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Temperature Dependences of Losses in High Frequency Dielectrics

Temperature is one of the important factors that affect to the coefficient of dielectric loss. Currently electronics is actively developing in the gigahertz frequency range. The frequency growth leads to the increasing of dielectric self-heating in the microwave electric field. Heating of dielectrics might be caused also by the external sources of heat. This paper presents the investigation of temperature dependences of the microwave dielectric losses for different mechanisms of polarization. The results of mathematical modelling are shown as well. References 3, figures 6.

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

I. Introduction

In modern electronics commonly use dielectric materials. They are allplied as insulators, substrates, resonators, filters, transmission lines, packaging, and gate insulator of transistors. Creation of new dielectric materials with specific properties is a difficult process that requires high material costs as the design stage and at the stage of manufacture. The need to reduce material costs and time-consuming to design and manufacture of dielectric materials requires the development and implementation to the production process simple reliable mathematical models of electrical parameters of dielectrics. The important parameter that characterizes the quality of the dielectric is a loss coefficient. The loss coefficient value depends on many factors such as the field intensity and frequency of the applied electromagnetic field, presence and concentration of structural defects in the dielectric, temperature, etc. Because the electronic devices can be used in different temperature conditions, a special attention is paid to the temperature influence on the properties of the materials. This is especially actual in connection with development of higher frequency intervals, as well as reducing the size of the structural elements, which increases the self-heating of the devices. Therefore, this paper is devoted to study of the temperature dependence of the dielectric materials loss factor.

II. Mechanisms of losses in high frequency dielectrics

There are three main parameters that characterize loss in dielectrics: absorbed heat power density p, loss coefficient ε'', and loss tangent $\tan\delta$: $\quad p = \sigma E^2, \varepsilon^* = \varepsilon' - i\varepsilon'', \tan\delta = \dfrac{\varepsilon''}{\varepsilon'},$

where σ is specific conductivity, ε^* is complex permittivity which consists of real (ε') and imaginary (ε'') parts. The magnitude of the losses, as well as their dependence on frequency and temperature indicate certain features of the mechanism of polarization. Dielectric losses mechanisms are quite different: as one case, the frequency dispersion of the dielectric permittivity has a resonant nature, and the other it has a relaxation nature.

The microscopic source of losses might be as conductivity so the anharmonicity in the polarization mechanisms. As a rule, conductivity influence at microwaves is minimal. The primary cause of the anharmonicity in crystalline dielectrics is determined by the asymmetry in the electron density distribution along the atomic bonds. This is conditioned by the differences in the electro-negativity of atoms. Sometimes the distinction of different atoms in their electro-negativity might be large. Atom with higher electro-negativity strongly attracts the electron-pair bond, so his true charge becomes more negative. Atom with a lower electro-negativity acquires, respectively, the increased positive charge. Together these atoms create a non-harmonic polar bond.

Dielectric losses at microwaves might be the footprints of:

1) Phenomenon of conductivity (σ).

2) Relaxation of slow polarization mechanisms (electronic defects, ionic defects, various kinds of dipoles, etc.) that are described by the Debye model of relaxation.

3) Different kinds of relaxors results in frequency-diffused dielectric spectrum that is depicted by Cole-Cole model.

4) Resonant of the fast mechanisms of dielectric polarization (optical and far infrared polarizations) that are described by the Lorentz oscillator model.

5) In the non-centre symmetric materials microwave loss factor governs by the very high frequency polar mechanism of losses.

In the case of the electronic conductivity the charge is transferred by the negatively charged electrons and positively charged holes. For some dielectrics and semiconductors a polaronic type of charge transfer is also possible. Typical for dielectrics is also an ionic transport of charge. The conductivity has influence upon loss as

$$\tan\delta = \frac{\sigma}{\varepsilon_0\varepsilon'\omega}. \qquad (1)$$

In a broad frequency range ($10^{-2}...10^7$ Hz) in many dielectrics (and in some semiconductors) the $\sigma(\omega)$ increases following the power law established by A.Ionscher: $\sigma \sim \omega^n$ where $0.7 < n < 1$.

