Lasers in Manufacturing Conference 2015

Crater shape dependence on pulse duration in crystalline silicon generated using an IR Gaussian laser beam: from femtosecond to microsecond regime

Stefano Buratin[a], Carol Kong[a,*]

[a]University of Birmingham,Birmingham, B15 2TT, United Kingdom

Abstract

Semiconductor micromachining is one of the most common industrial applications where laser has been used in the last few years. Laser ablation is widely applied in the microelectronic field and in the photovoltaic industry. These two applications typically require a non-contact method for welding, cutting and scribing and the laser is one of the most suitable solutions for them. The prediction of the crater shape is a relevant issue due to the surface requirements of these processes. Semiconductors are also very interesting to study in the infrared due to their electromagnetic penetration that is strongly dependent on the wavelength, because of the material band gap. At the same time the physical proprieties of semiconductors, in particular the thermal ones, are likely to affect the final crater shape. The dependence of final crater shape on the laser pulse duration is relevant in laser material processing because different phenomena occur at different time regimes; this is why a systematic study of the crater shape, depending on the pulse duration, has been carried out. Four different temporal regimes have been studied. In femtosecond regime, a 330 fs laser has been used, with central wavelength at 1032 nm with energies below 10 µJ per pulse. In the picosecond regime, a 10 ps laser has been used, with central wavelength at 1064 nm with energies below 200 µJ per pulse. In nanosecond regime, the range between 9 ns and 220 ns has been used, with central wavelength at 1064 nm with energies below 1.1 mJ per pulse. In microsecond regime, the range between 2µs ns and 20 µs has been used, with central wavelength at 1064 nm with energies below 1.6mJ regime. Different fitting functions have been suggested for the different crater shapes depending on the phenomena involved in the ablation process, considering the different pulse durations.

"Keywords:pulse duration; energy beam; ablation; surface shape."

* Corresponding author. Tel.: +00 0121 4147133.
E-mail address: C.Kong@bham.ac.uk.

1. Introduction

Since the laser has been introduced in the manufacturing process the laser material interaction models have been used to identify and explain the various phenomena which occur in laser material interaction (Bogaerts et al. 2003). It has been possible to identify the dominant role of the laser pulse duration and the laser fluence on phenomena occurring in laser material interaction. Considering the processes involved in material removal, models have been developed to predict crater depth and diameter. Two main approaches have been developed to model the laser material interaction. The first one is applicable on a macroscopic scale and is based on the thermal conduction heat equations (Yoo et al. 2000),(Watanabe & Iguchi 1999),(Liu et al. 1997). The second one is the two-temperature model and it is used in ps or fs ablation regime (Wu & Shin 2009),(Cheng et al. 2009)(Chen et al. 2006). The two temperatures correspond to the electron temperature and the lattice temperature respectively. This is due to the relaxation time during the energy transfer from the excited electron to the lattice phonons. When an electron absorbs the energy from one or more photons, it is excited to a higher energy state, and the time it takes for this energy to be transferred to the lattice is around few picoseconds depending on the material (Choi & Grigoropoulos 2002). Other kind of models are based on the Boltzmann electron transport equation or on molecular dynamic simulation (Qiu & Tien 1993),(Perez & Lewis 2002), but due to the high computational requirements they are usually used for small ablated volumes and very short pulses. Also some analytical models have been reported (Lunney & Jordan 1998),(Arnold et al. 1998),(Anisimov et al. 1999) where simple numerical models are developed to describe the main physical processes involved in the laser heating and vaporisation of the targets.

The majority of these models are not focused on the 3D crater prediction because of the high computational requirement for a 3D model or because the prediction of the 3D shape is not relevant for a certain kind of applications. Taking into account the previous models we identified two main equations to fit the crater shape and we compared the two fitting equations with the experimental results analysing the RMS error for each regime.

