Efficient Pocketing Simulation Model for Solid State Laser Micromachining and its Application to a Sol-gel Material

A.I. Onischenko, D.S. George, A.S. Holmes, Optical & Semiconductor Devices Group, Department of Electrical & Electronic Engineering, Imperial College London, Exhibition Road, London, SW7 2BT, United Kingdom; F. Otte, Laser Zentrum Hannover, Germany

ABSTRACT

Laser ablation using diode pumped solid state lasers shows great potential for a wide range of micromachining applications. We have been using a frequency quadrupled Nd:VO₄ laser (266 nm wavelength), with a pulse duration < 30 ns, to ablate a sol-gel Ormocer material. With a pulse energy of around 20 µJ, and a focal spot of the order of 10 µm diameter, single pulses were found to produce craters a few microns in depth and ~10 µm in diameter. A study of the variation of the crater profile with pulse energy and angle of incidence to the surface has enabled the development of an efficient method to simulate the ablation for a series of consecutive shots constituting a toolpath. Multiple pulses with varying degrees of overlap were simulated, and compared with experiment. Results show that the model accurately predicts the profiles of trenches and pocketed surfaces given parameters obtained from a single crater machined at normal incidence. The “self calibrating” feature of our approach significantly reduces the number of input parameters required for adequate simulations. In particular, it does not require knowledge of the beam profile or material ablation curve. The simplicity and practicality of the method make it promising for use in an industrial environment.

Keywords: Laser ablation; laser micromachining; diode pumped solid state laser; simulation; sol-gel

1. INTRODUCTION

Laser ablation for micromachining applications is a highly promising technique. Diode pumped solid state lasers (DPSSL) have recently been employed for this purpose due to the fact they are compact, powerful sources with high efficiency and good beam quality. Direct laser writing with a focussed beam has advantages especially for prototyping and complex 3D structures, being fast with direct transfer from computer to the work-piece, and not requiring an expensive mask. The features of DPSSL systems allow a high level of CAD integration which is instrumental in exploiting all the benefits of the DPSSL for micro-fabrication. The CAD integration dramatically improves flexibility and complexity of the 3D structure design. An adequate modelling of the ablation process is a key part of such integration. However, use of the DPSSL for fabrication of the 3D structures also imposes different challenges and more strict constraints in comparison with conventional laser material processing using broad area beams and masks.

Optimization of the traditional operations like cutting, drilling or surface cleaning usually requires modelling of general ablation parameters such as ablation threshold or, more generally the ablation curve. To date the majority of theoretical studies have been focussed on understanding how these fundamental characteristics of the ablation process are determined by physical mechanisms of the material decomposition and mass removal, heat transfer, plume/plasma effects, re-deposition, details of the solid/liquid phase transition, etc. Due to the relatively simple geometry of the heat transfer problem considered in relation to the traditional laser processing operations it is usually solved by means of various semi-analytical methods. Recently several attempts to introduce more universal methods for heat transfer simulations based on the finite difference \(^1\)\(^2\) and control-volume \(^3\) approaches have been made. More fundamental aspects of material mass removal are usually analysed by means of molecular dynamic (MD) methods\(^4\)+\(^6\).

Since in DPSSL systems CAD will be tightly imbedded into the fabrication process, modelling must be efficient and take a reasonable simulation time (of the order of minutes) on a mainstream computer. Recent research has shown that the conventional modelling methods of the laser processing yield simulation times of the order of days (if not weeks) \(^7\). Both heat transfer and MD simulations require substantial time and computational resources and, at the moment, are suitable mainly for general academic research.
The main objective of DPSSL ablation simulations is to predict a tool path of the laser beam for a given 3D design. The structure is created then by a series of laser pulses according to the tool path. In this case, optimisation must guarantee that the real structure size and shape are close enough to the intended design. The key feature of this class of fabrication process is the cumulative effect of the individual laser shots. An adequate model of the effect is central for understanding and optimisation while the physical processes mentioned above still play an important role. The modelling also has to allow for fine tuning of the simulation parameters within each material class since there is a growing demand for hybrid or designer materials with widely varying parameters, such as sol-gel for example. At the same time simulations have to provide quantitative accuracy. Thus, the model needs a consistent mechanism for adjustment from experimental feedback.

The advanced capabilities of DPSSL fabrication systems and especially the key role of CAD simulations require new modelling approaches that would meet the mentioned requirements. In this paper we present a phenomenological simulation method for predictive tool path generation. The method implements a consistent algorithm for self-calibrating the simulation parameters from experimental data resulting from ablation processing development. We report our recommendations on the minimal set of data that provides a parameter calibration suitable for quantitative modelling of the 3D structure ablation and, as an ultimate goal, predictive tool path simulation.