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

In some microwave dielectrics (for instance, in metal-polymer composites) effective conductivity becomes very high because of reactive current though the polymer millions times increases with frequency so conductivity of metallic grains begins dominative, and this mechanism can be use for high loss microwave dielectrics (in absorbing covers). Another increase in loss in such a composite is dissipated polar phase originated from double charged layers in the metal-dielectric boundaries.

The complex dielectric permittivity dispersion in the case of migratory polarization is described by the Debye equation similarly to the thermal relaxation polarization:

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

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

Setting time τ of this kind of polarization is temperature dependent that is determined by the structure of dielectric and by the type of defects (impurities). Generally, at the normal temperature (about 300 K) the relaxation time turns up in the interval of $\tau = 10{-}4...10{-}8$ s. Any delay of polarization always leads to increased absorption of electrical energy. Therefore, the thermally induced polarization can be a major cause of dielectric losses at the radio frequencies.

Loss factor maximum located near the frequency of 106 Hz presents a typical relaxation loss. The contribution to the microwave loss tangent from the relaxation polarisation is described by the equation:

$$\tan\delta = \frac{\left[\varepsilon(0) - \varepsilon(\infty)\right]\omega\tau}{\varepsilon(0) + \varepsilon(\infty)\omega^2\tau^2}. \qquad (2)$$

It is obvious that high-frequency $\tan\delta$ that is conditioned by the relaxation process decreases proportionally to frequency. Loss factor depends also on the size of relative contribution from given relaxation process to the dielectric permittivity.

For the high frequency dielectrics the ionic displacement polarization plays a decisive role. Among these dielectrics are the alkali-haloid crystals as well as the most of dielectric oxides, including paraelectrics, piezoelectrics, ferroelectrics and pyroelectrics, and some of semiconductors of AIIIBV and AIIBVI groups.

Ionic polarization mechanism is rather fast (install time is $\sim 10{-}13$ s) that is longer than the time setting of the electronic polarization ($\sim 10{-}16$ s) but still much less than the relaxation times for thermally activated relaxation ($\sim 10{-}6$ s) and migratory polarization ($\sim 10{-}1$ s). Dielectric dispersion for the ionic polarization should occur in the far-infrared frequency range so that in the GHz region the ionic polarization is completely installed. However, the low frequency tail from far-infrared the loss maximum is observed at microwaves, especially in the case of high-ε dielectrics where dispersion frequency ωTO is much lower then in other ionic crystals.

The dispersion of complex dielectric permittivity for ionic displacement polarization is described by the Lorentz equation:

$$\varepsilon^*(\omega) = \varepsilon(\infty) + \frac{\varepsilon(0) - \varepsilon(\infty)}{1 - \left(\omega/\omega_0\right)^2 + i\Gamma\left(\omega/\omega_0\right)}.$$

Here $\omega_0 = \sqrt{c/m}$ is the oscillator frequency that equals to ωTO that is a frequency of transverse optical phonon mode, Γ is relative damping coefficient, $\varepsilon(0)$ is dielectric permittivity quite below resonant frequency when $\omega/\omega_{TO} << 1$ that is microwave permittivity εmic, while $\varepsilon(\infty)$ is the permit-

tivity quite above resonant frequency (when $\omega / \omega_{TO} \gg 1$) that means the optical permittivity εopt.

The Lorentz equation enables also to find a contribution to the microwave loss tangent from the resonant ionic polarisation (its microwave tail below the resonant frequency):

$$\tan\delta = \Gamma \frac{\omega}{\omega_{TO}} \frac{\varepsilon_{mic} - \varepsilon_{opt}}{\varepsilon_{mic}} . \qquad (3)$$

It is seen that losses linearly increase with the frequency growth, and they are as big as the ω is close to the ωTO. Just this case is typical for high-ε dielectrics.

Among ionic compounds there are some crystals and ceramics (MgO, Al_2O_3, $LaAlO_3$, $Bi_{12}SiO_{20}$, AlN, etc) which losses are unexpectedly big that cannot be explained by any of simple loss mechanisms. These dielectrics have practically no conductivity that is depicted by eq. (1), a few probability of relaxation, described by eq. (2), and they have too high frequency of lattice resonance ωTO in order it might have noticeable affect to microwave losses that are described by the eq. (3).