2. Analytical equation

The thermal diffusion in the bulk can be described by the Fourier with the boundary conditions described in (1):

$$\begin{cases} u_t - a^2 \Delta u = f(\vec{r}, t) \\ u(\vec{r}, 0) = 0 \\ \frac{du}{dx}(x = 0, t) = 0 \end{cases} \quad -\infty < x < 0,\ -\infty < y, z < \infty,\ 0 < t \leq +\infty \,, \qquad (1)$$

where a is the thermal diffusivity, $\vec{r}$ the space tensor, t the time, u the solution and $f(\vec{r}, t)$ the laser source. For two semi-finite media (air/silicon) the heat kernel equation is defined by Eq. (2)

$$K(\vec{r}, t) = \frac{1}{(4\pi a^2 t)^{3/2}} e^{-\frac{x^2+y^2+z^2}{4a^2 t}} \qquad (2)$$

The laser beam has been modeled with a Gaussian energy profile and the electromagnetic penetration has been defined using the Lambert-Beer law Eq.(3). Considering the diffusion time at least 2 order of magnitude bigger than the pulse duration, the temporal shape of the laser pulse duration has been consider instantaneous

$$f(\vec{r},\tau) = \frac{Q}{2\sigma^2} e^{-\frac{y'^2+z'^2}{2\sigma^2}} e^{-kx'} \delta(\tau), \tag{3}$$

where k is the electromagnetic penetration depth and $\sqrt{2}\sigma$ is the beam waist. It is possible now to obtain the integral that gives the solutions of Eq. (3) by the integral on Eq. (4)

$$u(\vec{r},t) = \int_0^t \int_{R^3} K(\vec{r}-\vec{r}',t-\tau) f(\vec{r}',\tau) d\vec{r}' dt \tag{4}$$

The solution of (4) is given by Eq. (5).

$$u(\vec{r},t) = \frac{Q}{2\sigma^2+4a^2t} e^{a^2k^2t - \frac{y^2+z^2}{2\sigma^2+4a^2t}} \left(e^{-kx} erfc\left(\frac{x}{\sqrt{4a^2(t)}} - ka\sqrt{t}\right) + e^{kx} erfc\left(\frac{x}{\sqrt{4a^2(t)}} + k\sqrt{a^2t}\right)\right) \tag{5}$$

In the case of a long pulse regime, where the thermal diffusion is the most relevant phenomenon, the $erfc$ function can be approximated using the asymptotic expansion and the solution can be written as:

$$u(\vec{r},t) = \frac{Q}{2\sigma^2+4a^2t} \frac{1}{\sqrt{\pi a^2 t}} e^{-\frac{x^2}{4a^2t} - \frac{y^2+z^2}{2\sigma^2+4a^2t}} \tag{6}$$

From Eq. (6) the shape of the isothermal fitting equation was/has been identified, and it is defined by an ellipsoid equation described in (7)

$$\frac{x^2}{a} + \frac{y^2}{b} + \frac{z^2}{c} = k \tag{7}$$

In the case where the diffusion effects are negligible because of the short pulse duration with respect to the relaxation time, only the energy balance used to induce ablation is taken into account. Under these conditions is quite easy to obtain from Eq. (3) the following relation:

$$\frac{x^2}{a} + \frac{y^2}{b} + \frac{z}{c} = k \tag{8}$$

3. Material and methods

Laser ablation experiments were performed on an n-doped 4-inch single side polished 3 inches diameter Silicon (100) wafer (Semiconductor Wafer).

In Table 1 Laser parameter for the four temporal regimes are reported. For the micro- and microsecond regimes several pulse duration have been evaluate on the range specified in the table. The laser beam delivery for each laser system is composed by a galvanometric scanner and an x-y-z axis stages in order to provide a single pulse.

The geometrical shape of the craters created on micro- and nanosecond regime have been measured using InfiniteFocus v6.1 (Alicona) optical microscope system. This system creates a 3-dimensional profile of the

sample's surface, the vertical resolution of the system is 50 nm and lateral resolution is 2 µm and White Light Interferometry (WLI) system (Bruker) for pico-and femtosecond regime
For the 3D reconstruction a code has been written using MATLAB software, which compares the two fitting functions with the experimental results. The RMS error between the real crater and the two fitting function has been calculated singularly. The RMS error ratio is defined in equation (9)

$$RMS\ error\ ratio = \frac{RMS\ paraboloid}{RMS\ ellipsoid} \tag{9}$$

Table 1 Laser parameter for the four temporal regimes

	Femtosecond	Picosecond	Nanosecond	Microsecond
Pulse duration	310 fs	<10 ps	9<t<220 ns	2<t<20 µs
Repetition rate [KHZ]	200	200	10	10
Wavelength [nm]	1032	1064	1064	1064
M^2	<1.3	<1.2	<1.4	<1.4