2. PHENOMENOLOGICAL MODELS OF LASER ABLATION

Direct writing by a DPSSL creates structures by superposing focused laser pulses with various degrees of spatial and temporal overlap. Modelling of the process requires consideration of two key problems: (1) simulation of the shape and size of individual craters produced by the laser pulses with given spatial and temporal characteristics and (2) simulation of cumulative superposition of the craters on the work piece or, in other words, how the individual craters interfere at the material surface.

The starting point for our modelling method requires calculation of the single crater shape. Predictive modelling can be justified if the laser ablation creates the surface morphology in a “controlled manner”, i.e. when the laser pulses produce craters with repeatable and quantifiable characteristics. If the laser ablation causes material cracks or other stochastic surface features then the use of the particular ablation method for the particular material is questionable. Modelling in that case has different goals exceeding the scope of the methods described here. The modelling approach described in this work is most effective when the crater depth is less than its lateral size - the “shallow crater regime”. Modelling of the “deep crater regime” is more similar to traditional drilling and can use the conventional methods developed for that operation.

The most common way of describing the ablation process in phenomenological terms is based on the concept of the ablation curve (AC), which describes the dependence of the ablation depth on the laser fluence. This approach seems to be the best framework for developing an efficient and practical simulator for tool path optimisation. However, the AC was originally defined for the case of almost uniform fluence associated with excimer laser processing. In the case of ablation by DPSSL lasers the fluence profile is a major feature and the AC concept might need to be revised. For excimer systems the ablation curve is defined as the depth of the ablation, $h$ (usually along $z$ direction, normal to the surface) versus uniform fluence, $F$. In DPSSL systems material is ablated by a focussed beam with a diameter typically around 10µm. The laser pulse produces a crater $z(x, y)$ rather than uniform subsidence, $h$, of the material surface. In the most general case the dependence between them can be very complex – integral, for example, dependent on many factors such as heat diffusion, etc. The central assumption of our approach is that the crater depth at a given point $z(x_1, y_1)$ depends on the fluence value, $F(x_1, y_1)$, at this point only. Such a local dependence approximation (LDA) can be expressed mathematically as:

$$z(x_1, y_1) = h(F(x_1, y_1))$$ (1)
In this case the crater profile, \( z(x, y) \), can be modelled as a “projection” of the fluence profile, \( F(x, y) \) via a traditionally defined ablation curve, \( h(F) \). As will be shown below, for the materials investigated in this work simulations based on the LDA provide close agreement with experiment.

<table>
<thead>
<tr>
<th>Ablation Model</th>
<th>Expression, ( h(F) )</th>
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<tbody>
<tr>
<td>Logarithmic</td>
<td>( \frac{1}{\alpha} \ln\left(\frac{F}{F_{th}}\right) ) for ( F_{th} &lt; F )</td>
</tr>
<tr>
<td>Polynomial</td>
<td>( \frac{1}{\alpha} \left(\frac{F}{F_{th}} - 1\right)^{n} ) for ( F_{th} &lt; F )</td>
</tr>
<tr>
<td>Exponential</td>
<td>( \frac{1}{\alpha} \exp\left( -\gamma \ln\left(\frac{F}{F_{th}}\right) \right) ) for ( F_{th} &lt; F )</td>
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</table>

Table I summarizes the most common ablation curve models discussed in the literature. \( F_{th}[\text{Jcm}^{-2}] \) is the threshold fluence, \( \alpha[\text{cm}^{-1}] \) is the absorption coefficient, and \( n, \gamma \) are dimensionless parameters.

The most common AC model is logarithmic, sometimes called “Beer’s” model (see, for instance, ref. [7]). However, it might be confusing since Beer’s law just describes light absorption in a material and leads to the logarithmic ablation curve model only in the case of certain approximations about the ablation process. We have shown that in the framework of the moving ablation front approach, the same Beer’s law for absorption can lead to a linear AC as well [8]. The linear model [7] can be considered as an instance of the more general polynomial model [9] with \( n=1 \). The exponential model was proposed in reference [10] to explain AC saturation at high fluence values in polymer materials.

