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Numerical Simulations - A Versatile Approach for Better Understanding Dynamics in Laser Material Processing

Andreas Otto[a]*, Holger Koch[b,c], Karl-Heinz Leitz[b], Michael Schmidt[b]

[a]*Technical University of Vienna, Institute for Manufacturing Technology , Austria*
[b]*University of Erlangen-Nürnberg, Chair of Photonic Technologies, Erlangen, 91052, Germany*
[c]*Erlangen Graduate School in Advanced Optical Technologies (SAOT), Erlangen, 91052, Germany*

- Invited Paper -

Abstract

This paper gives an overview on the potentials of numerical simulations for understanding dynamics in laser material processing. After a short introduction into the model, simulation results on several processes like laser beam deep penetration welding, drilling or cutting are presented. Furthermore simulation results are compared with experimentally obtained data.

Keywords: Laser material processing; numerical simulation; fluid dynamics; beam-material interaction

1. Introduction

Numerical process simulations gain more and more importance both for industrial applications and for scientific purposes. In science these simulations enable for thorough process understanding as it is possible to separate different process or material parameters in their influence on the processing result. They also enable for a look inside the work piece also on very short time scales and thus allow the analysis of processes that can not or only hardly be observed by experimental means. In industrial production simulations serve as a tool for planning of single production steps or even of whole process chains. Furthermore, simulations are important for the development of production means like new machining tools.

Contrary to other technologies, like e.g. forming, simulations for laser material processing are not yet state of the art especially in industrial production. This is due to the complexity of laser processes where a variety of different physical phenomena are coupled with each other. To reduce this complexity in state of the art models most of these phenomena are regarded as decoupled or they are even neglected dependent on the process that is to be simulated. Thus these models are only capable to analyze certain effects of the processing like e.g. thermal distortion or residual stresses. Figure 1 gives an overview of a newly developed model that is capable for simulating many aspects of different laser processes. This model allows the simulation of process dynamics, for example during laser beam welding including keyhole oscillations or melt pool respectively vapor flows.

* Corresponding author. Tel.: +49 9131 8523240; Fax: +49 9131 8523234
E-mail address: Andreas.Otto@lpt.uni-erlangen.de.

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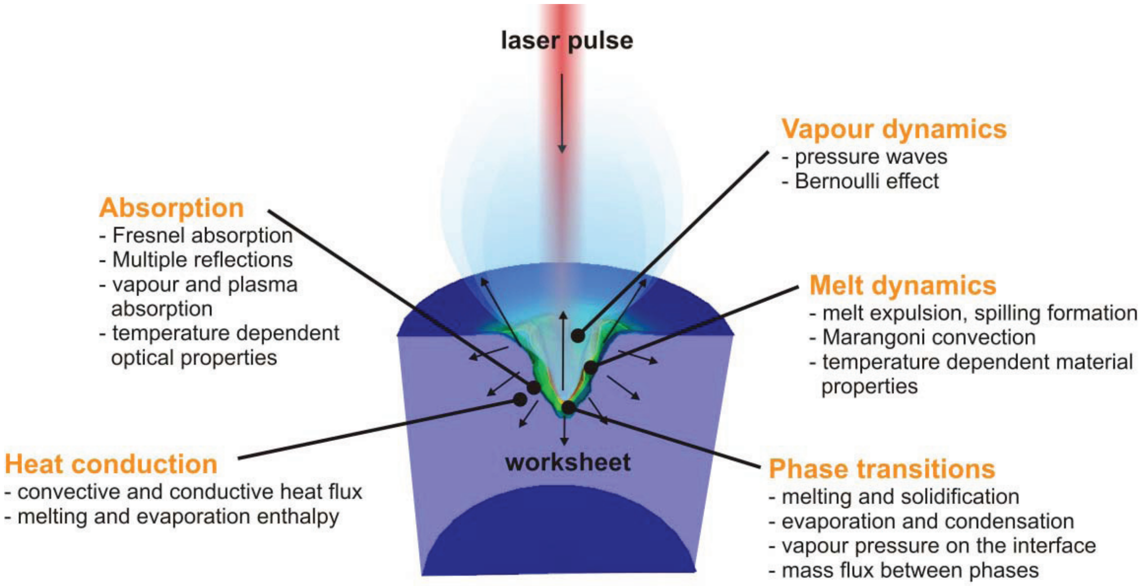

Figure 1: Overview of the model for simulating laser material processing (here on the example of laser beam drilling)

In the following a short introduction into this model will be given pointing out which new developments have been done compared to standard algorithms. After that, results of simulations concerning laser beam welding, laser beam drilling and laser beam cutting are discussed.

