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Effective conductivity of microwave dielectric materials

Dielectric losses, that characterize the transformation of electrical energy into heat energy, are an important electro-physical parameter of the dielectrics. In fact these losses are determined by the material's effective conductivity, so it is one of the most practical characteristics. Therefore, this article describes the main loss mechanisms and their contribution to the microwave effective conductivity of the dielectric materials. The frequency dependence of the effective conductivity is analyzed. References 3, figures 5.

Keywords: *dielectric materials; loss factor; loss angle tangent; dielectric permittivity; conductivity.*

I. Introduction

Analysis of modern trends in microelectronics shows that the main directions of development in this industry are increasing of integration degree, finding new circuit solutions, new materials and advanced technologies. Hence further progress need new materials with a given set of properties. However, creating such materials is impossible without a fundamental study of their physical properties. Research in this direction occurs all over the world. At the present moment, there are many models that describe different properties of dielectric materials. However, this area of investigations can't be considered as a complete.

There are two aspects of the losses as one of microwave dielectric parameter. Firstly, loss factor is used to describe a quality factor (Q) of dielectric material, in this case a loss-angle tangent ($\tan\delta = 1/Q$) is applied. This is very important parameter for the resonant circuits, such as dielectric resonators.

Secondly, in many microwave devises microwave heating is a key factor; in this case an effective conductivity (σ) should be used. Just this parameter describes the conversion of microwave energy into a heat. It concern to various microstrip devices, antennas, etc.

Clear understanding of effective conductivity nature needs to study the mechanisms of dielectric losses and their contribution to the conductivity of dielectric materials. Therefore, the aim of this paper is to study the physical mechanisms of dielectric materials microwave conductivity.

II. The effective conductivity mechanisms of dielectrics

There are three main parameters that characterize losses in dielectrics: electrically induces heat power density p, loss coefficient ε'' and loss tangent $\tan\delta$. They are depicted as:

$$p = \sigma E^2,\ \varepsilon^* = \varepsilon' - i\varepsilon'',\ \tan\delta = \frac{\varepsilon''}{\varepsilon'}, \quad (1)$$

where ε^* is the complex permittivity which consists of real (ε') and imaginary (ε'') parts and σ is specific conductivity which related to the loss coefficient as:

$$\sigma = \omega\varepsilon_0\varepsilon'', \quad (2)$$

where ω is cyclic (angular) frequency, ε_0 is dielectric permittivity of the vacuum.

Dielectric losses mechanisms are quite different. As one case, the frequency dispersion of the dielectric permittivity has a resonant nature and shows as a maximum so a minimum in the $\varepsilon'(\omega)$ dependence (Fig. 1 curve 2′). The other mechanism has a relaxation nature of dispersion that is characterized by the gradual decrease of in the $\varepsilon'(\omega)$ dependence while dispersion (Fig. 1 curve 1′).

However, in both cases, the loss factor $\varepsilon''(\omega)$ is characterized by a maximum that is very diffusive in the case of relaxation (Fig. 1 curve 1″) but rather sharp for the resonant spectrum (Fig. 1 curve 2″). As usual, in the selected gigahertz interval, the only tails of these mechanisms of dipersion are observed. However, in some ferroelectric materials the relaxation type or the resonant type of dielectric dispersion happens just at the microwaves.

In the gigahertz frequency domain the only fast mechanisms of dielectric polarization can determine the dielectric constant, namely, the elastic shift of electronic orbitals (optical polarization) and reciprocal elastic shift of ionic sublattices (far-infrared polarization). Dynamic properties of both fast polarization mechanisms are described by the Lorentz oscillator model.

However, in addition to the oscillator model (that corresponds to far- infrared polarization, Fig. 1, curve *2″*), dielectric losses at the microwaves might be the footprints of relaxation of a number of comparatively slow polarization mechanisms (electronic defects, ionic defects, various kind of dipoles, etc.) that are described by the Debye model of relaxation, Fig. 1, curves *1″*. All of these mechanisms give some contributions to conductivity.

