

Mathematical Methods for Indirect Visualization of the Electronic Structure of Diamond

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Abstract

Background/Objectives: The relevance of the work described in this study due to the fact that even the allotropic modification of carbon - diamond has a very complex internal structure and many of its physical and chemical properties still have no clear scientific interpretation. In this theoretical model that exist within the relevant field of knowledge on the one hand, more or less satisfactorily explain only some of the observed phenomena, often engaging in an insoluble contradiction with one another. In addition, the available experimental data and is clearly insufficient, since they do not allow real detail investigated the structure due to the practical impossibility of using technical means of modern microscopy. In this context, this article aims to identify the traditional paradigm of “composition - structure - properties”, implemented against the background of a clear link between the conservation of the original visual model of e-sample configuration and formed on its basis and the resulting mathematical description of the dynamic characteristics. **Method:** The basic approach to the study of physical and chemical properties of the material in question is their learning through computer modeling of continuous frequency spectrum of the imaginary part of a complex electronic polarizability. An important part of the method used is the indirect visualization of electron atomic structure of the unit cell of the diamond. This visualization of the structural features of the crystal parsed performed by the spatial geometric modeling nodal points of its nuclear atomic skeleton, surrounded by electron shells of a certain configuration. For indirect identification of necessary geometrical parameters include relatively simple computational methods that rely on the use of a small number of easily generated experimental data. In turn, the definition of geometric parameters of the electronic configuration of particulate matter can be realized by optimizing the frequency characteristics of an elastic electronic polarization. It is proposed to use the original “cybernetic” model of these processes, created on the basis of the classical theory of the polarization of the preconditions given explicit allocation of causality, objectively existing in the traditional description of the Lorentz local field strength. **Findings:** The article presents the results of simulation of continuous frequency spectrum of the imaginary part of a complex electronic polarizability of the diamond based on the consideration of physical models, which were calculated in the framework of the described techniques. Comparing the data of physical experiment, the traditional interpretation of covalent diamond connection with the results of a computational experiment, it should be noted that the use of the existing model does not allow to achieve high-quality real-compliance and the model spectra. The differences lie in the presence of the physical characteristics of a complex dual-output, and on the simulated curve - single output. In addition, the use of core-electron interpretation electronic diamond configuration does not allow to achieve high-quality real-compliance and the model spectra, obtained on the basis of a simulation of the spectrum. In this case, the differences lie in the displacement of the simulated electron emission caused by the polarization of core-electron pairs in the region of deep electronic resonances. However, the authors proposed a modified model of the carbon of the diamond connection allows you to get it close enough to the dielectric characteristics of the data of physical experiment. Thus, a modified model of the structure of the internal structure of the material allows for the most precise study of its optical properties. **Improvements:** Practical use the mathematical techniques of mediated visualization of the electronic structure of the diamond should be useful for the further evolution of the theoretical foundations of modern nanotechnology.

Keywords: Crystal Lattice Type, Cybernetic Model of Dielectric Permeability, Electronic Configuration

1. Introduction

It is now generally accepted that the development of modern nanotechnologies must be based on the reciprocal integration of research methods that are characteristic of scientific disciplines which until recently were considered independent. Clear knowledge of the characteristics of matter manifested at the level of the internuclear distances opens up effective possibilities for the development of new technological methods of physical-chemical synthesis of new structural materials and creation of high-tech devices designed on their basis¹.

Owing to the unique physical and chemical properties, diamond is a popular object research fulfilled in the most diverse science and technology fields. In addition, it is generally considered as a classical model of a crystal that is theoretically studied in the electron theory of the solid body, because of simple interatomic bonds and the structure of the unit cell being characteristic of diamond^{2,3}.

It is known that the most complete information about the features of the electronic structure of any test sample is enclosed in a complex of its fundamental optical functions, representing the frequency (or equivalent to them – long-wave, wave, and electron-volt) dependencies: transmission $T(\omega)$, absorption $A(\omega)$ and reflection $R(\omega)$ coefficients; the refractive $n(\omega)$ and absorption $\chi(\omega)$ indices; the real $\epsilon_1(\omega)$ and imaginary $\epsilon_2(\omega)$ characteristics of the complex dielectric permittivity $\epsilon(j\omega)$. All these functions are directly related to each other, and their physical essence and the mutual coherence are the result of classical Maxwell equations⁴.