2. The Model

The here presented model for simulating laser material processing has been implemented in the framework of the software package OpenFOAM® (Open Field Operation and Manipulation). This software package is a free open source toolbox mainly designed for solving fluid dynamical problems, but has also been used for solving mechanical problems. It mainly uses finite volume numerics to solve systems of coupled partial differential equations. Due to OpenFOAM's modular design it is quite easy to extend the existing toolbox with regard to the physics of laser material processing. Namely the propagation of the laser beam to the work piece, the interaction of the laser beam with the material (absorption, reflection etc.), conductive respectively convective heat conduction and the fluid flow in the melt and the surrounding medium are already implemented in the model. The free surface of the material is computed by means of a volume of fluid (VOF) [1] approach included in OpenFOAM®. To reduce the calculation effort automatic adaptive time step control and adaptive remeshing strategies are incorporated in the model.

The presented results concerning the electromagnetic wave propagation and the thermo-mechanical processes are obtained with the commercial multiphysics software COMSOL. For the future it is planned to tackle these topics also within OpenFOAM.

2.1. Propagation of the Laser Beam to the Work Piece

The straight forward approach for calculating the propagation of the laser beam to the work piece is the solving of Maxwell's equations. Though such calculations are possible on very short time scales in the order of some hundreds of femtoseconds and small calculation domains in the µm range [2-5], other methods have to be developed if more macroscopic effects on longer time scales are to be examined. Otherwise this direct approach results in very long calculation times as the calculation time step width is clearly below 1 fs and the spatial resolution must be at least one third of the wavelength.

Thus most models for laser material processing handle the beam propagation by means of ray tracing, e.g. [6, 7].

The drawback for this approach is again the quite high calculation time as the laser beam has to be discretized quite finely and many search operations have to be done during tracing the rays through the calculation domain. An alternative approach that is currently used in our model handles the beam propagation as a stationary diffusion problem based on the so called radiative transfer equation [8]. This approach allows calculating the beam propagation until the first reflection with reasonably low computational effort. Both absorption, calculated with Beer's law, and reflection, calculated with Fresnel's equations (see figure 2), are handled as sinks in the used stationary diffusion equation. While the reflective sink deals as a source for the calculation of the reflected beam, the absorbed part is used as source for the heat equation. Until now it is not possible to handle the propagation of reflected beams with this very efficient approach. Thus we combined the method with a ray tracing algorithm reducing the computational effort for simulating the whole beam propagation by about 70% compared with a pure ray tracing algorithm. Further research work has to be carried out to totally avoid the ray tracing by means of generalizing our diffusion based method.

