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Finite-Difference Time-Domain Calculation With All Parameters of Sellmeier's Fitting Equation for 12-fs Laser Pulse Propagation in a Silica Fiber

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Abstract—In order to both experimentally and numerically investigate nonlinear femtosecond ultrabroadband-pulse propagation in a silica fiber, we have extended the finite-difference time-domain (FDTD) calculation of Maxwell's equations with nonlinear terms to that including all exact Sellmeier-fitting values. We have compared results of this extended FDTD method with experimental results, as well as with the solution of the generalized nonlinear Schrödinger equation by the split-step Fourier method with a slowly varying-envelope approximation. To the best of our knowledge, this is the first comparison between FDTD calculation and experimental results for nonlinear propagation of a very short (12 fs) laser pulse in a silica fiber.

Index Terms—FDTD, femtosecond, GNLSE, monocycle optical pulse, nonlinear chirp, nonlinear fiber optics, nonlinear propagation, Raman, self-phase modulation, self-steepening, Sellmeier, silica fiber, SVEA, ultrabroad-band spectrum.

THERE WAS RECENTLY significant interest in the generation of single-cycle optical pulses by optical pulse compression of ultrabroad-band light produced in fibers. We reported some experiments on the ultrabroad-band pulse generation using a silica fiber [1], [2] and an Ar-gas filled hollow fiber [3], and the optical pulse compression by nonlinear chirp compensation [1], [3]. For these experiments on generating few-optical-cycle pulses, characterizing the spectral phase of ultrabroad-band pulses analytically as well as experimentally is highly significant.

Conventionally, the slowly varying envelope approximation (SVEA) has been used to describe the propagation of an optical pulse in a fiber [4]. However, if the pulse duration approaches the optical cycle regime ($<$10 fs), this approximation becomes invalid. It is necessary to use the finite-difference time-domain (FDTD) method [5], [6] without SVEA [4]. Previous reports [5] by Goorjian, Joseph, Taflove, and Hagness (GJTH) proposed an excellent FDTD algorithm considering combination of the linear dispersion with one resonant frequency and the nonlinear terms with Raman response function.

We performed an experiment of 12-fs optical pulse propagation [1][2]. In order to compare an FDTD calculation results with the experimentally measured ultrabroad spectra of such an ultrashort laser pulse, we extend the GJTH algorithm to that considering all exact Sellmeier's fitting values for ultrabroad spectra. Owing to broad spectrum of pulse propagating in a fiber, it becomes much more important to take accurate linear dispersion into account. It is well known that at least two resonant frequencies must be required for the linear dispersion to fit accurately to a refractive index data. Recent report by Kalosha and his coworker considers the linear dispersion with two resonant frequencies and the nonlinear terms without Raman effect [6]. For the single-cycle pulse generation experiment, we must use at least sub-5 fs [3], [7] or commercially available 12-fs pulses. Such a time regime is comparable to the Raman characteristic time of 5 fs [4] in a silica fiber. Therefore, it is very important to consider not only the accurate linear dispersion of silica but also the Raman effect in a silica fiber in the few-optical-cycles regime. In addition, owing to the high repetition rate and pulse intensity stability, in particular, ultrabroad-band supercontinuum light generation and few-optical-cycles pulse generation by nonlinear pulse propagation in photonic crystal fibers and tapered fibers [8], [9], which both are made of silica, have attracted much attention. In this work, we have extended the FDTD method with nonlinear polarization P_{NL} involving the Raman response function (GJTH-algorithm) to 12-fs ultrabroad-band pulse propagation in a silica fiber with consideration of linear polarization P_L including all exact Sellmeier-fitting values of silica with three resonant frequencies, in order to compare the calculation results with our experimental results [1], [2]. We also compare the extended FDTD method with the split-step Fourier (SSF) method which is the solution of the generalized nonlinear Schrödinger equation (GNLSE) with SVEA [4]. To the best of our knowledge, this is the first comparison be-

tween FDTD calculation and experimental results for nonlinear propagation of a very short (12 fs) laser pulse in a silica fiber.