Essentially increased microwave losses have sillenites ($Bi_{12}GeO_{20}$ and similar) that shows heightened permittivity ($\varepsilon \approx 40$), and even very firm nitrides (AlN, BN and others) in which permittivity is of usual value for ionic compounds ($\varepsilon < 10$), as well as semiconductors of $A^{III}B^{V}$ and $A^{II}B^{VI}$ groups. One of example is gallium arsenide in which the influence to microwave loss from the conductivity is very small, but one can see a significant growth of losses with frequency. We suppose that this is manifestation of internal polarity mechanism of absorption at the millimeter and submillimeter wavelengths. Due to the piezoelectric effect, in the GaAs arises a relaxation process conditioned by the interaction of acoustic and optical phonon's modes. This electromechanical coupling results in the "leakage" of electric energy from excited by the electric field optical phonons to the "heat reservoir" of the acoustic phonons. This is a reason why gallium arsenide losses increase with increasing frequency.

The object of this report is to determine the main mechanisms of microwave losses in the high-ε dielectrics by means of known mechanisms analyses.

II.1. Temperature dependences of losses given by conductivity

The conductivity that in the microwaves represents the charge transfer by the fast charge carriers (mostly electrons) provokes losses that are strongly dependent as on frequency so on temperature:

$$\tan\delta(\omega, T) = \frac{\sigma}{\varepsilon_0 \varepsilon \omega} \approx \frac{\sigma_0 \exp\left[a(T - T_0)\right]}{\varepsilon_0 \varepsilon \omega} , \qquad (4)$$

where σ_0 is specific conductivity at certain temperature T_0, parameter ε_0 is electric constant and ε is frequency independent permittivity, while a is peculiar parameter for a given semiconductor. This dependence is illustrated on the example of high-resistance silicon that at the millimetre waves at room temperature and below looks like a dielectric, Fig. 1.
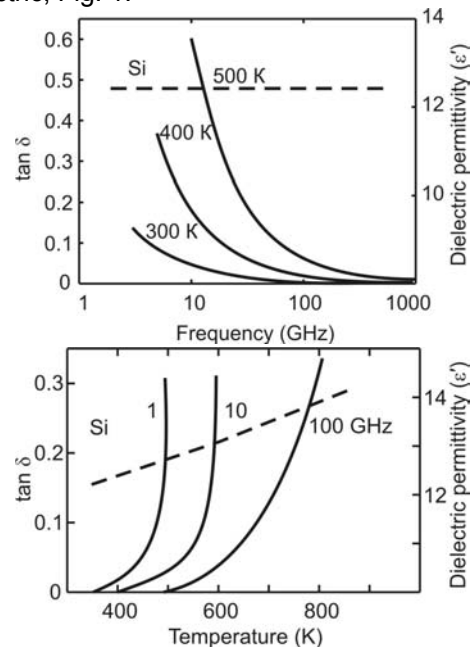

Fig. 1. Frequency and temperature dependence of microwave losses tan δ (solid lines) and permittivity ε′ (dashed lines) for the high-resistance silicon in the gigahertz range

In a good agreement with eq. (4), loss tangent given by conductivity exponentially increases with temperature but decreases linearly with frequency. So the conductivity` deposit to the losses might by important at rather high temperatures only.

II.2. Temperature dependences of losses given by slow relaxation polarization mechanism

Relaxation of the slow polarization mechanisms (electronic defects, ionic defects, various kinds of dipoles, etc.) are described by the Debye model of relaxation. Debye equation permits to find a deposit to microwave losses that looks like a tail from megahertz-frequency relaxation when $\omega\tau > 1$:

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

$$\tan\delta \approx \frac{1}{\omega\tau}\frac{\varepsilon(0) - \varepsilon(\infty)}{\left(\varepsilon(0)\big/\omega^{2}\tau^{2}\right) + \varepsilon(\infty)},$$

