Experimental and modelling investigations into the laser ablation with picosecond pulses at second harmonics

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ABSTRACT

Ablation threshold experiments on various materials are carried out using a picosecond laser generating second harmonic radiation in air at atmospheric pressure. Various materials are investigated which vary according to their different electronic band gap structure and include: silicon, fine grain polycrystalline diamond, copper, steel and tungsten carbide. Through the use of scanning electron microscopy and 3D confocal microscopy, the crater depth and diameter are determined and a correlation is found. The ablation thresholds are given for the aforementioned materials and compared with recent literature results. Picosecond laser-material interactions are modelled using the two-temperature model, simulated and compared with experimental results for metallic materials. An extension of the two-temperature model to semiconducting and insulating materials is discussed. This alternative model uses multiple rate equations to describe the transient free electron density. Additionally, a set of coupled ordinary differential equations describes the processes of multiphoton excitation, inverse bremsstrahlung, and collisional excitation. The resulting electron density distribution can be used as an input for an electron density dependent two-temperature model. This multiple rate equation model is a generic and fast model, which provides important information like ablation threshold, ablation depth and optical properties.

Keywords: ablation threshold, picosecond pulses, modeling, two-temperature model, multiple rate equations, band gap, simulation

1. INTRODUCTION

The choice of the best process parameters and accordingly the most efficient results during laser microprocessing are facilitated by understanding the physical interactions between light and matter. Investigating damage and ablation thresholds is a good way to understand these interactions and consequently, achieve efficient fabrication, since it is possible to determine the minimal laser energetic parameters. Even though the definitions of surface damage, bulk damage and damage threshold are described in ISO 21254-1, there is still an obstacle on experiments with determining ablation thresholds. The quasi-standard for determining the ablation threshold is according to the dependence of the squared crater diameter $D^2$ on the radius $w_0$ and peak fluence $\phi_0$ of the impeding laser beam:

$$D^2 = 2w_0^2 \ln \left( \frac{\phi_0}{\phi_{th}} \right) \text{ where } \phi_0 = \frac{2E_0}{\pi w_0^2}$$

Craters are generated according to various laser parameters and the peak threshold fluence $\phi_{th}$ is determined by setting the squared crater diameter to zero. It must be ensured that the threshold is determined for a peak fluence $\phi_0$ which in fact results in ablation, which in this paper is defined as a measurable ablation depth or crater diameter by confocal microscopy. Extensive variations in the crater’s morphology can be observed depending on the laser parameters resulting in behaviors which magnify the task to search for explanations and understanding. The appearance of surface ripples, residual thermal effects and different ablation phases are some of the features which add to the vague definition of the ablation threshold and misrepresent the measurements of the craters diameter.

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Furthermore, the ablation threshold varies according to focal spot size [1], wavelength [2], polarization state [3] and number of pulses [4], whereby thermal accumulations of the latter play an important role. Nevertheless, this approach is utilized extensively in the femtosecond [5] and picosecond [6] time regimes.

For the aforementioned reasons, the most comprehensive method to determine ablation thresholds and later on morphology is to make a correlation between experiments and simulation. Here, a focus is put on the picosecond time regime, i.e. $\tau_p = 10$ ps. This pulse duration marks the time period when electrons start to relax and conduct energy into the lattice, however, the electrons do not reach thermal equilibrium with the lattice. It is challenging to determine when electron-phonon coupling commences and how severe of a role it plays in terms of workpiece quality. This difficulty in understanding is further exacerbate for dielectric materials due to the presence of a bandgap and transparency. The instance when electrons start to relax followed by electron-phonon coupling for metals is well known and for steel as an example, starts at $\tau_p = 0.5$ ps [7]. Modelling of picosecond pulses is typically approached using the two-temperature scheme. Solving the models however vary, in which using a hybrid finite-difference and molecular dynamic is suggested by [8], while [9] suggests using a purely numerical approach. This paper intends to bring deeper insight to understand the picosecond time regime, both through experiments of ablation thresholds and through simulation of material removal. The model will put special emphasis on the difference between dielectric and metallic materials, such that suggestions of how to extend the model to accommodate dielectrics is presented.

2. METHODOLOGY

2.1 Materials

The materials investigated within the scope of this paper vary considerably according to the value of their bandgap, composition and surface roughness. A table of specifications of the materials is given in Table 1.

<table>
<thead>
<tr>
<th>Material</th>
<th>At % composition</th>
<th>Surface quality, $R_s$</th>
<th>Bandgap, $E_g$</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fine grained polycrystalline diamond (PCD)</td>
<td>C92.8 O5.5 Co1.0 W0.7</td>
<td>20 nm</td>
<td>0 eV (grains 5.5 eV)</td>
<td>From company Diamond Innovations</td>
</tr>
<tr>
<td>Silicon (Si)</td>
<td>Si100</td>
<td>20 nm</td>
<td>1.1 eV</td>
<td>Crystal orientation &lt;100&gt;</td>
</tr>
<tr>
<td>Copper (Cu)</td>
<td>Cu100</td>
<td>28 nm</td>
<td>0 eV</td>
<td>n/a</td>
</tr>
<tr>
<td>Steel (Fe)</td>
<td>C6 Fe63.8 Ni9.9 Si2.3 Cr 18</td>
<td>280 nm</td>
<td>0 eV</td>
<td>n/a</td>
</tr>
<tr>
<td>Tungsten carbide (WC)</td>
<td>C22.9 O19.9 Co7.9 W49.3</td>
<td>237 nm</td>
<td>0 eV</td>
<td>From company Diamond Innovations</td>
</tr>
</tbody>
</table>

Surface topography is measured using a confocal microscope at a 50×, 0.9NA objective. Afterwards, surface roughness is determined by averaging four profile measurements. The composition of each sample is determined by energy-dispersive X-ray spectroscopy (EDX) measurements.

2.2 Experimental

The focused laser beam is characterized according to its size, polarization state and power. To characterize the focused laser beam diameter, a beam analysis CCD camera is used. To characterize the polarization state, a free-space polarimeter is used whereby a $\lambda/2$ and $\lambda/4$ plate allows for exact setting of the polarization state. To characterize the power, a highly sensitive thermopile sensor is used. The sensor has a measurement range from 15 $\mu$W to 3 W with an accuracy of $\pm 3\%$. The picosecond laser system exhibits a MOPA laser architecture and outputs linear polarization at fundamental harmonics which can be frequency doubled and tripled. Details of the laser system and the utilized laser parameters are given in Table 2.