The problem of determining the fine structure parameters of optical transitions of a definite crystal (energies E_i and half-widths H_i of electron resonances, as well as the forces f_i of the appropriate electronic oscillators) is usually solved by one of two techniques of the modern quantum mechanical calculations⁵. First, by reproducing an integral curve $\epsilon_2(\omega)$ using the set of K Lorentzian oscillators set out by a large number of adjustable parameters $3K$ (up to 30 for $K=10$). Secondly, on the basis of the merged Argand diagrams, also based on the use of classical model of Lorentz electronic oscillator, but eliminating the need to adjust the dynamic parameters of the electronic polarization processes due to the simultaneous analysis of the spectra of $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$.

It is quite obvious that own parameters of the oscillation equations describing the studied processes depend

on the theoretical interpretation of the electronic configuration of chemical bond.

The considered chemical bonds are often described on the basis of theoretical ideas about the formation of hybrid orbitals. Under this common interpretation, diamond has sp^3 hybridization which is realized by mixing the electron shells of valent s- and p-orbitals⁶. In this case four formed hybrid orbitals providing physical existence of single carbon bonds of the form C – C (Figure 1), are directed to the vertices of a tetrahedron with an atomic core of carbon located in its center.

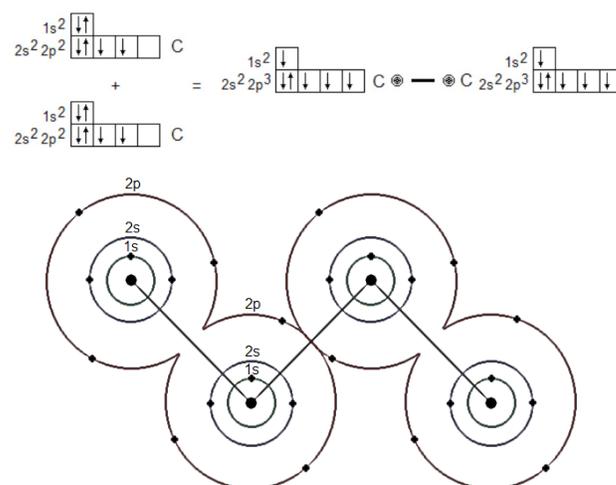


Figure 1. The traditional interpretation scheme of C – C carbon bond formation.

The results of rather recently performed applied research⁷ proved that efficiency of mathematical modeling of optical and dielectric spectra of substances possessing a polar covalent chemical bond can be considerably increased due to its purely ionic interpretation.

2. Concept Headings

Thus, within modified interpretation of the mechanism for implementation of the non-polar covalent bond arising for each couple of the neighboring atoms of diamond it is supposed that a half of them passes into a cationic condition of C^{4+} , and another half – into an anion condition of C^{4-} (Figure 2).

The main advantage of the modifications offered by the authors is that on their base it becomes possible to consider carbon particles in the form of the incompressible ionic spheres possessing a complicated electronic

structure. Rather adequate mathematical model of their elastic electronic polarization can be described by means of the relevant system of the linear differential equations such as:

$$\frac{d^2 \mu_k(t)}{dt^2} + 2\beta_k \frac{d\mu_k(t)}{dt} + \omega_{0k}^2 \mu_k(t) = \frac{2e^2}{m_e} E(t), \quad k = \overline{1, 6};$$

$$E(t) = E_0(t) - \frac{2}{3\epsilon_0} N \sum_{i=1}^6 \mu_i(t), \quad (1)$$

where $m_k(t)$ - temporal variation functions of induced dipole moments inherent in the electronic orbital of a particular type; β_k and ω_{0k} - attenuation coefficients and frequencies of their own fluctuations; q_k - the number of electrons inhabiting the electronic orbital; e and m_e - charge and mass of an electron; $E(t)$ - the function of effective field intensity; $E_0(t)$ - external field intensity; ϵ_0 - dielectric permeability of vacuum; N - volume concentrations of the C-C bonds.

