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FINAL REPORT

for

SUBCONTRACT NO. B23471

**Discrete Modeling of Optical Pulse Propagation in
Nonlinear Media**

by

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Discrete Modeling of Optical Pulse Propagation in Nonlinear Media

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SUMMARY

This report describes the efforts supported by LLNL under the Subcontract No. B234571 at the University of Arizona during the Fiscal Years 1993 and 1994.

We have successfully developed a finite difference time domain method that simulates the propagation of ultra-short optical pulses in nonlinear materials which can be described with a linear Lorentz dispersion model, an instantaneous nonlinear Kerr model and a retarded nonlinear Raman model.

We have used this NL-FDTD method to model and characterize several ultra-short optical pulse configurations including linear and nonlinear optical waveguides that could be used as all-optical output couplers and beam steerers.

submitted to Jeff Kallman
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FINAL REPORT

With the continuing and heightened interest in nonlinear semiconductor and optically integrated devices, more accurate and realistic numerical simulations of these devices and systems are in demand. Such calculations provide a testbed in which one can investigate new basic and engineering concepts, materials, and device configurations before they are fabricated. This encourages multiple concept and design iterations that result in enhanced performances and system integrations of those devices. They also provide a framework in which one can interpret complex experimental results and suggest further diagnostics or alternate protocols. Thus the time from device conceptualization to fabrication and testing could be enormously improved with numerical simulations that incorporate more realistic models of the linear and nonlinear material responses and the actual device geometries.

To date most of the modeling of pulse propagation in and scattering from complex linear and nonlinear media has been accomplished with one-dimensional, scalar models. These models have become quite sophisticated; they have predicted and explained many of the nonlinear as well as linear effects in present devices and systems. Unfortunately, they can not be used to explain many observed phenomena. Moreover, we and others have been able to demonstrate that the scalar models are not adequately modeling a variety of linear and nonlinear phenomena that are being proposed for new effects and devices. It has been shown that vector and higher dimensional properties of Maxwell's equations that are not currently included in existing scalar models in addition to more detailed materials models will significantly impact the scientific and engineering results. Moreover, because they are limited to simpler geometries, current modeling capabilities are not adequate for realistic linear/nonlinear optical-component engineering design studies. It is believed that our successful development of a general, linear and nonlinear electromagnetic modeling capability will significantly impact the concept and design stages associated with novel linear and nonlinear phenomena and the resulting optical components.

During the duration of this project, we have numerically constructed solutions to the multi-dimensional, full-wave, vector Maxwell's equations describing the interaction of ultrashort, pulsed beams with a dispersive, nonlinear material having a finite response time. These numerical solutions have been obtained¹⁻⁴ in two space dimensions and time with a nonlinear finite difference time domain (NL-FDTD) method which combines a generalization of a standard, FDTD, full-wave, vector, linear Maxwell's equations solver with a Lorentz linear dispersion model, a nonlinear (thermal) Raman model, and an instantaneous nonlinear Kerr model. In particular, we have developed a simulator that solves in a self-consistent manner the system of equations:

$$\frac{\partial}{\partial t} [\mu_0 \vec{H}] = -\nabla \times \vec{E} \quad (1)$$

Maxwell Curl Equations

$$\frac{\partial}{\partial t} [\epsilon_0 \vec{E}] = \nabla \times \vec{H} - \frac{\partial}{\partial t} \vec{P} \quad (2)$$

$$\frac{\partial^2}{\partial t^2} \vec{P}^L + \Gamma_L \frac{\partial}{\partial t} \vec{P}^L + \omega_L^2 \vec{P}^L = \epsilon_0 \chi_0 \omega_L^2 \vec{E} \quad (3)$$

Lorentz Model

$$\frac{\partial^2}{\partial t^2} \chi^{NL} + \omega_R^2 \left(\tau_R \frac{\partial}{\partial t} \chi^{NL} + \chi^{NL} \right) = \epsilon_R \omega_R^2 |\vec{E}|^2 \quad (4)$$

