Numerical Modeling of Nonlinear Beam Propagation Phenomena

G. A. Swartzlander, Jr.*, A. M. Deykoon*, D. W. Jackson*, and C. T. Law**
* Physics Dept., Worcester Polytechnic Institute, Worcester, MA 01609, grovers@wpi.edu
** ECE Dept., University of Wisconsin, Milwaukee, WI 53201

ABSTRACT

A user-friendly beam propagation program has been developed for use over the world-wide-web to aid the optical limiting community in modeling the transmission of light through nonlinear refractive and absorptive media having local intensity-dependent or nonlocal fluence-dependent mechanisms.

INTRODUCTION

We have developed software, complete with a user-friendly interface, which gives members in the optical limiting community device-independent access to a powerful computer program that models the propagation of light through an optical system containing a nonlinear optical material. Unlike most commonly available software packages, this program can be run from virtually any computer because the memory-intensive computing is performed on a remote computer. This is accomplished by making extensive use of the world wide web and electronic mail. A suite of simple optical systems has been developed to help facilitate the verification of the numerical codes with experimental measurements. Various nonlinear refractive and absorptive mechanisms are modeled, including Kerr, two-photon, bleaching, reverse-saturable absorption, and thermal heating processes. Presently, the optical system may be configured with a single thin lens having an f-number greater than 3.5 and either pill-box or partially apodized Gaussian beam profiles at the input aperture.

The design of any nonlinear optical device, e.g., limiters and rectifiers, cross-bar switches, logic gates, or soliton encoders, require that demanding engineering constraints be satisfied. As is generally characteristic of nonlinear systems, the performance of these devices may be sensitive to the characteristics of the input beam, the optical system, and the properties of the nonlinear medium. The marginal performance of current nonlinear optical materials requires one to optimize the device and material systems to achieve adequate limiting without sacrificing optical quality. Though partial differential equations governing the propagation of light in nonlinear media are known, analytic solutions are rare; hence, numerical methods are required to determine parameter values which provide acceptable levels of exposure at the sensor. Whereas such information may be experimentally measured for a given set of optical and material parameters, only numerical solutions are capable of providing data for arbitrary parameters. Thus, numerical modeling may be used as a powerful guide in the development of nonlinear materials and systems for sensor protection.

While many system and material parameters can be included in the numerical model, it is not practical to scan over all permutations of the parameter values to determine the optimal combination. Instead, a few special cases can provide significant insight into the underlying optical processes which occur as the beam propagates through the system. Several optical schemes have been incorporated into the numerical package to facilitate the development of a qualitative understanding, while at the same time, allowing quantitative comparisons with experiments. These schemes are (1) an f/5 optical system with a uniformly illuminated aperture (i.e., a pillbox profile), (2) an f/20 optical system, also with a pillbox intensity profile, (3) an f/5 system with a Gaussian input beam whose waist is truncated by an aperture, and (4), an f/20 system, also slightly apodized at the waist position (planar wavefronts are assumed in this report). The computer program simulates the propagation of light through the optical system so that intensity profiles of the propagating and far-field beams can be viewed. Thus, the user is able to rapidly determine the most important aspect of optical limiting, namely, how the beam intensity is being redistributed. Public domain software may be used to visualize the propagation dynamics of the beam.

The user interface takes advantage of the world-wide-web, using the standardized Hypertext Markup Language (HTML) which most computers can read with the aid of a standard browser program such as Netscape or Mosaic. This interface allows the user to enter material and optical parameters and then to submit the job to a remote computer workstation. The user is notified when the job is complete via electronic mail. Using the web browser, the user then retrieves the data from the workstation. Finally, the user may view the data. The image sequences may be easily converted to ASCII data for further analysis by the user.

