Modeling and Analysis of Wave Packet Scattering and Generation for a Nonlinear Layered Structure

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Abstract – Nonlinear dielectrics with controllable permittivity are the subject of intense studies and have begun to find broad applications in device technology and electronics. We develop a model of resonance scattering and generation of waves on an isotropic, nonmagnetic, nonlinear, layered dielectric structure excited by a packet of plane waves in the resonance frequency range in a self-consistent formulation. Various effects caused by the nonlinearity of the structure are investigated using analytical and numerical techniques.

Introduction

The elaboration of mathematical models of wave propagation in nonlinear media is a key issue in multiphysics modeling of microwave processing of materials. We investigate scattering and generation of waves for an isotropic, nonmagnetic, nonlinear, layered dielectric structure in the resonance frequency range excited by a packet of plane waves [1–3]. Here, both the radio [4] and optical [5] frequency ranges are of interest. Our mathematical model reduces to a system of nonlinear boundary value problems (BVPs) of the Sturm-Liouville type or, equivalently, to a system of nonlinear Fredholm integral equations (IEs). Here, for the first time, the solution to BVPs is obtained rigorously in a self-consistent formulation and without using approximations of the given field, slowly varying amplitudes etc. [4, 5]. The analytical continuation of the complex frequency region allows us to turn to the analysis of spectral problems and to reveal various resonance phenomena related to the nonlinearity of the structure. We present and discuss results of calculations of the scattered field, taking into account the third harmonic generated by the nonlinear layer. We show that the portion of total energy generated in the third harmonic may reach up to 36%, which significantly exceeds the known results [5].

Technique

Consider layered nonlinear media in the region $\mathbf{r} = \{(x, y, z) \in \mathrm{R}^3 : |z| \le 2\pi\delta\}$, $\delta > 0$ (cf. Fig. 1).

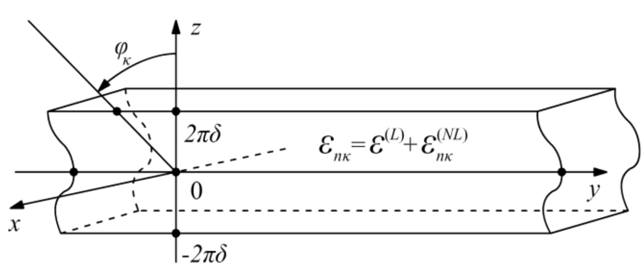


Fig. 1. Nonlinear dielectric layered structure

It is assumed that the vector of polarization moment $\mathbf{P}$ can be expanded as follows:

$$\mathbf{P} = \boldsymbol{\chi}^{(1)}\mathbf{E} + (\boldsymbol{\chi}^{(2)}\mathbf{E})\mathbf{E} + ((\boldsymbol{\chi}^{(3)}\mathbf{E})\mathbf{E})\mathbf{E} + \ldots,$$

where $\boldsymbol{\chi}^{(1)}$, $\boldsymbol{\chi}^{(2)}$, $\boldsymbol{\chi}^{(3)}$ are the media susceptibility tensors. In the case of isotropic media, the quadratic term disappears. It is convenient to split $\mathbf{P}$ into its linear and nonlinear parts $\mathbf{P} = \mathbf{P}^{(L)} + \mathbf{P}^{(NL)} := \boldsymbol{\chi}^{(1)}\mathbf{E} + \mathbf{P}^{(NL)}$. Similarly, with $\boldsymbol{\varepsilon} = \mathbf{I} + 4\pi\boldsymbol{\chi}^{(1)}$ and $\mathbf{D}^{(L)} = \boldsymbol{\varepsilon}\mathbf{E}$, the electric displacement field can be decomposed as

$$\mathbf{D} = \mathbf{D}^{(L)} + 4\pi\mathbf{P}^{(NL)}. \tag{1}$$

Furthermore, if the media under consideration are non-magnetic, isotropic, and transversely inhomogeneous with respect to z, i.e. $\boldsymbol{\varepsilon} = \varepsilon^{(L)}\mathbf{I}$ with a scalar, possibly complex-valued function $\varepsilon^{(L)} = \varepsilon^{(L)}(z)$; if the wave is linearly E-polarized, i.e.