Raman Model ,

where the polarization $\vec{P} = \vec{P}^L + \vec{P}^{NL}$ is composed of the linear contribution $\vec{P}^L$ and the nonlinear contributions

$$\vec{P}^{NL} = \epsilon_0 \chi^{NL} \vec{E} + \epsilon_0 \chi^{Kerr} |\vec{E}|^2 \vec{E}, \quad (5)$$

χ^{Kerr} being the instantaneous Kerr susceptibility. The susceptibility χ^{NL} encompasses all of the retarded nonlinear effects. For simplicity only, we treat the nonlinearities as being thermal rather than electronic. Goorjian and his coworkers⁵⁻⁷ have also developed a similar capability to model pulse propagation under the influence of linear and nonlinear dispersive, linear and nonlinear diffractive, and time retardation effects in the medium.

By coupling the linear and nonlinear dispersion models together simultaneously, as

well as using the natural boundary conditions arising from dielectric discontinuities, for example, at gratings and corrugated interfaces, we have demonstrated the ability to design all-optical switching devices and beam steerers for ultrashort pulses. The NL-FDTD approach can readily handle complex, realistic structures. This allows a thorough investigation of the wave propagation in the presence of complicated scatterers built into a nonlinear waveguiding structure. In contrast to standard approaches such as the beam propagation method, the NL-FDTD approach allows one to study the effects of the reflected and longitudinal field components, which become significant when complex scatterers or nonlinearities are present, and the nonlinear coupling between the longitudinal and transverse components, which becomes significant depending on the polarization of the fields. For the straightforward 1D or 2D waveguide structures treated in Refs. 5-7, the full-wave, vector Maxwell results recover those expected from NLS studies⁸. The NL-FDTD technique is, however, more potent than the NLS method; it can be applied to much more complex situations and can provide new information not obtainable with the standard linear-nonlinear modeling methods.

We have found, as expected, that the NL-FDTD approach is not a panacea for all optical modeling problems. It is useful because it can incorporate straightforwardly complicated structures and all of the relevant physics one is willing to build into the material models. The Raman and instantaneous Kerr nonlinearities used in the current NL-FDTD simulator are idealized, phenomenological models; but they have been chosen because of their widespread use. Additionally, because of the bandwidth of the pulses that are used in the cases we have examined, one could argue that more than one resonance line should be included in the models. Multiple resonance Lorentz and Raman models could be designed to mimic the behavior of most materials. However, we typically choose not to run problems in which the optical pulses have frequency spectra that are centered directly on the resonance lines; these models simply absorb most of the energy presented to them, hence, generally lead only to modest scattering results. More realistic multi-level atom

models of the materials can be incorporated into the NL-FDTD simulator; these models are currently under development in cooperation with John Arnold at Glasgow University. Despite the ability of the approach to handle complicated structures and material models, our NL-FDTD simulation model is memory and time bound. It is an explicit approach whose timestep is connected to the spatial discretization through the Courant stability condition. The amount of memory required is directly proportional to the number of unknowns which is determined by the number of grid cells and the number of equations in the combined fields-materials models. Finer spatial resolution or more complex material models requires more memory and more time steps for a given time record length. Even two-dimensional problems dealing with nonlinear structures that are millimeters in size and with pulses that are picosecond long and have wavelengths on the order of a micron are truly enormous and task the largest machines available today. Larger problems simply await larger simulation platforms. Despite the ability of the NL-FDTD approach to handle reasonably sized design problems of current interest, we have emphasized with our test-validation cases the design and simulation of futuristic output couplers and beam steerers - those appropriate for ultrashort optical pulses and structures that are on the order of several wavelengths in size.