THEORY

Modeling the propagation of electromagnetic waves through time-integrated or fluence dependent materials is particularly challenging, primarily because large amounts of computer memory and/or time are required for accurate (3+1) dimensional simulations. Current computer processing speeds and the cost of computer memory are no longer prohibitive barriers against such modeling efforts. Given these advances, we developed a numerical code to predict the spatio-temporal propagation of a laser beam through an absorbing and/or refracting nonlinear material. In this report we describe the more complicated thermal model which couples the heat and wave equations.

Since nearly the advent of the laser, it was noticed that a small amount of absorption in a liquid would induce a laser beam to undergo "thermal lensing" or "blooming"[1]. This phenomenon occurs because the absorbed light heats the liquid, thereby reducing the mass density in the volume of the beam path. The refractive index is proportional to the density of the liquid, and therefore, light is refracted radially out of the beam toward regions of higher refractive index, i.e., toward the cooler, more dense material. If the beam continues to illuminate the material, the temperature continues to rise over time, creating a temperature profile in the transverse cross-section of the beam. Owing to diffusion, the heat also spreads radially outward so that the refractive index distribution varies in both space and time. Hence the intensity profile of the beam will also vary with time. Unlike "local" nonlinear effects where the refractive index profile is identical to the intensity profile (e.g., Kerr materials), here we see that diffusion produces a "non-local" refractive index change.

To model the propagation of light through such thermal materials, one must simultaneously solve the wave equation and the heat equation. The wave equation must include an absorption term and an inhomogeneous refractive index term. For optical systems have an f-number exceeding 3.5, the paraxial ray approximation may be assumed, and thus the wave equation may be written:

$$2ik\partial E / \partial z + \partial^2 E / \partial x^2 + \partial^2 E / \partial y^2 + 2k^2 n_0^{-1} \Delta n(x,y,z;t) E = -ik\alpha E \tag{1}$$

where E is the envelope of the oscillating electric field, z is the axis of propagation, (x,y) are transverse coordinates, k is the wavenumber in the material, n_0 is the linear refractive index of the material (at ambient temperature), Δn is the refractive index profile (we assume $\Delta n << n_0$), and α is the absorption coefficient. The so-called "Split-Step" or "Beam Propagation" method [2] may be used to numerically solve Eq. (1) for a given incident field distribution, E(x,y,z=0;t), at the boundary, z=0, and at a fixed time, t. For thermal media, the refractive index profile, Δn, is assumed to be proportional to the local temperature of the medium:

$$\Delta n(x,y,z;t) = (dn / dT) \Delta T(x,y,z;t) \tag{2}$$

where (dn/dT) is an experimentally determined coefficient that may be found in scientific reference books or tables of material properties. (We ignore pressure-dependent effects which dominate over shorter time scales than temperature-dependent effects).

For a laser heat source, the temperature change, $\Delta T = T - T_0$, may be determined from the heat equation

$$\frac{\partial T(x,y,z;t)}{\partial t} = D \nabla^2 T(x,y,z;t) + \frac{\alpha}{c_p \rho} I(x,y,z;t) \tag{3}$$

where we assume an arbitrary ambient temperature of $T_0=0$, c_p is the heat capacity at constant pressure, ρ is the density, and

$$D = \kappa / c_p \rho \tag{4}$$

is the diffusion coefficient, where κ is the heat conductivity. If the intensity profile varies slowly along the longitudinal direction (the z-axis) compared to the transverse gradients (e.g.,$\alpha w_0' << 1$ where w_0' is the transverse beam size) then we may ignore changes of temperature along z:

$$^{2}T \approx \partial^2 T / \partial x^2 + \partial^2 T / \partial y^2 . \tag{5}$$

For a given initial incident field distribution, E(x,y,z=0;t=0), a numerical solution may be found for E(x,y,z;t) using the following approach:

1. At t=0 determine the electric field and intensity throughout the material using numerical solutions of the wave equation, Eq. (1) with Δn=0.
2. Determine the incremental temperature change over a small time step, δt, using the heat equation, Eq. (3), with the heat source determined in Step 1. Calculate the temperature profile, Δn, using Eq. (2).
3. Store the resulting distributions for intensity and temperature to a file on the hard disk of the computer.
4. Advance the time by δt, and determine the electric field and intensity, taking into account the temperature-dependent refractive index profile calculated in Step 2.
5. Repeat Steps 2, 3, and 4, until the desired time has elapsed.