$$\mathbf{E} = (E_x, 0, 0)^{\top}, \ \mathbf{H} = (0, H_y, H_z)^{\top}, \tag{2}$$

and if the electric field $\mathbf{E}$ is homogeneous with respect to the coordinate x, i.e. $\mathbf{E}(\mathbf{r},t) = (E_x(t; y, z), 0, 0)^{\top}$, then Maxwell's equations together with (1) reduce to

$$\nabla^2\mathbf{E} - \frac{\varepsilon^{(L)}}{c^2}\frac{\partial^2}{\partial t^2}\mathbf{E}(\mathbf{r},t) - \frac{4\pi}{c^2}\frac{\partial^2}{\partial t^2}\mathbf{P}^{(NL)} = 0, \tag{3}$$

where $\nabla^2 = \partial^2/\partial y^2 + \partial^2/\partial z^2$. A stationary electromagnetic wave with oscillation frequency $\omega > 0$ propagating in a nonlinear dielectric structure gives rise to a field containing all frequency harmonics. Therefore, representing $\mathbf{E}, \mathbf{P}^{(NL)}$ via Fourier series ($\mathbf{F} \in \{\mathbf{E}, \mathbf{P}^{(NL)}\}$),

$$\mathbf{F}(\mathbf{r},t) = \frac{1}{2}\sum_{s\in\mathbb{Z}} \mathbf{F}(\mathbf{r}, s\omega)\exp(-is\omega t),$$

we obtain from (3) an infinite system of coupled equations with respect to the Fourier amplitudes. In the case of a three-component E-polarized electromagnetic field (cf. (2)) this system reduces to a system of scalar equations with respect to E_x:

$$\nabla^2 E_x(\mathbf{r}, s\omega) + \frac{\varepsilon^{(L)}(s\omega)^2}{c^2} E_x(\mathbf{r}, s\omega) + \frac{4\pi(s\omega)^2}{c^2} P_x^{(NL)}(\mathbf{r}, s\omega) = 0, \quad s \in \mathbb{N}. \tag{4}$$

We assume that the main contribution to the nonlinearity is introduced by the term $\mathbf{P}^{(NL)}(\mathbf{r}, s\omega)$ (cf. [1–3]), and we take only the lowest-order terms in the Taylor series expansion of the non-linear part $\mathbf{P}^{(NL)}(\mathbf{r}, s\omega) = (P_x^{(NL)}(\mathbf{r}, s\omega), 0, 0)^{\top}$ of the polarization vector in the vicinity of the zero value of the electric field intensity. In this case, the only non-trivial component of the polarization vector is determined by the susceptibility tensor $\boldsymbol{\chi}^{(3)}$, and we have that

$$P_x^{(NL)}(\mathbf{r}, s\omega) \cong \frac{1}{4}\sum_{j\in\mathbb{N}} 3\chi^{(3)}_{xxxx}(s\omega; j\omega, -j\omega, s\omega)\,|E_x(\mathbf{r}, j\omega)|^2 E_x(\mathbf{r}, s\omega) +$$
$$+ \frac{1}{4}\sum_{\substack{n,m,p\in\mathbb{Z}\setminus\{0\};\ n\neq -m,\ p=s\\ m\neq -p,\ n=s;\ n\neq -p,\ m=s\\ n+m+p=s}} \chi^{(3)}_{xxxx}(s\omega; n\omega, m\omega, p\omega)\, E_x(\mathbf{r}, n\omega) E_x(\mathbf{r}, m\omega) E_x(\mathbf{r}, p\omega) \tag{5}$$

where the symbol $\cong$ means that higher-order terms are neglected.

If we study nonlinear effects involving the waves at the first three frequency components of E_x only, it is possible to restrict the system (4), (5) to three equations. Using Kleinman's rule (i.e., equating all coefficients $\chi^{(3)}_{xxxx}$ at multiple frequencies, [5]), we obtain the system

$$\nabla^2 E_x(\mathbf{r}, n\kappa) + (n\kappa)^2 \varepsilon_{n\kappa}\big(z, \alpha(z), E_x(\mathbf{r},\kappa), E_x(\mathbf{r},2\kappa), E_x(\mathbf{r},3\kappa)\big) E_x(\mathbf{r}, n\kappa) = \\ -\delta_{n1}\kappa^2\alpha(z) E_x^{2}(\mathbf{r},2\kappa) E_x^{*}(\mathbf{r},3\kappa) - \delta_{n3}(3\kappa)^2\alpha(z)\left\{\frac{1}{3}E_x^{3}(\mathbf{r},\kappa) + E_x^{2}(\mathbf{r},2\kappa)E_x^{*}(\mathbf{r},\kappa)\right\},\ n=1,2,3, \quad (6)$$

