Large scale simulation of optical-material interaction to determine laser ablation in liquid and spectral absorptivity of perfect light absorber

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Introduction

A range of important physical mechanisms can happen when light strikes a surface. For example, absorption and transmission of light can happen at the surface, which can result in heating of the target either at the surface or beneath the surface depending on the absorption coefficient of the target and the depth of penetration. The optically induced heating, when it is strong enough, can cause mass removal from the target with micron (or even sub-micron) scale precision. With this high level of resolution, optical laser ablation is valuable in radiative-energy detection and harvest for different renewable energy applications. In this paper, we summarized a portion of our previous work relating to the utilization of wave optics to determine the optical-material interactions and the associated joule heating/phase change behavior of the material. The presentation is divided into two portions, namely (a) optical induced vapor bubble formation/evaporation in water-like materials. Such phenomenon is called micro-cavitation in bio-tissues, and is important in a wide range of laser-surgeries; (b) design of multiband perfect light absorbers (PCLA) which can be achieved with appropriate materials to harvest the volumetric-scales patterns. When Maxwell’s equations are applied to handle the wave type simulations, required mesh size can be equal or less than 1/50 to 1/200. More than a few millions of meshes are commonly required in such simulations. Therefore, we mainly rely on the ADG cluster at TAMU especially for cases requiring parametric sweep parallel simulations.

Theory

The numerical results presented in the following sections are based on solving the following governing equations under: (a) evolutionary symmetries or 3D conditions with either different finite element method (FEM); (b) wave optical simulation with Maxwell’s equations in frequency domain

\[ \nabla \times \mathbf{H} = j \omega \mathbf{D} + \mathbf{J}_0; \quad \mathbf{E} = -\nabla \phi \]

where \( \nabla \), \( \mathbf{H} \), \( \mathbf{D} \) and \( \mathbf{J}_0 \) represent the gradient operator, magnetic induction, electric induction and magnetic field in the frequency domain, respectively. \( \phi \) is the relative permittivity of the material, \( \epsilon_0 \) is the permittivity of free space, \( \mathbf{J}_0 \) is the induced electric current density, \( \eta \) is the speed of light. \( \mathbf{E} \) is the electric field vector and \( \mathbf{H} \) is the magnetic field vector.

(c) heat transfer with two temperature model for heat diffusion in the solid/liquid/vapor phases

\[ \nabla \times \mathbf{H} = j \omega \mathbf{D} + \mathbf{J}_0; \quad \nabla \cdot \nabla \mathbf{T} = \frac{\rho_c}{\epsilon_0} \left( \frac{\partial \mathbf{E}}{\partial t} - \mathbf{J}_0 \right) \]

where \( \epsilon_0 \) is the permittivity of vacuum, \( J \) is the electron and photon flux density, \( \rho_c \) is the heat capacity per unit volume, and \( \epsilon_0 \) is the relative permittivity of the material.

The induced current density \( \mathbf{J}_0 \) is given by:

\[ \mathbf{J}_0 = \eta \mathbf{E} \]

The heat transfer coefficient is

\[ h = \frac{1}{R} = \frac{1}{\frac{1}{h_1} + \frac{1}{h_2} + \frac{1}{h_3}} \]

where \( h_1 \), \( h_2 \), and \( h_3 \) are the convective and radiative heat transfer coefficients respectively.

Optically induced vapor bubble in water

The simulation of optically induced vapor bubble in water as well as its expansion process can be divided into two stages. First, we simulate a flat top laser light delivered to a water-like target through a hemispherical lens. The resulting joule heating in the target especially around the focal point can be extracted from

\[ \mathbf{J}_0 \quad \text{joule heating} \]

with \( \mathbf{J}_0 \) is the induced current density.

The obtained joule heating rate per unit volume from the full wave simulation is then inserted into the energy equation as the \( \phi \) term to determine the induced heating. The temperature increment of the target during the EM joule heating indicates the deformation velocity, field phase change of the target, which can be described with conservation equations and equation of state of the target. To properly handle the deformation of the target due to the expansion of the vapor bubble, arbitrary Lagrangian-Eulerian (ALE) method and moving meshes to trace the movement of the top boundary is adopted. The obtained results are listed in the following figures 1-4.

Design of multiband perfect light absorber

A perfect light absorber is a device which absorbs all the energy that is incident upon it at a particular wavelength. A perfect absorber can be achieved with metamaterial composed of micro/nanoscale surface patterns. It was shown in a previous study that perfect light absorber could be realized using a gold cross electric ring resonator (ERR) separated from a conducting gold layer using a thin Gallium Antimonide dielectric layer. When light with appropriate wavelength strikes the metal cross shape ERR, standing electric field with high intensity will be induced in the ERR, which will in turn cause strong magnetic field resonance in the dielectric layer confined by the top metallic ERR and the bottom metal base. By adjusting the amplitude of the electric and magnetic resonance, the impedance of the metamaterial can be fine tuned to provide zero reflection at selected wavelengths (i.e., perfect absorber). To achieve this critical condition for perfect light absorption, the size of each ERR and the thickness of the dielectric layer should be well designed. To determine the required size of the ERR when it is made with Au as well as the required thickness of the dielectric layer to achieve perfect light absorption at specific wavelength, we have to carry out a parametric sweep simulation, using full wave simulation based on Maxwell’s equations to test the light absorptivity of this specific type of metamaterial with different sizes of Au crossed shape ERR and different dielectric thickness with full wave simulation. Figure 8A shows the simulation domain and the results are presented in Figure 8B for design of metal superabsorbers providing perfect light absorption at 1-12 mum with aluminium as the dielectric layer.

In many applications, however, more than one perfect absorption band is required. Based on this motivation, we aim to attain multiband perfect light absorber by combining different sizes of cross-shaped electric ring resonators (ERR) on one planar ERR. On one plan, based on Maxwell’s equations, we calculated the light absorptivity of this specific type of metamaterial/with different sizes of Au crossed shape ERR and different dielectric thicknesses with full wave simulation. Figure 8A shows the simulation domain and the results are presented in Figure 8B for design of metal superabsorbers providing perfect light absorption at 1-12 mum with aluminium as the dielectric layer.

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All the presented results are accomplished with COMSOL 5.1 and lab-made multiphase two-temperature modules on ADA cluster of TAMU. Each light induced vapor bubble formation simulation requires 4 nodes with 20 CPUs each with a total simulation time less than 48 hours. Each parametric sweep simulation for the design of multiband perfect light absorbers requires 10 nodes with 50 CPUs each with a total simulation time of 72 hours.