where τ is relaxation time, $\varepsilon(0)$ is permittivity quite below relaxation frequency ($\omega\tau << 1$), $\varepsilon(\infty)$ is permittivity quite above the relaxation frequency ($\omega\tau >> 1$). It is obvious that high-frequency $\tan\delta$ (that is conditioned by the relaxation process) decreases proportionally to the frequency $\omega = 2\pi\nu$ and increases with temperature, Fig. 2.
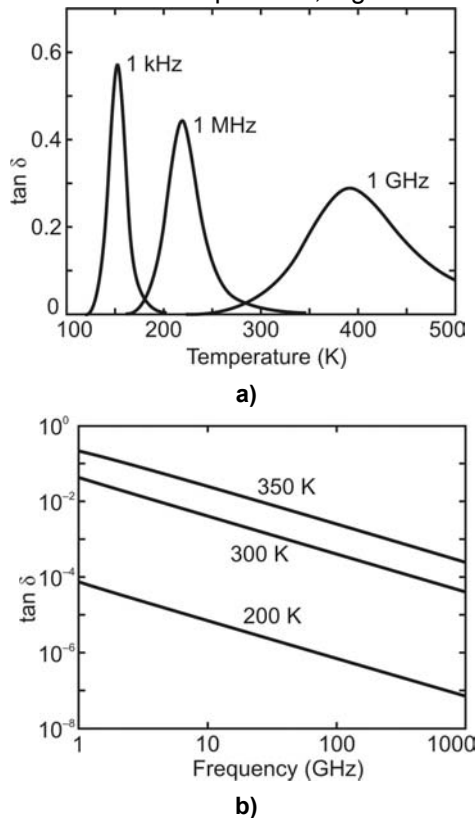

a)

b)

Fig. 2. Temperature (*a*) and frequency (*b*) dependences of relaxation losses for rutile with oxygen vacancies

II.3. Dielectric dispersion for the lattice (ionic) polarization

This mechanism is described by the Lorentz equation and takes place in the far-infrared fre-

quency range. Thus, the only low-frequency tail from the loss maximum is observed at gigahertz region:

$$\varepsilon^{*}(\omega) = \varepsilon(\infty) + \frac{\varepsilon(0) - \varepsilon(\infty)}{1 - (\omega/\omega_0)^{2} + i\Gamma(\omega/\omega_0)},$$

$$\tan\delta = \Gamma\frac{\omega}{\omega_0}\frac{\varepsilon(0) - \varepsilon(\infty)}{\varepsilon(0)}.$$

Here ω_0 is oscillator frequency that equals to transverse optical phonon mode frequency, Γ is relative damping coefficient, $\varepsilon(0)$ is dielectric permittivity quite below resonant frequency, while $\varepsilon(\infty)$ is the permittivity quite above resonant frequency. Figure 3(a) shows lattice damping influence to losses in the gigahertz frequencies.
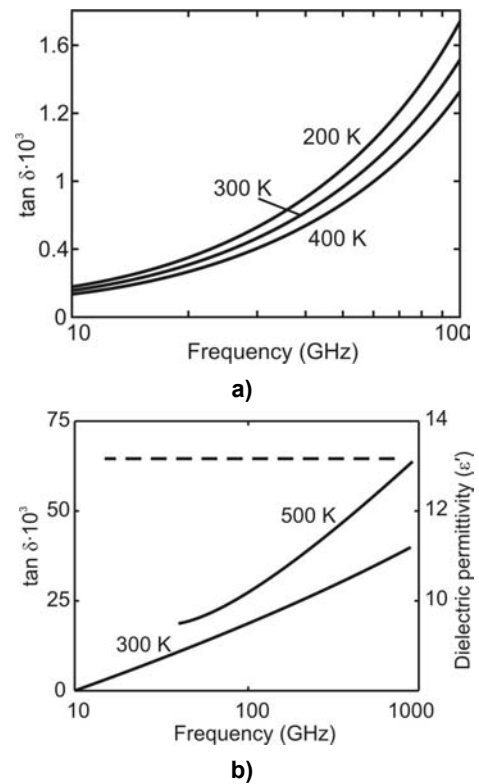

a)

b)

Fig. 3. Loss tangent frequency dependence: *a* – low-frequency tail from lattice loss maximum; *b* – impact of quasi-Debye mechanism on the losses in polar crystal GaAs (dotted line is permittivity)

II.4. Temperature dependences of losses given by fast relaxation polarization (quasi-Debye mechanism)

In the non-centre symmetric (polar) materials microwave loss factor governs by the very high frequency mechanism of losses that theoretically is described by the quasi-Debye losses. Frequency and temperature dependences of these losses, shown in Fig. 3 (b), are conditioned by the fast re-

laxation polarization mechanism; at the condition when $\omega\tau < 1$:

$$\tan\delta \approx \frac{\omega}{2\nu_D}\exp\frac{U}{kT}\frac{\varepsilon(0)-\varepsilon(\infty)}{\varepsilon(0)},$$

where ν_D is Debye frequency, k is Boltzmann constant, U is potential barrier. In this case loss factor increases as with frequency so with temperature; experimental data is given for polar crystal gallium arsenide in Fig. 3(b). Therefore, the loss tangent increases as frequency so with temperature.

