

A 'collimated' laser beam has a slight divergence (the beam expands) as it propagates through a material or a vacuum. This effect is a result of diffraction of the beam at the output aperture of the laser. The SimphoSOFT mathematical model has a designated term to simulate diffraction. However, if a user specifies a very large discretization grid, the numerical integration of the diffraction term may become very time consuming. A user has a choice to turn 'OFF' diffraction in certain cases.

## When is this diffraction effect important and when can it be ignored?

For a laser beam having  $1/e$  radius  $R_0$  and wavelength  $\lambda_0$  propagating through a material having a linear refractive index  $n_0$ , the 'diffraction length ( $L_{df}$ )' or 'Rayleigh Length' is defined as

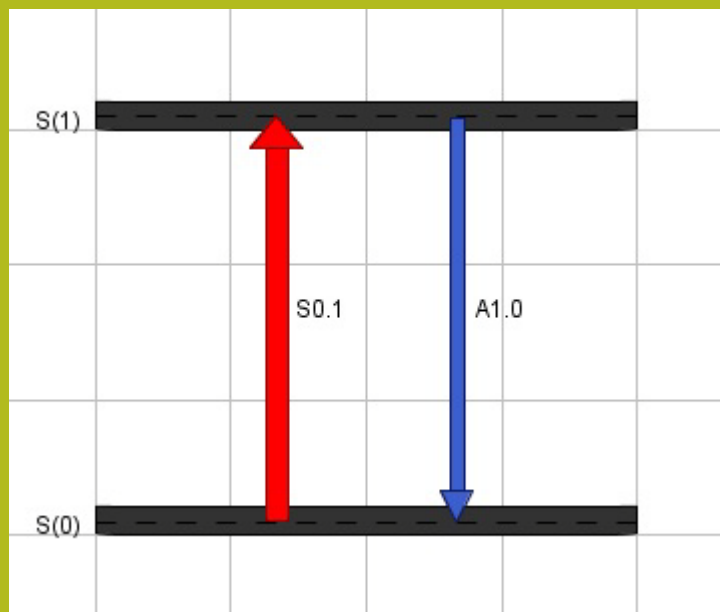
$$L_{df} = \pi (R_0)^2 n_0 / \lambda_0.$$

If the sample thickness is less than  $L_{df}$ , then the divergence of the beam as it passes through the sample is small and can probably be ignored. If the sample thickness is greater than  $L_{df}$ , then the divergence of the beam may need to be taken into consideration for the simulation.

## Example SimphoSOFT calculation with the diffraction feature turned 'OFF' or 'ON':

The sample is composed of molecules dispersed in a host material. The molecules have two important singlet energy states,  $S(0)$  and  $S(1)$ , for optical transitions.

Screenshot of SimphoSOFT® M-CAD with 2-level energy level diagram of the molecules



One-photon absorption (1PA) cross-section in the example 2-level model:  $1 \times 10^{-20} \text{ cm}^2$  from  $S(0)$  to  $S(1)$

Relaxation time for the example 2-level model: 1 ns from  $S(1)$  to  $S(0)$

Other sample properties	
Molecular dopant density (concentration) in the host material	$3.0 \times 10^{18}$ molecules/cm <sup>3</sup>
The host material linear refractive index	$n_0 = 1.4$
Host material linear absorption	$\alpha = 0.001 \text{ cm}^{-1}$
Host material nonlinear refractive index	$n_2 = 0$
Sample length	30 mm

For this example,  $L_{df}$  is 9.096 mm for the given laser wavelength and radius. Since the 30 mm sample length corresponds to 3.30  $L_{df}$ , divergence of the beam is important.

