A Mathematical Model for Process Control in Laser Chemical Vapor Deposition

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ABSTRACT

Laser chemical vapor deposition is a free form technique capable of producing high aspect ratio microstructures of arbitrary shape. The process does not yet have a high resolution required for microfabrication. For this study, we develop a mathematical model that can be used for predicting the scanning pattern of the laser beam on the surface of deposit in order to produce a microstructure with the desired geometry. We demonstrate the applicability of the model by simulating the deposition of a concave microlens using nickel on a graphite substrate.

Keywords: Chemical vapor deposition, mathematical model.

1 INTRODUCTION

Microtechnology is a critical technology with an enormous potential for new products and product enhancement. Current micromanufacturing techniques have some drawbacks in that the microstructures produced are planar, somewhat fragile, and not suitable for building robust three-dimensional structures. For further development of the technology, it is necessary to develop new processes suitable for the manufacture of high aspect ratio microstructures. High aspect ratio microstructures improve the rigidity of microparts and allow coupling to them thus enabling the manufacture of complex mechanisms such as microactuators, and micromotors. Among the new techniques for free-form production of high aspect ratio microstructures is laser chemical vapor deposition (LCVD). The LCVD process is capable of producing high aspect ratio microstructures of arbitrary shape and is rapid, flexible, and relatively inexpensive to operate. The process does not yet have the high resolution required for microfabrication. Part of the problem is not knowing how to scan the surface in order to produce a microstructure conforming to a desired geometry with accuracy. To achieve a process with high resolution, accurate predictive models must be developed for process control and optimization.

In this work, we develop a mathematical model for predicting the scanning pattern of the laser beam on the surface of deposit in order to produce accurate microstructures with the desired geometry. Work on simulating solid deposition using laser chemical vapor has included solid deposition at a focal spot or direct writing of lines [1,2,3,4]. The present model is the first attempt at predicting the laser pixel dwell time on the surface to be scanned in order to deposit a solid conforming to a pre-specified geometry.

2 MATHEMATICAL MODEL

The governing equations which describe the heat flow through the deposit and substrate are the heat conduction equations:

$$C_D\rho_D\frac{fT^D}{ft}=\frac{f}{fx}(K_D\frac{fT^D}{fx})+\frac{f}{fy}(K_D\frac{fT^D}{fy})+\frac{f}{fz}(K_D\frac{fT^D}{fz})+Q_{in} \quad (1)$$

$$C_S\rho_S\frac{fT^S}{ft}=\frac{f}{fx}(K_S\frac{fT^S}{fx})+\frac{f}{fy}(K_S\frac{fT^S}{fy})+\frac{f}{fz}(K_S\frac{fT^S}{fz}) \quad (2)$$

where T_D and T_S are the temperatures of the deposit and substrate, respectively. Q_{in} is the heat source at or within the deposit boundaries due to absorption of the laser light. Also, c_D, c_S, ρ_D, ρ_S, K_D and K_S are the specific heat, mass densities, and conductivities of the deposit and substrate, respectively. The interfacial equations between the deposit and substrate are

$$T^D(x,y,0,t)=T^S(x,y,0,t) \quad \text{and}$$
$$K_D\frac{fT^D(x,y,0,t)}{fz}=K_S\frac{fT^S(x,y,0,t)}{fz} \quad (3)$$

On the surface of the deposit,

$$-K_D\frac{fT^D}{fz}=J_{loss},\ z=h_0(x,y) \quad (4)$$

where J_{loss} describes the energy loss to the gas phase at $z=h_0(x,y)$. Likewise, at the interface between deposit

and substrate, $J_{loss}(z=0) = K_S \frac{fT^S}{fz}$.

