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Uncertainty quantification for modeling pulsed laser ablation of aluminum considering uncertainty in the temperature-dependent absorption coefficient

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ABSTRACT

In this paper, an extension of the result of Wang et al. ("Modeling pulsed laser ablation of aluminum with finite element analysis considering material moving front," *Int. J. Heat & Mass Transfer*, 113, 1246–1253, 2017) concerning the problem of uncertainty quantification for pulsed laser ablation (PLA) of aluminum is considered, when the source of uncertainty is due to an inherent randomness of the temperature-dependent absorption coefficient. In particular, we use a generalized polynomial chaos (gPC) method to incorporate the parameter uncertainty for the temperature-dependent absorption coefficient within the representation of the laser heat conduction phenomena. Furthermore, numerical simulation studies for the PLA of aluminum, with nanosecond Nd:YAG 266 nm pulsed laser, that demonstrate the proposed gPC predictions are presented. Finally, a sensitivity study is performed to identify whether small changes in the lower and/or upper parameter values of the absorption coefficient provide the most variance in the thermal and ablation responses.

1. Introduction

In recent years, a number of research efforts have been devoted to understand the working mechanisms and develop accurate simulation models for laser ablation of solid materials [1–9]. Despite these efforts, the problem of uncertainty quantification (UQ) for laser ablation of solid materials, when the sources of uncertainty are due to (inherently stochastic) variability of material and optical properties of target materials at various elevated temperatures, is not sufficiently understood or addressed, while recognizing their critical impact on guiding experimental efforts and advanced manufacturing. This further necessitates the need for developing efficient UQ methods for laser ablation of solid materials that establish confidence intervals in the computed temperature predictions and/or ablation response, the assessment of the suitability of model formulations for laser ablation of solid materials and/or the support of decision-making analysis. In this paper, we extend our recent work [8] to address the problem of UQ for pulsed laser ablation (PLA) of aluminum, when the source of uncertainty is due to an inherent randomness of the temperature-dependent absorption coefficient. In particular, we use a generalized polynomial chaos (gPC) method to incorporate the parameter uncertainty of the temperature-dependent absorption coefficient within the representation of the laser heat conduction phenomena. Note that the fundamental concept, where the gPC expansions are used for representing random fields and/or stochastic variables, is to consider the uncertainty as generating a new stochastic dimension and observing the solutions as being dependent on this dimension [10–15]. A convergent expansion along the new stochastic dimension is then sought in terms of a set of orthogonal basis functions, whose coefficients can be used to characterize and quantify the uncertainty.

Here it is worth mentioning that the gPC based method has been extensively used for UQ in engineering problems of solid and fluid mechanics (e.g., see Refs. [12,16] in the context of elastic structures; see Ref. [17] in the context of flow through porous media; and see Refs. [18,19] in the context of thermal problems). The main motivation behind the PC expansions includes the suitability for models expressed in terms of a set of coupled partial differential equations, the ability to deal with situations exhibiting steep nonlinear dependence of the solution on random model data, and the promise of obtaining efficient and accurate estimates of uncertainty. Moreover, such an information provides a format that

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permits itself to be readily used to probe the dependence of specific observables on particular components of the input data and/or to design experiments in order to better calibrate and test the validity of postulated model representation. In this paper, numerical simulation studies for the PLA of aluminum, with nanosecond Nd:YAG 266 nm pulsed laser, that demonstrate the proposed gPC predictions are presented. Moreover, a sensitivity study is performed to identify whether small variations in the lower and/or upper parameter values of the absorption coefficient provide the most variance in the thermal and ablation response and also integrate the effect of uncertainty ranges of the parameters on the thermal and ablation response.

The remainder of this paper is organized as follows. In Section 2, we outline the mathematical model of the laser heat conduction that accounts for the uncertainty in the absorption coefficient. The uncertainty is incorporated into the laser heat conduction through gPC expansions. In Section 3, the temperature-dependent material properties and the absorption coefficient uncertainty used for the UQ of the PLA model are presented. Section 4 briefly discusses the computational method used, where such a method captures the coupling between the material progressive surface recession and the laser heat conduction that also considers the material parameter uncertainties. Results and discussions demonstrating the applicability of the gPC based UQ for the PLA of aluminum are given in Section 5. Finally, our findings are summarized in Section 6.

2. Mathematical model for laser heat conduction considering uncertainty in the Temperature-dependent absorption coefficient

In the absence of convective and radiative heat exchanges, the thermal response of the solid material is governed by the following energy balance equation [1,20,21]

$$\rho C_p\left(\frac{\partial T}{\partial t}-\dot{s}\frac{\partial T}{\partial z}\right)-\nabla\cdot(k\nabla T)=\dot{q}, \tag{1}$$

where T is the temperature, the dependent variables are t (time) and z, the spatial coordinate normal to the material surface (see also Fig. 1), and the material properties are ρ, the solid density, k, the thermal conductivity, and C_p, the specific heat. $\dot{s}$ is the surface recession rate (i.e., the ablation rate due to material removal) and $\dot{q}$ is the rate of energy density input from the laser beam, which is essentially a laser-induced body heat flux, and expressed as:

$$\dot{q}=\alpha(1-R_f)I_0(t)e^{-\alpha z'}, \tag{2}$$

where α and R_f are, respectively, the absorption coefficient and the reflectivity, z' is the vertical distance from any points to the surface of the target material (i.e., $z' = z\text{-}d$, with d is the corresponding ablation depth), and I_0 is the instantaneous laser irradiance at time t. Specifically, the temporal profile of the laser irradiance for the