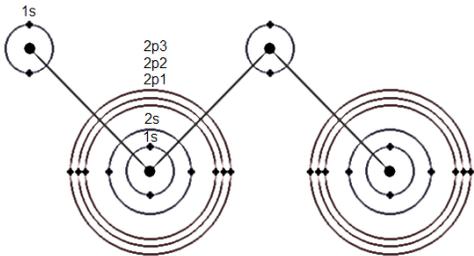
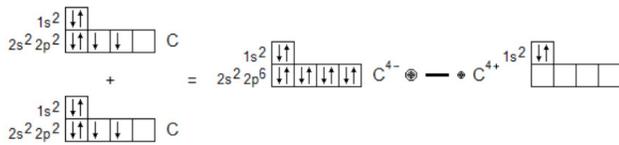


Figure 2. The modified interpretation scheme of C - C carbon bond formation.

The initial description of the studied processes of the type (1) results in the cybernetic model of complex dielectric permeability of diamond using the equations of complex polarizabilities of $\alpha_k(j\omega)$ of each considered electronic couples⁸⁻¹²:

$$\epsilon(j\omega) = 1 + \frac{2}{3\epsilon_0} N \sum_{i=1}^6 \alpha_i(j\omega);$$

$$\alpha_k(j\omega) = \frac{2e^2/m_e}{\omega_{0k}^2 - \omega^2 + j2\beta_k\omega}, \quad k = \overline{1, 6}. \quad (2)$$

To perform utilitarian calculations of eigen frequencies of forced electromagnetic oscillations of each orbital it is possible to apply the following formulas:

$$\omega_{0k}^2 = \frac{Q_k e^2}{4\pi\epsilon_0 m_e r_k^3}, \quad r_k = \frac{n_k^2 \hbar^2}{Q_k e^2 m_e}, \quad k = \overline{1, 6}, \quad (3)$$

where Q_k - the effective charge of the atomic core influencing the preset electronic orbital; r_k - the spherical electronic orbit radius; n - the main quantum number of an orbital; \hbar - the Planck constant.

In turn, to determine the values of atomic core charges influencing effectively electrons of certain orbitals it is possible to apply the methods for description of a linear combination of atomic orbitals (MD LCAO) characterizing well the internal energy of various crystals. Slater-type atomic orbitals are considered to be the best MD LCAO. Moreover, the value of an effective charge Q is connected with serial number Z of a chemical element and the value s of its kernel shielding with internal electron shells.

Numerical value of s is calculated by grouping orbitals according to shells ($1s$), ($2s$, $2p$), ($3s$, $3p$), ($3d$), ($4s$, $4p$), ($4d$), ($4f$), etc., representing the sum of the shielding contributions made by electrons of each group.

Taking into consideration that the empirical Slater's technique was initially developed for stationary atoms of substance, its modified option should be used to increase the efficiency of the performed calculations^{8,13,14}. On the basis of this option effective charges of electronic orbitals of diamond particles can be presented as:

$$Q_{1s^2} = Z - \sigma_1; \quad (4)$$

$$Q_{2s^2} = Z - \sigma_2; \quad Q_{2p_x^2} = Z - \sigma_3; \quad Q_{2p_y^2} = Z - \sigma_4; \quad Q_{2p_z^2} = Z - \sigma_5,$$

where s_1 - the standard value of the shielding contribution of electrons of a $1s$ -orbital equal 0.30; $s_2 \dots s_5$ - the shielding contributions of external (optical) electrons of C^+ anion optimized with regard to the appropriate quantity of internal electrons on the basis of physical experiment data.

Calculation of attenuation coefficients of electronic fluctuations β_k according to classical formulas is not quite accurate, so it is expedient to consider their values in general:

$$\beta_k = b_k \omega_{0k}, \quad k = \overline{1, 6}, \quad (5)$$

where b_k - proportionality coefficients optimized on the basis of physical experiment data.

Concentration of single-point carbon bonds C-C existing for the unit of volume of the studied sample can be calculated as:

$$N = \rho / m, \quad (6)$$

where ρ – material density; m – total mass of the bonded particles.

Besides, the optimized values s_k and b_k can be presented in the following form (Table 1):

It should be noted that traditional disclosure of internal structure of substance is based on the direct fixing of an electronic and nuclear structure of certain nanostructures which is carried out by means of the expensive instrument equipment and requires special technological processing of the studied samples. On the other hand, visualization of structural features of nano systems can be executed by spatial geometrical modeling the location of the nodal points of their atomic and nuclear frame surrounded with electron shells of a certain configuration.

Taking the position of any particle of a crystal as the beginning of a three-dimensional orthogonal reference system, coordinates of the particles of its immediate environment making the structure of the considered type can be rather simply expressed through the value of internuclear distance in its formula unit. Besides, the stereochemical formulas considering the type of a crystal lattice can be applied to calculate internuclear distances R .

