



# Thermal modeling of chemical vapor deposition on the particle surface subjected to nanosecond laser heating

Quan Peng<sup>a</sup>, Yuwen Zhang<sup>a,b,\*</sup>, Yaling He<sup>a</sup>, Yijin Mao<sup>b</sup>

<sup>a</sup> Key Laboratory of Thermal-Fluid Science and Engineering of MOE, School of Energy and Power Engineering, Xi'an Jiaotong University, Xi'an, Shaanxi 710049, China

<sup>b</sup> Department of Mechanical and Aerospace Engineering, University of Missouri, Columbia, MO 65211, USA

## ARTICLE INFO

### Article history:

Received 27 September 2012

Accepted 14 February 2013

Available online 15 March 2013

### Keywords:

Laser chemical vapor infiltration

Numerical simulation

Heat and mass transfer

Thermal modeling

Integral approximate method

## ABSTRACT

A thermal model of chemical vapor deposition of titanium nitride (TiN) on the spherical particle surface under irradiation by a nanosecond laser pulse is presented in this paper. Heat and mass transfer on a single spherical metal powder particle surface subjected to temporal Gaussian heat flux is investigated analytically. The chemical reaction on the particle surface and the mass transfer in the gas phase are also considered. The surface temperature, thermal penetration depth, and deposited film thickness under different laser fluence, pulse width, initial particle temperature, and particle radius are investigated. The effect of total pressure in the reaction chamber on deposition rate is studied as well. The particle-level model presented in this paper is an important step toward development of multiscale model of LCVI.

© 2013 Elsevier Ltd. All rights reserved.

## 1. Introduction

Gas-phase Solid Freeform Fabrication (SFF) with Laser Chemical Vapor Deposition (LCVD) or Laser Chemical Vapor Infiltration (LCVI) is an emerging manufacturing technology that can directly produce three dimensional (3-D) parts from CAD data [1]. The LCVD/LCVI technique, which based on reactions initiated pyrolytically, photolytically or a combination of both [2], can build functional structure via deposition of solid materials from gas precursors irradiated by a laser beam in an environmentally controlled chamber. In the pyrolytically LCVD/LCVI process, a laser beam locally heats the substrate to create a hot spot where a thermally activated chemical reaction is induced; the resulting product, which is a thin film of material, deposits on the substrate due to chemisorption. In the photolytically LCVD/LCVI process, the laser is tuned to an electric or vibrational level of the gas; the irradiated gaseous substance decomposes and the products stick to the substrate surface to form the thin film. During these two processes, lines can be formed by multiple laser scans and are subsequently interwoven to form a part layer. Consecutive layers can be deposited to create a three-dimensional part according to the CAD design. The most recent LCVD/LCVI advances as reported in various journals and proceedings are well documented by Zhang [3].

While the LCVD technique uses precursors to directly create free-standing part, the LCVI, on the other hand, uses gas precursors and powder particles to build three-dimensional parts, which is similar to other powder-based SFF techniques, such as Selective Laser Sintering (SLS). In the LCVI process, powder particles are bounded together through deposition of solid material on the particle surface by decomposition of gas precursors. During the LCVI process, a thin powder layer (100–250  $\mu\text{m}$  thick) is scanned by laser to form the two-dimensional slice to an underlying solid piece, which consists of a series of stacked two-dimensional slices. A fresh powder layer is spread after laser scanning and the process is repeated. Loose powder is removed after the part is extracted from its bin, and the finished part has a composite structure consisting of starting powder bonded into a matrix of the deposited materials [4]. The advantages of LCVI over LCVD include (a) uninfilted powder provides support for producing overhangs, (b) confining the deposition to thin powder layers provide dimensional control in the direction of growth, and (c) it is possible to tailor local chemistry and microstructures [5]. Much experimental work on LCVI has been conducted and various applications of this new technique have been discovered. Sun et al. [6] fabricated in situ thermocouples into micro-components using LCVI to build the bulk shape. Crocker et al. [7–9] presented LCVI of SiC into metal and ceramic powders to fabricate composite parts.

Accurate prediction and control of LCVI require a thermal model of the process. The physical and chemical phenomena occurred in LCVI are similar to that in LCVD, which has been investigated extensively and detailed works can be found in Refs. [10–14]. The only difference is that deposition occurs on the powder

\* Corresponding author at: Key Laboratory of Thermal Fluid Science and Engineering of MOE, School of Energy and Power Engineering, Xi'an Jiaotong University, Xi'an, Shaanxi 710049, China. Tel.: +1 573 884 6936; fax: +1 573 884 5090.

E-mail address: [zhangyu@missouri.edu](mailto:zhangyu@missouri.edu) (Y. Zhang).

