# Modeling of Terahertz Radiation Generation By Femtosecond Laser Pulse of FEW Cycles

G.D. Hovhannisyan<sup>1</sup>, A.H. Vardanyan<sup>1\*</sup>, A.V. Sahakyan<sup>2</sup>

<sup>1</sup>"National Institute of Metrology" National body of metrology Closed Joint-Stock Company (CJSC), 49/4 Building Komitas Ave. 0051, Yerevan, Armenia
<sup>2</sup>Nuclear Physics Department of Yerevan State University, 1 Alex Manoogian, 0025, Yerevan, Armenia \*E-mail: s vardanyan@hotmail.com

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Abstract: In this paper, we study the spectrum and time profile of terahertz radiation that generated during the propagation of an extraordinary linearly polarized laser pulse of a few optical cycles in the direction normal to the optical axis of a nonlinear uniaxial crystal of 3m symmetry group. We solve Maxwell's equations describing the propagation of the laser pulse using the FDTD method. As an example, we calculate the spectrum and time profile of terahertz radiation for laser pump pulse with duration  $10 f_s$  at 850nm wavelength. As an example, we apply our model to study the propagation of a femtosecond laser pulse in a *LiNbO*, crystal of  $390\mu m$  thickness.

Keywords: terahertz, few optical cycles, uniaxial crystal

# 1. Introduction

The very first process put to use for the generation of microwave pulses from picosecond's duration laser pulses was optical rectification. Yang et al [1] demonstrated in 1971 the generation of far-infrared radiation in  $LiNbO_3$ . In 1984 Auston et al. [2] demonstrated the high-bandwidth capabilities of optical rectification by the generation of frequencies up to 4 THz in lithium tantalate. The generation of terahertz radiation through optical rectification has subsequently been demonstrated in a variety of materials, such as lithium tantalate ( $LiNbO_3$ ) [3], semiconductors [4, 5] and organic crystals [6].

The rapid development of the generation techniques of powerful femtosecond laser pulses of a few optical cycles has recently created interest in generation of terahertz radiation. During the last decade, time-domain THz spectroscopy and imaging have become widely used techniques in various fields of physics, chemistry and biology. The access to the interesting THz spectral region, which has remained almost unexplored for a long time, has been enabled by rapid progress in the development of powerful THz sources such as optical rectification of femtosecond laser pulses in nonlinear crystals [7,8]. Probably one of the most important present challenges of THz technology is up-scaling of the THz pulse energy to a level suitable for nonlinear spectroscopy.

As compared with powerful THz sources such as photoconductive switches irradiated by ultrashort laser pulses, THz sources based on optical rectification is more direct since it simply requires one to focus the laser beam on a nonlinear crystal. The transient polarization is generated at a microscopic level, directly through the material response, unlike that in photoconductive switching, which involves the realization of an optoelectronic device. The advantage of photoconductive switching is obviously its much greater efficiency, as very large voltages can be switched by the laser pulse, unlike optical rectification, which must rely on existing nonlinear coefficients. On the other hand, optical rectification is truly instantaneous. As a result, while photoconductive switching is limited to a few terahertzes, optical rectification has been demonstrated to allow the generation of frequencies up to 50THz [9], well into the mid-infrared spectral domain. The conversion efficiency in optical rectification depends primarily on the material's nonlinear coefficient and the velocity-matching conditions.

More recent technique is termed time-resolved THz spectroscopy (TRTS). TRTS have enabled the measurement of the electric field of a nearly single-cycle THz pulse after it propagates through a photoexcited medium with subpicosecond resolution [10]. This new visible pump, far-infrared (FIR) probe spectroscopy, has opened up the FIR region of the spectrum to time-resolved studies. The FIR region contains important information relevant to chemistry, physics, and biology, and time-resolved studies in the FIR will provide new insights. Consequently, it is of considerable practical interest to use femtosecond laser pulse of a few optical cycles duration to generate broadband THz pulses for TRTS applications.

Now more than ever, new methods of modeling femtosecond laser pulses are needed. The slowly varying amplitude (SVA) approximation cannot be used to model such processes [11]. Therefore, modeling the propagation process of a femtosecond laser pulse of a few optical cycles in an anisotropic optical crystal requires either numerical methods or special analytical methods. The numerical finite-difference time domain (FDTD) method for nonlinear optics is completely general. FDTD is an explicit full-wave finite-difference solution of the time dependent Maxwell's equations that yields both electric and magnetic fields with a spatial resolution much finer than one wavelength.