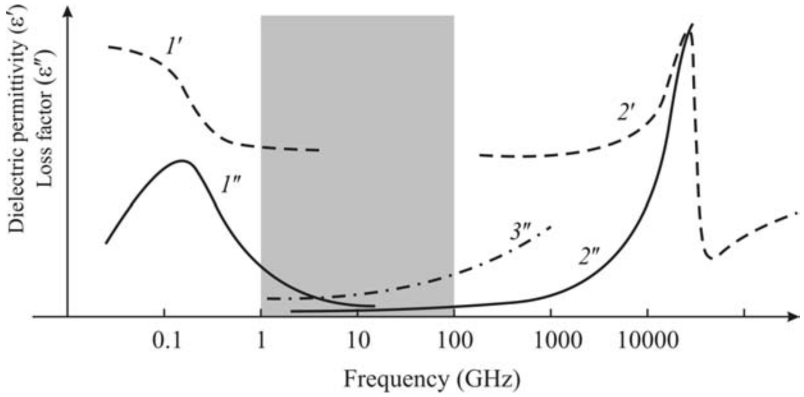

Fig. 1. Typical dielectric relaxation (*1*) and resonant (*2*) dielectric spectra where ε′(ω) are curves *1′* and *2′* while ε″(ω) are marked by the *1″* and *2″*. Gigahertz diapason is shaded, and the curve *3″* shows polar phase losses

II.1. Relationship between conductivity and losses

In dielectrics, the only a small portion of electric charge (free carries) contributes to the conductivity, whereas the polarization is the result of the displacement (separation) of practically all charges existing in dielectric. A clear distinction between the electrical conductivity and polarization is possible only in a static electric field. In an alternating electric field, the difference between these processes is conditional.

In the case of the electronic conductivity the charge is transferred by negatively charged electrons and positively charged electron vacancies (holes). For some dielectrics and semiconductors a polaron type of charge transfer is also possible – when electrons or holes are strongly associated with the crystal lattice and, therefore, they have relatively low mobility. Typical for dielectrics is the ionic transport of charge – the flow of positively charged cations, negatively charged anions or charged ion vacancies of both signs.

The sluggishness of all mentioned processes is quite different so the conductivity of dielectric might have rather complicated frequency dependence. Figure 2(a) shows typical for dielectrics frequency dependence of the conductivity in comparison with very simple case σ(ω) for semiconductor. Fast electronic conductivity in semiconductors shows no frequency dependence up the gigahertz region. In this case the dispersion σ(ω) is expected only in a terahertz diapason.

Generally, charge transfer through dielectric (conductivity) and charge separation in dielectric is possible to divide at the direct voltage only. At the alternating voltage, particularly at increased frequency both of these “charges moving mechanisms” become mixed. The point is that slow mechanism of charge separation has no enough time to come to the end when voltage polarity is changed. Similarly, at the alternating voltage change carrier which provide for conductivity are forced to change their movement onto the opposite direction. That is why in the case of alternating voltage it possible to distinguish only “active part of current” (that corresponds to conductivity σ′(ω)) and “reactive part of current” (that corresponds to polarization: ε′(ω) or σ″(ω)). As a result, it possible to introduce a conception of complex conductivity σ*(ω) = σ′(ω) – iσ″(ω) on the analogy of complex dielectric permittivity ε*(ω) = ε′(ω) – iε″(ω). Both of these representations are equivalent.

That is why the lagging polarization, that is the dispersion ε*(ω) while ε′ decreases with frequency (Fig. 2(a), curve 2′), generates a deposit to the effective conductivity (Fig. 2(a), curve σ).

In a broad frequency range (10^{-2}...10^{7} Hz) in many dielectrics (and in some semiconductors) σ(ω) increases following the power law established by A. Ionscher: $\sigma \sim \omega^{n}$ where $0.7 < n < 1$. Such dependence is typical for many mechanisms of the local movement of charged particles in the electric field. Ions and polarons during their "hopping"-type movement between states of their localization, dipoles in the process of rotational vibrations between the equilibrium positions separated by potential barriers, as well as other charged particles and complexes under the influence of electric field can be moved in the dielectric in a confined space. The thermal motion of charged particles which partial localization is determined by a set of potential minima and barriers in the external electric field leads to both the conductivity and to polarization. At low frequency ($\omega \to 0$) polarization predominates. While frequency increases, this movement becomes limited, and low-frequency (slow) polarization looks like conductivity.