In turn, knowing g coefficient of lattice compactness of the studied crystal, as well as values of its molecular weight and tabular value of physical density it is possible to use equation:

$$R = \sqrt[3]{\frac{\gamma \cdot m}{\rho}}. \quad (7)$$

Moreover, on the basis of alternative interpretation of C-C carbon bond formation each couple of neighboring

atomic nodes will be populated with the ionized particles of C^{4+} and C^{4-} carbon.

It should be mentioned that the theoretical calculation of internuclear distances of diamond realized by the formula (7) for the g value = $3\sqrt{3}/16$ corresponding to a diamond-like lattice gives value $R = 1.545 \cdot 10^{-10}$ m that completely coincides with data of the corresponding physical measurements.

In this case, considering formulas of the type (3), a direct definition of the geometrical dimensions of electron shells of C^{4+} and C^{4-} particles formed by the set of the corresponding electronic orbitals can be realized on the basis of the calculated data given in Table 2.

Results of the mediated visualization of an electronic and nuclear structure of an elementary cell of diamond are shown in Figure 3.

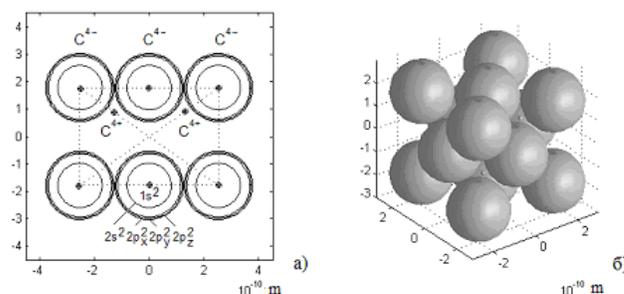


Figure 3. The mediated visualization of a diamond crystal lattice: a) the diagonal plane section; b) three-dimensional structure model.

Thus, the main advantage of the approach offered by the authors is the possibility of rather reasonable visualization of the nanostructure of materials, which is carried

Table 1. Optimized values s_k and b_k

Value	Electronic orbitals				
	$1s^2$	$2s^2$	$2p_x^2$	$2p_y^2$	$2p_z^2$
s_k	0,30	3,38	4,16	4,24	4,30
b_k	0,001	0,100	0,050	0,150	0,100

Table 2. Calculation data

Value	Electronic orbitals				
	$1s^2$	$2s^2$	$2p_x^2$	$2p_y^2$	$2p_z^2$
$w_{0k}, 10^{16}$ rad/s	134,32	3,5473	1,7496	1,6007	1,4935
$r_k, 10^{-10}$ m	0,0928	0,8079	1,1504	1,2027	1,2451

out using its easily measured macro parameters realized in its framework. Besides, this method is almost acceptable for studying the samples in various aggregate states, thus the level of specification of internal structure of substance is higher, than at modern means of high resolution electronic microscopy.

3. Result

On the basis of a visual picture of the physical model (Figure 1) with regard to the corresponding configuration of the electronic orbitals of the individual particles of carbon which determines the specific numeric values of its own parameters q_k , within the structure of the system of equations of the general form (1), it becomes possible to form the following initial mathematical description:

$$\begin{cases} \frac{d^2 \mu_{1s}}{dt^2} + 2\beta_{1s} \frac{d\mu_{1s}}{dt} + \omega_{01s}^2 \mu_{1s} = \frac{e^2}{m_e} E(t) \\ \frac{d^2 \mu_{2s}}{dt^2} + 2\beta_{2s} \frac{d\mu_{2s}}{dt} + \omega_{02s}^2 \mu_{2s} = \frac{2e^2}{m_e} E(t) \\ \frac{d^2 \mu_{2p}}{dt^2} + 2\beta_{2p} \frac{d\mu_{2p}}{dt} + \omega_{02p}^2 \mu_{2p} = \frac{3e^2}{m_e} E(t). \end{cases} \quad (8)$$

