

# Effect of Absorption on the Efficiency of Terahertz Radiation Generation in the Metal Waveguide Partially Filled with Nonlinear Crystal $\text{LiNbO}_3$ , Dast or ZnTe

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**Abstract**—The influence of terahertz (THz) radiation absorption on the efficiency of generation of coherent THz radiation in the system ‘nonlinear-optical crystal partially filling the cross section of a rectangular metal waveguide’ has been investigated. The efficiency of the nonlinear frequency conversion of optical laser radiation to the THz range depends on the loss in the system and the fulfillment of the phase-matching (FM) condition in a nonlinear crystal. The method of partially filling of a metal waveguide with a nonlinear optical crystal is used to ensure phase matching. The phase matching is achieved by numerical determination of the thickness of the nonlinear crystal, that is the degree of partial filling of the waveguide. The attenuation of THz radiation caused by losses both in the metal walls of the waveguide and in the crystal was studied, taking into account the dimension of the cross section of the waveguide, the degree of partial filling, and the dielectric constant of the crystal. It is shown that the partial filling of the waveguide with a nonlinear crystal results in an increase in the efficiency of generation of THz radiation by an order of magnitude, owing to the decrease in absorption.

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## 1. INTRODUCTION

Waveguides containing dielectric inserts are used in many waveguide components [1]. In THz spectroscopy, it was shown that the method of measuring the absorption of a dielectric, which partially fills the waveguide [2], is 50 times more sensitive than the traditional method of single-layer reflection. The efficient generation of ultrashort GHz and THz pulses in a nonlinear crystal, partially filling a rectangular waveguide, using pico- or femtosecond laser pulses was proposed and performed in [3–5]. The generation of GHz and THz radiation is based on the mixing of the spectral components of a pico- or femtosecond laser pulse in a nonlinear crystal (the method of optical rectification). The method of partially filling a metal waveguide with the nonlinear optical crystal was used to fulfill the phase matching condition, that is to achieve the efficient generation of THz radiation.

The generation efficiency for a given difference frequency in the spectrum of a THz pulse in the absence of absorption of optical laser radiation, but taking into account the absorption of a THz wave,

when the crystal is in free space, is determined by the expression [6,7]:

$$\eta_{\text{THz}} = \frac{2\omega^2 d_{\text{eff}}^2 L^2 I}{\varepsilon_0 n_{\text{NIR}}^2 n_{\text{THz}} c^3} \exp[-\alpha_{\text{THz}} L / 2] \frac{\sinh^2[\alpha_{\text{THz}} (L / 4)]}{[\alpha_{\text{THz}} L / 4]^2}. \quad (1)$$

At insignificant absorption ( $\alpha_{\text{THz}} L \ll 1$ ), equation (1) is converted to (2), and in the case of a large absorption ( $\alpha_{\text{THz}} L \gg 1$ ) – to (3)

$$\eta_{\text{THz}} = \frac{2\omega^2 d_{\text{eff}}^2 L^2 I}{\varepsilon_0 n_{\text{NIR}}^2 n_{\text{THz}} c^3}, \quad (2)$$

$$\eta_{\text{THz}} = \frac{8\omega^2 d_{\text{eff}}^2 I}{\varepsilon_0 n_{\text{NIR}}^2 n_{\text{THz}} c^3 \alpha_{\text{THz}}^2}, \quad (3)$$

where  $\omega$  is the angular frequency of the THz wave,  $d_{\text{eff}}$  is the effective nonlinear optical coefficient,  $L$  is the nonlinear crystal length,  $I$  is the near-infrared light intensity,  $\varepsilon_0$  is the dielectric constant of vacuum,  $c$  is the velocity of light in free space,  $\alpha_{\text{THz}}$  is the THz radiation absorption coefficient, and  $n_{\text{THz}}$  and  $n_{\text{NIR}}$  are the crystal refractive indices for terahertz (from 0.1 to 0.03 mm) and near-infrared radiation (from 780 to 2500 nm), respectively. It follows from the expression (1) that the length of the crystal should not exceed the value  $L = \alpha_{\text{THz}}^{-1}$ , and from the condition for the fulfillment of phase matching it follows that it also should not be greater than the coherence length  $L_{\text{coh}}$  [6].