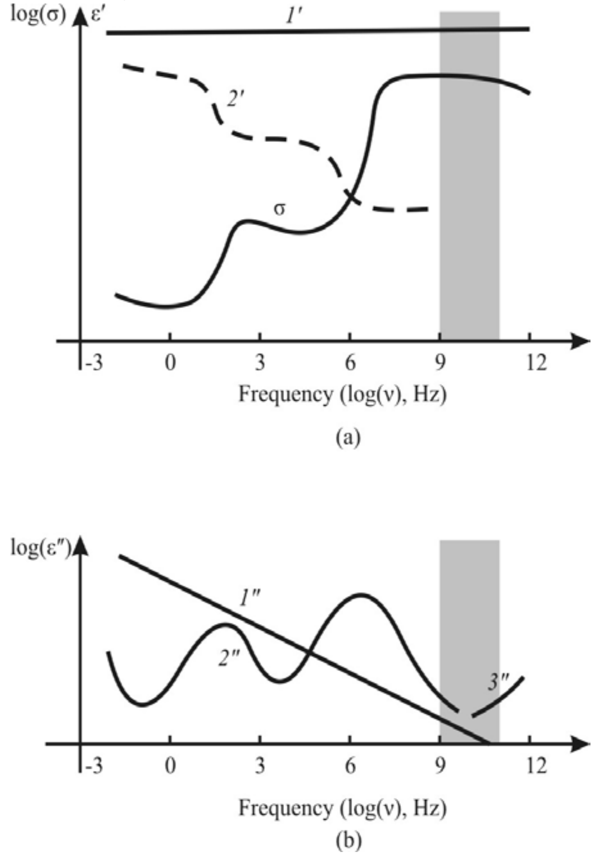

Fig. 2. Conductivity and correspondent dielectric losses frequency dependences, diapason of interest is shaded. (a): *1′* – fast electronic conductivity; *2′* – dielectric permittivity dispersion at the time of migratory and at relaxation mechanisms; σ – impact to conductivity from the retarded migration and relaxation polarization, (b): *1″* – loss factor from fast conductivity, *2″* – losses from migration from relaxation polarizations, *3″* – losses inserted by non centre symmetric phase

The point is that the motion of charged particles at the almost constant field is limited to the space potential barriers that impede to transfer of electric charges from electrode to electrode. With the increasing frequency some of charged particles do not have time for the quarter period of the applied voltage to reach their places of localization and continuously following to the change of electric field, and this movement contributes to the conductivity.

II.2. Slow polarization impact onto microwave conductivity

Migratory polarization arises in dielectrics owing to macroscopic heterogeneity or inclusions. This polarization is delayed at very low frequencies ($10^{-3}...10^{3}$ Hz, Fig. 2(a) curve *2′*) and is associated with a significant dispersion of $\varepsilon(\omega)$ that is accompanied by the increase of losses on these frequencies, Fig. 2(a) curve σ. Plausible reason of this polarization is the presence of layers with different conductivity and permeability as well as the presence of impurities in the technical dielectrics.

Possible mechanism of migratory polarization might be as such: in the electric field free electrons and ions of semi-conductive inclusion can move within this inclusion, which becomes like a huge polarized molecule. Another possible mechanism is conditioned on the border layers of laminates (or near electrode layers) that can accumulate the charges of slowly moving ions, and this process also has the effect of migratory polarization.

Dielectric permittivity is increased in the range of very low frequency that is the evidence of material structural heterogeneity. This might be a reason of increased losses as well in the all frequency range because loss maximum which is inspired by this polarization transforms into increased conductivity, Fig. 2(a), curve σ), and this conductivity results in a loss heat power: $p = \sigma E^2$.

Complex dielectric permittivity dispersion in the case of migratory polarization is described by the Debye equation similarly to the thermal relaxation polarization.

$$\varepsilon^*(\omega) = \varepsilon' - i\varepsilon'' = \varepsilon(\infty) + \frac{\varepsilon(0) - \varepsilon(\infty)}{1 + i\omega\tau}, \quad (3)$$

where $\omega = 2\pi\nu$ is electric field frequency, τ is relaxation time, $\varepsilon(0)$ is permittivity quite below relaxation frequency when $\omega\tau << 1$, $\varepsilon(\infty)$ is permittivity quite above the relaxation frequency when $\omega\tau >> 1$.

Thermally activated relaxation polarization is inspired by the electrons (as well as by ions and dipoles). If the electron (dipole or ion) is a loosely coupled in the structure of the dielectric, the thermal motion of these particles can have a big impact on the process of polarization. Being localized in a micro-volume, these particles under the influence of the thermal motion can make heat hopping, moving to a distance of the order of atomic dimensions.