## Nomenclature

$C$	concentration ( $\text{kg/m}^3$ )	$T$	temperature (K)
$D$	mass diffusivity ( $\text{m}^2/\text{s}$ )	$x$	coordinate (m)
$E$	activation energy (J/mol)	Greek symbols	
$k$	thermal conductivity ( $\text{W}/(\text{m}\cdot\text{K})$ )	$\alpha$	thermal diffusivity ( $\text{m}^2/\text{s}$ )
$K'_0$	Arrhenius constant	$\gamma$	sticking coefficient
$K_0$	$(C_{\text{H}_2})_i(C_{\text{N}_2})_i^{1/2}K'_0$ (m/s)	$\delta$	thickness of the deposited film (m)
$M$	molecular weight (g/mol)	$\delta_h$	heat penetration depth (m)
$\dot{m}$	mass flux ( $\text{kg}/\text{m}^2$ )	$\delta_m$	mass penetration depth (m)
$p$	total pressure in the reaction chamber (Pa)	$\theta$	temperature rise ( $T - T_i$ ) ( $^\circ\text{C}$ )
$q''$	heat flux ( $\text{W}/\text{m}^2$ )	$\rho$	density ( $\text{kg}/\text{m}^3$ )
$q''_0$	maximum heat flux ( $\text{W}/\text{m}^2$ )	$\tau$	relative time, $t/t_p$
$r_0$	particle radius (m)	Subscripts	
$R_u$	universal gas constant ( $8.314 \text{ J}/(\text{mol} \cdot \text{K})$ )	$i$	initial
$t$	time (s)	$s$	particle surface
$t_p$	half width of the laser beam pulse at $q''_0/2$ (s)		

particle surface during LCVI, instead of on the top of non-porous flat substrate in LCVD. Laser processing in LCVI is complicated since the irradiated material responds differently from that in the case for a simple, fully dense material. Thermal modeling of the LCVI process requires knowledge about heat and mass transfer in the precursors and the porous powder bed, and chemical reaction on the particle surface. Convective heat transfer in porous material has been extensively investigated in the past and detailed reviews are available in Refs. [15–16]. In addition, radiation heat transfer in the powder bed also plays an important role in thermal analysis due to the high temperature involved. The distinctive feature of heat transfer in the LCVI process is that the porosity is not constant. During the entire process, the porosity may change from a value up to 0.6 to nearly zero.

Dai et al. [17] presented numerical simulation of LCVI using a finite element commercial code ANSYS. The effect of variational porosity on the powder bed properties was taken into account. The density of the powder bed was directly correlated to the temperature and thus the chemical reaction model was not necessary. Dai et al. [18] introduced a finite element model with the same method and the laser power was modified from one time step to the next to ensure that the powder bed temperature was constant. The models in Refs. [17–18] were improved later through incorporating a densification model by infiltration based on experimental growth rate [19].

Compared to LCVD, the efforts on simulation of LCVI are extremely limited at this time. Moreover, most of the existing works on LCVI were conducted on the powder bed level, and mass transfer in the precursors and powder bed was not taking into account in any of them. In this paper, a thermal model will be developed to investigate heat and mass transfer during chemical vapor deposition on the surface of a single powder particle irradiated by a nanosecond laser pulse. The particle surface temperature distribution, thermal penetration depth, and the thickness of deposited film will be obtained through numerical simulation. In addition, the effects of laser fluence and pulse width, particle radius, initial particle temperature, and total pressure in the reaction chamber on the simulation results will also be investigated.

## 2. Physical model

During the LCVI process, the diameter of the particle is much smaller than that of the laser beam, which is in turn much smaller than the dimension of the final part. Since the laser irradiates the powder bed from a distance of several powder-sphere diameters away, a nearly homogeneous distribution of the heat flux within

the penetrated layer can be assumed due to multiple scattering of the radiation [20]. The physical model of LCVI on a single powder particle surface subjected to temporal Gaussian heat flux from a nanosecond pulsed laser beam is illustrated in Fig. 1; a metal powder particle made of Incoloy 800 is surrounded by a mixture of  $\text{H}_2$ ,  $\text{N}_2$ , and  $\text{TiCl}_4$ . Because of symmetry of the spherical particle as well as the assumption of uniform heat flux distribution, the problem can be simplified to be one-dimensional in the  $r$ -direction. The origin of time is chosen to be when the heat flux is at its maximum, thus the time-dependent heat flux is expressed as

$$q''(t) = q''_0 e^{-\ln 2 \frac{t^2}{t_p^2}} \quad (1)$$

where  $q''_0$  is the maximum heat flux, and  $t_p$  is the half-width of the laser pulse at half maximum.

After the onset of the laser pulse, the particle surface temperature raises rapidly due to sensible heat absorption. The vapor deposition starts when the surface temperature reaches the chemical reaction threshold temperature of 1173 K, and the concentration difference resulting from chemical reaction on the particle surface becomes the driving force of mass transfer. The surface heat flux reaches its peak value at the time  $t=0$ , after which the heat flux will decrease. The deposition process finishes when the surface temperature decreases to the threshold temperature. The laser energy absorbed by the particle surface will be distributed to two parts during the chemical reaction: the first part goes into the powder grain through conduction, and the second part is consumed by the chemical reaction [12]. Thus the physical model of the LCVI process includes: heat transfer in the powder particle, chemical reaction on the particle surface, and mass transfer in the gases. After the pulse is off, the internal temperature distribution of the particle will be uniform well before the next laser pulse is launched. Consequently, the whole process can be modeled as a recurrence of the two stages by using the uniform temperature from the previous pulse as the initial condition in the preheating stage of the next pulse [21]. All physical properties of the materials, such as density, conductivity and so on, are independent of temperature and pressure during the whole process.

### 2.1. Governing equations for heat transfer in the powder particle

The heat transfer within the powder particle can be described as a pure conduction problem. The heat conduction equation within the particle is

Download English Version:

<https://daneshyari.com/en/article/7058953>

Download Persian Version:

<https://daneshyari.com/article/7058953>

[Daneshyari.com](https://daneshyari.com)