We consider a one-dimensional problem with electric field E_y and magnetic field H_x propagating in the z direction with electric displacement D_y. In this case, Maxwell's equations are written as

$$\frac{\partial H_x(t, z)}{\partial t} = \frac{1}{\mu_0} \frac{\partial E_y(t, z)}{\partial z} \tag{1-a}$$

$$\frac{\partial D_y(t, z)}{\partial t} = \frac{\partial H_x(t, z)}{\partial z} \tag{1-b}$$

$$E_y(t, z) = (1/\varepsilon_0) \cdot [D_y(t, z) - P_L(t, z) - P_{NL}(t, z)]$$

$$P_L(t, z) = \sum_{i=1}^{3} P_i(t, z) \tag{1-c}$$

where ε_0, P_L, and P_{NL} are the vacuum permittivity, and the linear and nonlinear polarizations, respectively. For simplicity, we omit hereafter the expression of z dependence, that is, we simplify (t, z) and (ω, z) to (t) and (ω), respectively. In the FDTD calculation algorithm, the electromagnetic field values are repetitively renewed using (1) in alphabetical order with increasing time steps. In the frequency domain, P_L of (1-c) is defined as

$$\tilde{P}_L(\omega) = \varepsilon_0 \tilde{E}_y(\omega) \sum_{i=1}^{3} \tilde{\chi}_i(\omega) \tag{2}$$

where the Fourier transform of all values is expressed with a tilde and $\tilde{\chi}_i(\omega)$ is the linear susceptibility. Here, we assume that, using Sellmeier's equation, $\tilde{\chi}_i(\omega)$ ($i = 1$, 2, and 3) or dielectric constant $\tilde{\varepsilon}_r(\omega)$ is expressed by

$$\tilde{\varepsilon}_r(\omega) = 1 + \sum_{i=1}^{3} \tilde{\chi}_i(\omega) = \tilde{n}(\omega)^2 = 1 + \sum_{i=1}^{3} \frac{b_i \omega_i^2}{\omega_i^2 - \omega^2} \tag{3}$$

where ω_i is the resonance frequency and b_i is the strength of the ith resonance. Equations (1-c), (2), and (3) lead to the following differential equations:

$$\frac{\partial^2 P_i(t)}{\partial t^2} + \omega_i^2 P_i(t) = \omega_i^2 b_i \left(D_y(t) - \sum_{i=1}^{3} P_i(t) - P_{NL}(t) \right) \tag{4}$$

where $i = 1$, 2, and 3, and $P_{NL}(t)$ has the current value. We can solve three equations with past values of $P_i(t)$ and obtain each new value of $P_1(t)$, $P_2(t)$, and $P_3(t)$ in order to obtain a new linear polarization of $P_L(t) = P_1(t) + P_2(t) + P_3(t)$ using (1-c). Using this new $P_L(t)$ and the past value of $P_{NL}(t)$, we can obtain a new value of $P_{NL}(t)$ by solving the differential equation [5], obtained from (1-c) and Fourier transformation of the following equation which defines $P_{NL}(t)$:

$$P_{NL}(t) = \varepsilon_0 \chi^{(3)} E \cdot \int_{-\infty}^{\infty} [\alpha \delta(t - \tau) + (1 - \alpha) g_R(t - \tau)]$$
$$\cdot [E(\tau)]^2 \, d\tau \tag{5}$$

where $\chi^{(3)}$ is the electronic third-order susceptibility divided by α, $\delta(t)$ is the delta function, $g_R(t) =$
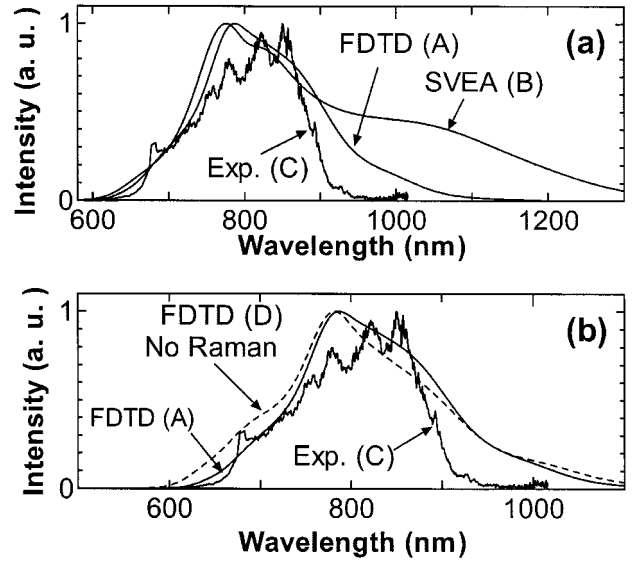

