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Simulation-based process development for laser processing with ultra-short pulses

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Abstract

Computer-aided, mathematical modeling and numerical simulation are indispensable for modern process and product development. In particular, the non-linear radiation-material interactions that occur especially in laser processing using ultra-short-pulsed laser systems can be better understood, visualized and brought into line with the processing results by using suitable numerical techniques. This opens up new possibilities for using the laser as a universal tool for the robust, industrial-grade high-precision processing of a multitude of materials. Using applications in the fields of glass processing, stent cutting and black-marking as an example, the choice of an adequate model, the inclusion of experimental knowledge and the reduction of the numerical solution methods to a manageable measure for the use of ultra-short pulses is exemplarily demonstrated.

Keywords: mathematical modeling, simulation, laser process development, ultra-short pulses

1. Simulation-based process development

Numerical simulation techniques have become a well-established means for gaining process understanding and supporting if not enabling laser process development. Demonstration examples of simulation-based process development that are presented here are the focus position dependence in filament cutting which has led to new designs for filamentation optics, the gas dynamics and melt ejection in stent cutting which has motivated new process gas nozzle designs and a basic understanding how the black-marking process works which enabled a process parameter optimization leading to a better acid resistance of the produced markings.

Each of the shown use-cases provides its own mathematical model and numerical implementation, but there is something in common to all of those, that is the ability to check if a reduced set of physical mechanisms implemented is already enough to reproduce the basic experimental observations and thus showing that these mechanisms are responsible for the processing result and even turning them addressable for further process optimization.

2. Use cases for simulation-based process development

The following description of application cases gives an exemplary review for modeling and simulation in the context of process development in an industrial environment. It does so exemplarily for the applications of laser glass processing, stent cutting and black marking.

2.1. Laser glass processing

Laser processing of semi-transparent materials (like silicate glasses) with ultrashort pulses (see Fig. 1 a) is a technology strongly asked for these days. Although there are diagnostic methods to have a closer look at the in-volume modification (but without a deep quantitative understanding of the underlying ultra-short processes) with quite laborious and expensive pump-and-probe setups (see Flamm et al. (2015)), modeling and simulation offers

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a much cheaper and time-effective method to investigate the physical mechanisms and exploit them for process optimization. A reduced but yet effective model for the simulation of the essential mechanisms like bulk ionization, beam propagation and material modification is presented in (Sun, Eppelt, et al. (2012)) which was already proven to be valid for glass ablation has now been modified to account for the high-NA focusing optics used in filament cutting and applied to simulate the material modification within and in the vicinity of a filament.

The model allows for the prediction of void formation (which is essential for cutting) as well as damage patterns where the glass is not ablated yet still damaged by the incident radiation (see Fig. 1 b). With these features it is possible to evaluate the strength of the produced filament and thereby estimate its ability for later separation.

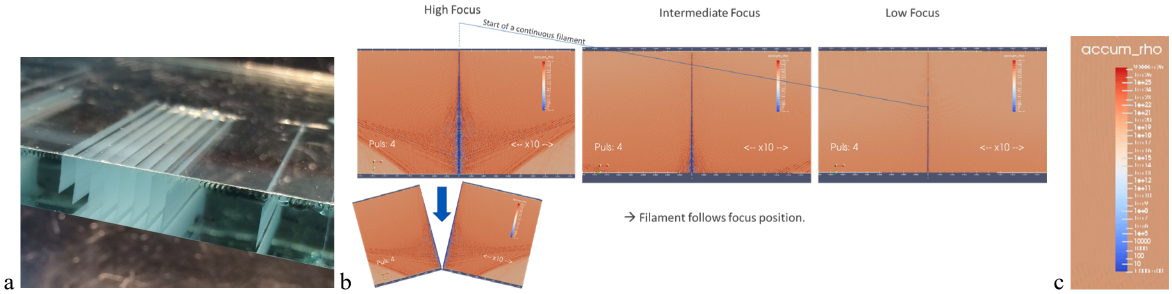

Fig. 1. (a) Filament curtain inside a glass bulk volume (b) Simulation of bulk ionization inside the glass material for filament cutting (pseudo-color shows electron density and thus damage (in red) as well as void formation (in blue)); the change of the filament structure due to a change in focal position is shown in the different pictures from left to right where the working distance is continuously decreased (c) common logarithmic legend of the accumulated electron density in $1/cm^3$

This way via modeling and simulation, filament separation and how to influence it becomes fully transparent.