The majority of the DPSSL systems are expected to have Gaussian beams in which case the fluence shape should have a form:

\[
F(x, y) = F_{pk} \cdot \exp\left[ -2 \left( \frac{2x}{w_x} \right)^2 + \left( \frac{2y}{w_y} \right)^2 \right]
\]

(2)

where \( F_{pk} \) is the peak fluence; the \( z \) axis of the coordinate system is chosen to be perpendicular to the material surface. \( w_x, w_y \) are the Gaussian beam diameters in the \( x \) and \( y \) direction respectively. In reality, however, the beam shape is often truncated or otherwise distorted and so for practical simulations a choice of other shapes for \( F(x, y) \) might be required. Airy or 2D sinc functions are appropriate choices if the collimated beam is flattened. Uniform fluence of elliptical or rectangular shape can be used for modelling of the deep crater regime.

The central problem of DPSSL ablation modelling is the calculation of crater superposition caused by multiple laser pulses. Since the majority of the pulses are applied to the already pre-processed surface, the crater formation can be affected by previous laser shots. The most obvious factors are the surface morphology and possible residual heat in the Heat Affected Zone (HAZ) and/or material modification due to that heat. If the surface morphology has weak influence on the individual crater formation then the “flat” surface crater can be linearly added to the surface. The degree of influence of surface structure on the crater formation can be estimated from analysis of the relation between size and shape of the craters for normal incident pulses and pulses at angled incidence. In a recent study of angle dependence [4] we have shown that, for certain sol-gel and polymer materials, the crater shape under angled ablation can be constructed from the normal incidence crater by a simple coordinate transformation combining a shear and a rotation. This is
illustrated in Figure 1, where the solid line is the crater profile at normal incidence, the dashed line is the crater profile at 60 degrees, and the crosses represent the fit obtained by transforming the normal incident crater. The close match to the observed crater profile implies that the angular dependence of the ablation depth along the direction of the incident laser beam is negligible in this case. Due to this fact, and in combination with LDA, the surface propagation can be modelled as a superposition of the individual flat surface craters.

The superposition however can be affected by another important factor: the residual heat left by the previous laser shots. If the time between pulses is sufficiently short then the material at each successive ablation site will be preheated and the AC parameters could differ from their “cold” values. Heating can also cause a permanent material modification in the HAZ. Taking into account such “thermal memory” effects has two aspects: (1) identifying a measurable parameter of the degree of the laser shot overlap that would be convenient for calculations and feasible physically; (2) modification of the AC models to include the overlap parameter. The modified AC model would also have additional phenomenological constants, $a_1, a_2, a_3, \ldots$ reflecting the specific form of the thermal effects.

A convenient overlap parameter, $d$, is the distance between the point $(x, y)$ of the calculated crater and a centre of the previous crater $(X_0, Y_0)$:

$$d = \left( (x - X_0)^2 + (y - Y_0)^2 \right)^{1/2}$$

In the case of the logarithmic AC, the thermal memory effects are most likely to change $F_{th}$ rather than $\alpha$ and, thus, the modified AC is:

$$h(x, y) = \frac{1}{\alpha} \ln \left( \frac{F(x, y)}{F_{th}(d, \{a_i\})} \right)$$

The explicit form for $F_{th}(d, \{a_i\})$ could be the subject for extensive research in its own right. This however exceeds the scope of this paper. In our simulation we used the Gaussian type:

$$F(d, \{a_i\})_{hh} = F_{th}\left( 1 - a_1 \exp\left( -\frac{d^2}{a_2^2} \right) \right)$$
where $F_{0,th}$ is the “cold” threshold fluence, $0 < a_1 < 1$ is the first fitting parameter, and $a_2 [\mu m]$ is the second fitting parameter.

3. IMPLEMENTATION OF THE NUMERICAL ALGORITHM

The method was implemented as a plug-in module for AlphaCAM (Licom Ltd) computer-aided design software. The module has a VBA interface for parameter input with a C/C++ DLL mathematical engine. The results were visualized by the native AlphaCAM API.

Any predictive simulation based on a phenomenological approach is only useful if the model parameters are known a priori or can be derived in a way much easier than actual trial ablation of the complete structures. The accuracy of the parameter values has to be adequate for quantitative modelling. Ideally parameters of the models should be calibrated from ablation of relatively simple shapes like a series of single shot craters, for instance. For all our simulations fitting of the single crater profile was used for calibration of the AC parameters. To find the best fit each model was tried in turn. An initial tool path for the intended structure was generated by standard tools of AlphaCAM. The tool path was converted into a laser shot map by setting the feed rate of the scanner and the laser repetition rate. The resulting simulated surface was compared with the intended design. The tool path, feed rate and repetition rate were modified until the simulated shape replicated the design.

4. RESULTS AND DISCUSSION

To test our approach we fabricated a number of shot lines with various degree of overlap. We then modelled trenches formed by superposition of single craters on a flat surface. A typical shot map test pattern is shown in Figure 2.