From the Arrhenius equation, one may express the local growth, $\Delta\vec{z}$, at a point on the surface of deposition during a time increment Δt as

$$\Delta\vec{z}_n(x,y) = K_0 e^{-\frac{E_a}{RT^D}} \hat{n}(x,y)\Delta t \qquad (5)$$

where K_0 is a rate constant, T^D is the surface temperature, E_a and R are the activation energy and the universal gas constant, respectively. Here, $\vec{n}(x,y)$ is the unit outward normal vector on the deposit surface, $z = h_0(x,y)$,

$$\vec{n}(x,y) = \frac{1}{\varphi}[-\frac{fh_0}{fx}\hat{x} - \frac{fh_0}{fy}\hat{y} + \hat{z}],$$

$$\varphi = \sqrt{1 + (\frac{fh_0}{fx})^2 + (\frac{fh_0}{fy})^2}$$

where $\hat{x}$, $\hat{y}$ and $\hat{z}$ are the unit vectors on the x, y, z coordinates, respectively.

Equations (1)-(5) are used to predict the scanning pattern of the laser beam on the surface of the deposit. One may consider obtaining a microstructure with a pre-specified geometry by depositing a solid layer by layer.

Let $z = h_0(x,y)$ and $z = h_1(x,y)$ be two consecutive layers of deposition, where $z = h_0(x,y)$ and $z = h_1(x,y)$ are the deposited layer and the next layer to be deposited, respectively. We wish to determine the laser beam dwell time at each point on the surface of deposit $z = h_0(x,y)$ in order to obtain the next surface $z = h_1(x,y)$.

We decompose the total region into a number of small subelements, $\Delta_{i,j}$, $i = 1,...,M$ and $j = 1,...,N$. We assume that temperatures are the same everywhere in each subelement $\Delta_{i,j}$. Let $\Delta t_{i,j}$ be the time duration where the laser beam is focused in subelement $\Delta_{i,j}$ and let the temperature at subelement $\Delta_{p,q}$ be $T^D_{i,j}(x_p, y_q, h_0(x_p, y_q))$ when the laser beam is focused in subelement $\Delta_{i,j}$. Here, (x_p,y_q) is the center of $\Delta_{p,q}$, and we assume that the temperature is at steady state (in this process, steady state is reached quite rapidly [3]). Thus, the laser beam dwell time at each subelement can be obtained by solving the following linear system:

$$\sum_{i=1}^{M}\sum_{j=1}^{N} K_0 e^{\frac{-E_a}{RT^D_{i,j}(x_p,y_q,h_0(x_p,y))}} \Delta t_{i,j} = \left|\Delta\vec{z}_n(x_p, y_q)\right|,$$

$$p = 1,...,M \ , q = 1,...,N \qquad (6)$$

In principle, the temperature distribution, T^D, on the surface of $z = h_0(x,y)$ can be obtained by solving Eqs. (1)-(4) in the steady state case. For the solution, we ignore heat loss to the gas phase, and at the interface (z=0), we let

$$J_{loss}(z=0) = K_S \frac{fT^S}{fz}$$

The laser light was assumed to have a Gaussian distribution and to be totally absorbed within the deposit. Hence, at (x,y)

$$\int_0^{h_0} Q_{in}\, dz = \frac{P_0(1-\Gamma(\phi))}{2\pi\sigma^2} e^{-\frac{(x-x_i)^2+(y-y_i)^2}{2\sigma^2}} (\hat{z},\hat{n})_{(x,y)}$$

where P_0 is the laser intensity, σ is the standard deviation of the intensity distribution of the laser beam, and $\langle\vec{z},\vec{n}\rangle$ is the inner product of $\vec{z}$ and $\vec{n}$. Here, Γ(ϕ) is the angular spectral reflectance defined by [4]:

$$\Gamma(\phi) = \frac{1}{2}\left[\frac{\cos\phi - \sqrt{n_i^2 - \sin^2\phi}}{\cos\phi + \sqrt{n_i^2 - \sin^2\phi}}\right]^2 + \left[\frac{n_i^2\cos\phi - \sqrt{n_i^2 - \sin^2\phi}}{n_i^2\cos\phi + \sqrt{n_i^2 - \sin^2\phi}}\right]^2$$

where n_i is the deposit index of the refraction and ϕ is the local incidence angle.