2.2. Stent Cutting

One of the most prominent USP laser applications (see the top ten ranking by Nördinger (2018)) of ultra-short laser pulses is the production of medical stents via micro cutting of small hollow tubes. However, the process result from laser stent cutting still needs to be cleaned from the remaining debris after laser processing, although ultra-short pulsed laser processes are usually regarded as clean processes. Reaching the limits of the process window (e.g. via feed rate), the debris of the ablation which is up to a great extent still bulk material (and not evaporated) needs to go somewhere and forms clustering structures on the workpiece (see Fig. 2). Without a highly-demanding and also expensive diagnostic apparatus for the imaging of ultrashort processes it remains unknown how and where the bulk debris is produced.

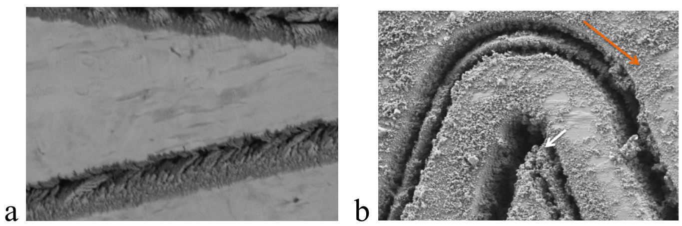

Fig. 2. Experimental observations in stent cutting (a) Top-view of feather-like structures on the cutting edge (b) Top-view of "Dust-Blade" inside the cutting kerf (marked by white arrow) and debris on the workpiece surface (marked by orange arrow)

Simulation on the other hand explains commonly observed features like the "dust-blade" phenomenon, feather-like debris structures that appear with increasing process speeds based on the physical debris ejection mechanism (see Fig. 3) and shows the effectiveness of conventional nozzle designs for debris ejection within these tiny dimensions (see Fig. 4).

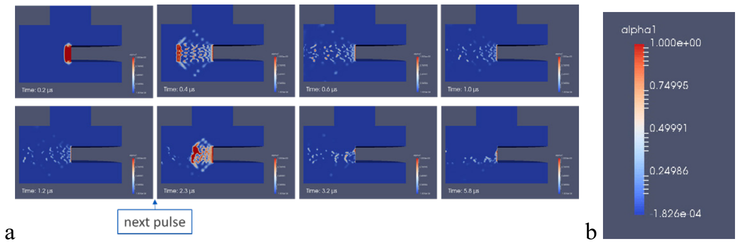

Fig. 3. (a) Debris ejection from the cutting front in stent cutting with ultra-short pulses at different time steps; debris shown in red color, void areas in blue; gas flow out of a nozzle at the top is injected into the cutting kerf, but is not able to properly eject the high-speed debris out of the cutting kerf. The bigger pile of debris of each pulse is collected in the wake of the cutting kerf, forming a dust-blade; the smaller feather-like structures form due to surface tension effects (i.e. elongated droplet formation) (b) legend of the shown volume-fraction for all plots ranging from 0 to 1

Reaching the cutting limit (given a certain pulse energy and repetition rate while increasing the feeding velocity) the appearance of a so-called dust blade is significant in ultra-short pulsed micro cutting, which is similar to the appearance of a closed kerf in high-speed laser fusion cutting or remote cutting (see Otto (2010)).