II.5. Lattice polarization mechanism impact for paraelectrics

There are crystals with the special temperature dependence of the dielectric permittivity described by the Curie-Weiss law:

$$\varepsilon(T) = \varepsilon_i + \frac{C}{(T-\theta)},$$

where $C \approx 10^4\ldots10^5$ is Curie-Weiss constant and θ is Curie-Weiss temperature while ε_i represents the optical and other very high frequency contributions. In such crystals at the critical temperature there is a phase transition to the ferroelectric or antiferroelectric state.

Dispersion of ε caused by the elastic displacement of the ion lattice usually observed in the crystals at frequencies of about 10^{13} Hz, but in some ferroelectrics in the vicinity of phase transition the frequency of the "soft mode" lattice vibrations may decrease to 10^{11} Hz.

In the vicinity of the phase transition the temperature dependence of the "soft mode" frequency is determined by the relation W. Cochran:

$$\omega_{TO} = A\sqrt{T-\theta},$$

where A is the temperature coefficient of frequency.

The damping of lattice mode is weakly dependent on temperature:

$\gamma = \Gamma\omega_{TO} = \gamma_0 + aT + bT^2$. Here, γ_0 describes two-phonon absorption, in which connection parameters a and b correspond to three and four phonons absorptions mechanisms. In the vicinity of the phase transition the relatively weak temperature dependence of γ can be neglected.

Temperature-frequency dependence of dielectric constant for ferroelectrics that have displacement-type phase transitions is characterized by the following expression:

$$\varepsilon^*(\omega,T) = \varepsilon_\infty + \frac{C}{T-\theta}\frac{\omega_{TO}^2}{\omega_{TO}^2 - \omega^2 + i\gamma\omega},$$

where $\varepsilon(\infty)$ is permittivity at very high frequency, C is Curie-Weiss constant, θ is Curie-Weiss temperature. From this relation it is possible to obtain an expression for the calculation of the dielectric loss tangent:

$$\tan\delta = \frac{CA^2\gamma\omega}{\left[A^2(T-\theta)-\omega^2\right]\left\{\varepsilon(\infty)\left[A^2(T-\theta)-\omega^2\right]+CA^2\right\}+\varepsilon(\infty)\gamma^2\omega^2}$$

Figure 4 shows the frequency (a) and temperature (b) $\tan\delta$ dependences for barium titanate in the paraelectric phase. It can be seen that the losses increase with frequency and decrease with temperature growth.

a)   b)

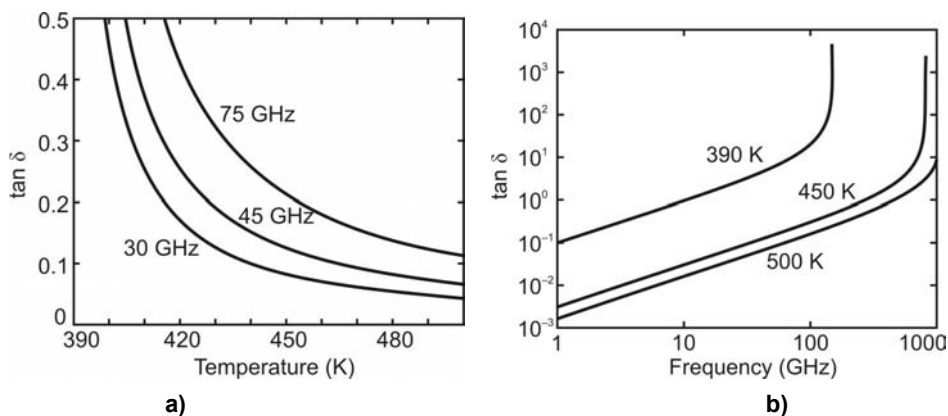**Fig. 4. Temperature (a) and frequency (b) dependences of microwave losses tan δ for the lattice polarization mechanism in paraelectrics**