The heat equation may be solved using various algorithms. We use an explicit approach called the Forward Time Centered Space scheme [3] because it applies to a wide variety of cases, is simple to program, and has a simple stability criterion that can be satisfied for a given set of initial parameters. The algorithm is represented by the expression

$$\boxed{\begin{aligned} \frac{T(t_n+\delta t)-T(t_n)}{\delta t} &= \frac{\alpha}{c_p \rho} I(x,y,z,t_n) + \\ & D\left[\frac{T(x+\delta x)+T(x-\delta x)-2T(x)}{\delta x^2} + \frac{T(y+\delta y)+T(y-\delta y)-2T(y)}{\delta y^2}\right] \end{aligned}}$$

(6)

where δx and δy are discrete transverse spatial intervals on the numerical grid. This explicit scheme allows one to calculate the temperature distribution everywhere in space at time, $t_n+\delta t$, once the temperature distribution at time t_n is known. For example, we assume the initial temperature distribution is uniform. The stability criterion for this scheme is

$$2D\delta t / (\delta x)^2 \leq 1 \quad \text{and} \quad 2D\delta t / (\delta y)^2 \leq 1 \tag{7}$$

The numerical data may be compared against a known analytic solution; for example, the case of a collimated Gaussian intensity profile, where the induced temperature profile is

$$\Delta T(r;t) \;=\; \frac{1}{8}\frac{\alpha \;\; w_0'^2 \;\; I_0}{\kappa}\left\{ Ei\left(-2(r/w_0')^2\right) - Ei\left(-\frac{2(r/w_0')^2}{1+t/t_c}\right)\right\} \tag{8}$$

where $r=(x^2+y^2)^{1/2}$ is the transverse radial coordinate, w_0' is the radial beam size, I_0 is the peak incident intensity, *Ei* is the exponential integral function, and

$$t_c \equiv w_0'^2 / 8D \tag{9}$$

The on-axis temperature simplifies to a logarithmic function:

$$\Delta T(r=0,t) = T_c \ln\left(1+2\frac{t}{t_c}\right) \tag{10}$$

where $T_c = \alpha w_0'^2 I_0 / 8\kappa = \alpha P / 4\pi\kappa$ is approximately the temperature increase at $t=t_c$, for a given beam power, P.

Let us now determine an appropriate value for the absorption coefficient. If the absorption length, L_a, is significantly shorter than the cell length, L_{cell}, the device may have unacceptable linear transmission properties, whereas a weakly absorbing cell would produce little heating. A benchmark value for the absorption length is the diffraction length,

$$L_a = \alpha^{-1} \approx L_d = kw_0'^2 / 2 \tag{11}$$

where w_0' is the radial spot size of a collimated Gaussian beam of size, w_0, after passing through a lens with a focal length, f, and an effective f-number, $f^{\#}=f/2w_0$:

$$w_0' \approx (2\lambda/\pi) f^{\#} \tag{12}$$

(for a pillbox or severely apodized beam, $w'_0 \approx 1.22\lambda f^{\#}$). For the case, $L_a = L_d$, the product $\alpha w'_0 = \lambda / \pi w'_0 = \theta_d / 2$ is related to the divergence angle of the beam, θ_d. Thus, paraxial rays satisfy the assumption discussed above; namely, that the temperature varies slowly along the propagation direction, which requires $\alpha w'_0 << 1$. We also note that the f-number of the optical system is also related to the divergence angle: $\tan(\theta_d / 2) = 1/(2 f^{\#})$, and thus, the benchmark absorption coefficient may be written,

$$\alpha \approx \pi / \left[4\lambda (f^{\#})^2\right] \tag{13}$$

Therefore a desirable absorption coefficient may be determined, given only the wavelength and the f-number of the optical system. For example, if $f^{\#}=5$ and $\lambda=1$ μm, we calculate a benchmark absorption coefficient of approximately $\alpha=300$ cm^{-1} (or an absorption length of $L_a=32$ μm).