## Results of SimphoSOFT simulations of beam propagation with diffraction 'OFF':

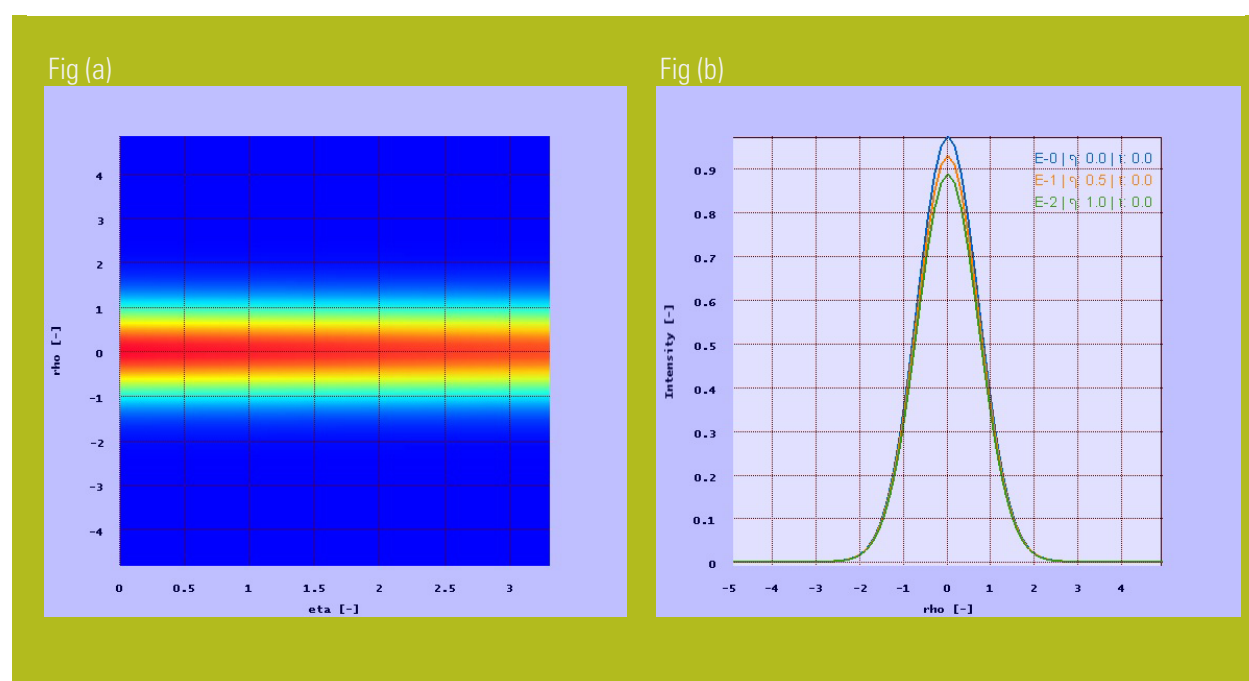


Figure (a): Graph of pulse intensity with diffraction 'OFF' calculated at the center of the pulse's moving frame (time=0) for a beam which propagates through the sample with length  $\eta = 3.3$  (in units of  $L_{df}$ ).

Figure (b): With diffraction 'OFF', the cross-section of the beam intensity does not expand as it propagates from the sample input surface (blue curve) to the sample midpoint (orange curve) and finally to the sample output surface (green curve). However, the beam intensity drops slightly due to weak 1PA absorption. The horizontal axis is the normalized radial dimension ' $\rho$ ' of the beam in units of  $R_0$ .

Laser properties	
Pulse energy	13.3 $\mu\text{J}$
Pulse radius (HW1/e2M)	56.8 $\mu\text{m}$
Pulse FWHM	175 fs
Wavelength	780 nm

Results of SimphoSOFT simulations of beam propagation with diffraction 'ON':

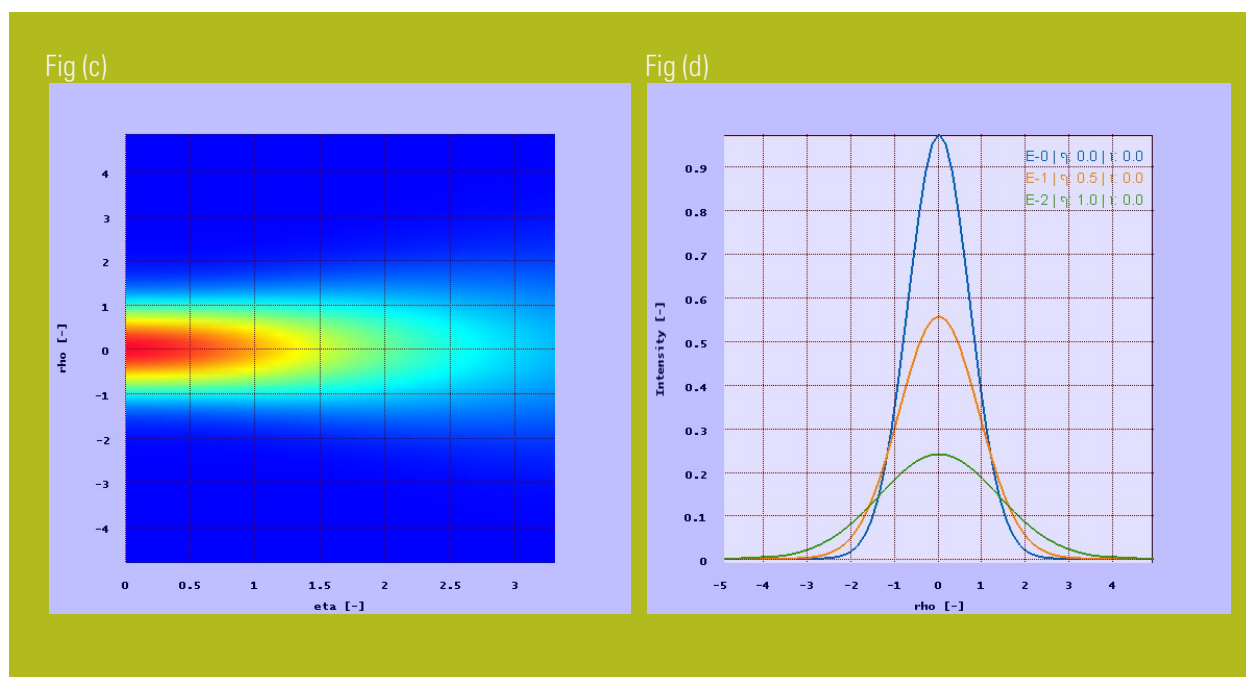


Figure (c): Graph of pulse intensity with diffraction 'ON' calculated at the center of the pulse's moving frame (time=0) for a beam which propagates through the sample with length  $\eta = 3.3$  (in units of  $L_{\text{diff}}$ ).

Figure (d): With diffraction 'ON', the cross-section of the beam intensity expands significantly as it propagates from the sample input surface (blue curve) to the sample midpoint (orange curve) and finally to the sample output surface (green curve). The beam also undergoes a significant drop in intensity due mainly to the beam expansion that results from diffraction. The horizontal axis is the normalized radial dimension ' $\rho$ ' of the beam in units of  $R_0$ .