = \overline{1,K},$$
$$W_\varepsilon(s) = \frac{1}{1 + \frac{2}{3\varepsilon_0}\sum_{i=1}^{K}W_i(s)N_i},$$

where $\mu_k(s)$, $E(s)$ and $E_0(s)$ – Laplace's description of similar functions; s – complex variable; $W_k(s)$ and $W_\varepsilon(s)$ – imposed transfer function.

In addition, the cybernetic description of formulas (11) makes it possible to generate quite proper visualization of causal relationships between every single element of the formulas, units of physical systems, common entrance and output (see Figure 2) by means of well-known engineering methodology for constructing block diagrams and their equivalent transformations [Smith, 1980].

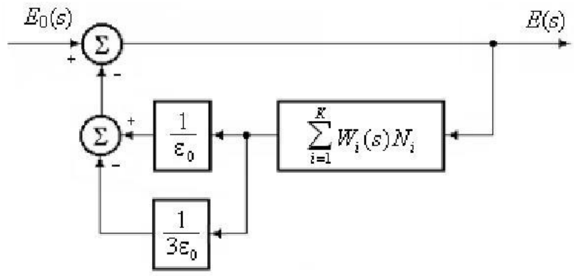

Figure 2. Block diagram corresponding to the cybernetic model of effective field strength, based on the concept of Lorentz's sphere.

To understand the physical nature of the entered transfer functions $W_k(s)$, describing the individual micro processes, as well as the transfer function for the mismatch $W_\varepsilon(s)$, which characterize the macroscopic interconnection of the external and effective fields, we can use their frequency analogues by implementing the replacement $s \to j\omega$ in complex formula (11):

$$W_k(j\omega) = \frac{q_k^2/m_k}{\omega_{0k}^2 - \omega^2 + j2\beta_k\omega}, \; k = \overline{1,K}; \quad (12)$$
$$W_\varepsilon(j\omega) = \frac{1}{1 + \frac{2}{3\varepsilon_0}\sum_{i=1}^{K}W_i(j\omega)N_i}.$$

After analyzing the overall structure of the functions $W_k(j\omega)$, we can conclude, that they are equivalent to the complex polarizability of particles (7). In turn, the frequency transfer function of $W_\varepsilon(j\omega)$ is not used in traditional physics of dielectrics, since it is a complex coefficient of intensifying, reversed to historical concept of the complex dielectric permittivity. However, considering the singularity of its numerator, the denominator $W_\varepsilon(j\omega)$ can objectively be regarded as a complete analogue of $\varepsilon(j\omega)$.

Thus, continuous deterministic mathematical transformations of the initial description of the processes of the formula (10), which is realized by means of automated control theory, enables to form cybernetic model of complex-dielectric constant for condensed sample [16, 17]:

$$\varepsilon(j\omega) = 1 + \frac{2}{3\varepsilon_0}\sum_{i=1}^{K}\alpha_i(j\omega)N_i. \quad (13)$$

Evaluating the formula as the dependence $\varepsilon(P)$, you will notice that this function is continuous and monotonically increasing. In other words, cybernetic can efficiently demonstrates the observed dependence of the dielectric constant of the sample on the polarization of the total quantity of its particles (Figure 3).

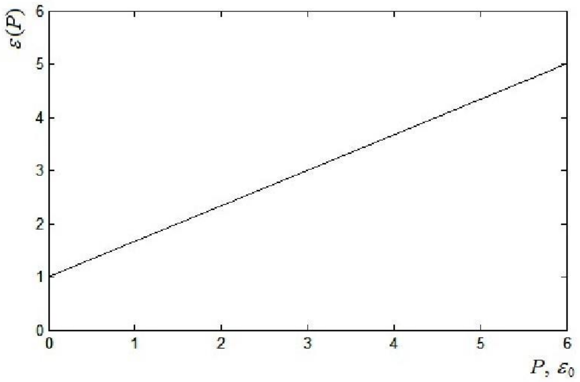

Figure 3. The dependence of permittivity according to formula (13).

Consequently, there is a fundamental fact, that excludes the possibility of “Mossotti disaster”, while considering any material. This has become evident by clarifying the mathematical description of causal relationships between the electric fields, operated in the condensed polarized dielectric, as the proposed cybernetic interpretation of the complex permittivity formula (13) entirely eliminates the drawbacks of Lorenz-Lorentz-Clausius-Mossotti formula (8).