In [12], we apply the FDTD method for the solution of the propagation of a laser pulse of a few optical cycles duration in a uniaxial crystal, taking into account the medium linear dispersion. We consider an extraordinary linearly polarized laser pulse with a plane wave front propagating along the *y*-axis, normal to the optical *z*-axis of a uniaxial crystal of 3*m* symmetry group. We calculate the conversion efficiency to the second harmonic as a function of crystal length, pump energy, and pulse duration. As a concrete example, we numerically solve for the propagation of a femtosecond laser pulse of  $\tau_0 = 10 fs$  duration at  $\lambda = 810 nm$  and energy  $\Delta E = 40 nJ$  (electrical field  $6.1 \cdot 10^8 V/m$ ) in a *LiNbO*<sub>3</sub> crystal of  $25 \mu m$  thickness. In [12] the length of selected crystal was choosing so that the partially stationary second harmonic oscillation mode occurs. At the same time it must be noted that in this geometry a phase mismatch between the pump and second-harmonic pulses for the entire pulse spectrum takes place.

In this paper, we study the generation of terahertz radiation in frequency range (66-85)THz that occur during the propagation of an extraordinary linearly polarized laser pulse of a few optical cycles in the direction normal to the optical axis of a nonlinear uniaxial crystal of 3m symmetry group. We solve Maxwell's equations describing the propagation of the laser pulse using the FDTD method. As an example, we calculate the spectrum and time profile of terahertz radiation generated during the propagation of laser pulse with duration 10 fs at 850nm wavelength. We apply our model to study the propagation of a femtosecond laser pulse in a  $LiNbO_3$  crystal of  $390\mu m$  thickness.

## 2. Physical Problem

Consider a linearly polarized laser pulse of a few optical cycles with field components  $E_z$ and  $H_x$  with a plane wave front propagating along the *y*-axis, normal to the optical axis of a uniaxial crystal of 3m symmetry group. Maxwell's equations in this case are written as

$$\frac{\partial H_x}{\partial t} = -\frac{1}{\mu_0} \frac{\partial E_z}{\partial y}$$

$$\frac{\partial D_z}{\partial t} = -\frac{\partial H_x}{\partial y}$$

$$E_z = \frac{D_z - (P_{zL} + P_{zNL})}{\varepsilon_0}$$
(1)

where  $D_z$  is the electric flux density,  $\mu_0$  is the free-space permeability,  $\varepsilon_0$  is the free-space permittivity, and  $P_{zL}$  and  $P_{zNL}$  are the induced linear and nonlinear electric polarizations, respectively.

The induced linear electric polarization can be written as

$$P_{zL}(t) = \varepsilon_0 \int_{-\infty}^{\infty} \chi^{(1)}(t - t_1) E_z(t_1) dt_1$$
(2)

In the nonlinear part of the polarization of a uniaxial optical crystal of 3m symmetry group, such as  $LiNbO_3$ , which is responsible for second order-nonlinearities, we shall confine ourselves to the quasistatic approximation

$$P_{zNL}(t) = \varepsilon_0 \cdot d_{33} \cdot E_z^2(t) , \qquad (3)$$

where  $d_{33}$  is the non-zero component of the second-order crystal susceptibility tensor. The quasistatic approximation in the nonlinear part of the medium's polarization fits the assumption about the inertia less nature of the crystal nonlinear response, which takes place in the near-infrared spectrum range [13].

The corresponding frequency-domain response function,  $\chi^{(1)}(\omega)$ , is related to the linear index of the extraordinary wave of the medium, by

$$\chi^{(1)}(\omega) = n_e^2(\omega) - 1 \tag{4}$$

For optical frequencies that are far from the resonant frequencies of the medium  $(0.35-5.5\mu m)$ , the index of refraction of the *LiNbO*<sub>3</sub> uniaxial nonlinear crystal can be approximated by the Sellmeier equation [13]. This equation is based on the classical Lorentz model of an atom and is written as

