NUMERICAL AND EXPERIMENTAL STUDIES OF DISPERSIVE, ACTIVE, AND NONLINEAR MEDIA WITH ACCELERATOR APPLICATIONS*

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Abstract

Current advanced accelerator modeling applications require a more sophisticated treatment of dielectric and paramagnetic media properties than simply assuming a constant permittivity or permeability. So far active media have been described by a linear, frequency-dependent, single-frequency, scalar dielectric function. We have been developing and testing algorithms to model the high frequency response of dispersive, active, and nonlinear media. The work described also has applications for modeling of other electromagnetic problems involving realistic dielectric and magnetic media. Using these algorithms as a starting point we plan to develop a software library and database of material parameters to solve for constitutive relations in conjunction with third party and in house FDTD codes.

INTRODUCTION

As accelerator technology moves towards the use of accelerating fields in the THz, IR, and optical frequency bands, the accurate modeling of dielectric properties becomes increasingly important. The PASER [1] is one of the first advanced accelerator modeling applications that requires a more sophisticated treatment of dielectric and paramagnetic media properties than simply assuming a constant permittivity or permeability.

So far the PASER medium has been described by a linear, frequency-dependent, single-frequency, scalar dielectric function or by direct transfer of energy from excited atoms or molecules to the accelerated particles (collisions of the second kind).

The active media for PASER applications is inherently dispersive. An interaction between the high charge beam and active media with high stored energy density leads to nonlinear effects as well.

We are developing and testing a set of algorithms to treat dispersive lossy and active medium as well as various types of nonlinearities (Kerr, Raman). These algorithms will be incorporated into a wakefield code, like Arrakis and form a generic tool for simulations of particle interaction with nonlinear and dispersive medium.

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In this paper we will overview the algorithms implemented so far. A report on our recent work on microwave active media can be found in another paper presented at this conference [2].

DISPERSIVE AND ACTIVE MEDIA

In the context of our work on developing a microwave PASER [3, 4], we have been investigating algorithms for modeling a medium with a complex frequency dependent permeability in a finite difference time domain (FDTD) framework using the auxiliary differential equation

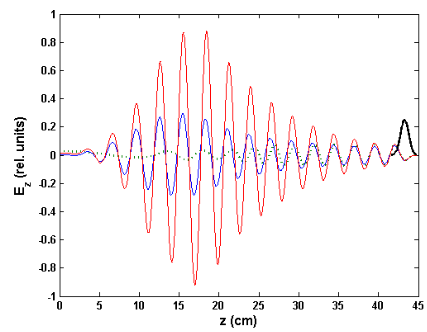

Figure 1. Arrakis simulation of the longitudinal wakefield of a beam in X-Band structures loaded with conventional dielectric and with a single Lorentz resonance active medium. Black: beam pulse; green: wake from dielectric; Red: wake from active structure; Blue: wake from active structure with lossy dielectric.

(ADE) method [5]. (The approach for a dielectric medium is completely analogous.) An active medium is one in which the imaginary part of the susceptibility χ'' is negative.

NONLINEAR MEDIA IMPLEMENTATON

We implemented and tested FDTD algorithms for treating Kerr and Raman (Brillouin) nonlinear media. The goal of the work is to develop a simulation tool for treating nonlinear effects in wakefield formation in high gradient dielectric loaded structures. Dielectric materials are likely to exhibit a nonlinear behavior in high RF fields before the actual breakdown.

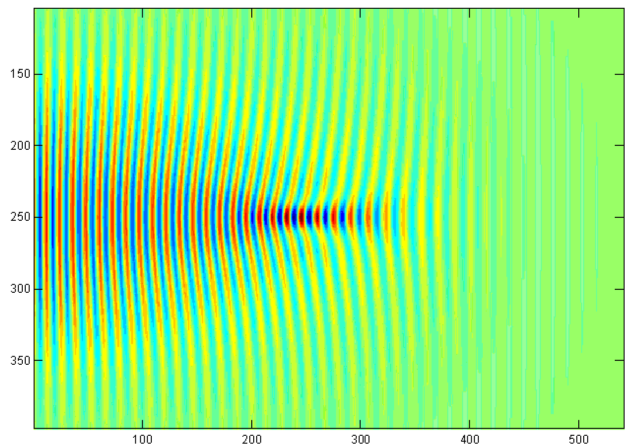

Figure 2. Kerr medium; Self focusing (H_z component of the field is plotted).