![Figure 2: Typical Shot Maps](image)

The experimental setup used for this investigation is shown in Figure 3. The laser system produced 266 nm (frequency quadrupled Nd:VO4) Q switched pulses < 40 ns in duration, with a pulse energy ranging from 10 to 100 µJ measured at the laser. It had an $M^2$ value < 1.3, beam divergence < 0.3 mrad, diameter ~ 2.5 mm, and polarisation >100:1 horizontal. The repetition rate was varied from 1 kHz to 100 kHz, but for most measurements was set to 20 kHz. The laser output was expanded X3 and stopped down with an iris of about 7 mm diameter. After the scanning mirror, the beam was focussed down using an f0 lens (f=160 mm). The spot size was approximately 10 µm diameter and depth of focus ~ 350 µm. Single craters and overlapped structures were formed using different pulse energies, repetition rates and scan speeds.
The samples were measured with a Zygo New View 200 surface profiler, based on scanning white light interferometry. In addition SEM images of the samples were analysed to provide more information about the surface detail and crater characteristics. To improve image quality the samples were coated with a very thin layer of gold. The samples consisted of thin (~ 100 µm) films of the Sol-gel material (Ormocer 4) deposited on a borofloat glass. The craters had a maximum depth up to ~ 3 µm. The sol-gel appears to have a rough surface after ablation, particularly at pulse energies in excess of 30 µJ. It also became cracked at higher energies. The porous surface may be due to local absorption by organic groups causing highly concentrated ablation points in the hybrid material. The process at lower energies appeared more predictable, and therefore these surface profiles were analysed below.

Figure 4 shows the experimental single crater on a flat surface fitted with the Gaussian fluence profile and logarithmic type of AC.

The model parameters derived from the fit in Figure 4 were:
The single crater parameters were then used to simulate a number of trenches with various crater separations, which were then compared with actual fabricated trenches. These are shown in Figures 5, 6 and 7 for single crater centre-centre separations of 10, 5, and 1.8 μm respectively. Picture sets a) and b) in Figures 5 - 7 show the side views and end views of the trenches respectively. In all figures the simulated trench is shown as a grey mesh and for comparison the experimental measured trench is superimposed as a black mesh. Each mesh is a 2-D view constructed by overlaying cross-sections taken at different positions across or along the trench structure.

For parts a) and b) of each figure the simulations consistently predicted smaller trenches than those observed experimentally (grey mesh is shallower than black mesh). The difference increases with the increase of the crater overlap suggesting the importance of thermal memory effects in sol-gel ablation.

The exponential model for the “hot” threshold fluence, based on eq.(5) with the parameters $a_1 = 0.65$ and $a_2 = 8\mu m$, accurately corrects the above differences, as illustrated by sets c) and d) in Figures 5 – 7. The same values of the parameters $a_1$ and $a_2$ have been used to fit all trenches.

![Figure 5: Cross-sections of a trench formed by equidistant craters with a separation of 10 μm in sol-gel material: Black mesh – experimental data, grey mesh – modelling. Simulations in (a), (b) are with no thermal effects; (c), (d) are with thermal effects](image-url)
Figure 6: Cross-sections of a trench formed by equidistant craters with a separation of 5 µm in sol-gel material: Black mesh – experimental data, grey mesh – modelling. Simulations in (a), (b) are with no thermal effects; (c), (d) are with thermal effects.

Figure 7: Cross-sections of a trench formed by equidistant craters with a separation of 1.8 µm in sol-gel material: Black mesh – experimental data, grey mesh – modelling. Simulations in (a), (b) are with no thermal effects; (c), (d) are with thermal effects.

To test the method further we simulated a simple square pocket. The modelling parameters were calibrated by fitting a number of trenches as described above. The simulated and real pockets are compared in the Figure 8. The simulation has accurately predicted the size and depth (~35 µm) of the pocket.
4. CONCLUSION

We have proposed a quantitative method for laser ablation simulation by means of DPSSL systems. The method is based on the phenomenological approach and is sufficient to assist computer generation of the tool paths for practical 3D structures. The accuracy of the method relies on the adequate knowledge of the simulation constants. The method allows calibration of the phenomenological constants by fitting of a crater formed by a single laser shot on a flat surface. Our experimental results demonstrate that, in the correct operating regime, the complete structure can be modelled as a superposition of single shot craters. We have tested the method by ablating 3D structures in a sol-gel (Ormocer 4) by 40 ns pulses at 266nm. The structures show close agreement with the modelled prototypes. The method provides the best results for “shallow” crater ablation, when the maximal depth of a single shot crater is less than its characteristic diameter.

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