$$\varepsilon_{e}(\omega) = n_{e}^{2}(\omega) = 4.5567 + 2.605 \cdot 10^{-7} \cdot T^{2} + \frac{\frac{(0.097 + 2.7 \cdot 10^{-8} \cdot T^{2}) \cdot \omega^{2}}{(2\pi \cdot c)^{2}}}{1 - \frac{(0.201 + 5.4 \cdot 10^{-8} \cdot T^{2})^{2} \cdot \omega^{2}}{(2\pi \cdot c)^{2}} , \qquad (5)$$
$$-2.24 \cdot 10^{-2} \cdot \frac{(2\pi \cdot c)^{2}}{\omega^{2}}$$

where T is the temperature by Kelvin and c is the light velocity in vacuum in  $\mu m/\text{sec.}$ Refraction index was calculated at  $T = 293^{\circ}K$ .

Equations (4) and (5) show that the linear frequency-domain response function  $\chi^{(1)}(\omega)$  can be presented in the following form

$$\chi^{(1)}(\omega) = \left(a_{e} - \frac{b_{e}}{c_{e}^{2}}\right) + \frac{\left(b_{e}/c_{e}^{2}\right)}{1 - c_{e}^{2} \cdot \omega^{2}} - \frac{q_{e}}{\omega^{2}} , \qquad (6)$$

where

$$a_{e} = (3.5567 + 2.605 \cdot 10^{-7} \cdot T^{2}), b_{e} = \left(\frac{0.097}{(2\pi \cdot c)^{2}} + \frac{2.7 \cdot 10^{-8} \cdot T^{2}}{(2\pi \cdot c)^{2}}\right)$$
(7)  
$$c_{e} = (0.201 + 5.4 \cdot 10^{-8} \cdot T^{2})/(2\pi \cdot c), q_{e} = 2.24 \cdot 10^{-2} \cdot (2\pi \cdot c)^{2}$$

The three terms for the linear response function in (6) lead to the following decomposition for the corresponding temporal polarization:

$$P_{zL}(t) = \mathcal{E}_0 \cdot \mathcal{E}_c \cdot E_z(t) + F(t) + G(t) , \qquad (8)$$

where  $\varepsilon_c = a_e - b_e / c_e^2$ , F(t) and G(t) are solutions of the following ordinary differential equations

$$c_{e}^{2} \cdot \frac{\partial^{2} F(t)}{\partial t^{2}} + F(t) = \varepsilon_{0} \cdot \frac{b_{e}}{c_{e}^{2}} \cdot E_{z}(t, y)$$

$$\frac{\partial^{2} G(t)}{\partial t^{2}} = \varepsilon_{0} \cdot q_{e} \cdot E_{z}(t, y)$$
(9)

The equations (9) describe the linear dispersion properties of the medium in the passband according to the Lorentz classical model.

Taking into account (1), (3), and (8) the electric induction  $D_z$  could be represented as

$$D_z = \mathcal{E}_0 \cdot \mathcal{E}_z + \mathcal{E}_0 \cdot \mathcal{E}_c \cdot \mathcal{E}_z + F + G + \mathcal{E}_0 \cdot \mathcal{d}_{33} \cdot \mathcal{E}_z^2 .$$
(10)

The classical model of interaction between a laser pulse of a few optical cycles and a nonlinear dispersive uniaxial crystal of 3m symmetry group described above was used by us for the description of the parametric near infrared radiation generation [14].

In this paper we use this model for the analysis of terahertz radiation generation in (66-85)THz spectral range by femtosecond laser pulse of a few optical cycles propagated in nonlinear dispersive uniaxial crystal of 3m symmetry group. As an example, we calculate the spectrum and time profile of terahertz radiation generated by laser pump pulse with duration 10 fs at 850nm wavelength. We apply our model to study the propagation of a femtosecond laser pulse in a  $LiNbO_3$  crystal of  $390\mu m$  thickness.

# 3. Numerical Implementation

In this paper the modified finite-difference solution model of nonlinear Maxwell equations is used for the numerical integration of the system of nonlinear Maxwell equations. This schematic model, as shown in [15], has increased stability, good dispersive characteristics and does not require heavy computing facilities.