Electronic thermal mechanism of polarization is the characteristic of only solid dielectrics. Assume that in the vicinity of a particular type of structural defects weakly bounded electron (or hole) is present, and it has two or more equivalent positions (traps that is separated by a potential barrier). Usually it is the electrons captured by crystal defects or impurity ions. These centers generate the irregular distribution of electric charge in the crystal lattice. The relaxation time of this polarization mechanism is rather big: $10^{-2}...10^{-7}$ s, so such a polarization is late to show itself at radio frequencies, Fig. 2(a), curve *2′*). However, high-frequency “tail” of $\varepsilon''(\nu)$ maximum noticeably affects onto microwave losses.

Thermally induced electronic polarization plays a significant role in many technically important microwave dielectrics, such as rutile (TiO_2), perovskite ($CaTiO_3$) and similar complex oxides of titanium, zirconium, niobium, tantalum, lead, cerium, bismuth etc, that are used as a components of microwave dielectrics. In these substances, especially in the polycrystalline state, a high concentration of defects in the crystal structure usually is present. During the synthesis of ceramics (or in process of crystal growth) from the mixture of oxides a high temperature is used, and therefore it is very likely the emergence of oxygen defects (that are anion vacancies). Electrical compensation of these defects is realized due to lower-valence cations, located near the anion vacancies. Thus, there exist the conditions for electron exchange between neighboring vacancy cations which leads to the polarization and losses.

Ionic thermally induced polarization is caused by the hoping of the impurity ions that are weakly bonded in the crystal lattice. That is why this polarization is mainly inherent to solid dielectrics with pronounced irregularity of structure. Such, for example, are glasses, glass-ceramics and ceramics. The fact that structural defects concentration of in these dielectrics is very great: the glass is characterized by the disordering of the ions positions, while in ceramics and glass-ceramics this disordering is peculiar properties of crystallite boundaries. However, thermal ionic polarization is observed in the single crystals as well in the vicinity of structural defects.

Ions in the interstices as well as ionic vacancies (voids in the regular structure) may change their positions under the influence of thermal vibrations and its fluctuations. The area of this movement is usually limited by the structural defects (dislocations, for example) but ions can overcome potential barriers and turn out in the new positions. External electric field changes the distribution of weakly bounded ions between defect sites and stimulates as polarization so losses.

Setting time τ of this kind of polarization is temperature dependent, and it is determined by the characteristics of dielectric structure and by the type of defects (or impurities). Generally, at the normal temperature (about 300 K) the relaxation time is $\tau = l0^{-4}\ldots10^{-8}$ s. Any delay of polarization always leads to increased absorption of electrical energy. Therefore, the thermal polarization can be a cause of dielectric losses at radio frequencies for such common technique dielectrics as ceramics, glass and glass ceramics.

Shown in the Fig. 2(b) loss factor maximum located near the frequency of 10^6 Hz presents a typical relaxation loss. The contribution to the microwave loss coefficient from the relaxation polarisation is described by the equation:

$$\varepsilon''(\omega) = \omega\tau\frac{\left[\varepsilon(0)-\varepsilon(\infty)\right]}{1+(\omega\tau)^2} \tag{4}$$

or below the relaxation frequency where $\omega\tau < 1$:

$$\varepsilon''(\omega) = \omega\tau\left[\varepsilon(0)-\varepsilon(\infty)\right]. \tag{5}$$

A high-frequency tail of these losses might have an influence upon gigahertz diapason. The loss coefficient is noticeable above the relaxation frequency, where $\omega\tau > 1$

$$\varepsilon''(\omega) = \frac{1}{\omega\tau}\left[\varepsilon(0)-\varepsilon(\infty)\right]. \tag{6}$$

It is obvious that high-frequency loss coefficient that is conditioned by relaxation process decreases proportionally to frequency $\omega = 2\pi\nu$. Loss factor depends also on the size of relative contribution from given relaxation process to dielectric permittivity: $[\varepsilon(0) - \varepsilon(\infty)]$.

In accordance with eq. (2) and (4) one can obtain the equation for conductivity which conditioned by relaxation losses:

$$\sigma(\omega) = \frac{(\omega\tau)^2}{1+(\omega\tau)^2}\frac{\left[\varepsilon(0)-\varepsilon(\infty)\right]\varepsilon_0}{\tau}, \tag{7}$$

Figure 3 shown frequency dependences of the normalized effective conductivity for different relaxation times.