Standard conversions of the presented system of equations allow obtaining the imaginary frequency response of the electronic polarizability of the test material:

$$\begin{aligned} \alpha_{1s}''(\omega) &= \frac{e^2}{m_e} \cdot \frac{2\beta_{1s}\omega}{(\omega_{01s}^2 - \omega^2)^2 + 4\beta_{1s}^2\omega^2} \\ \alpha_{2s}''(\omega) &= \frac{2e^2}{m_e} \cdot \frac{2\beta_{2s}\omega}{(\omega_{02s}^2 - \omega^2)^2 + 4\beta_{2s}^2\omega^2} \\ \alpha_{2p}''(\omega) &= \frac{3e^2}{m_e} \cdot \frac{2\beta_{2p}\omega}{(\omega_{02s}^2 - \omega^2)^2 + 4\beta_{2p}^2\omega^2}. \end{aligned} \quad (9)$$

On the basis of the considered mathematical model a computational experiment has been carried out aimed at complex crystal permittivity simulation, within which the numerical values of dynamic parameters β_k and ω_{0k} of the considered processes can be defined by abstract values proceeding from the mutual ratio of the radii of the appropriate electronic orbits. It is necessary to take into account that the lower natural vibration frequency and higher attenuation coefficient are typical of an orbit with a larger radius¹⁵.

The results of the simulation that was carried out in the MatLAB software environment based on equations (8) and (9) are shown in Figure 4.

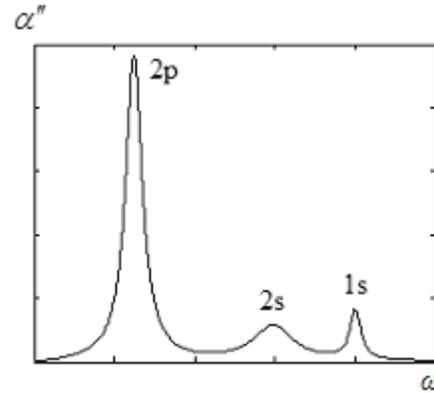


Figure 4. The simulation spectrum of the electronic polarizability of the diamond corresponding to the traditional interpretation of the covalent bond.

Spanning-electronic approach as a theoretical foundation for the explanation of the constitution and properties of minerals is based on the idea that any mineral, regardless of the type of chemical bond, consists of positively charged atomic cores (both metal and non-metal) and bonding or shared valence electrons¹⁶.

To clarify the physical meaning of the model, the crystal structure can be represented in the form of a “skeletal frame” formed by positive atomic cores that are localized in the lattice and cemented with binding electronic clouds. The latter, having certain volume negative charges function as a kind of spacers between the positive atomic cores. The requirement of comprehensive environment (screening) of the atomic cores with binding electronic clouds is obligatory when it is violated, the structure cannot be considered stable by the virtue of mutual repulsion of equally charged atomic cores (Figure 5).

On the basis of a visual picture of the physical model (Figure 5), given a corresponding proportion of the electronic cores binding the atomic cores of the individual particles of carbon and equal to 2:1, it becomes possible to form the following initial mathematical description:

$$\begin{cases} \frac{d^2 \mu_{1s}}{dt^2} + 2\beta_{1s} \frac{d\mu_{1s}}{dt} + \omega_{01s}^2 \mu_{1s} = \frac{2e^2}{m_e} E(t) \\ \frac{d^2 \mu_{2e}}{dt^2} + 2\beta_{2e} \frac{d\mu_{2e}}{dt} + \omega_{02e}^2 \mu_{2e} = 2 \frac{2e^2}{m_e} E(t). \end{cases} \quad (10)$$

The simulation results are shown in Figure 6.

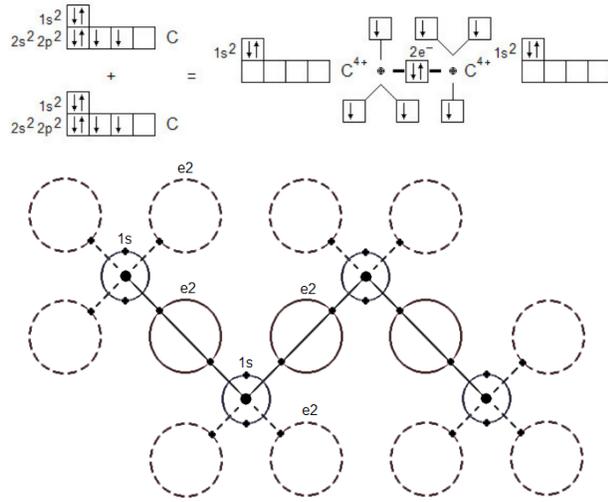


Figure 5. Scheme of spanning-electronic interpretation of the electronic configuration of diamond.