where $\kappa := \dfrac{\omega}{c} = \dfrac{2\pi}{\lambda}$, $\varepsilon_{n\kappa} := \varepsilon^{(\mathrm{L})}(z) + \varepsilon^{(\mathrm{NL})}_{n\kappa}$, at $|z| \le 2\pi\delta$; 1, at $|z| > 2\pi\delta$ and $\varepsilon^{(\mathrm{L})}(z) := 1 + 4\pi\chi^{(1)}_{xx}(z)$,

$$\varepsilon^{(\mathrm{NL})}_{n\kappa} := \alpha(z)\left[\sum_{m=1}^{3}|E_x(\mathbf{r}, m\kappa)|^2 + \delta_{n1}\frac{\big(E_x^{*}(\mathbf{r},\kappa)\big)^2}{E_x(\mathbf{r},\kappa)}E_x(\mathbf{r},3\kappa) + \delta_{n2}\frac{E_x^{*}(\mathbf{r},2\kappa)}{E_x(\mathbf{r},2\kappa)}E_x(\mathbf{r},\kappa)E_x(\mathbf{r},3\kappa)\right] \quad (7)$$

with $\alpha(z) = 3\pi\chi^{(3)}_{xxxx}(z)$, and δ_{nm} is the Kronecker delta. In addition, the following conditions are met:

(C1) $E_x(n\kappa; y, z) = U(n\kappa; z)\exp(i\Phi_{n\kappa} y)$, (the quasi-homogeneity condition with respect to y),

(C2) $\Phi_{n\kappa} = n\cdot\Phi_{\kappa}$, (the condition of phase synchronism of waves),

(C3) $\mathbf{E}_{\mathrm{tg}}(n\kappa; y, z)$ and $\mathbf{H}_{\mathrm{tg}}(n\kappa; y, z)$ are continuous at the boundary layers $\varepsilon_{n\kappa}$,

(C4) $E_x^{\mathrm{scat}}(n\kappa; y, z) = \begin{Bmatrix} a^{\mathrm{scat}}_{n\kappa} \\ b^{\mathrm{scat}}_{n\kappa}\end{Bmatrix}\exp\big(i(\Phi_{n\kappa} y \pm \Gamma_{n\kappa}\cdot(z \mp 2\pi\delta))\big),\ z \gtrless \pm 2\pi\delta$, (the radiation condition).

Where $\Phi_{n\kappa} = n\kappa\sin\varphi_{n\kappa}$ and $\Gamma_{n\kappa} = \sqrt{(n\kappa)^2 - \Phi_{n\kappa}^{2}}$, with $\mathrm{Re}\,\Gamma_{n\kappa} > 0$ and $\mathrm{Im}\,\Gamma_{n\kappa} = 0$. Obviously (C2) yields $\varphi_{n\kappa} = \varphi_{\kappa}$. Condition (C4) provides [6] physically consistent behavior of the energy scattering characteristics and guarantees absence of waves coming from infinity ($z = \pm\infty$). The desired solution is of the form ($n = 1, 2, 3$):

$$E_x(n\kappa; y, z) = U(n\kappa; z)\exp(i\Phi_{n\kappa} y) = \\ = \begin{cases} a^{\mathrm{inc}}_{n\kappa}\exp\big(i(\Phi_{n\kappa} y - \Gamma_{n\kappa}(z - 2\pi\delta))\big) + a^{\mathrm{scat}}_{n\kappa}\cdot\exp\big(i(\Phi_{n\kappa} y + \Gamma_{n\kappa}(z - 2\pi\delta))\big), & z > 2\pi\delta, \\ U(n\kappa; z)\exp(i\Phi_{n\kappa} y), & |z| \le 2\pi\delta, \\ b^{\mathrm{scat}}_{n\kappa}\cdot\exp\big(i(\Phi_{n\kappa} y - \Gamma_{n\kappa}(z + 2\pi\delta))\big), & z < -2\pi\delta. \end{cases} \quad (8)$$