We followed the work [5] and references therein. Kerr nonlinearity ($\boldsymbol{P} = \chi_0 |\boldsymbol{E}|^2\boldsymbol{E}$) is local and can be treated via traditional differencing:

$$J_{Kerr}^{n+1/2} = \frac{\alpha\varepsilon_0\chi_0^{(3)}}{\Delta t}\left[\left|E^{n+1}\right|^2 E^{n+1} - \left|E^n\right|^2 E^n\right], \text{ while}$$

Raman nonlinearity is non-local in time:

$$\vec{P}_{NL}\left(\vec{r},t\right) = \varepsilon_0\chi_0^{(3)}\vec{E}\int_{-\infty}^{\infty} g\left(t-t'\right)\left|\vec{E}\left(t'\right)\right|^2 dt$$

where $g_{Raman}(t) = \left(\frac{\tau_1^2+\tau_2^2}{\tau_1\tau_2^2}\right)\sin\left(\frac{t}{\tau_1}\right)\exp\left(\frac{-t}{\tau_2}\right)U\left(t\right)$

and U(t) is the step function. Parameters τ_1 and τ_2 are determined from the measurement of the Raman gain spectrum. Following refs. [6, 7] we can write out the Raman polarization integral as a convolution, take the Fourier transform and transform the result back into the time domain. This yields a difference equation for auxiliary variable S:

$$S^{n+1} = \left[\frac{2-\omega_{Raman}^2(\Delta t)^2}{\delta_{Raman}\Delta t+1}\right]S^n + \left[\frac{\delta_{Raman}\Delta t-1}{\delta_{Raman}\Delta t+1}\right]S^{n-1} + \left[\frac{(1-\alpha)\chi_0^{(3)}\omega_{Raman}^2(\Delta t)^2}{\delta_{Raman}\Delta t+1}\right]\left|E^n\right|^2$$

where $\omega_{Raman}^2 = \frac{\tau_1^2+\tau_2^2}{\tau_1\tau_2^2}$ and $\delta_{Raman} = \frac{1}{\tau_2}$.

The Raman polarization current differencing relation is:

$$J_{Raman}^{n+1/2} = \frac{\varepsilon_0}{\Delta t}\left[E^{n+1}S^{n+1} - E^n S^n\right].$$

These effective currents enter Maxwell's equations along with the beam current. The update for E^{n+1} is given by:

$$\nabla\times H^{n+1/2} = \frac{\varepsilon_0}{\Delta t}\left[E^{n+1}-E^n\right] + J_{Particle}^{n+1/2} + J_{Kerr}^{n+1/2} + J_{Raman/Brillouin}^{n+1/2} + J_{Dispersion}^{n+1/2}.$$

Note that the Kerr and Raman currents (and dispersive contributions which are not considered in this analysis) have an implicit form. These currents depend on E^{n+1} which we are trying to obtain. These systems can be solved efficiently via Gauss Newton regression iteration, similar to the approach in ref. [6]. This approach has a better numerical stability and better accuracy than explicit schemes. We also explored an explicit scheme for this problem that did not involve solving a nonlinear system of equations, but found it was prone to numerical instabilities and required smaller time steps.

We benchmarked the approach by simulating 2D TM mode propagation in a Kerr – Raman nonlinear medium. Results are identical to those of ref. [7]. We observe standard nonlinear phenomena like wave beam self focusing and self phase modulation (steepening) (Figs. 2-3). If we take the FFT of the time domain signal on Fig. 3, we will see spectrum broadening, presence of the weak third harmonic and Raman shifted spectrum peak.

Because Kerr and Raman are $\chi(3)$ nonlinearities a direct third order harmonic generation is possible due to nonlinearity. This is a weak effect. We observe third harmonic generation in our simulations (Fig. 5). To avoid other spectrum effects in this case we simulated Kerr-nonlinearity only. The third harmonic also broadens due to self phase modulation and also has a "fresh" narrowband portion.