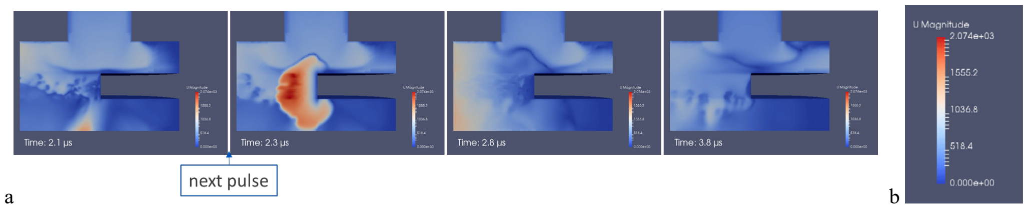

Fig. 4. (a) Gas flow around the cutting kerf in stent cutting with ultra-short pulses (b) legend of the shown flow velocity in m/s for all plots

It was found that at the process window limits the gas flow from a standard nozzle is too weak to change the direction of the bigger debris significantly that is ejected from the cutting front.

2.3. Black Marking

The process of laser black marking of metals (see Wang (2018)) works by two different mechanisms (shown in Fig. 5), meaning that there are (at least) two physical mechanisms that lead to a blackening effect. One of those is the blackening by a sort of dye with the help of the oxidation products that are mostly of a sort of blackish color and that are produced (more or less deliberately) during the heating of the metal material within an oxygen atmosphere. In Fig. 5 it is shown that with an increasing layer thickness of the oxidation layer, the reflection degree of the thus coated surface goes down (to the level of a grey of black surface of less than 10% reflection degree).

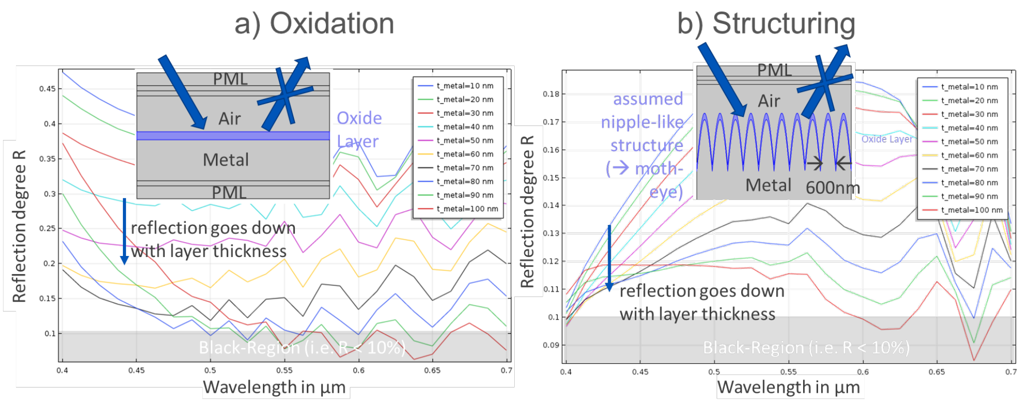

Fig. 5. There are two different mechanisms (analyzed on the left and right), by which the blackening effect in black marking is achieved: (a) oxidation and (b) structuring; for both mechanisms the basic (functional) simulation setup is shown in the graph inset, where the computational domain with different materials occupying different areas as well as a Perfectly-Matched-Layer (PML, see Taflove (2005)) for numerical absorption of the transmitted or reflected wave is illustrated; the effect itself is shown by the reflection spectra of each surface for different oxide layer thicknesses; note that the max. reflection degree in (b) is smaller than the maximum reflection degree in (a) proving that the additional structure in (b) decreases the reflection degree further

The other mechanism is blackening by structure, i.e. the reduction of the reflection degree by sub-micron structures that are proven to disguise a reflection (e.g. like a moth-eye, thus called moth-eye effect).

The effect of both mechanisms on the reflection degree of a surface can be calculated in a so-called functional simulation, in which the propagation of a plane wave onto a black-marked surface under different angles and with different wavelengths is modelled.