Fig. 1. (a) Spectra of 12-fs laser transmission through a 2.5-mm silica fiber, calculated by (A) the extended FDTD Maxwell equation method considering all orders of dispersions and the Raman response [$\alpha = 0.7$ in (5)], (B) the solution of GNLSE obtained using the SSF method with SVEA (considering up to the third-order dispersion terms and the Raman term using the parameter $T_R = 5$ fs [4]), and (C) our previously reported experimental result [2]. (b) Comparison between spectra calculated by (D) the FDTD Maxwell equation method without the Raman response [$\alpha = 1$ in Eq. (5)] and (A) with the Raman response. (A) and (C) are the same data as those in (a).

$[(\tau_1^2 + \tau_2^2)/\tau_1 \tau_2^2] e^{-t/\tau_2} \sin(t/\tau_1)$ and parameter α represents the relative strengths of Kerr and Raman interactions. As we can obtain both new $P_L(t)$ and $P_{NL}(t)$, the new electric field $E_y(t)$ is obtained by substituting $P_L(t)$ and $P_{NL}(t)$ into Newton's iteration algorithm [5], with a new value of $D_y(t)$ obtained from (1-b). In our calculation, the parameters for a fused silica fiber in (3) are set as $b_1 = 0.696\,166\,3$, $b_2 = 0.407\,942\,6$, $b_3 = 0.897\,479\,4$, $\lambda_1 = 0.068\,404\,3$ μm, $\lambda_2 = 0.116\,241\,4$ μm, and $\lambda_3 = 9.896\,161$ μm [4], where $\lambda_i = 2\pi c/\omega_i$ and c is the velocity of light in vacuum. We used the value of the nonlinear refractive coefficient $n_2^I = 2.48 \times 10^{-20}$ m^2/W from [10], and the third-order susceptibility $\chi^{(3)}$ was found to be $\chi^{(3)} = 1.85 \times 10^{-22}$ m^2/V^2 at 800 nm, given by $\chi^{(3)} = (4/3)\varepsilon_0 cn(\omega_0)^2 n_2^I$, where ω_0 is the center angular frequency of the optical pulse. The parameters α, τ_1, and τ_2 in (5) are set to be $\alpha = 0.7$, $\tau_1 = 12.2$ fs and $\tau_2 = 32$ fs. A single time step of the finite difference is set as $\Delta t = 4.447\,521\,5 \times 10^{-17}$ s.

In the extended FDTD calculation, we set all parameters to be the same as in our experiment [1], [2]. The total fiber length of $L = 2.5$ mm corresponds to 136 500 spatial steps which means that $L = 136\,500 \times \Delta z$, where Δz is a unit spatial step in the z direction. We need 293 000 time steps to measure the electric field until the pulse tail passes completely. The peak power of an input pulse is set to be 175 kW (soliton number $N = 2.09$). The effective core area A_{eff} is set to be 5.47 μm^2. Fig. 1(a) shows the results calculated by the extended FDTD Maxwell equation method (A), the solution of GNLSE obtained using the SSF method with SVEA (B) (up to the third-order dispersion terms with the Raman term using the Raman time constant of $T_R = 5$ fs [4] which is related to the slope of the Raman gain), and our previously reported experimental result
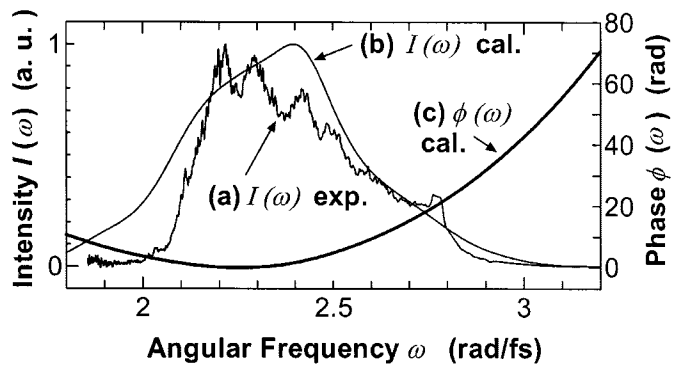
Fig. 2.   Spectral intensity obtained (a) experimentally and (b) numerically, and (c) spectral phase obtained numerically as a function of angular frequency for 12-fs laser transmission through a 2.5-mm silica fiber.