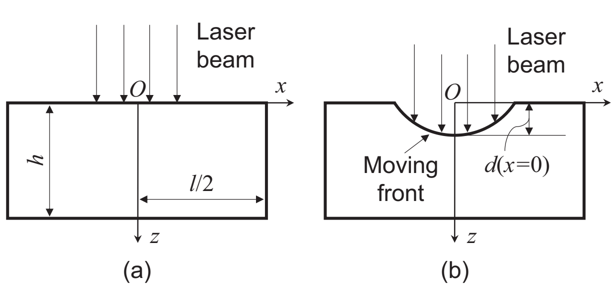

Fig. 1. Laser-material interaction considering moving front due to material removal: (a) at the beginning of laser ablation, and (b) during laser ablation.

Nd:YAG laser pulse is assumed to follow the form proposed by Refs. [20,22]:

$$I_0(t)=I_{\max}\left(\frac{t}{t_{\max}}\right)^7\exp\left[7\left(1-\frac{t}{t_{\max}}\right)\right], \tag{3}$$

where $I_{\max}$ is the peak irradiance of the laser pulse and $t_{\max}$ is the time when the laser irradiance reaches to its peak value.

The ablation rate $\dot{s}$ in Eq. (1) represents the rate of material removal during the PLA process. In particular, under low laser fluence conditions (i.e., without considering material phase explosion), the material removal is predominantly attributed to evaporation, where the corresponding ablation rate $\dot{s}$ can be described by using the Hertz-Knudsen equation [6]:

$$\dot{s}=\beta\sqrt{\frac{m}{2\pi k_B T}}\frac{P_b}{\rho}\exp\left[\frac{mL_v}{k_B}\left(\frac{1}{T_b}-\frac{1}{T}\right)\right], \tag{4}$$

where β is the vaporization coefficient, m is the atomic mass of the target solid material, k_B is the Boltzmann constant, L_v is the latent heat of vaporization of the material, and T_b is the boiling temperature at the pressure P_b, and $P_b = 1.01 \times 10^5$ Pa [23,24].

Note that, in this paper, the ablation depth due to the material phase explosion, under high laser fluence conditions including plasma formation, is not considered. Moreover, the initial and boundary conditions for the current 2D problem are:

$$T(x,z,t)|_{t=0}=T_a, \tag{5}$$

$$\left.\frac{\partial T(x,z,t)}{\partial x}\right|_{x=-l/2}=\left.\frac{\partial T(x,z,t)}{\partial z}\right|_{z=h}=0, \tag{6}$$

$$k\left.\frac{\partial T(x,z,t)}{\partial z}\right|_{z=0}=L_V\rho\dot{s}, \tag{7}$$

where T_a is the room temperature, i.e., $T_a = 300$ K, l and h are, respectively, the length and thickness of the target domain. Eq. (6) represents the adiabatic boundary conditions on both the vertical side and the bottom surfaces, while Eq. (7) represents the heat loss on the top surface of the target material due to vaporization. Such boundary conditions have also been used by Refs. [1,20,21]. Note that the surface radiation to the ambient boundary condition is ignored due to the extreme short duration of the laser pulse. The heat loss due to surface radiation was found to be insignificant, when compared to the heat loss due to material vaporization and heat conduction (see also Ref. [21] for additional discussions).

In what follows, we assume that the uncertainty is associated with absorption coefficient and we provide the gPC representation for the governing equation for the laser heat conduction (see Eq. (1)), in terms of a single random variable ξ, $\alpha=\sum_{i=0}^{P}\alpha_i\psi_i$, where ψ_i denotes the Legendre polynomial basis functions of order i. The first four Legendre polynomials are: $\psi_0(\xi)=1$, $\psi_1(\xi)=\xi$, $\psi_2(\xi)=(3\xi^2-1)/2$, and $\psi_3(\xi)=(5\xi^3-3\xi)/2$ (see Ref. [14] for more details regarding Legendre polynomial basis functions), where ξ denotes all conceivable values within the lower ($\xi_{\min}$) and upper bounds ($\xi_{\max}$) of absorption coefficients at a certain temperature. Furthermore, α_i denotes the coefficients of Legendre polynomials, which represent the projections of absorption coefficients to different polynomial chaos modes. α_i can be obtained using:

$$\alpha_i=\frac{2\int_{\xi_{\min}}^{\xi_{\max}}\xi\psi_i d\xi}{(\xi_{\max}-\xi_{\min})\|\psi_i\|^2}, \tag{8}$$

where $\|\psi_i\|^2$ is the normalization corresponding to the Legendre polynomial of order i and is given by $\|\psi_i\|^2=\frac{2}{2i+1}$. Here, the integral in Eq. (8) is calculated using the trapezoidal rule (the numerical