4 Objective Reason for the Classic “Mossotti Disaster”

Let us try to identify the true cause of “Mossotti disaster”, using dielectric polarization representation by means of logical scheme, corresponding to the formula of Clausius-Mossotti. Firstly, let us present it as complex analogue to formula (8):

$$\varepsilon(s) = \frac{E_0(s)}{E(s)} = 1 + \frac{\frac{1}{\varepsilon_0}\sum_{i=1}^{K}\alpha_i(s)N_i}{1 - \frac{1}{3\varepsilon_0}\sum_{i=1} + K\alpha_i(s)N_i} \quad (14)$$

$$\alpha_k(s) = \frac{q_k^2/m_k}{s^2 + 2\beta_k s + \omega_{0k}^2}.$$

As it was mentioned above, a common function of the complex permittivity of the material is denominator of transfer function reflecting the dielectric mismatch fields, which numerator is equal to one. Therefore, complex formula by Lorenz-Lorentz-Clausius-Mossotti can be fully represented as a transfer functions:

$$W_\varepsilon(s) = \frac{E(s)}{E_0(s)} = \frac{1}{1 + \frac{\frac{1}{\varepsilon_0}\sum_{i=1}^{K}W_i(s)N_i}{1 - \frac{1}{3\varepsilon_0}\sum_{i=1}^{K}W_i(s)N_i}}; \quad (15)$$

$$W_k(s) = \frac{q_k^2/m_k}{s^2 + 2\beta_k s + \omega_{0k}^2}.$$

It should be noted that, the numerator of the transfer functions $W_\varepsilon(s)$ with feedback connections describes the direct channel elements, and its denominator expresses the amount and composition of forward and reverse channel units. In addition, it is necessary to take into account that the arithmetic sign inside the considered algebraic sum is determined by the type of feedback. For the positive connection it is a minus, and for negative it is a plus [Egupov et al., 2000].

Thus, using the method of structural schemes, based on the formula (15), we can receive a block diagram of the dielectrics polarization process (Figure 4), which completely coincides with Clausius-Mossotti formula.

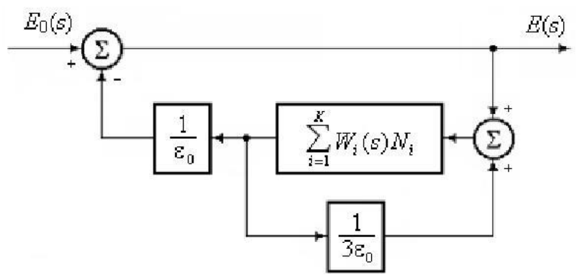

Figure 4. The block diagram corresponding to the classical Lorenz-Lorentz-Clausius-Mossotti formula.

On the one hand, it is obvious, that if following the overall structure of the formula (8), the first additional component of local field E_1 is included in the channel of main negative feedback (NFB), in the system being studied. In addition, the same element comes into its own positive feedback (PFB) with sum polarization of the sample. It is well known that the presence of the PIC between any of the elements of the system makes it unstable.

On the other hand, a block diagram of a cybernetic model of complex permittivity includes the same typical blocks. However, in the framework of its field, strength E_1 is only an optional module, which has no fundamental impact on the overall reverse channel configuration of the main NFG for physical system with a high degree of stability. In addition, the block diagram (Figure 2) is more consistent with the principle of superposition of fields, declared in the Lorentz model, as on the basis of its impact, the average macroscopic local fields are considered parallel. The structure of the second scheme (Figure 4) subjectively rated priority contribution to local field in relation with the depolarizing field, which contradicts the superposition principle.

It should be noted that the cybernetic model of the complex dielectric permittivity of condensed sample within the form (13), can be regarded as quite efficient in terms of practical modeling of polarization spectra, made of wide range of different materials [Kostyukov and Eremin, 2008; Eryomin, 2013; Eremin et al., 2010; Eremin et al., 2011; Eremin et al., 2014; Zhilindina and Eremin, 2012; Eremin, Zhilindina and Bartoshin, 2014; Eremin, Eremina and Zhilindina, 2014; Eremin, Eremina and Zhilindina, 2016]. Thus, we can conclude that the objective reason of "Mossotti disaster" is not the proposed approximation, but the formal misrepresentation of casual relationships between the components of the field, effectively operating within the polarized sample, arose as of inductive inference procedures of static formulation by dielectric permittivity according to Clausius-Mossotti formula.

5 Selecting of Low-Frequency Polarization Process

The essence of the polarization phenomena, excited by the changed electromagnetic field of low amplitude to any dielectric system, is regarded as a deviation of its constituent charged micro particles from their original state. All this leads to the forced electromagnetic-induction of the dipole moments, weakening the tension of electric field, induced in the test sample, quite effectively. At the same time, taking into account the different levels of persistence of certain processes, caused by significant difference of elementary mass particles involved, the traditional modeling of dielectric spectra have to be synthesized with detailed mathematic description of the system under study, realized within the sequence transition from the fastest physical reactions to slow ones.

On the other hand, if the interests of the researchers are limited by only inertial processes, eg. elastic electron oscillations of so-called dielectric particles, than such an approach is considered entirely effective in terms of overall labor costs. On the other hand, if the researcher's purpose is to study any inertial processes, for example, elastic ionic, dipole or elastic relaxation polarization of the sample, then the description of the previously established electromagnetic oscillations is an additional difficulty, overcoming which does not fundamentally affect the final scientific results.