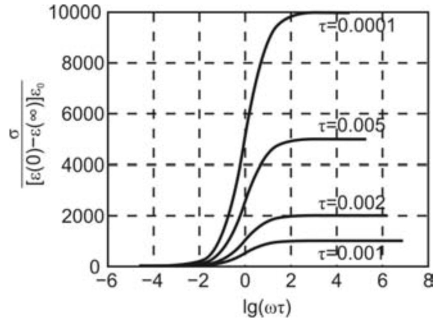

Fig. 3. Typical frequency dependence of conductivity conditioned by relaxation losses

If in microwave dielectric there are particles with different relaxation time or the interaction of relaxing particles is occurs, the dispersion spectrum becomes smeared. Due to this the probability of thermal relaxation contribution to the microwave conductivity increases. This can be considered by the Cole-Cole equation:

$$\varepsilon^{*}(\omega)-\varepsilon(\infty)=\frac{\varepsilon(0)-\varepsilon(\infty)}{1+(i\omega\tau_0)^{1-\alpha}}, \qquad (8)$$

where α is a parameter which characterizes the heterogeneity in the relaxation times (0 < α < 1).

From the eq. (8) it is easy to obtain an expression for correspondent loss factor:

$$\varepsilon''=(\omega\tau_0)^{\beta}\frac{\left[\varepsilon(0)-\varepsilon(\infty)\right]\sin\left(\frac{\beta\pi}{2}\right)}{1+2(\omega\tau_0)^{\beta}\cos\left(\frac{\beta\pi}{2}\right)+(\omega\tau_0)^{2\beta}}, \qquad (9)$$

where $\beta=(1-\alpha)$. Therefore the equation that describs conductivity dispersion taking into account equation (9) is (Fig. 4):

$$\sigma(\omega)=\omega(\omega\tau_0)^{\beta}\frac{\varepsilon_0\left[\varepsilon(0)-\varepsilon(\infty)\right]\sin\left(\frac{\beta\pi}{2}\right)}{1+2(\omega\tau_0)^{\beta}\cos\left(\frac{\beta\pi}{2}\right)+(\omega\tau_0)^{2\beta}}. \qquad (10)$$

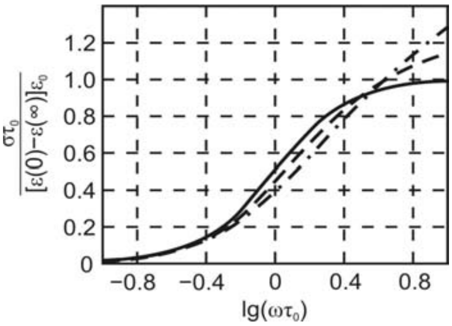

Fig. 4. Typical frequency dependence of conductivity conditioned by relaxation losses taking into account Cole-Cole distribution: β = 1 (solid line); β = 0.92 (dashed line); β = 0.84 (dash-and-dot line)

II.3. Fast polarization impact onto microwave conductivity

For high frequency ionic dielectrics the ionic displacement polarization plays a decisive role. Among these dielectrics there are alkali-haloid crystals and the most of oxides, including paraelectrics, piezoelectrics, ferroelectrics and pyroelectrics, as well as the semiconductors of $A^{III}B^{V}$ and $A^{II}B^{VI}$ groups. However, in the covalent semiconductors (such as silicon) the ionic polarization is absent.

Ionic polarization mechanism is rather fast (install time is ~ 10^{-13} s) that is longer than the time setting of the electronic polarization (~ 10^{-16} s) but still much less than typical relaxation time for thermally activated relaxation (~ 10^{-6}) and migratory (~ 10^{-2} s) polarizations. Dielectric dispersion for the ionic mechanism should occur in the far-infrared frequency range, Fig. 1, so that in the microwave region the ionic polarization is completely installed. However, low frequency tail from the loss maximum is possible to observe at the microwaves, especially in the case of high-ε microwave dielectrics where dispersion frequency of transverse optical phonon mode (ω_{TO}) is much lower.

Complex dielectric permittivity dispersion in the case of ionic displacement polarization is described by the Lorentz equation:

$$\begin{aligned}\varepsilon^{*}(\omega)&=\varepsilon'-i\varepsilon''=\\&=\varepsilon(\infty)+\frac{\varepsilon(0)-\varepsilon(\infty)}{1-(\omega/\omega_0)^2+i\Gamma(\omega/\omega_0)}\end{aligned} \qquad (11)$$

Here $\omega_0=\sqrt{c/m}$ is the oscillator frequency that equals to ω_{TO}, Γ is relative damping coefficient, ε(0) is dielectric permittivity quite below resonant frequency (when $\omega/\omega_{TO} \ll 1$), and ε(∞) is a permittivity quite above the resonant frequency (when $\omega/\omega_{TO} \gg 1$).