In accordance with the equations (2) and (3), the indicators of the quality of nonlinear crystal are introduced ((the figures of merit) – (FOM)) [8]:

$$\text{FOM}_{\text{NA}} \equiv \frac{d_{\text{eff}}^2 L^2}{n_{\text{NIR}}^2 n_{\text{THz}}}, \quad (4)$$

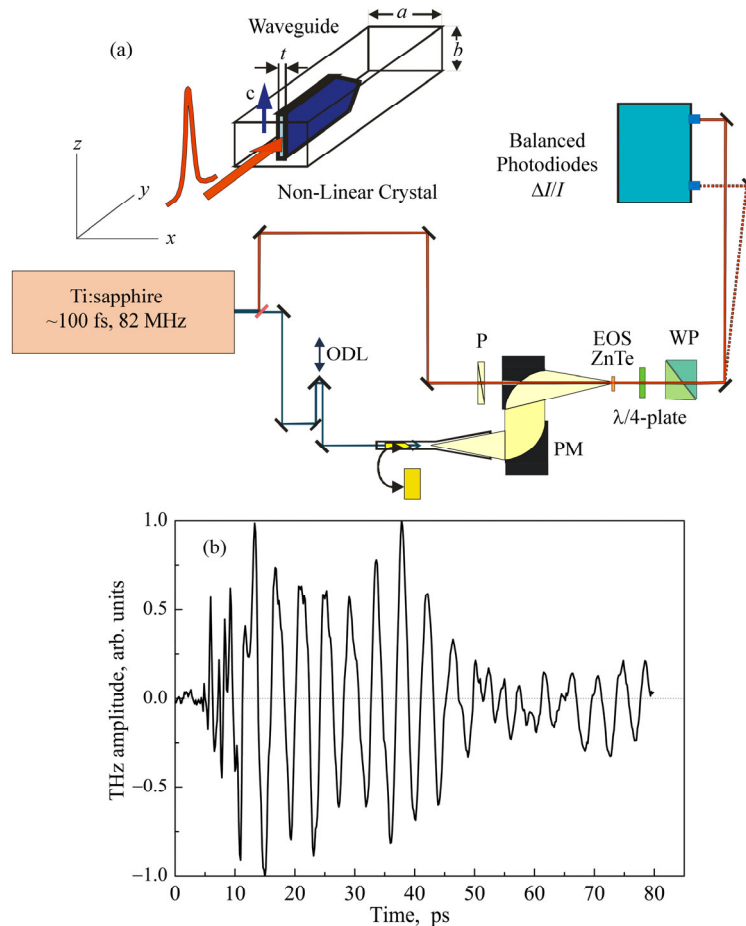
$$\text{FOM}_{\text{A}} \equiv \frac{4d_{\text{eff}}^2}{n_{\text{NIR}}^2 n_{\text{THz}} \alpha_{\text{THz}}^2}. \quad (5)$$

The values  $\text{FOM}_{\text{NA}}$  and  $\text{FOM}_{\text{A}}$  are the indicators of energy conversion efficiency in an optical rectification in weakly and strongly absorbing crystals, respectively. It was proposed in [8] to consider the FOM to be equal to  $\text{FOM}_{\text{A}}$  if  $\alpha_{\text{THz}} > 5 \text{ cm}^{-1}$  with a crystal length  $L = 2 \text{ mm}$ , and to  $\text{FOM}_{\text{NA}}$  for small values of  $\alpha_{\text{THz}}$ .

To ensure the efficient generation of the THz radiation under conditions of phase matching, the nonlinear crystals with the high values of FOM are used in experiments. So, for example, from the following nonlinear crystals CdTe, GaAs, GaP, ZnTe, GaSe, sLiNbO<sub>3</sub>, sLiNbO<sub>3</sub> 100 K, DAST and others, the DAST crystals have the highest value of  $\text{FOM} = 41.5 \text{ pm}^2 \text{cm}^2 / \text{V}^2$ . At pumping the wavelength of 1.55  $\mu\text{m}$ , when the FOM is smaller and equal to  $6.6 \text{ pm}^2 \text{cm}^2 / \text{V}^2$ , the THz pulses were generated with a focused field strength of  $\sim 50 \text{ kV/cm}$  [9], despite the fact that  $\alpha_{\text{THz}} = 50 \text{ cm}^{-1}$  [10]. The stoichiometric crystal sLiNbO<sub>3</sub> (sLN) has the second highest FOM, equal to  $18 \text{ pm}^2 \text{cm}^2 / \text{V}^2$ , which is more than twice that of ZnTe –  $7.27 \text{ pm}^2 \text{cm}^2 / \text{V}^2$  and other semiconductor crystals (despite the high absorption coefficient of LiNbO<sub>3</sub>  $\alpha_{\text{THz}} = 17 \text{ cm}^{-1}$  [11] as compared with the  $\alpha_{\text{THz}} = 1.3 \text{ cm}^{-1}$  of ZnTe [12]). The stoichiometric crystal sLiNbO<sub>3</sub> differs from LiNbO<sub>3</sub> crystal by a lower doping level Mg, approximately – 0.7% instead of 5%. Owing to this, the absorption coefficient of the sLiNbO<sub>3</sub> is significantly reduced, and the difference becomes more significant at low temperatures, at  $T = 100^\circ \text{ K}$   $\alpha_{\text{THz}} = 4.8 \text{ cm}^{-1}$  [13]. As a result, the FOM of the sLiNbO<sub>3</sub> crystal becomes equal to 48.6, that is, more than that of the DAST. At low