II.6. Cole-Cole model for relaxation time distribution

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

$$\varepsilon^*(\omega) = \varepsilon(\infty) + \frac{\varepsilon(0) - \varepsilon(\infty)}{1 + (i\omega\tau_0)^{1-\alpha}}, \qquad (5)$$

where α is a parameter which characterizes the distribution in the relaxation times ($0 < \alpha < 1$) and τ_0 is the average relaxation time:

$$\tau_0 = \frac{1}{2\upsilon}\exp\left(\frac{U}{kT}\right) = A\exp\left(\frac{B}{T}\right).$$

From (5) it can be obtained an expression for the temperature dependence of the dielectric loss tangent (taking into account the distribution relaxation times):

$$\mathrm{tg}\,\delta(T) = \frac{\left[\varepsilon(0) - \varepsilon(\infty)\right]\left[\omega A\exp\left(\frac{B}{T}\right)\right]^{\beta}\sin\left(\frac{\beta\pi}{2}\right)}{\left[\varepsilon(0) - \varepsilon(\infty)\right]\left[\omega A\exp\left(\frac{B}{T}\right)\right]^{\beta}\cos\left(\frac{\beta\pi}{2}\right) + \varepsilon(0) + \varepsilon(\infty)\left[\omega A\exp\left(\frac{B}{T}\right)\right]^{2\beta}}$$

where $\beta = 1 - \alpha$.

This dependence is illustrated on the example of rutile ceramics in Fig. 5. As in the case of the Debye mechanism, the loss tan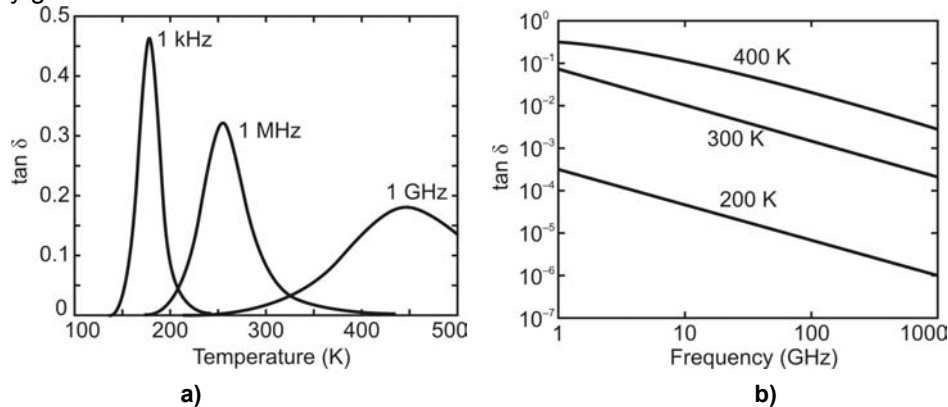gent decreases with frequency growth and increases with temperature. At the same time there is a decrease of the maximum loss values, a smearing of temperature curves, and a shift of the maxima towards higher temperatures.

Fig. 5. Temperature (a) and frequency (b) dependences of microwave losses tan δ taking into account Cole-Cole distribution (α = 0.15)

II.7. Losses in dielectric-metal composites

Composite materials consist of two or more substances. Each of the components contributes to the properties of the composite material in accordance with its volume part. The complex dielectric permittivity of the composite can be calculated using Lichtenecker's equation:

$$\varepsilon_c^* = \left(\varepsilon_m^*\right)^{1-q}\left(\varepsilon_d^*\right)^{q},$$

$$\varepsilon_c^* = \left(\varepsilon_m'\right)^{1-q}\left(\varepsilon_d'\right)^{q}\left[\cos\left(q\tan\delta_d + (1-q)\tan\delta_m\right) - i\sin\left(q\tan\delta_d + (1-q)\tan\delta_m\right)\right],$$

$$\tan\delta_c = \frac{\varepsilon_c''}{\varepsilon_c'} = \tan\left[q\tan\delta_d + (1-q)\tan\delta_m\right].$$

where q is volume part of the disperse phase in the composite, ε_m^*, ε_d^* are the complex dielectric permittivity of matrix and disperse phase respectively.