Substituting this representation into (6) results in a system of semilinear BVPs of the Sturm–Liouville type [1–3], $n = 1, 2, 3$:

$$\frac{d^2}{dz^2}U(n\kappa; z) + \Big[\Gamma^2_{n\kappa} - (n\kappa)^2\big(1 - \varepsilon_{n\kappa}\big(z, \alpha(z), U(\kappa; z), U(2\kappa; z), U(3\kappa; z)\big)\big)\Big]U(n\kappa; z) = \\ = -(n\kappa)^2\alpha(z)\left(\delta_{n1}U^2(2\kappa; z)U^{*}(3\kappa; z) + \delta_{n3}\left\{\frac{1}{3}U^3(\kappa; z) + U^2(2\kappa; z)U^{*}(\kappa; z)\right\}\right), \quad |z| \le 2\pi\delta. \quad (9)$$

By elementary calculations, from (C3) we obtain the boundary conditions for (9) ($n = 1, 2, 3$):

$$i\Gamma_{n\kappa}U(n\kappa; -2\pi\delta) + \frac{d}{dz}U(n\kappa; -2\pi\delta) = 0, \quad i\Gamma_{n\kappa}U(n\kappa; 2\pi\delta) - \frac{d}{dz}U(n\kappa; 2\pi\delta) = 2i\Gamma_{n\kappa}a^{\mathrm{inc}}_{n\kappa}. \quad (10)$$

Problem (6), (C1)–(C4) can also be reduced to finding solutions of one-dimensional nonlinear IEs (cf. [1–3], [6]) with respect to $U(n\kappa; \cdot) \in L_2(-2\pi\delta, 2\pi\delta)$, $n = 1, 2, 3$:

$$U(n\kappa;z)+\frac{i(n\kappa)^2}{2\Gamma_{n\kappa}}\int_{-2\pi\delta}^{2\pi\delta}\exp\left(i\Gamma_{n\kappa}|z-\xi|\right)\left[1-\varepsilon_{n\kappa}\left(\xi,\alpha(\xi),U(\kappa;\xi),U(2\kappa;\xi),U(3\kappa;\xi)\right)\right]\times$$
$$\times U(n\kappa;\xi)\,d\xi=\delta_{n1}\frac{i(n\kappa)^2}{2\Gamma_{n\kappa}}\int_{-2\pi\delta}^{2\pi\delta}\exp\left(i\Gamma_{n\kappa}|z-\xi|\right)\alpha(\xi)U^2(2\kappa;\xi)U^*(3\kappa;\xi)\,d\xi+ \tag{11}$$
$$+\delta_{n3}\frac{i(n\kappa)^2}{2\Gamma_{n\kappa}}\int_{-2\pi\delta}^{2\pi\delta}\exp\left(i\Gamma_{n\kappa}|z-\xi|\right)\alpha(\xi)\left\{\frac{1}{3}U^3(\kappa;\xi)+U^2(2\kappa;\xi)U^*(\kappa;\xi)\right\}d\xi+U^{\text{inc}}(n\kappa;z)$$

Here $U^{\text{inc}}(n\kappa;z)=a^{\text{inc}}_{n\kappa}\exp\left[-i\Gamma_{n\kappa}\cdot(z-2\pi\delta)\right]$. Application of suitable quadrature rules to (11) leads to a system of complex-valued nonlinear algebraic equations

$$\left(\mathbf{I}-\mathbf{B}_{n\kappa}(\mathbf{U}_{\kappa},\mathbf{U}_{2\kappa},\mathbf{U}_{3\kappa})\right)\mathbf{U}_{n\kappa}=\delta_{n1}\mathbf{C}_{\kappa}(\mathbf{U}_{2\kappa},\mathbf{U}_{3\kappa})+\delta_{n3}\mathbf{C}_{3\kappa}(\mathbf{U}_{\kappa},\mathbf{U}_{2\kappa})+\mathbf{U}^{\text{inc}}_{n\kappa},\quad n=1,2,3, \tag{12}$$