temperatures, for the sLiNbO<sub>3</sub>,  $\eta_T$  increases with the increasing crystal length in proportion to  $L^2$ .

Below we present a study of the influence of the absorption of the THz radiation on the generation efficiency of the coherent THz radiation in a nonlinear optical crystal placed in a metal rectangular waveguide and partially filling its cross section (Fig. 1). The efficiency of nonlinear conversion of optical laser radiation in the THz range also depends on the fulfilment of the FM condition in a nonlinear crystal, that is, on the equality of the group velocity of the optical pulse and the phase velocity of the THz pulse at the difference frequency. The phase matching is achieved by numerical determination of the thickness of a nonlinear crystal, that is, of the degree of partial filling of the waveguide [3–5]. Each thickness of the crystal corresponds to a series of specific frequencies for which the FM occurs.



**Fig. 1.** (a) The nonlinear LiNbO<sub>3</sub> crystal in a rectangular metal waveguide, and experimental setup for generating and detecting the THz pulses; (b) the temporal form of the radiated THz pulse generated when the crystal is illuminated with the Ti: sapphire laser pulse of 100 fs duration at the wavelength of 800 nm.

The THz radiation attenuation caused by the losses both in the metal walls of the waveguide and in the crystal was calculated taking into account the cross-sectional dimensions of the waveguide, the crystal thickness (the degree of partial filling) and its dielectric constant. The DAST, LiNbO<sub>3</sub> and ZnTe crystals are studied owing to their high conversion efficiency of optical radiation to the THz range. These crystals have the high nonlinear second-order susceptibilities and various dielectric constant, for which the condition of the FM is satisfied.

## 2. THE ATTENUATION OF THE THz RADIATION CAUSED BY THE LOSSES IN THE METAL WALLS OF THE WAVEGUIDE AND IN THE CRYSTAL

The attenuation coefficient in the metal walls of the waveguide  $\alpha_m$ , partially filled with a nonlinear crystal defined by the expression  $\alpha_m = P_m / 2P$  [14], was calculated numerically from the expression (6):

$$\alpha_m = m \frac{a}{b} \left\{ \left( \frac{\varepsilon_0 \mu_0}{m^2} - 1 \right) \frac{1}{R_1} \left[ R_2 + 2 \frac{b}{a} \left( \frac{\cos \beta t}{\sin \alpha d} \right)^2 \right] + 1 \right\} \frac{R_3}{a Z_0}, \quad (6)$$