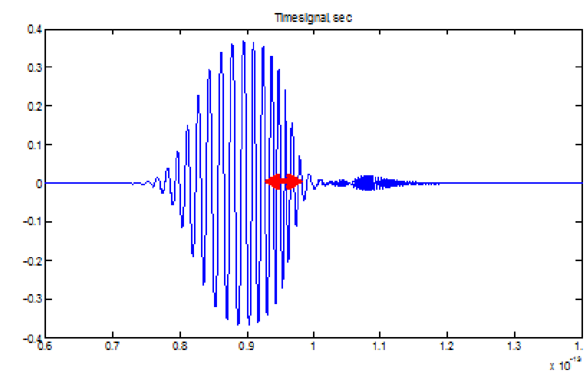

Figure 3. Time domain signal measured by a probe as the pulse propagates. Self phase modulation (self steepening) with daughter pulse are observed. The arrow marks the compressed region of the leading edge of the pulse.

The Raman effect occurs when photon inelastically scatters of the molecule. A photon excites the molecule from ground state to a higher energy state. As the molecule relaxes it can go to a different intermediate rotational or vibrational state. A photon of a different energy will be emitted and we will observe a corresponding Raman frequency shift. The frequency shift can be negative (a lower frequency is emitted) if the final state is more energetic than the original one. Such shift is called the Stokes shift. If the opposite happens the shift will be positive (toward higher frequency): antiStokes shift occurs.

The Raman effect occurs together with the Kerr effect. Kerr effect results from instantaneous response of electrons. Raman effect is not instantaneous as it occurs due to vibrations of the material. When these vibrations are optical phonons the effect is called Raman scattering. If the vibrations are acoustical phonons the effect is called Brillouin scattering. In simulation, depending on the parameters we will get Raman or Brillouin scattering.

We simulated self – induced effects of the intense wave packet. In this simulations Brillouin spectrum shifts are very small. We present the results for larger, Raman shifts.

In our simulations besides the pump signal as expected we observe a satellite with shift 35 THz. The time signal exhibits a typical beating due to appearance of extra spectral components. In another simulation parameters corresponded to larger shift of ~ 80 THz which was also observed (Fig. 4). It is important to notice, that due to filamentation the placement of a field probe is sensitive to the spectrum. Some probes don't see the Raman scattered light as well as others. It requires unrealistic propagation times to resolve Brillouin shifts in these self induced experiments.

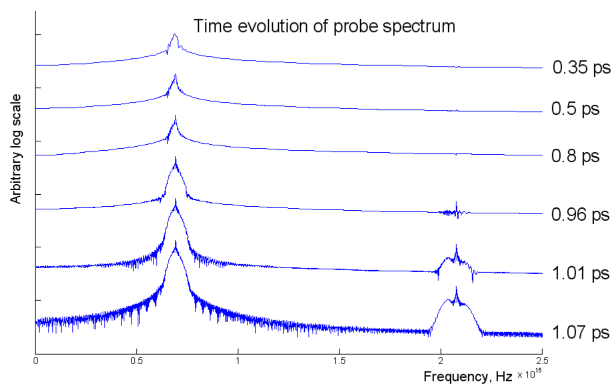

Figure 4. Spectra taken from a probe signal at successive intervals as the pulse propagates. Third harmonic generation is observed at 0.96 ps and later. Note spectrum broadening as a result of self phase modulation.

SUMMARY

We reported on the development of algorithms for modeling the high frequency and nonlinear optical properties of dielectric and paramagnetic materials with an emphasis on problems relevant to the PASER. The applicability of this work however is not limited to PASER related problems. One example is the expanding research area of metamaterials [8]. Numerical modeling of systems involving bulk metamaterials requires the accurate handling of dispersive permittivities and permeabilities. Simulations of particle interaction with nonlinear dielectrics may become relevant for dielectric loaded accelerating structures as they reach high (hundreds of MV/m) gradients.

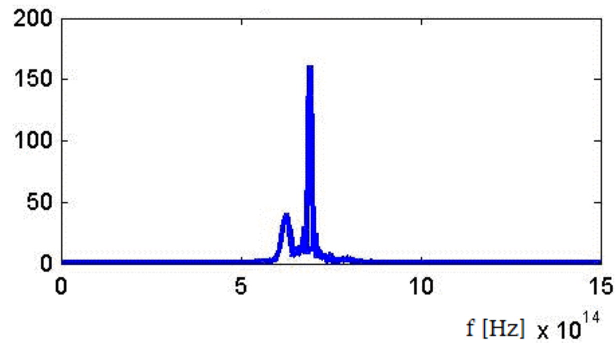

Figure 5. Spectrum showing Raman scattering with media shift frequency 80 THz.

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