Let us now estimate the values of other material parameters. To achieve significant nonlinear refraction over a length of the material, an induced phase change of roughly $kL_{cell}\Delta n \approx \pi$ is required and thus, for $L_{cell} = L_d$, an index change of roughly

$$\Delta n \approx 3.2 / (f^{\#})^2 \tag{14}$$

is needed [4]. Thus, for an f/5 system, an index change in the range of $\Delta n=0.1$ is desirable. The parameters required to achieve a given index change may be estimated by ignoring diffusion and calculating the index change under continuous illumination at the characteristic time, t_c:

$$\Delta n(t = t_c) = \alpha \eta t_c I_0 = \left\{ \frac{\alpha \lambda^2}{2\pi^2 \kappa} \left(f^{\#}\right)^2 \frac{dn}{dT} \right\} I_0 \equiv n_2^{(eff)} I_0 \tag{15}$$

where $\eta = (dn/dT)/\ c_p\rho$ is a thermal nonlinear figure of merit, and

$$t_c = w_0'^{\,2} / 8D \approx (\lambda f^{\#})^2 c_p \rho / 2\pi^2 \kappa \tag{16}$$

and $n_2^{(eff)}$ is an effective Kerr nonlinear coefficient at the instant $t=t_c$, which may be expressed:

$$n_2^{(eff)} = \left(\lambda L_d / 8\pi L_a \kappa\right)\left(dn/dT\right). \tag{17}$$

To achieve the strongest nonlinearity, irrespective of the response time, t_c, materials having large values of (dn/dT) and α, and small values of κ are desirable. Furthermore, large diffraction lengths and wavelengths exhibit stronger nonlinear responses. That is, the heat should remain in the beam path so that a large index change may be induced. To minimize the response time, materials having small values of density, ρ, and heat capacity, c_p, are desirable.

For a given material with known thermal parameters, the intensity required to achieve a significant index change may be calculated. Let us consider an f/5 system, a wavelength $\lambda = 1$ [μm], and a cell containing dyed methanol: $L_{cell} = L_d = L_a$. The thermal parameters for methanol are $dn/dT = -3.9\times10^{-4}$ [K^{-1}], $c_p = 2.5\times10^3$ [J/ kg − K], $\kappa = 0.2$ [J / s − m − K], $\rho \approx 790$ [kg/ m^3], and $D = \kappa / c_p\rho = 10^{-7}$ [s / m^2]. The calculated thermal figure of merit is $\eta = -1.9\times10^{-10}$ [m^3 / J], the beam waist is $w_0' = 3.2$ [μm], and the critical time is $t_c = 12.5\times10^{-6}$ [s]. We calculate $n_2^{(eff)} = -7.4\times10^{-7}$ [cm^2 / W] Thus, to achieve $|\Delta n| = 0.1$, a peak intensity of $\mathrm{I}_0 \approx 130$ [kW / cm^2] or a power of $\mathrm{P} = (\pi w_0'^2 / 2)\mathrm{I}_0 = 21$ [mW] is required.