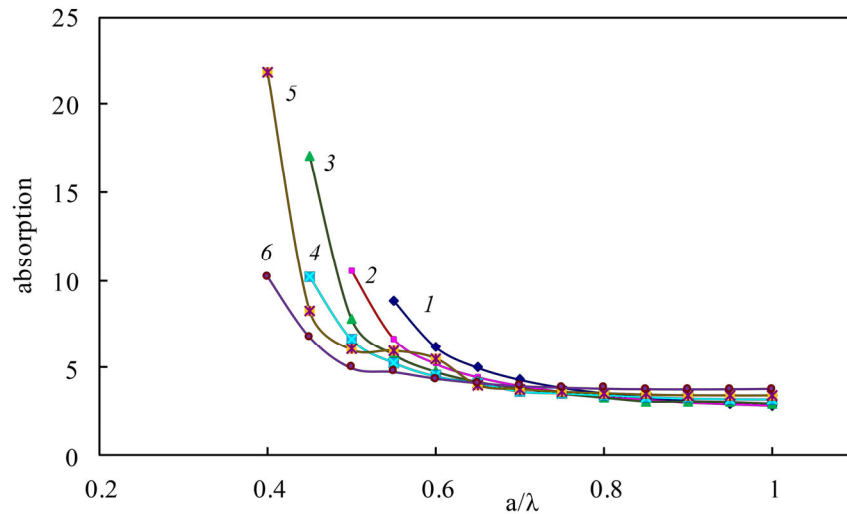
where

$$R_1 = \frac{2t}{a} \left( 1 + \frac{\sin 2\beta t}{2\beta t} \right) + \left( 1 - \frac{2t}{a} \right) \left( \frac{\cos \beta t}{\sin \alpha d} \right)^2 \left( 1 - \frac{\sin 2\alpha d}{2\alpha d} \right),$$

$$R_2 = \frac{2t}{a} \left( \frac{\beta}{\alpha} \right)^2 \left( 1 - \frac{\sin 2\beta t}{2\beta t} \right) + \left( 1 - \frac{2t}{a} \right) \left( \frac{\cos \beta t}{\sin \alpha d} \right)^2 \left( 1 + \frac{\sin 2\alpha d}{2\alpha d} \right),$$

$$R_3 = \sqrt{\omega \mu / 2\sigma}.$$

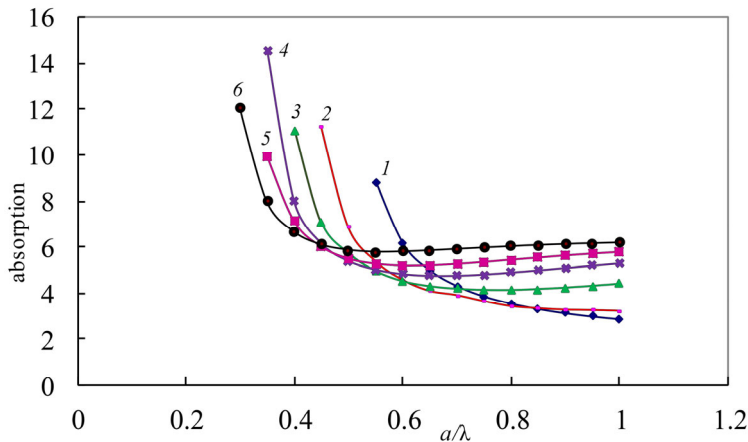
Here  $P$  is the power transmitted through the waveguide,  $P_m$  are the losses in metal walls per unit length,  $m = \lambda / \lambda_{\text{WG}}$  is the electromagnetic wave deceleration coefficient,  $\lambda$  is the free space wavelength,  $\lambda_{\text{WG}}$  is the wavelength in the waveguide,  $a$  and  $b$  are the width and height of the rectangular waveguide, respectively,  $d$  is the distance from the narrow wall of the waveguide to the crystal,  $2t$  is the crystal thickness,  $\alpha = 2\pi / \lambda \sqrt{\varepsilon_0 \mu_0 - m^2}$ ,  $\beta = 2\pi / \lambda \sqrt{\varepsilon \mu - m^2}$ ,  $R_3$  is the surface resistance,  $Z_0 = 377 \Omega$  is the free space resistance,  $\sigma$  is the conductivity of the waveguide walls. The attenuation is determined as a function of the ratio  $a/\lambda$ , for given relative crystal thicknesses  $2t/a$ . The nonlinear crystals DAST ( $\varepsilon_{\text{THz}} = 5.2$ ), ZnTe ( $\varepsilon_{\text{THz}} = 10.1$ ), and LiNbO<sub>3</sub> ( $\varepsilon_{\text{THz}} = 26.5$ ) are investigated for given relative thicknesses of crystals with different dielectric constants and the high indexes of quality (FOMs [6]). Losses in an empty waveguide depend on the ratio of the width of the waveguide to its height and are minimal when  $a/b = 2$ . The values of  $a = 2.4$  mm, and  $b = 1.2$  mm are substituted into expression (6). It should be noted that in the case of low dielectric constant (DAST ( $\varepsilon_{\text{THz}} = 5.2$ )) and partial filling, there are cases when losses in the metal



**Fig. 2.** The attenuation in a metal waveguide partially filled with the DAST crystal,  $\varepsilon_{\text{THz}} = 5.2$ , at (1)  $2t/a = 0$ , (2)  $2t/a = 0.025$ , (3)  $2t/a = 0.05$ , (4)  $2t/a = 0.075$ , (5)  $2t/a = 0.1$ , (6)  $2t/a = 0.15$ .