In order to simplify the given situation, i.e. for obvious understanding of arbitrarily chosen polarization process K, it is proposed to replace the cybernetic complex of dielectric constant of the general form of the sample (13) into more private interpretation:

$$\varepsilon(j\omega) = 1 + \sum_{i=1}^{K-1} \chi_i(j\omega) + \frac{2}{3\varepsilon_0}\alpha_k(j\omega)N_k; \quad (16)$$

$$\alpha_K(j\omega) = \frac{q_K^2/m_K}{\omega_{0K}^2 - \omega^2 + j2\beta_K\omega},$$

where $\chi_i(j\omega)$ – table data of frequency functions for complex dielectric susceptibility, characterizing polarization contributions before low-inertia processes settings.

Using the method described above, with the help of formula (16) we can form a structural diagram of field-emitted polarization process (Figure 5). It should be noted that the proposed scheme can not only be directly used for imitation modeling of transient process, characterizing the studied type of oscillations, but also its resulting graph won't include transients processes of less inertial oscillations, which are specified by their static contributions.

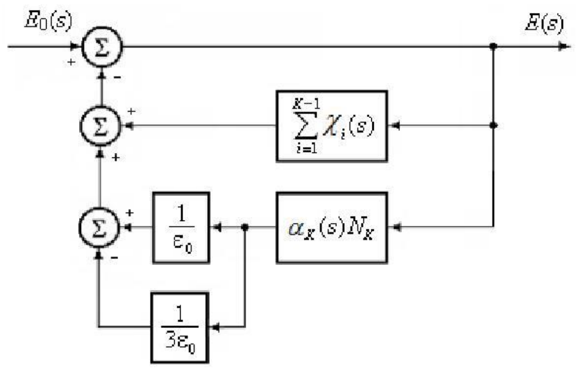

Figure 5. Block diagram, identifying the resulting contribution of dedicated low-frequency polarization process.

It is quite obvious that the described approach complicates the technology of preparation of input data. In turn, optical measurements as indicators of dielectric materials are considered physically accessible for practical researching. But in definite form they carry the necessary information about the missing parameters of electromagnetic oscillations for each individual dielectric particles. That's why they require more detailed processing of experimental quantities, conducted on the basis of theoretical models [Zolotarev et al., 1984]:

$$\varepsilon_{\mathrm{Re}}(\omega) = n^2(\omega) - X^2(\omega); \qquad (17)$$
$$\varepsilon_{\mathrm{Im}}(\omega) = 2n(\omega)X(\omega),$$

where $\varepsilon_{\mathrm{Re}}(\omega)$ and $\varepsilon_{\mathrm{Im}}(\omega)$ – real and imaginary parts of the complex dielectric transmittivity; $n(\omega)$ and $X(\omega)$ – table data, showing the frequency dependence on fraction and absorption, based on the quality of absorbing material and luminous flux. This data was formed according to physical experiments available in the existing scientific literature, see eg. [Li, 1976].

Thus, the complex of formulas (16) and (17) allows generating the following final formula for the frequency dependencies of physical characteristics that can be used directly for the application of scientific and technological calculation of the resulting spectra:

$$\begin{aligned} \varepsilon_{\mathrm{Re}}(\omega) &= n^2(\omega_{\min}) - X^2(\omega_{\min}) + \\ &+ \frac{2N_k q_k^2}{3\varepsilon_0 m_k} \cdot \frac{\omega_{0K}^2 - \omega^2}{\left(\omega_{0K}^2 - \omega^2\right)^2 - \left(2\beta_K\omega\right)^2}; \\ \varepsilon_{\mathrm{Im}}(\omega) &= 2n(\omega_{\min})X(\omega_{\min}) + \\ &+ \frac{2N_k q_k^2}{3\varepsilon_0 m_k} \cdot \frac{2\beta_K\omega}{\left(\omega_{0K}^2 - \omega^2\right)^2 - \left(2\beta_K\omega\right)^2}, \end{aligned} \qquad (18)$$

where $\omega_{\min}$ – left border of the frequency range under study.

In conclusion of this section, we must note that the particular quantity of $n(\omega_{\min})$ and $X(\omega_{min})$ should be chosen in such a way, that their complex can guarantee the minimum quantity of function $\varepsilon_{\mathrm{Re}}(\omega)$.

6 Conclusion

It is obvious that any real physical process is always non-linear. However, mathematical models of forced electric deformation of crystalline micro particles, which are under study, can be quite properly represented by formulas of linear harmonic oscillation with friction. This, on the one hand, stimulates the integration of the fundamental provisions of the classical physics of dielectrics with mathematical methods of classical control theory. On the other hand, it makes overall perspective of dielectric spectra of crystals modeling more efficient for further observations.

Generally, any theoretical concept is the result of instrumental studies of the world in case of using fundamental laws and principles that connect the studied physical phenomenon with its internal characteristics. This connection also determines the relationship between the properties of the object being studied with internal structure. In other words, the proposed approach of constructing cybernetic description of the interaction dielectric substances with weak electromagnetic fields can be valuable not only for the development of traditional polarization theory, but also can be used in the formation of a modern system of knowledge on condensed matter physics as a whole.

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