(C) [2]. It is seen that, with SVEA (B), the spectrum intensity at long wavelengths is much higher than those for FDTD (A) and the experimental result (C). This indicates that the extended FDTD Maxwell equation is superior to GNLSE by SSF with SVEA. A linear approximation of the actual Raman gain curve and only up to the third-order dispersion terms are included in GNLSE by SSF with SVEA (B). Furthermore, in GNLSE by SSF with SVEA, the second derivative of the electric field with respect to z, $\partial^2 E_y / \partial z^2$, is neglected, which corresponds to neglecting the backward propagation wave. In contrast to this, our extended FDTD Maxwell equation method (A) accurately includes the delayed Raman response and all orders of the dispersion in silica using Sellmeier's equation, and does not use SVEA. Thus, the difference between (A) and (B) is considered to be due to the Raman effect, the higher order dispersion effect, or the backward propagation wave. In order to clarify this, we performed a calculation using (D) the FDTD Maxwell equation method without the Raman response [$\alpha = 1$ in (5)], as shown in Fig. 1(b), where (A) and (C) show the same data as those in Fig. 1(a). In Fig. 1(b), the spectrum for case (A) is closer to the experimental result (C) than that of the case of FDTD which does not consider the Raman effect (D). It is evident that by including the Raman term (A), the spectral intensity at a shorter wavelength is smaller and the agreement between the experimental and calculated results becomes better than that in the case of (D). For example, the spectral intensity at 700 nm in (D) is 48% higher than that in (A), which is almost same as that in the experimental result (C). On the other hand, at a longer wavelength, for example, 850 nm, the spectral intensity of (A) is 15% higher than that of (D). This feature of (A) shows a tendency analogous to (C) because there is a larger peak at 850 nm than at the center wavelength of 800 nm in (C). These tendencies of the spectral characteristics indicate that it is important to include the Raman term.

Fig. 2 shows the spectral intensities obtained (a) experimentally and (b) numerically, and (c) the spectral phase obtained numerically as a function of angular frequency for 12-fs laser

transmission through a 2.5-mm silica fiber. From our calculation corresponding to Fig. 2(c), we determine the GDD, the TOD, and the fourth-order dispersion (FOD) values to be 136.5 fs^2, 80.65 fs^3, and -35.59 fs^4, respectively. These values are very important for single-cycle pulse generation via phase compensation of the nonlinear-chirped supercontinuum generated in a silica fiber.

In conclusion, we have extended the nonlinear FDTD method with GJTH algorithm to that with exact sellmeier's fitting values in order to compare the experimental and calculated results of nonlinear femtosecond ultrabroadband-pulse propagation in a silica fiber, and analyzed spectral characteristics for the propagated pulse. This extended method is robust for the breakdown of the SVEA. The spectrum obtained in our previous experiment agrees better with the spectrum calculated by the extended FDTD method than that calculated by the solution of GNLSE obtained using the SSF method with SVEA. To the best of our knowledge, this is the first comparison between FDTD calculation and experimental results for nonlinear propagation of a very short (12 fs) laser pulse in a silica fiber. We also obtained the spectral phase of propagated pulses, which will be highly significant for single-cycle optical pulse generation via compensation of the nonlinear-chirped supercontinuum generated in silica fibers with a spatial light modulator.

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