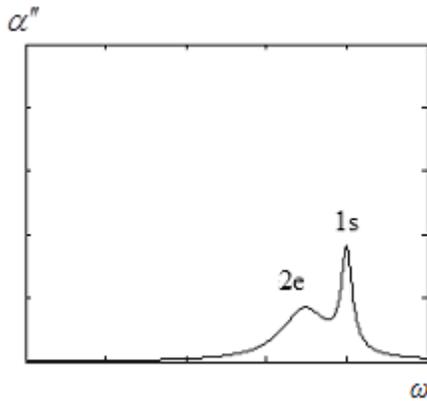


Figure 6. The simulation spectrum of the electronic polarizability of diamond corresponding to the spanning-electronic interpretation of covalent bonds.

$$\left\{ \begin{aligned} \frac{d^2 \mu_{1s}}{dt^2} + 2\beta_{1s} \frac{d\mu_{1s}}{dt} + \omega_{01s}^2 \mu_{1s} &= \frac{2e^2}{m_e} E(t) \\ \frac{d^2 \mu_{2s}}{dt^2} + 2\beta_{2s} \frac{d\mu_{2s}}{dt} + \omega_{02s}^2 \mu_{2s} &= \frac{1}{2} \frac{2e^2}{m_e} E(t) \\ \frac{d^2 \mu_{2p1}}{dt^2} + 2\beta_{2p1} \frac{d\mu_{2p1}}{dt} + \omega_{02p1}^2 \mu_{2p1} &= \frac{1}{2} \frac{2e^2}{m_e} E(t) \\ \frac{d^2 \mu_{2p2}}{dt^2} + 2\beta_{2p2} \frac{d\mu_{2p2}}{dt} + \omega_{02p2}^2 \mu_{2p2} &= \frac{1}{2} \frac{2e^2}{m_e} E(t) \\ \frac{d^2 \mu_{2p3}}{dt^2} + 2\beta_{2p3} \frac{d\mu_{2p3}}{dt} + \omega_{02p3}^2 \mu_{2p3} &= \frac{1}{2} \frac{2e^2}{m_e} E(t). \end{aligned} \right. \quad (11)$$

On the basis of a visual picture of the physical model (Figure 2), with regard to the appropriate proportions of electron pairs, occupying the electronic orbitals of allocated types, it becomes possible to form the following initial mathematical description:

With reference to expression (11) the imaginary frequency response of the complex electronic polarizability takes the form:

$$\begin{aligned} \alpha''_{1s}(\omega) &= \frac{2e^2}{m_e} \cdot \frac{2\beta_{1s}\omega}{(\omega_{01s}^2 - \omega^2)^2 + 4\beta_{1s}^2\omega^2} \\ \alpha''_{2s}(\omega) &= \frac{e^2}{m_e} \cdot \frac{2\beta_{2s}\omega}{(\omega_{02s}^2 - \omega^2)^2 + 4\beta_{2s}^2\omega^2} \\ \alpha''_{2p1}(\omega) &= \frac{e^2}{m_e} \cdot \frac{2\beta_{2p1}\omega}{(\omega_{02p1}^2 - \omega^2)^2 + 4\beta_{2p1}^2\omega^2} \\ \alpha''_{2p2}(\omega) &= \frac{e^2}{m_e} \cdot \frac{2\beta_{2p2}\omega}{(\omega_{02p2}^2 - \omega^2)^2 + 4\beta_{2p2}^2\omega^2} \\ \alpha''_{2p3}(\omega) &= \frac{e^2}{m_e} \cdot \frac{2\beta_{2p3}\omega}{(\omega_{02p3}^2 - \omega^2)^2 + 4\beta_{2p3}^2\omega^2}. \end{aligned} \quad (12)$$

The simulation results are shown in Figure 7.

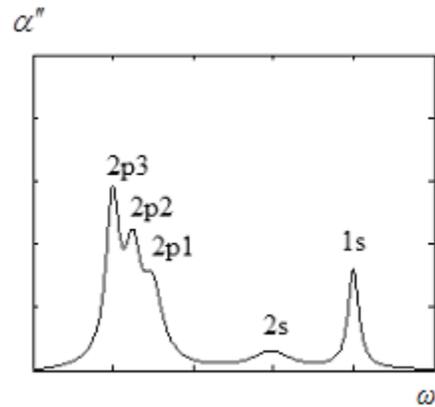


Figure 7. The simulation spectrum of the electronic polarizability of diamond corresponding to the pure ionic interpretation, covalent bonds.