RESULTS

As an example, we have solved the coupled heat and wave equations for a Gaussian beam in an f/5 optical system, using a transverse grid of size $N_x \times N_y = 128\times128$, and longitudinal grid size of $N_z = 320$ (corresponding to a cell thickness of $L_{cell}=L_d=31.8$ [μm]). The simulation ran for $N_t = 402$ time steps, which corresponds to 100 [μs] of laser heating. The CPU time required to run the simulation was 8.5 [hr], and the memory requirement for single precision was roughly 20 Mb. The diffusion coefficient for methanol was used, $\mathrm{D} = 10^{-7}$ [s/ m^2], and an absorption coefficient of $\alpha \approx 218$ [cm^{-1}] $= 0.69/\ \mathrm{L_d}$ was assumed. A laser of wavelength, $\lambda = 1$ [μm], and power of $P = 7.9$ [mW] was also assumed. The intensity profiles at the output face of the cell, as well as the corresponding far-field profiles, are depicted at different times in Fig. 1. The beam was focused at the input face of the nonlinear cell. Within the characteristic time, $t_c=12.5$ [μs] the near and far-field beams have expanded only slightly. For limiting purposes, we are most interested in the far-field profile, where we do not see a significant redistribution of energy until $t \approx 8t_c = 100$ [μs].

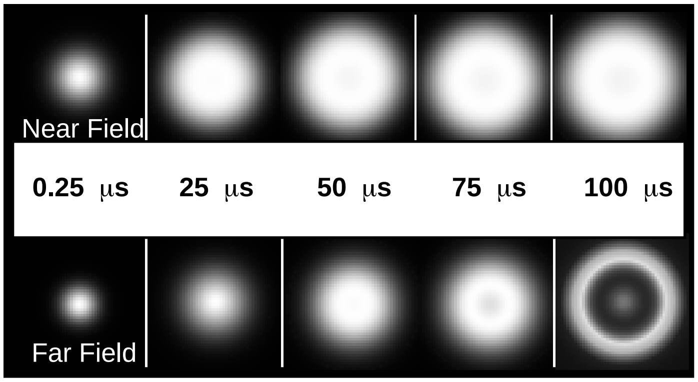

Fig. 1. Time evolution of the near and far field intensity profiles for a beam at the output face of a thermal nonlinear cell in an f/5 optical system.

As another example, we demonstrate that optical systems having large f-numbers require a significantly lower change in the refractive index to induce a π phase change across the beam. Using the same design principle as in the f/5 case above, $L_a = L_d = L_{cell}$, let us now investigate an f/20 system. In this case, the focal spot size of the beam will be $w_0' = (2\lambda / \pi) f^{\#} = 12.7$ [μm] and the lengths will be set at $L_a = L_d = L_{cell} = 509$ [μm] (again we assume λ=1 μm). The thermal response time is $t_c = w_0'^2 / 8D = 0.2$ [ms] is now 16 times larger than it is for the f/5 case. To achieve a benchmark index change, $|\Delta n| \approx 3.2 / (f^{\#})^2 \approx 0.01$ (and noting from Eq. (17) that the effective Kerr coefficient is the same for any f-number if the ratio, L_d / L_a, is unchanged), a peak intensity of $I_0 = \Delta n / n_2^{(eff)} = 13[\mathrm{kW/\ cm^2}]$ is required (or P = 33[mW]). We have numerically calculated intensity profiles, shown in Fig. 2, for an f/20 system with a relatively short absorption length, $L_a = 0.57 L_d$. The transverse grid size in this case was 256x256 pixels, and the code ran for 16.6 hr. As expected, strong nonlinear diffraction was observed in both the near and far-field regions within t_c. Though large f-number systems exhibit stronger nonlinearity, and hence, enhanced limiting capabilities, they suffer from having a small optical field-of-view.