4. Results and discussion

In Figure 1 is shown the RMS error ratio between the paraboloid function and the ellipsoid function at different fluences. Four pulse durations are represented in the pictures. Each pulse duration represents one of four temporal regimes evaluated.
In the fs regime the RMS error ratio is close to one for several fluences, so it means that the two functions fit the craters with a similar error. This is probably due to the non-linear interaction in these time regimes, in particular the non-linear absorption (Cheng et al. 2009). For the ultrafast regime the absorption and consequently the crater depth is strongly dependent on the pulse peak power which permits to ablate a thin film of material independently from the electromagnetic penetration; however, with an increase in fluence (from x to y), the RMS error ratio start to be over 1.
In the picosecond regime the RMS error ratio it's about 1.2. It means that the paraboloid function fits substantially better than the ellipsoid one at fluences close to the threshold. With an increase in fluence the two functions start to be comparable so it results that increasing the energy per pulse the thermal regimes cannot be neglected.
In the nanosecond regime, the paraboloid function has an RMS error close to 1.5 times bigger than the ellipsoid one for the pulses longer than 100 ns and with a fluence couple than the threshold. However decreasing the pulse duration and the fluence the RMS error starts to be close and lower to one. This behavior can be explain by the fact that for shorter pulses than 100 ns and energies close to the threshold there is no enough energy to induce a thermal diffusion in the material. Oppositely increasing the energy fluence the ratio is stable to 1.5, in this case the plasma absorption has a fundamental role to reduce the energy absorbed by the bulk and decrease the effect of the heat diffusion.

In the microsecond regime the RMS error ratio is stable around 1.2. In this regime thermal diffusion it is significant, but his contribution is not as relevant as expected, also for fluences bigger than the ablation threshold the RMS ratio doesn't overcame 1.3.