For the numerical modeling of the processes described by equations (1), (9), (10), let's pass on to the mesh functions for  $E_z$  and  $H_x$  fields, electric induction  $D_z$ , linear and nonlinear responses, for which the grids are set over the  $k \cdot \Delta y$  coordinate and  $n \cdot \Delta t$  time. The step of spatial grid  $\Delta z$  was chosen equal to 15nm. The step of time grid is determined by Kurant's condition  $\Delta t = \Delta y/(2 \cdot c)$  and is equal to 0.025 fs. For such time step the linear part of the scheme has a dispersion that is approached the Lorentz dispersion of the medium as much as possible. The magnetic field's values are set between the mesh points in Y-direction and on the intermediate layer over the time. The difference schemes, corresponding to the equations (1), (3), (9), and (10), are written down for the following normalized quantities

$$\overline{E}_{z} = \sqrt{\frac{\varepsilon_{0}}{\mu_{0}}} \cdot E_{z}, \overline{D}_{z} = \frac{1}{\sqrt{\varepsilon_{0} \cdot \mu_{0}}} \cdot D_{z}, \overline{H}_{x} = H_{x},$$

$$\overline{P}_{zL} = \frac{1}{\sqrt{\varepsilon_{0} \cdot \mu_{0}}} \cdot P_{zL}, \overline{P}_{zNL} = \frac{1}{\sqrt{\varepsilon_{0} \cdot \mu_{0}}} \cdot P_{zNL}, \qquad (11)$$

$$\overline{G} = \frac{1}{\sqrt{\varepsilon_{0} \cdot \mu_{0}}} \cdot G, \overline{F} = \frac{1}{\sqrt{\varepsilon_{0} \cdot \mu_{0}}} \cdot F$$

At the beginning of iteration process the given values are  $E_z$ ,  $D_z$  on time layer n and  $H_x$ on time layer n-1/2. At the first step of calculation by the given values  $E_z$ ,  $D_z$ , and  $H_x$  the values  $D_z$  and  $H_x$  are found on a new time layer n+1 and n+1/2 accordingly

$$\overline{H}_{x}\Big|_{k+1/2}^{n+1/2} = \overline{H}_{x}\Big|_{k+1/2}^{n-1/2} - \frac{c \cdot \Delta t}{\Delta y} \cdot \left(\overline{E}_{z}\Big|_{k+1}^{n} - \overline{E}_{z}\Big|_{k}^{n}\right),$$

$$\overline{D}_{z}\Big|_{k}^{n+1} = \overline{D}_{z}\Big|_{k}^{n} - \frac{c \cdot \Delta t}{\Delta y} \cdot \left(\overline{H}_{x}\Big|_{k+1/2}^{n+1/2} - \overline{H}_{x}\Big|_{k-1/2}^{n+1/2}\right)$$
(12).

Before proceeding to the next step of calculation let's consider the difference schemes corresponding to the differential equations (9). The difference scheme defining the linear response of a medium  $F_i$ ,  $G_i$  on n+1 time layer according to (9) is determined in the following way

$$\overline{F}\Big|_{k}^{n+1} = aL1 \cdot \overline{F}\Big|_{k}^{n} - \overline{F}\Big|_{k}^{n-1} + cL1 \cdot \overline{E}_{z}\Big|_{k}^{n}$$
$$\overline{G}\Big|_{k}^{n+1} = 2 \cdot \overline{G}\Big|_{k}^{n} - \overline{G}\Big|_{k}^{n-1} + dL \cdot \overline{E}_{z}\Big|_{k}^{n}, \qquad (13)$$

where  $\overline{F}\Big|_{k}^{n-1}$ ,  $\overline{F}\Big|_{k}^{n}$ ,  $\overline{G}\Big|_{k}^{n-1}$ ,  $\overline{G}\Big|_{k}^{n}$  - are the values of linear polarization of the medium on time layers n-1 and n,  $\overline{E}_{z}\Big|_{k}^{n}$  - is the value of electrical field on time layer n,

$$aL1 = 2 - \frac{\Delta t^2}{c_e^2}, cL1 = \frac{b_e}{c_e^4} \cdot \Delta t^2, dL = q_e \cdot \Delta t^2 .$$

$$(14)$$

At the second step of calculation the linear polarization of the medium  $\overline{F}\Big|_{k}^{n+1}, \overline{G}\Big|_{k}^{n+1}$  on time layer n+1 is determined according to (13).