walls are comparable to losses in the walls of an unfilled metal waveguide. Figure 2 shows that for the DAST crystal with the low dielectric constant, the losses in the metal wall are comparable to the losses in the empty waveguide in the case of  $2t/a \leq 0.15$  and  $a/\lambda > 0.65$ , that is, the waveguide does not distort the pulse shape in the frequency range of the main type waves. In addition, in the case of a thin crystal, the damping may be weaker than in an unfilled waveguide with the value of  $a/\lambda$  from 0.4 to 0.8. In a partially filled waveguide, this effect is caused by the decrease in the cut-off frequency of the waveguide.

In the case of a high dielectric constant of a crystal, the losses in the waveguide walls are higher, and the damping depends more on the degree of filling with a crystal  $2t$ , than on the ratio  $a/\lambda$ , that is, on the frequency (Fig. 3, Fig. 4).



**Fig. 3.** The attenuation in a metal waveguide partially filled with the ZnTe crystal,  $\epsilon_{\text{THz}}^e = 10.1$ , at (1)  $t/a = 0$ , (2)  $2t/a = 0.025$ , (3)  $2t/a = 0.05$ , (4)  $2t/a = 0.075$ , (5)  $2t/a = 0.1$ , (6)  $2t/a = 0.15$ , and  $a = 2.4$  mm.

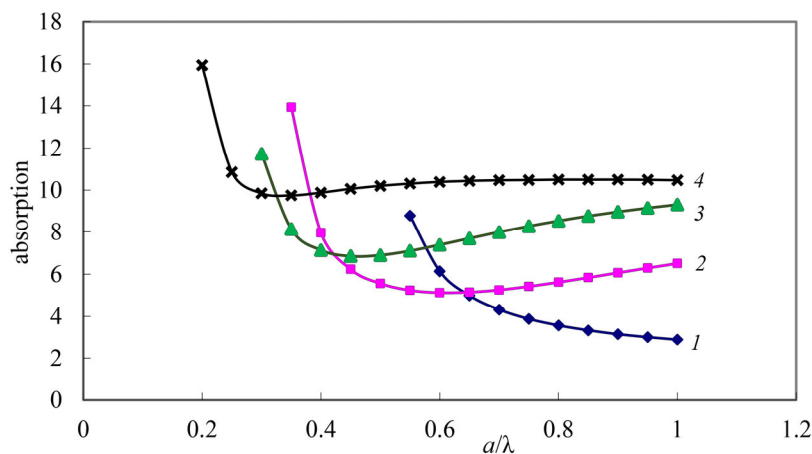
The attenuation in the walls of a waveguide with a thin LiNbO<sub>3</sub> crystal is less than in an empty waveguide in the wavelength range  $0.5 < a/\lambda < 0.65$ . Consequently, the periodic THz pulses or continuous radiation of a given frequency in a certain narrow frequency range can be generated with the attenuation less than in an empty waveguide, with a crystal length equal to the waveguide length. In this frequency band, the losses in metal walls will not weaken and expand the THz pulse.

The attenuation due to the losses in the crystal, partially filling the waveguide, was determined from the expression (7)

$$\alpha_d = \epsilon \frac{\pi a}{m \lambda R_1} \frac{1}{a} \frac{2t}{a} \left( 1 + \frac{\sin 2\beta t}{2\beta t} \right) \tan \delta / a, \quad (7)$$

where  $\tan \delta = \epsilon''/\epsilon'$ . The attenuation constant of THz radiation, shown in Fig. 5, equals to  $\alpha = \alpha_d \tan \delta / a$  ( $\alpha_d$  in a units of  $Np/m$ ) increases with the increasing degree of filling of the waveguide cross-section.

The data obtained show that a threefold decrease in attenuation for a given frequency is possible, if instead of a completely filled waveguide, a partially filled waveguide is used. From (3) it can be seen that the conversion efficiency of optical radiation in the THz range depends on the square of the attenuation coefficient. The reducing of the attenuation in a partially filled waveguide, in turn, means that there can be used the longer crystals to generate high-intensity THz radiation as compared to the case of completely filling the waveguide with the crystal. It is known that when the phase-matching condition is satisfied, the



**Fig. 4.** The attenuation in a metal waveguide partially filled with the LiNbO<sub>3</sub> crystal,  $\varepsilon_{\text{THz}}^e = 26.5$  at (1)  $2t/a = 0$ , (2)  $2t/a = 0.025$ , (3)  $2t/a = 0.05$ , (4)  $2t/a = 0.15$ .