Thus, for obtaining the laser beam dwell time at each point on the surface of $z = h_0(x,y)$ in order to obtain the next deposited layer $z = h_1(x,y)$, one may calculate $T^D_{i,j}$ in equation (6) from the heat equations. With $T^D_{i,j}$ and the distance along the normal vector between the two layers $z = h_0(x,y)$ and $z = h_1(x,y)$ known, one can solve the linear system in (6) to obtain the dwell time $\Delta t_{i,j}$'s. A micro-object with a pre-specified geometry can then be obtained by repeating the process layer by layer.

3 NUMERICAL EXAMPLE

We use the model to calculate the dwell times for manufacturing a concave microlens from nickel deposited on graphite. Parameters used in the calculation are listed in Table 1.

We chose 40 × 40 subelements (or pixels) on the xy-surface of the substrate. Also, a mesh of $40 \times 40 \times 40$ was chosen for the substrate. The solution for the temperature was obtained when $\left|\frac{T_S^{(n+1)} - T_S^{(n)}}{T_S^{(n)}}\right| \le 1.0 \leftarrow 10^{-2}$ was satisfied.

This solution was obtained on a Sun workstation using the Jacobi iteration method. Eq. (6) was solved for the dwell times using the Gauss-Seidel iteration method.

Figure 1 shows a concave microlens resulting from 20 layers of deposition. Figure 2 presents the total corresponding dwell times for 20 layers. As expected, dwell times agree with the deposit shape in Figure 1.

Parameter	Value
E_a	$9.4 \leftarrow 10^4 (J/mol)$
R	$8.314 (J/mol\,?K)$
K_0	$1.37 \leftarrow 10^4 (mm/\sec)$
K_D	$6.55 \leftarrow 10^{-2} (W/mm\,?K)$
K_S	$1.7 \leftarrow 10^{-3} (W/mm\,?K)$
$T_\times$	$475 (K)$
P_0	$0.10 (W)$
σ	$0.0005 (mm)$
n_i	3.95

Table 1. Values for parameters used in the numerical example

Figure 3 presents the change in the maximum and minimum temperatures at the surface with layers of deposit. It is seen that the temperature decreases with an increase in the number of layers or thickness of the deposit. This is as expected since nickel has a higher heat conductivity than graphite. This result indicates that as the thickness of the deposit increases the surface temperature decreases to the point where no growth may be possible. As such, it may become necessary to increase the laser intensity with an increase in the number of layers or deposit thickness.

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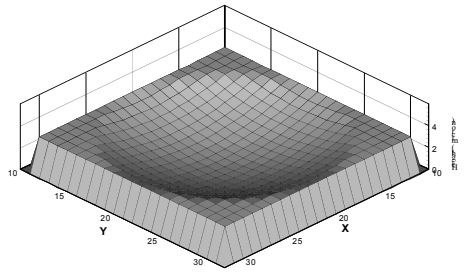

Figure 1: A concave microlens resulting from 20 layers of deposit. The height of the microlens is 1 micron at the center and 3 microns at the edge.

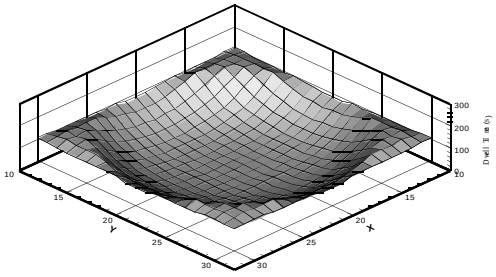

Figure 2: Total dwell time for each pixel on the x-y surface that corresponds to the concave microlens in Figure 1.

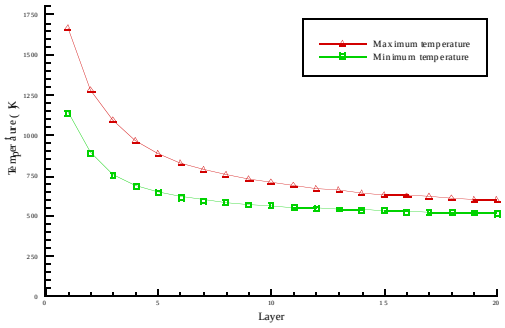

Figure 3: Change in the maximum and minimum surface temperatures over layers.