4. Discussion

Comparing the simulation spectrum of the electronic polarizability of the diamond corresponding to the physical model (Figure 1), with their physically observable counterparts (Figure 8) it should be noted that:

- resonance ejection of the 1s-orbital, being a part of the atomic core, should be located in the X-ray spectrum, therefore, it cannot be considered during the analysis of the general adequacy of the studied model since the control data cover only the area of ultraviolet frequencies.
- simulated 2s-orbital resonance ejection can be correlated with weakly pronounced absorption band of the diamond, physically observed in the right part of the spectrum in the region of 23 electron volts.
- the applied traditional interpretation of hybridized orbitals (Figure 2) determines the feasibility of simulating a single strongly pronounced resonance ejection characterizing the elastic deformations of the 2p-orbitals. At the same time physical experiment indicates the presence of more complex spectral pattern, namely the existence of another small absorption band observed in the region of 7.5 electron volts.

Analyzing the overall effectiveness of the practical application of the spanning - electronic interpretation of the carbon bond formation (Figure 2), it can be stated first, introduction similar electronic cores represented by the electron pairs into the consideration leads to the mathematical generation of a single resonance ejection superseding the absorption bands formed by the oscillation of 2s- and 2p-orbitals; second, the simulated resonance ejection of the electronic cores (taking into account the possible geometric size of the respective spheres) is revealed objectively in the region of high frequencies included in the X-ray spectrum or the deep ultraviolet.

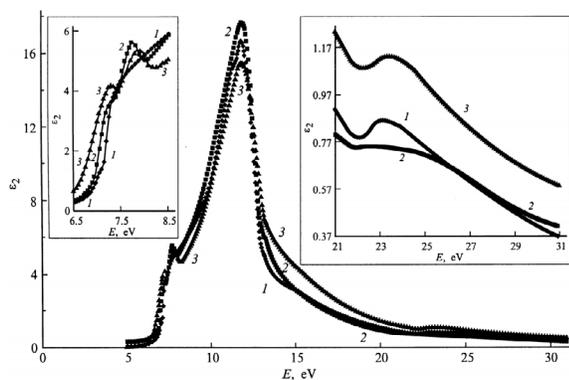


Figure 8. Electron-volt spectra of the imaginary part of the dielectric permeability of diamond.

Comparing the general view of absorption bands of specific electronic orbitals occurring on the theoretical curve with their physically observable counterparts, it should be noted that the considered ion interpretation of the carbon bond formation, on the one hand, retains the previously mentioned advantages of the model of hybridized orbitals concerning the location of the resonant ejections of the 1s - and 2s-electrons; and on the other hand, it also corrects the identified deficiency of the traditional interpretation, as it enables to model complex spectral picture of electronic polarization of the 2p-orbitals.

Figure 8 shows reflection spectra of three different samples of diamond (Nos. 1, 2, 3), the inserts illustrate spectra in the regions of 6.5 – 8.5 and 21 – 31 eV¹⁷.

5. Conclusion

As is known, computer simulation represents one of the types of theoretical study of physical reality. In most cases, any cognitive activity is based on the generalization of empirical knowledge obtained as a result of a series of experiments, including computing. It should be noted that the results of computational experiments directly depend on the used mathematical models describing the studied system, and accordingly taken in the course of its construction assumptions.

Thus, any theoretical concept becomes a productive tool of cognition of the surrounding world only when it is established laws or regularities linking specific physical phenomenon and its inner essence, and defined the relationship between the properties of the studied object and its structure. From this point of view proposed a systematic approach to the construction of efficient mathematical description of electronic polarization of a crystal may be useful not only for the theory of polarization of dielectrics, but also to improve the system of knowledge in physics of condensed state as a whole. In addition, the key value of this publication is the possibility of a well-founded visualization of the nanostructure of the materials conducted on the basis of the use of its easily measurable macroparameters. In addition, this method is practically acceptable for studies of samples in different states of aggregation, the level of detail of the internal structure of the substance is higher than that of modern means of electronic microscopy of high resolution.

6. Acknowledgement

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