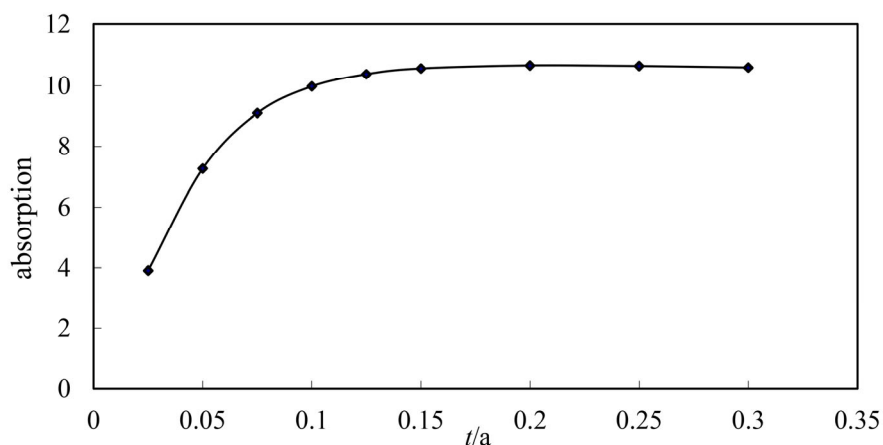
THz radiation power grows quadratically with the increasing length of a nonlinear crystal [6]. Therefore, there is a double effect. A waveguide partially filled with a nonlinear crystal allows one to ensure both the phase matching condition and the reduction of the THz radiation absorption in the generated crystal. This cannot be achieved in other ways that provide phase matching when a nonlinear crystal is in free space, where the attenuation coefficient is constant. Thus, a waveguide, partially filled with the non-linear crystal, ensures the efficient generation of the THz radiation owing to both phase matching and a decrease in the absorption of THz radiation in the crystal. A further increase in the energy conversion efficiency of optical radiation in the THz range is possible, if the generation is carried out not at room temperature, but at cryogenic temperatures. With a decrease in temperature to 100 K in LiNbO<sub>3</sub> [15, 16], when the phase matching condition is satisfied, an increase in the energy conversion efficiency of more than 2.5 times is achieved, because of the decrease in the absorption.

A greater increase in the conversion efficiency (5–10 times) than with a decrease in temperature was achieved in [17] by giving the output crystal wedge-shaped form with a wedge angle equal to the Brewster angle.

### 3. CONCLUSION

The generation efficiency in the process of converting the frequency of ultrashort laser pulses to the THz range depends on the fulfillment of the phase matching condition, as well as on the losses ( $\alpha = \alpha_m + \alpha_d$ ) for a given crystal length. The DAST, LiNbO<sub>3</sub> and ZnTe crystals were studied due to the high efficiency of conversion of optical radiation into the THz range in a waveguide partially filled with one of these crystals.

It is shown that the attenuation of a THz pulse increases with the corresponding increase in the degree of filling of a given cross section of the waveguide with a crystal (Fig. 5). However, in the case of a small dielectric constant and partial filling, the losses in the metal walls are comparable to the losses in the walls of an unfilled metal waveguide. Moreover, in the case of a thin crystal with the low dielectric constant, the damping may be weaker than in an unfilled waveguide. In a partially filled waveguide, this phenomenon occurs owing to the decrease in the dominant mode cut-off frequency, which is more



**Fig. 5.** The attenuation in a metal waveguide partially filled with the LiNbO<sub>3</sub> crystal at  $2t/a$  changing in the (0; 1) interval.

obvious when the waveguide is completely filled with the crystal. In the case of high dielectric constant of a crystal, the higher losses are observed in the walls of the waveguide, which is more due to the degree of filling with the crystal than the ratio  $a/\lambda$ , that is, with the frequency dependence. In all crystals, the minimum attenuation is observed for a certain frequency band.

Thus, optical rectification in organic crystals (DAST, DSTMS OH1, [18, 19]), and in the crystal LiNbO<sub>3</sub> is the most promising method for generating the extremely strong THz field [15]. The results are important for the rapidly growing field of high-performance THz sources [20, 21] with promising applications in various fields in the interaction of GHz and THz waves with matter [22] and for a significant reduction of dielectric losses which is the main cause of attenuation in the waveguides integrated on the substrate (SIW) [23].

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