where we use a discrete set $\{z_l\}_{l=1}^N$ of nodes such that $z_1=-2\pi\delta<z_2<\ldots<z_l<\ldots<z_N=2\pi\delta$. $\mathbf{U}_{n\kappa}:=\{U_l(n\kappa)\}_{l=1}^N\approx\{U(n\kappa;z_l)\}_{l=1}^N$, $\mathbf{U}^{\text{inc}}_{n\kappa}=\{a^{\text{inc}}_{n\kappa}\exp\left[-i\Gamma_{n\kappa}(z_l-2\pi\delta)\right]\}_{l=1}^N$, $\mathbf{I}=\{\delta_{lm}\}_{l,m=1}^N$ is the identity matrix, $\mathbf{B}_{n\kappa}(\mathbf{U}_{\kappa},\mathbf{U}_{2\kappa},\mathbf{U}_{3\kappa})$, $\mathbf{C}_{\kappa}(\mathbf{U}_{2\kappa},\mathbf{U}_{3\kappa})$ and $\mathbf{C}_{3\kappa}(\mathbf{U}_{\kappa},\mathbf{U}_{2\kappa})$ are the matrices and the right-hand side vector, respectively, generated by the quadrature method. A solution of (12) can be found iteratively, where at each step a system of linearized algebraic equations is solved.

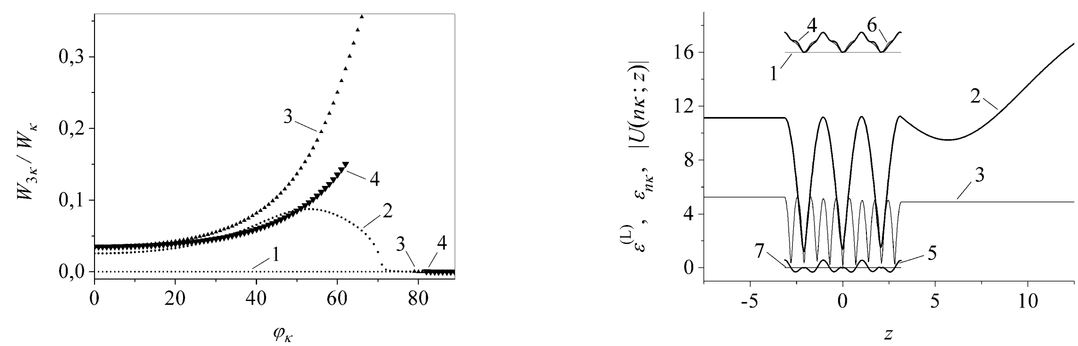
The analytic continuation of these linearized nonlinear problems into the region of complex values of the frequency parameter allows us to switch to the analysis of spectral problems [3]. Then we obtain in a similar manner a set of independent systems of linear algebraic equations depending nonlinearly on the spectral parameter: $\left(\mathbf{I}-\mathbf{B}_{n\kappa}(\kappa_n)\right)\mathbf{U}_{\kappa_n}=\mathbf{0}$, where $\kappa_n\in\Omega_{n\kappa}\subset H_{n\kappa}$, at $\kappa\equiv\kappa^{\text{inc}}$, $n=1,2,3$, $\Omega_{n\kappa}$ are the sets of eigenfrequencies and $H_{n\kappa}$ denotes two-sheet Riemann surfaces (see [3]). The spectral problem of finding eigenfrequencies κ_n and eigenfields $\mathbf{U}_{\kappa_n}$ reduces to the following equations ($n=1,2,3$):

$$\begin{cases} f_{n\kappa}(\kappa_n)=\det\left(\mathbf{I}-\mathbf{B}_{n\kappa}(\kappa_n)\right)=0, & \\ \left(\mathbf{I}-\mathbf{B}_{n\kappa}(\kappa_n)\right)\mathbf{U}_{\kappa_n}=\mathbf{0}; & \kappa\equiv\kappa^{\text{inc}};\quad \kappa_n\in\Omega_{n\kappa}\subset H_{n\kappa}. \end{cases} \tag{13}$$