Equation (11) enables to find a contribution to the microwave loss coefficient from the resonant ion polarisation (its microwave tail below resonant frequency is shown in Fig. 1, curve *2″*):

$$\varepsilon''(\omega)=\Gamma\frac{\omega}{\omega_0}\frac{\left[\varepsilon(0)-\varepsilon(\infty)\right]}{\left(1-\left(\frac{\omega}{\omega_0}\right)^2\right)^2+\Gamma^2\left(\frac{\omega}{\omega_0}\right)^2}, \qquad (12)$$

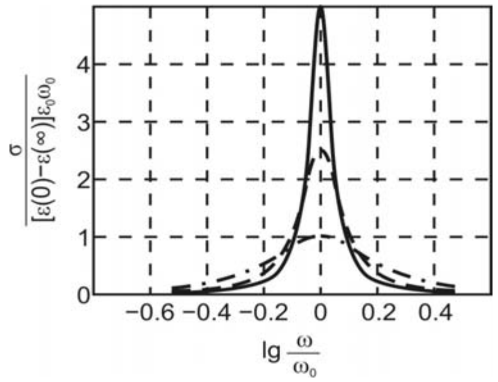

Fig. 5. Typical frequency dependence of conductivity conditioned by Lorentz oscillator: Γ = 0.2 (solid line); Γ = 0.4 (dashed line); Γ = 1 (dash-and-dot line)

In accordance to eq. (2) and (12), it is possible to obtain the equation for effective conductivity which is conditioned by the oscillatory loss:

$$\sigma(\omega)=\frac{\left[\varepsilon(0)-\varepsilon(\infty)\right]\omega_0\varepsilon_0}{\Gamma}\frac{\Gamma^2\left(\frac{\omega}{\omega_0}\right)^2}{\left[1-\left(\frac{\omega}{\omega_0}\right)^2\right]^2+\Gamma^2\left(\frac{\omega}{\omega_0}\right)^2}, \quad (13)$$

Figure 5 shows normalized conductivity frequency dependences for different relative damping coefficients. It is obvious that the impact to σ will be as much as damping factor Γ and dielectric power of oscillator [ε(0) – ε(∞)] values.

It is worth to notice also that effective conductivity σ(ω) has a maximum exactly at the resonant frequency $\omega_{TO} = \omega_0$ and position of this maximum is independent on damping factor Γ. Opposite, the maxims of another resonant characteristics of oscillator (eq. 11), such as ε' and ε", are strongly dependent on the damping factor. That is why the σ(ω)-dependence is the best way to establish an agreement between experimental data and their theoretical decryption.

Conclusions

The factual losses are determined by the effective conductivity of the material, so from the parameters that describe the microwave losses ($\tan\delta$, ε'', σ) the effective conductivity is one of the most practical. In the case of resonant loss namely effective conductivity determines the resonant frequency of the equivalent oscillator.

It is the fact that small absorption of electric power at the frequencies of 1...100 GHz can be realized only by the low inertia polarization mechanisms which provide low contribution to losses. These mechanisms of polarization are optical and infrared polarization only. Another mechanisms of polarization give rise to losses that might be analyzed and predicted by several polarization mechanisms.

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Ефективна провідність діелектричних матеріалів НВЧ

Діелектричні втрати, які характеризують перетворення електричної енергії в теплову, є важливим електрофізичним параметром діелектриків. Фактично ці втрати визначаються ефективною провідністю матеріалу. Тому в даній статті описані основні механізми втрат і їх внесок в ефективну провідність діелектричних матеріалів НВЧ. Проаналізовано частотну залежність ефективної провідності. Бібл. 3, рис. 5.

Ключові слова: *діелектричні матеріали; фактор втрат; тангенс кута втрат; діелектрична проникність; провідність.*

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СВЧ свойства композитных структур металл-диэлектрик

Диэлектрические потери, характеризующие преобразование электрической энергии в тепловую, являются важным электрофизическим параметром диэлектриков. Фактически эти потери определяются эффективной проводимостью материала. Поэтому в данной статье описаны основные механизмы потерь и их вклад в эффективную проводимость диэлектрических материалов СВЧ. Проанализированы частотную зависимость эффективной проводимости. Библ . 3, рис. 5.

Ключевые слова: *диэлектрические материалы; фактор потерь; тангенс угла потерь; диэлектрическая проницаемость; проводимость.*

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