According to (3), the second order nonlinear instantaneous response of a medium  $P_{zNL}$  on n+1 time layer is determined by the following way

$$\overline{P}_{zNL}\Big|_{k}^{n+1} = d_{33} \cdot \left(\overline{E}_{z}\Big|_{k}^{n+1}\right)^{2} .$$
(15)

According to (10), (13), and (15), the electric induction can be represented as

$$\overline{D}_{z}\Big|_{k}^{n+1} = \left(1 + \varepsilon_{c}\right) \cdot \overline{E}_{z}\Big|_{k}^{n+1} + \overline{F}\Big|_{k}^{n+1} + \overline{G}\Big|_{k}^{n+1} + d_{33} \cdot \overline{E}_{z}^{2}\Big|_{k}^{n+1} .$$

$$(16)$$

At the third step of calculations the value of electric field  $E_z$  on n+1 time layer is derived from the constitutive equation (16), which is used during the difference approximation (15).

At the last step, using the given values of linear and nonlinear polarization, the value of  $\overline{E}_{z}\Big|_{v}^{n+1}$  is calculated by the following recurrence formula

$$\overline{E}_{z}\Big|_{k}^{p+1} = \frac{\overline{D}_{z}\Big|_{k}^{n+1} - \overline{F}\Big|_{k}^{n+1} - \overline{G}\Big|_{k}^{n+1}}{1 + \varepsilon_{c} + d_{33} \cdot \left(\overline{E}_{z}\Big|_{k}^{p}\right)^{2}} , \qquad (17)$$

where  $\overline{E}_{z}\Big|_{\kappa}^{p} = \overline{E}_{z}\Big|_{\kappa}^{n+1}$  at the beginning of the iteration. The iteration process is repeated up to the getting of the root of an equation and is used in the program for calculation accuracy control.

### 4. Results of Computational Modeling

We are now in a position to compute the spectrum evolution of a femtosecond laser pulse of a fewoptical cycles through  $LiNbO_3$  taking into account the medium linear dispersion. In the nonlinear part of the medium polarization of uniaxial crystal of 3m group, that is responsible for the second order nonlinearity, we will confine ourselves to the quasi-static approximation. The quasi-static approximation in the nonlinear part of the medium polarization actually fits the assumption about the inertia less nature of the crystal nonlinear response, which takes place in the infrared spectrum range. Particularly we will consider the energy redistribution process in the spectral region  $(3\mu m - 5\mu m)$  of laser pulse spectrum at the nonlinear crystal output.

In figure 1 we show the results of numerical computations of equations (12), (13), (15), (16), and (17) which describe the nonlinear propagation of femtosecond pulse with linear extraordinary polarization in a uniaxial optical crystal  $LiNbO_3$ , with the following boundary condition for the pulse field at the input of the crystal

$$E_{zINP}(t, z=0) = E_{Z0} \cdot \exp\left(-\frac{t^2}{\tau_0^2}\right) \cdot \cos\left(\frac{2 \cdot \pi \cdot c}{\lambda_0} \cdot t\right), \qquad (18)$$

where  $E_{z0}$  – is the initial amplitude value of a pulse,  $\tau_0$  is the duration and  $\lambda_0$  is the central wavelength.

In this paper, the results of the computational modeling of propagation process of linearly polarized pulse with central wavelengths  $\lambda_0 = 0.85 \mu m$  and duration  $\tau_0 = 10 fs$  are presented. The length of the medium in calculations is considered equal to  $L = 390 \mu m$ , the pulse energy are equal to  $\varepsilon = 7.317 nJ$ . The initial value of the amplitude of linearly polarized electric field  $E_{z0}$  is determined according to the expression [14]

$$E_{z0} = 27 \cdot \sqrt{\frac{\mathcal{E}}{S \cdot \tau_0}} \quad , \tag{19}$$

where  $S = \pi \cdot d^2/4$  is the cross-section of a beam, d – beam diameter. The beam diameter is considered in calculations equal to  $d = 100 \mu m$ . As it is not difficult to notice, for the given value of energy and cross-section of pulse, the initial value of pulse amplitude is equal to  $E_{z0} = 260 MV / m$ . And this corresponds to the intensity value  $I \approx 9.3 GW / cm^2$  and peak power value  $P_0 = 731.71 kW$ .