The temperature properties of the matrix-composite are determined by the type of dielectric, and they can be described by using the above-mentioned models. Temperature properties of the metallic phase can be described using the temperature dependence of the conductivity. Taking into account that loss tangent of the matrix-composite material is small, it can be obtained:

In the case of very small size of the metal parti-

cles, the temperature dependence of loss tangent of the composite material is:

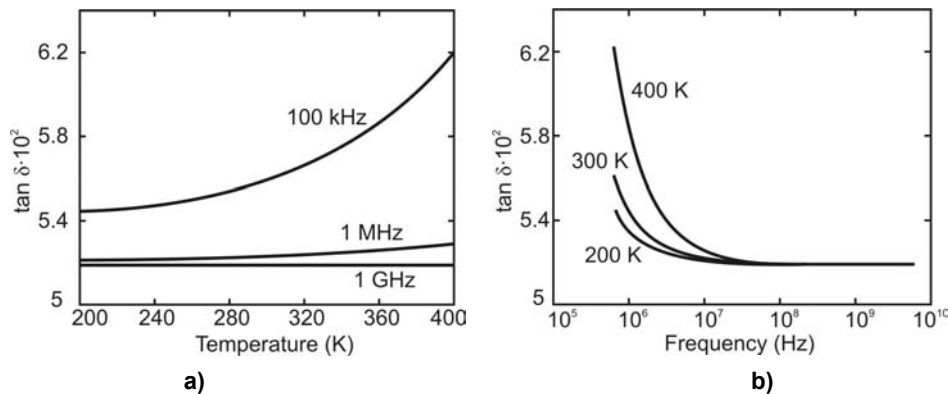$$\tan\delta_c = \frac{\varepsilon_c^{''}}{\varepsilon_c^{'}} = \tan\left[(1-q)\tan\delta_m(T)\right].$$

Fig. 6. Temperature (a) and frequency (b) dependences of microwave losses (tanδ) for dielectric-metal composites

In Fig. 6 the temperature and frequency dependences of the loss tangent for a composite material Al-epoxide with $q = 0,2$ and particles size of 80…200 nm are shown. For modeling of the epoxide temperature properties Debye model was used.

Conclusions

Experimental and theoretical investigations show that dominating loss mechanism for high-ε dielectrics arises from the polar phase existence. In the case of polar bonds between atoms, the atomic equilibrium potential manifests a pronounced anharmonicity that is the main microscopic channel to transfer electrical energy into a heat (dielectric losses). In crystal dynamic theory the anharmonic potential results in a coupling between optical phonons (that are excited by the electric field) and acoustical phonons (that represents heat reservoir).

With increasing temperature, and, consequently, with the increase in the amplitude of vibration of the atoms, the manifestation of anharmonicity becomes more noticeable, and losses increase. Consequently, with the object of microwave dielectrics elaboration or application one need to avoid or to suppress any polar (non-centre symmetric) components in the dielectric composition.

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Температурні залежності втрат у НВЧ діелектриках

Температура є одним з важливих факторів, що впливають на коефіцієнт діелектричних втрат. В даний час електроніка активно освоює гігагерцовий діапазон частот. Зростання частоти призводить до збільшення саморозігріву діелектрика в електричному полі НВЧ. Нагрівання діелектриків також може бути викликане зовнішніми джерелами тепла. У цій статті представ-

лено дослідження температурних залежностей НВЧ діелектричних втрат для різних механізмів поляризації та наведено результати математичного моделювання. Бібл. 3, рис. 6.

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

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Температурные зависимости потерь в СВЧ диэлектриках

Температура является одним из важных факторов, влияющих на коэффициент диэлектрических потерь. В настоящее время электроника активно осваивает гигагерцовый диапазон частот. Рост частоты приводит к увеличению саморазогрева диэлектрика в электрическом поле СВЧ. Нагрев диэлектриков также может быть вызван внешними источниками тепла. В этой статье представлено исследование температурных зависимостей СВЧ диэлектрических потерь для различных механизмов поляризации. Также показаны результаты математического моделирования. Библ. 3, рис. 6.

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

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