Results

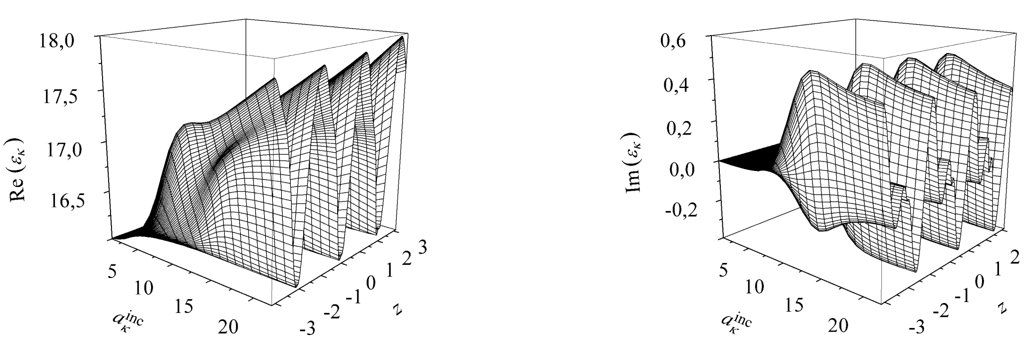
Consider excitation of the nonlinear structure by a strong electromagnetic field at the basic frequency only, i.e. with $a^{\text{inc}}_{\kappa}\neq 0,\ a^{\text{inc}}_{2\kappa}=0,\ a^{\text{inc}}_{3\kappa}=0$. In this case, the number of equations in the systems in (6) can be reduced to two by deleting the second equations and setting $E_x(\mathbf{r},2\kappa)\equiv 0$. Also, the permittivity (7) of the nonlinear layer simplifies, because here $U(2\kappa;z)\equiv 0$. Thus, we investigate problem (6), (7) at $n=1,3$ and $U(2\kappa;z)\equiv 0$, as in [2, 3], and consider a nonlinear dielectric structure with the parameters $\varepsilon^{(L)}(z)=16$, $\alpha(z)=+0.01$, and $\delta=0.5$; the excitation frequency is $\kappa=0.375$.

Let $W_{n\kappa}=\left|a^{\text{scat}}_{n\kappa}\right|^2+\left|b^{\text{scat}}_{n\kappa}\right|^2$ denote the total energy of the scattered field at frequency $n\kappa$, $n=1,3$. Consequently, W_{κ} is the total energy scattered at frequency κ and $W_{3\kappa}$ is the total energy generated at frequency 3κ. The ratio $W_{3\kappa}/W_{\kappa}$ characterizes the relative part of the energy generated in the third harmonic at the value a_κ^{inc}; see Fig. 2(a). In particular, $W_{3\kappa}/W_\kappa = 0.3558$ for $a_\kappa^{\text{inc}} = 14$ and $\varphi_\kappa = 66^0$; i.e., $W_{3\kappa}$ generated in the third harmonic constitutes 35.58% of the energy W_κ (see [3]). The function $\text{Im}(\varepsilon_\kappa)$ in Figs. 2(b) (curve 5) and 3(b) characterizes energy losses in the nonlinear layer (w.r.t. excitation frequency κ) spent on generation of electromagnetic field of the third harmonic (at frequency 3κ); $\text{Re}(\varepsilon_\kappa)$ is shown in Fig. 3(a). Note that at the frequency 3κ the permittivity $\varepsilon_{3\kappa}$ is real; see Fig. 2(b) (curves 6, 7). Scattering and generation properties of the nonlinear structure are described by means of the reflection and transmission/generation coefficients $R_{n\kappa} = \left|a_{n\kappa}^{scat}\right|^2 / \left|a_\kappa^{inc}\right|^2$, $T_{n\kappa} = \left|b_{n\kappa}^{scat}\right|^2 / \left|a_\kappa^{inc}\right|^2$; see Fig. 4(a), problem (12). Here we present results corresponding to the case of energy channeling [3], cf. the curve 1 where $R_\kappa \approx 0$ at $\varphi_\kappa = 60^0$. The results of calculations are validated numerically with the help of the energy balance equation $R_\kappa + T_\kappa + R_{3\kappa} + T_{3\kappa} = 1$. Solutions (13) are shown in Fig. 4(b). Comparing Figs. 4 (a) and (b) we see that a local maximum in generated energy at the tripled frequency (curves 3 – $R_{3\kappa}$, 4 – $T_{3\kappa}$, 5 – $W_{3\kappa}/W_\kappa$) corresponds to characteristic behavior of the curve 5.2 – $\text{Im}(\varepsilon_1^{\text{NL}})$ in a vicinity of its local minimum.