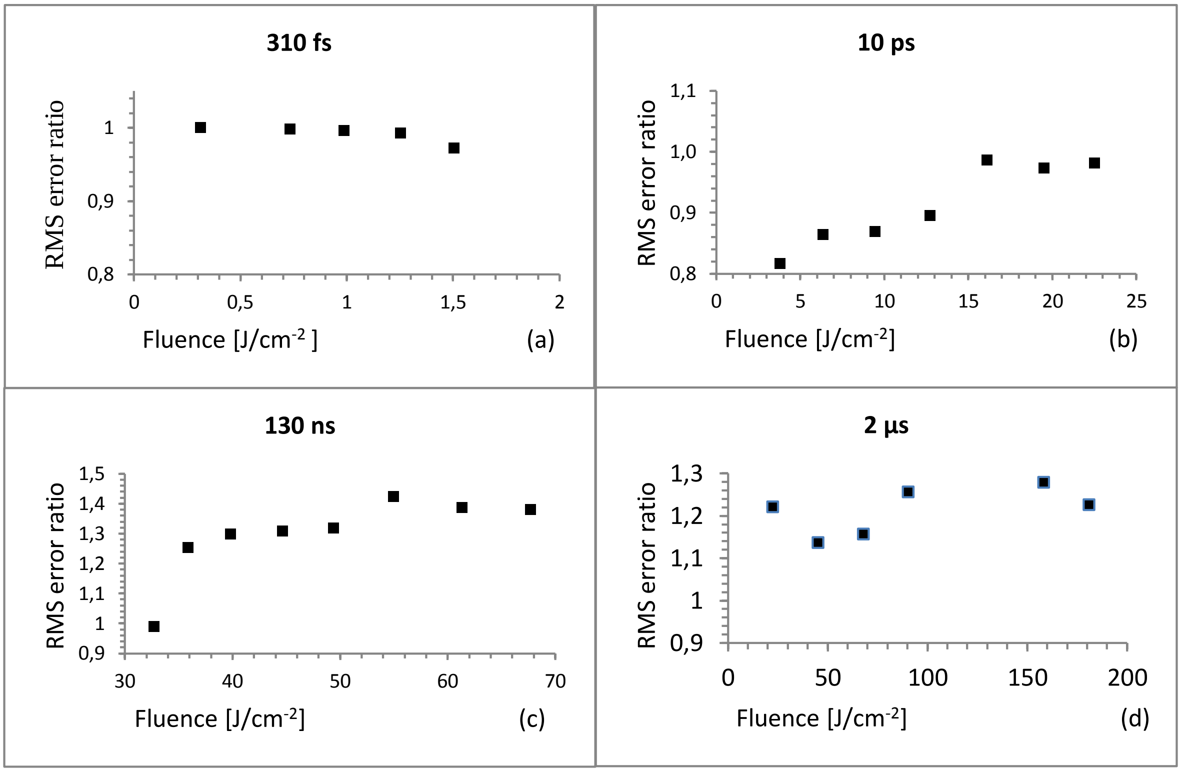

Figure 1 RMS error ratio at 310 fs (a), 10 ps (b), 130 ns (c) and 2us (d)

5. Conclusion

In this study a comparative study on the crater shape of several pulse regimes has been performed, starting from 300 fs to 20 µs and for different fluences. Two fitting equations, one based on the thermal diffusion and one based on the energy balance neglecting the effects of the thermal diffusion are used to fit the crater shape. As expected for long pulses (over 100 ns) thermal effects are driving the ablation process. For pulses in nanosecond regime but shorter than 100ns the shape is strongly dependent on the fluence, however for high energies the thermal effect are still dominant. In the picosecond regime the function based on the energy balance has a lower RMS error than the other, but prevalently for energy pulse close to the ablation threshold instead the fs regime, where the thermal effects are supposed to not contribute, the two equations present a similar RMS error probably due to the no-linear absorption.

Acknowledgements

I would like to acknowledge the funding support of EU FP7-ITN (Grant no. 316560) for the works presented as a part of the STEEP project. I thank Rocio Ortiz, for assistance with the picosecond laser experiment, and Eva Rodriguez for assistance with the microsecond laser experiment. I also thank Kateryna Bashtova for the advice on the analytical equation and Simina Rebegea for the discussions on the surface analysis.

References

Anisimov, S.I. et al., 1999. Pulsed laser evaporation: equation-of-state effects. *Applied Physics A: Materials Science & Processing*, 69(6), pp.617–620.

Arnold, N., Luk'yanchuk, B. & Bityurin, N., 1998. A fast quantitative modelling of ns laser ablation based on non-stationary averaging technique. *Applied Surface Science*, 127-129, pp.184–192.

Bogaerts, A. et al., 2003. Laser ablation for analytical sampling: what can we learn from modeling? *Spectrochimica Acta Part B: Atomic Spectroscopy*, 58(11), pp.1867–1893.

Chen, J.K., Tzou, D.Y. & Beraun, J.E., 2006. A semiclassical two-temperature model for ultrafast laser heating. *International Journal of Heat and Mass Transfer*, 49(1-2), pp.307–316.

Cheng, J. et al., 2009. Ablation mechanism study on metallic materials with a 10ps laser under high fluence. *Applied Surface Science*, 255(18), pp.8171–8175.

Choi, T.Y. & Grigoropoulos, C.P., 2002. Plasma and ablation dynamics in ultrafast laser processing of crystalline silicon. *Journal of Applied Physics*, 92(9), p.4918.

Liu, C.L. et al., 1997. Computational modeling of physical processes during laser ablation. *Materials Science and Engineering: B*, 47(1), pp.70–77.

Lunney, J.G. & Jordan, R., 1998. Pulsed laser ablation of metals. *Applied Surface Science*, 127-129, pp.941–946.

Perez, D. & Lewis, L.J., 2002. Ablation of Solids under Femtosecond Laser Pulses. *Physical Review Letters*, 89(25), p.255504.

Qiu, T.Q. & Tien, C.L., 1993. Heat Transfer Mechanisms During Short-Pulse Laser Heating of Metals. *Journal of Heat Transfer*, 115(4), p.835.

Watanabe, K. & Iguchi, T., 1999. Modeling of vaporization processes of resonant laser ablation. *Applied Physics A: Materials Science & Processing*, 69(7), pp.S845–S848.

Wu, B. & Shin, Y.C., 2009. A simplified predictive model for high-fluence ultra-short pulsed laser ablation of semiconductors and dielectrics. *Applied Surface Science*, 255(9), pp.4996–5002.

Yoo, J.H. et al., 2000. Explosive change in crater properties during high power nanosecond laser ablation of silicon. *Journal of Applied Physics*, 88(3), p.1638.