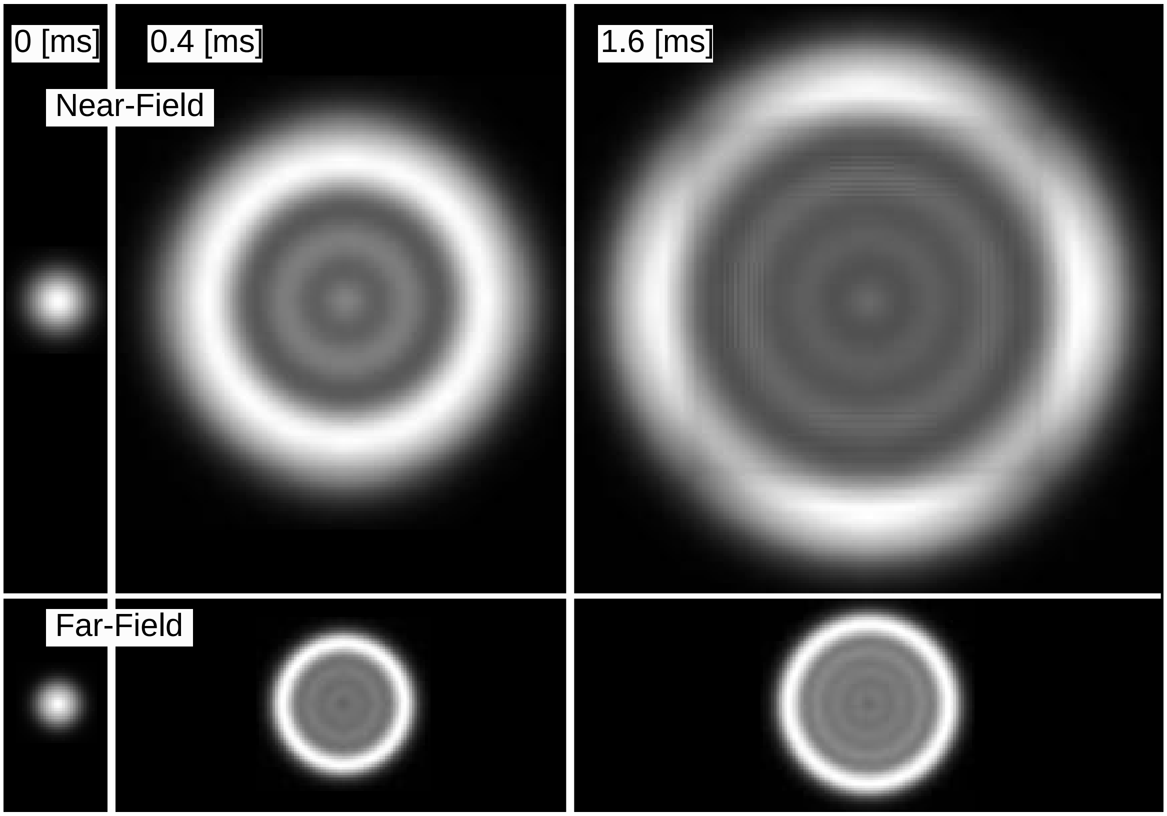

Fig. 2. Time evolution of the near and far field intensity profiles for a beam at the output face of a thermal nonlinear cell in an f/20 optical system.

Finally, to verify our code, we compare numerical solutions with the analytic result given in Eq. (8) for a collimated Gaussian beam. Excellent agreement, shown in Fig. 3, is found between the two over a time scale of at least $4t_c$. The parameters used in this comparison are: w_0=1 [mm], α=1.026 [m^{-1}], D=10^{-7} [m^2/s], I_0=63.3 [W/cm^2], and κ=0.202 [W/m-K]. We calculate the following characteristic temperature and time from these parameters: T_c=0.404 [K] and t_c=2.5 [s].