As the structuring mechanism for blackening does not rely on oxides (which are mostly soluble in acids) this is the preferred mechanism for black marking. Unfortunately, not any sub-micron structure is doing the job of preventing any reflection. To find out, if the typical surface structure (i.e. laser-induced periodic surface structure, LIPSS, see Sipe et al. (1983)) that results from an ultra-short pulse ablation process is doing that, the generation of such a structure has to be modelled and simulated (see Fig. 6, for the method used see Skolski (2014)). It was found, that the typical nano-ripple structure that evolves from an ultrashort pulsed black marking application is not performing well with respect to reflection prevention. So, it is actually the first mechanism of oxide layers that (for the conventional black marking processes) is taking a greater part in blackening, although the nano-ripples may be more prominent.

By tweaking the marking process via parameter optimization into the direction of a more suitable nano-structure for back-reflection suppression it was possible to achieve a major improvement on the robustness and resistance

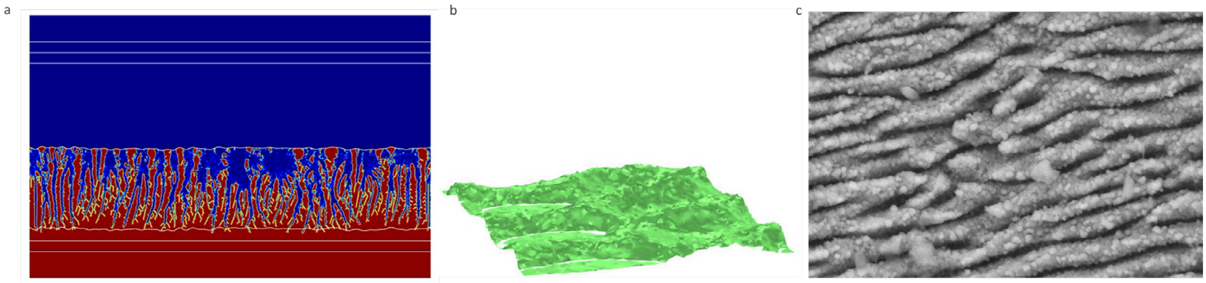

Fig. 6. (a) Simulation result of ripple formation in a 2D cross-section, in red color the bulk material that was not ablated, in blue the void area, white lines show different locations in the simulation domain (initial surface, PML area, sender line); (b) Simulation result of ripple formation in 3D; (c) Actual ripple structures in photographic measurement (from Zhu Liu (2019)).

of a black marking against household acids (see Fig. 7), which is especially suitable for the marking of household-goods, which may at some point in their product life cycle come into contact with household acids e.g. contained in cleaning agents.

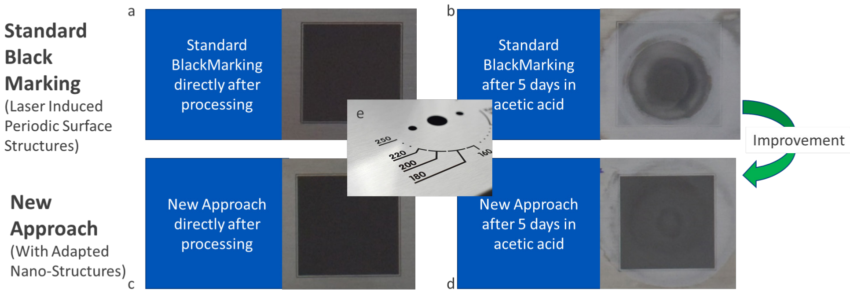

Fig. 7. Achieved improvement due to simulation-based process development (e.g. for the black-marking of household [white] goods like shown in sub-figure e)

3. Conclusion

The presented use cases involving the cutting of glass with filaments, the cutting of stents and the black-marking of metals show the successful modeling and simulation of typical ultrashort-pulsed laser applications, which lead us to the conclusion that mathematical modeling and numerical simulation are techniques that are applicable and useful just as well for an industrial environment as for scientific researchers. They have become a ubiquitous means for gaining process understanding and supporting if not enabling laser process development. In fact, numerical tools are even more suitable for companies with less research & development resources, as they can in many cases save the expense of valuable diagnostics equipment that is rather part of a university infrastructure than available in industrial R&D labs.

Acknowledgements

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