Corrugated waveguides were chosen as a primary example of a two-dimensional scattering structure that requires inclusion of both the transverse and the longitudinal field components in its design. These structures have been of considerable interest in integrated optics because of their potential applications as couplers, converters, filters, or steering devices of the Bragg type. However, they have been analyzed mainly in the linear regime as infinite periodic structures⁹⁻¹³ using Floquet mode theory. To design a useful nonlinear corrugated structure that is only a few wavelengths long for any of these applications, one must resort to a numerical modeling tool such as the NL-FDTD approach that allows the dielectric waveguide or the corrugations themselves to be nonlinear materials; allows for arbitrary groove spacings and depths; allows for tapering of the corrugations; allows

for single-cycle or multi-cycle pulses; and allows for either TE or TM polarizations. One rapidly realizes that the currently available analysis tools such as the BPM and NLS methods can not provide the desired results. The inadequacy of analytical approaches such as perturbation techniques even in the general linear case has been recognized^{11,12}. In addition, the NL-FDTD approach permits one to visualize all of the physical scattering processes involved in the interaction of the pulses with the corrugated structure. It has been the one of the applications goals of our research efforts to demonstrate the efficacy of using the NL-FDTD approach to design finite corrugated waveguide structures as output couplers and beam steerers for ultrashort pulses.

The NL-FDTD approach can handle single-cycle cases as readily as multiple-cycle cases having an intrinsic carrier wave. Since most current optical systems deal directly with a carrier-wave type signal, the NL-FDTD simulator was used primarily to investigate the propagation and scattering effects associated with those signals. It can also simulate the behaviors of single-cycle optical devices and systems as shown in Ref. 2. The single cycle results represent behaviors that should be observed with optical systems currently under investigation and those being developed for future studies by the international optics community. However, in either case, the full pulse is modeled with the NL-FDTD approach rather than only the envelope of the carrier wave, as it is with the NLS models. The increase in computational costs associated with the NL-FDTD approach over the NLS models is warranted by the corresponding increase in phase and vector information maintained by the former and generally ignored or included only in an approximate sense in the latter. The NL-FDTD approach handles the corrugations directly without any of the standard assumptions which are necessitated by the BPM or NLS methods. This enhanced modeling capability of the NL-FDTD approach allows one to model and distinguish the effects that arise in both the single- and multiple-cycle TE and TM polarization cases.

The NL-FDTD approach can readily handle very complex, realistic structures. The *TE* and *TM* nonlinear optics problems that have been treated with the NL-FDTD simulator

highlight the differences between the scalar and the vector approaches and the effects of the finite response time of the medium. The NL-FDTD method is beginning to resolve several very basic physics and engineering issues concerning the behavior of the full electromagnetic field during its interaction with a nonlinear, finite response time medium. In particular, during the contract period we have

- (1) shown the viability of combining the linear Lorentz dispersion model, the instantaneous Kerr nonlinear model and the Raman nonlinear model with the FDTD engine;
- (2) have studied one and two dimensional solitary waves with this improved NL-FDTD simulator;
- (3) have revisited the TM and TE models of an optical diode (linear-nonlinear interface switch) with the improved NL-FDTD simulator;
- (4) have characterized the performance of various linear-nonlinear slab waveguide structures;
- (5) have characterized the performance of grating assisted output couplers and have shown that these coupler geometries can be designed to achieve beam-steering that is intensity dependent; i.e., the output coupling angle is directly dependent on the intensity of the exciting wave; and
- (6) have characterized the performance of corrugated nonlinear waveguides in terms of their polarization selectivity properties and their generation of higher order modes and changes in propagation speeds through the corrugation regions.

In all of these analyses we have identified the role of the longitudinal field component and the resulting transverse power flows in the associated scattering-coupling processes. Comparisons between the nonlinear structures and their linear counterparts were performed for all cases to quantify the effects of the nonlinear response of the medium on the basic device designs.

Our work has been reported in a variety of refereed journals and professional meetings. The journal papers generated in the contract period are attached below. The work to

date has been extremely well-received. Our follow-on efforts will include extending the NL-FDTD model to more complex propagation and scattering geometries.

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12. R. W. Ziolkowski and J. B. Judkins, "NL-FDTD modeling of linear and nonlinear grating-assisted couplers", Session THa-01, EUROEM International Symposium, Bordeaux, France, June 1994.
13. R. W. Ziolkowski and J. B. Judkins, "NL-FDTD simulations of dielectric waveguide, ultrashort optical pulse output couplers formed by linear and nonlinear corrugated sections", Session W-J5, IEEE Antennas and Propagation Society and URSI Radio Science Meeting, Seattle, Washington, June 1994.

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