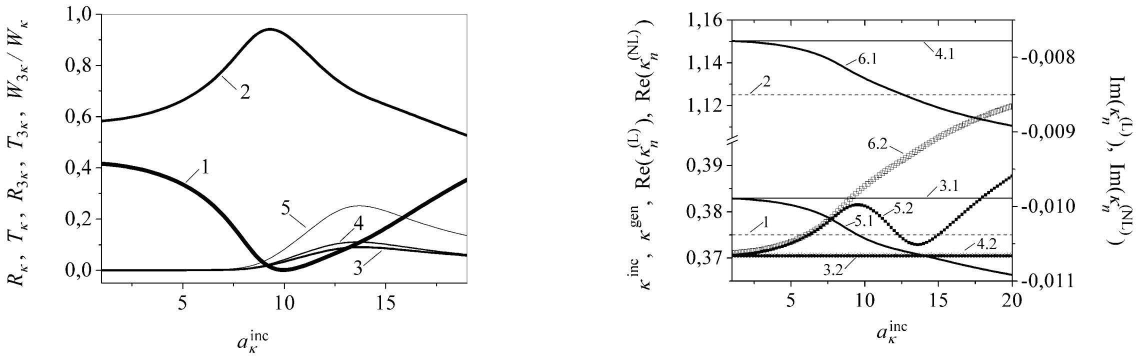
(a) (b)

Fig. 2. (a) $W_{3\kappa}/W_\kappa$ for: 1 – $a_\kappa^{\text{inc}} = 1$, 2 – $a_\kappa^{\text{inc}} = 9.93$, 3 – $a_\kappa^{\text{inc}} = 14$, 4 – $a_\kappa^{\text{inc}} = 19$;
(b) Curves at $a_\kappa^{\text{inc}} = 14$ and $\varphi_\kappa = 66^0$: 1 – $\varepsilon^{(L)}$, 2 – $|U(\kappa; z)|$, 3 – $|U(3\kappa; z)|$, 4 – $\text{Re}(\varepsilon_\kappa)$, 5 – $\text{Im}(\varepsilon_\kappa)$, 6 – $\text{Re}(\varepsilon_{3\kappa})$, 7 – $\text{Im}(\varepsilon_{3\kappa}) \equiv 0$.



(a) (b)

Fig. 3. The nonlinear permittivity at $\varphi_\kappa = 60^0$: (a) $\text{Re}(\varepsilon_\kappa(a_\kappa^{\text{inc}}, z))$; (b) $\text{Im}(\varepsilon_\kappa(a_\kappa^{\text{inc}}, z))$.



(a) (b)

Fig. 4. The curves at $\varphi_\kappa = 60^0$: (a) 1 – R_κ, 2 – T_κ, 3 – $R_{3\kappa}$, 4 – $T_{3\kappa}$, 5 – $W_{3\kappa}/W_\kappa$; (b) 1 – $\kappa \equiv \kappa^{inc}$, 2 – $\kappa^{gen} = 3\kappa^{inc}$, the curves for $\alpha = 0$: 3.1 – $\mathrm{Re}\left(\kappa_1^{(L)}\right)$, 3.2 – $\mathrm{Im}\left(\kappa_1^{(L)}\right)$, 4.1 – $\mathrm{Re}\left(\kappa_3^{(L)}\right)$, 4.2 – $\mathrm{Im}\left(\kappa_3^{(L)}\right)$; and for $\alpha = +0.01$: 5.1 – $\mathrm{Re}\left(\kappa_1^{(NL)}\right)$, 5.2 – $\mathrm{Im}\left(\kappa_1^{(NL)}\right)$, 6.1 – $\mathrm{Re}\left(\kappa_3^{(NL)}\right)$, 6.2 – $\mathrm{Im}\left(\kappa_3^{(NL)}\right)$.

Conclusion

Based on a model that utilizes analytical continuation of the complex frequency region, we have discovered resonance phenomena related to medium nonlinearity involving the waves at the first three frequency components. In numerical experiments we have reached intensities of the excitation field such that the relative portion of total energy generated in the third harmonic is up to 36%, which exceeds the known data [5] by a factor of about 3.6. The results indicate the possibility of designing a frequency multiplier and nonlinear dielectrics with controllable permittivity. The transformation of the frequency and angular spectra, and the rapid control of amplitude and phase of the waves form the basis of a broad class of technical systems [7].

Acknowledgement

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