In figure 1 (a) we show the temporal profile of the 10 fs duration pulse field at the input of the crystal. In figure 1 (b) we show the initial pump pulse normalized power spectrum of the 10 fs duration pulse at the input of the crystal. In figure 1 (c) we show the temporal profile of the pulse at the crystal output  $E_{OUT}(t)$ . In figure 1 (d) we show the normalized power spectrum of the pulse at the crystal output. In figure 1 (c), we can see that during pulse propagation in a

nonlinear crystal, asymmetric broadening of the pulse's time profile occurs. In figure 1 (c) it is seen that the amplitude of the output pulse is 36.39MV / m, duration of the output pulse is about 120 fs and the peak power of output pulse is 61kW. As shown in figure 1 (d) and from the results of numerical computations for the above mentioned values of parameters, during pulse propagation in a nonlinear crystal the sum and difference spectral components generation occurs.



Figure 1. The evolution of the femtosecond laser pulse with a duration 10 fs at wavelength 850 nm and electrical field  $E_z = 260 MV / m$  as it propagates in a uniaxial optical crystal  $LiNbO_3$  with  $390 \mu m$  length.

In this figure is shown the spectrum of the pump pulse at the crystal output normalized to initial pulse spectrum

$$10 \cdot \lg(S_{OUT}(\lambda)) = 10 \cdot \lg\left(\frac{P_z}{P_{z0}}\right) = 10 \cdot \lg\left(\frac{\left|\int_{-\infty}^{\infty} E_z(t, y = L) \cdot \exp\left\{j \cdot \frac{2 \cdot \pi \cdot c \cdot t}{\lambda}\right\} \cdot dt\right|^2}{\left|\int_{-\infty}^{\infty} E_z(t, y = 0) \cdot \exp\left\{j \cdot \frac{2 \cdot \pi \cdot c \cdot t}{\lambda}\right\} \cdot dt\right|^2}\right).$$
(20)

According to calculations results the power spectrum for high order harmonics is about - 60dB whereas the power spectrum for terahertz spectral components (66-85THz) doesn't exceed ~ -75dB.

It is obvious from the figure 1 (d) that from a practical perspective, extremely short femtosecond pulses of a few optical oscillations centered at one frequency and propagating in nonlinear dispersive uniaxial crystal can be used to generate terahertz radiation. The generated radiation can be subsequently filtered to select a specific band of frequencies. Such a femtosecond pulse generator at tunable wavelengths is practically realizable, and is expected to be useful in the research of the interaction between materials and terahertz radiation.

Consequently it is of practical interest to consider filtering process of the specific band of frequencies in the spectral super continuum that occur in the output pulse spectrum. For this purpose we will consider two different filters with the Gaussian transmission functions

$$H_i(\mathbf{v}) = \exp\left(-\frac{(\mathbf{v} - \mathbf{v}_{i0})^2}{\delta \mathbf{v}_i^2}\right),\tag{21}$$

where  $v_{10} = 85.757THz \ (\lambda_{10} = 3.4982 \,\mu m), \ \delta v_1 = 18.7695THz, \ v_{20} = 66.341THz \ (\lambda_{20} = 4.5221 \,\mu m), \ \delta v_2 = 7.6858THz.$ 

In figures 2 (a), (d) the filters transmission functions in logarithmic scale are shown. In figures 2 (b), (e) in logarithmic scale are shown the spectral bands of supercontinuum that are transmitted by corresponding filters. In figures 2 (c), (f) are shown the temporal profiles of pulses with central frequencies in infrared spectral region obtained by filtering.



Figure 2. (a), (d), the filters transmission functions in logarithmic scale; (b), (e), the spectral bands of supercontinuum transmitted by corresponding filters in logarithmic scale; (c), (f), the temporal profiles of pulses with central frequencies in terahertz (mid infrared) spectral region obtained by filtering.

The duration of the pulse (figure 2 (c)) at the  $v_{10} = 85.757THz$  ( $\lambda_{10} = 3.4982\mu m$ ) central frequency obtained by filtering is about 113.4 *fs*, the maximum value of electric field amplitude is 5.811kV/m. The peak power of obtained pulse in a case when the beam diameter is considered in calculations equal to  $d = 100\mu m$  is  $363.80\mu W$ . Conversion efficiency

$$\gamma = 10 \cdot \lg \left( \frac{P(\lambda_i)}{P_0} \right)$$
(22)

in this case is -93.035dB. The duration of the pulse (figure 2 (f)) at the  $v_{20} = 66.341THz$  ( $\lambda_{20} = 4.5221\mu m$ ) central frequency obtained by filtering is about 138.5 fs, the maximum value of electric field amplitude is 2.2498 kV/m. The peak power of obtained pulse in a case when the beam diameter is considered in calculations equal to  $d = 100\mu m$  is  $54.5221\mu W$ . Conversion efficiency in this case is -101.278dB.