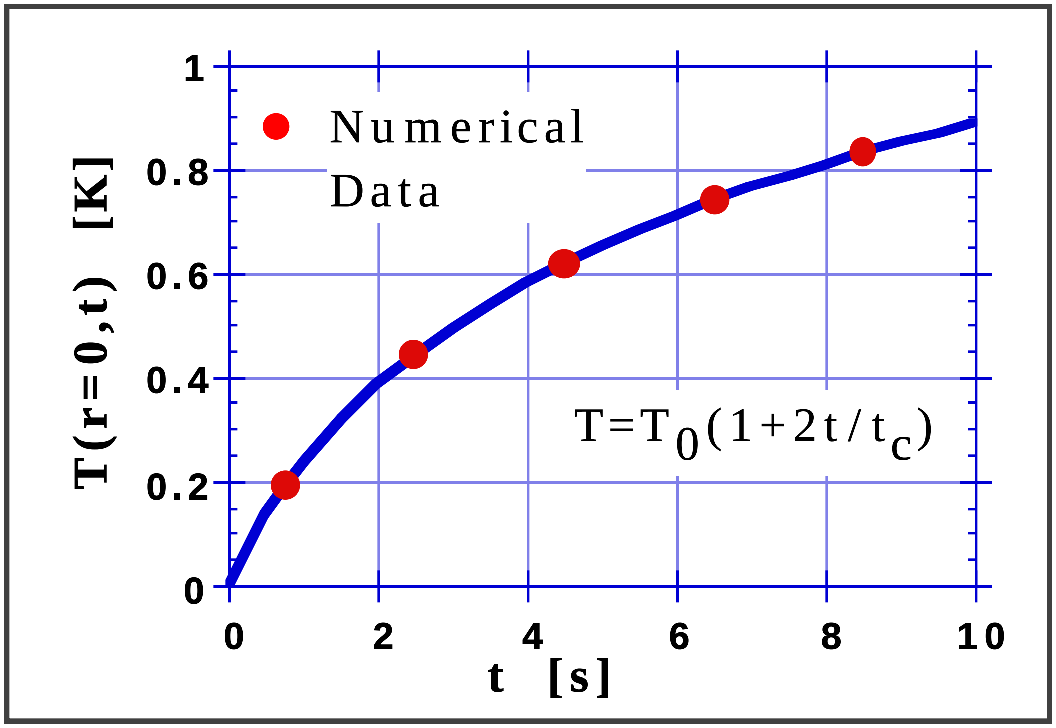

Fig. 3. On axis temperature (or refractive index) profile owing to heating of a liquid with a Gaussian laser beam.

CONCLUSIONS

We have successful launched a powerful beam propagation program on the world-wide web for use by the optical limiting community. We have verified the thermal and Kerr nonlinear codes against analytic solutions. Other mechanism will require experimental verification. The web site demonstrates that users can have immediate access to sophisticated modeling tools without the need to install the software on their own computer. The numerical models described here are valid for paraxial rays, which include systems having f-numbers down to roughly 3.5. For thermal nonlinear systems, large nonlinearities may be achieved by choosing highly absorbing materials having large values of (dn/dT) and low heat conduction. Fast response times require low density materials with a low heat capacity.

ACKNOWLEDGMENTS

We are grateful to Gregg Anderson (Material Directorate, Wright Laboratory, Air Force Systems Command, United States Air Force, Wright-Patterson AFB Ohio 45433-6533) for providing guidance, and James Shirk (US. Naval Research Laboratory, Code 5613, 4555 Overlook Ave. SW, Washington, DC. 20375) for suggesting improvements. This research was supported by funds supplied from the US. Air Force under Contract No. F33615-92-D-5000 through Subcontract Number 96-5000-71-1 from Anteon Corporation. The research results and the interpretation thereof do not necessarily reflect the views or opinions of either the Government or Anteon and represent those of the authors of this publication.

REFERENCES

1. R. C. C. Leite, R. S. Moore, and J. R. Whinnery, *Low absorption measurements by means of the thermal lens effect using a He-Ne laser*, Appl. Phys. Lett. 5, 141 (1964).

2. J. A. Fleck, Jr., J. R. Morris, and M. D. Feit, *Time-dependent propagation of high energy laser beams through the atmosphere*, Appl. Phys. 10, 129 (1976).

3. W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, Numerical Recipes, The Art of Scientific Computing, (Cambridge University Press, New York, 1989).

4. G. A. Swartzlander, Jr., B. L. Justus, A. L. Huston, A. J. Campillo, and C. T. Law, *Characteristics of a low f-number broadband visible thermal optical limiter*, International J. of Nonlinear Opt. Phys. 2, 577 (1993).