The quasistatic interaction length limited by group velocity mismatch for the transformlimited initial femtosecond pulse with extraordinary polarization is determined as in [16] by

$$Lg(\omega) = \frac{2 \cdot \pi}{\Delta \omega} \cdot \left(\frac{\partial k_e(\omega)}{\partial \omega} - \frac{\partial k_e(\omega_{IR})}{\partial \omega}\right)^{-1}$$
(23)

where  $k_e(\omega)$ ,  $k_e(\omega_{lR})$  are the wave numbers for extraordinary polarized waves at the first harmonic and infrared harmonics, respectively. For the predetermined numerical values of the extraordinary polarized femtosecond pulse duration and central frequency  $\omega_0$ , the group velocity mismatch length for  $LiNbO_3$  crystal at the difference infrared central wavelengths are:  $Lg(\omega_1 = 2 \cdot \pi \cdot v_{10}) = 82.872 \mu m$ ,  $Lg(\omega_2 = 2 \cdot \pi \cdot v_{20}) = 350.374 \mu m$ . The length of the crystal in our simulations is  $y \approx Lg(\omega_2 = 2 \cdot \pi \cdot v_{20})$ . This means that in this particular case<sub>2</sub> the stationary infrared harmonic oscillation mode occurs only at  $\lambda_2 = 4.5221 \mu m$  central wavelength. At the same time it is necessary to notice that in our geometry, due to the first order dispersion of the linear index of refraction, a phase mismatch between the fundamental and terahertz pulses for the entire pulse spectrum takes place. In another word in our case we have the terahertz radiation generation by non-phase-matched interaction of femtosecond laser pulse of a few optical cycles with nonlinear crystal.

According to the numerical calculations of the system of equations (12), (13), (15)-(17), at the predetermined numerical values of the parameters, both difference frequencies and summary frequencies appear in the transmitted spectrum of a femtosecond pulse during the propagation of extraordinary polarized femtosecond laser pulse of a few optical oscillations in a negative uniaxial crystal in the direction normal to optical axis.

It can be noticed that in non-phase-matched interaction case for the realization of the tunable laser source in the terahertz (mid infrared) region by means of using the spectrum of few optical cycles' duration laser pulse at the nonlinear crystal output the medium length must be chosen equal to the quasistatic interaction length for the desired value of central wavelength.

# 5. Conclusions

Thus, in this paper, we apply the nonlinear FDTD model to study the process of terahertz (mid infrared) radiation generation to solve Maxwell's equations that describe the propagation of a femtosecond laser pulse of a fewoptical cycles in a negative uniaxial crystal in the direction normal to the optical axis, taking into account medium linear dispersion and second order nonlinearity. The modified finite-difference solution model of nonlinear Maxwell equations is used for the numerical integration of the system of nonlinear Maxwell equations. This schematic model has heightened stability, good dispersive characteristics and does not require heavy computing facilities. We have considered an extraordinary linearly polarized laser pulse with a plane wave front propagating along the y-axis, normal to the optical z-axis of a uniaxial crystal of 3m symmetry group. In the nonlinear part of the polarization of a uniaxial crystal of the 3m group we confine ourselves to considering the quasistatic approximation that takes place in the near infrared spectrum range. The nonlinear crystal length is chosen so that the stationary infrared harmonic oscillation mode occurs for the spectral components near the  $\sim 4.5 \mu m$  wavelength. At the same time we note that in our geometry a phase mismatch between the pump and infrared harmonic pulses for the entire pulse spectrum takes place.

As the final result it is shown that in non-phase-matched interaction case, for realization the tunable laser source in the terahertz (mid infrared) region by means of using the spectrum of few optical cycles duration laser pulse at the nonlinear crystal output the medium length must be chosen equal to the quasistatic interaction length for the desired value of central wavelength. The generated radiation can be subsequently filtered to select a specific band of frequencies.

We obtain the time profiles of filtered pulses in the terahertz (mid infrared) spectral region for 10 fs duration pump pulse at  $0.85 \mu m$  central wavelength.

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