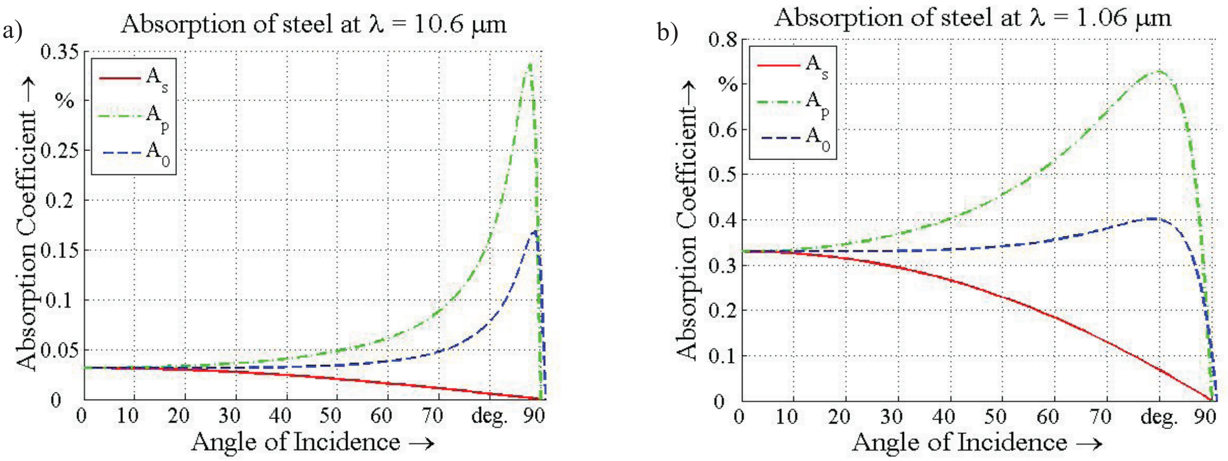

Figure 2: Angle dependent absorption coefficients at room temperature for vertical and parallel polarized components [12]. a): Absorption coefficient for $\lambda = 10.6$ µm. b): Absorption coefficient for $\lambda = 1.06$ µm

2.2. Heat Transfer and Fluid Flow

Solving the heat equation for computing the convective and conductive heat transfer and deriving the temperature field is a standard problem for numerical simulations. Most challenging in this context is the incorporation of the latent heats during phase transitions like melting respectively solidification, evaporation and condensation or even ionization. For our model an approach quite similar to the method proposed in [9] has been developed, where latent heats are iteratively corrected within the heat equation. The basic heat equation to be solved is given by

$$\frac{\partial \rho H}{\partial t} + \nabla \bullet (\rho \vec{u} H) - \nabla \bullet \lambda \nabla T = Q \quad (1)$$

with $H = c_p T + L$

For iteratively solving this equation with regard to the total enthalpy H we start with neglecting the latent heat L of the phase changes. From the result we can estimate the latent heat and solve the differential equation again. This leads to a corrected estimation of the latent heat. These calculation steps are repeated until the difference of the result of two subsequent calculation steps is less than a certain threshold. In our implementation convergence is typically reached after 5 to 10 iteration steps if phase changes are included. The source term Q as heat input is calculated from the above described beam propagation module. From the acquired solution for H the final temperature field and the contained latent heat can be derived.

Fluid flow must be taken into account if the material is molten or even vaporized during the laser material processing. If material is vaporized it expands into the surrounding medium and the recoil pressure deforms the surface of the molten material. The calculated latent heat of evaporation is used to calculate the mass flow due to evaporation and the corresponding recoil pressure. The mass flow is then used as a source term in the Navier-Stokes equation which is solved with standard methods of OpenFOAM (PISO scheme, see e.g. [10]). Of course mass conservation and temperature dependent surface tension are also taken into account.

Up to know both the work piece material and the surrounding medium is handled as incompressible. This is reasonable as long as the flow velocity is below about one half of the speed of sound. As this limit is exceeded in the vapor if processing with high laser intensities, the implementation of a model for mixed compressible and incompressible flows is planned.

2.3. Free Surface Handling

To track deforming surfaces respectively free boundaries in computational fluid dynamics several methods have been developed in the past. Most prominent are the Level Set Method [11] and the Volume of Fluid Method (or in short VOF method)[1]. As the VOF method is capable to conserve the mass of the traced fluid also if its interface changes topology, this method has been chosen within the model for laser material processing.

In this method a so called fraction function is defined. This function is zero if there is no traced fluid within one computational cell and one if the cell is full. At the interface between the material and the surrounding medium the function is between zero and one. To avoid unwanted smearing of the interface special compression algorithms are available within OpenFOAM. Consequently the fraction function is discontinuous and it is not possible to trace the expanding vapor. Therefore the original VOF method has been slightly modified by means of switching off the compression algorithm for material that is marked as vapor. Thus, evaporating material may cross the interface and vapor flow can be traced throughout the calculation domain.

2.4. Course of the calculation

Within each simulation time step the single modules for the calculation of the free surface movement, the beam propagation, the heat transfer and the fluid flow are solved sequentially. The calculation starts with the evaluation of the so called Courant number from which the time step width is according Courant-Friedrichs-Lewy condition [12] derived. Then the adaptive remeshing is started that is based on an analysis of the temperature field and the locations of the laser beam respectively the material's surface. The mesh is refined where the beam hits the surface, where phase changes take place and where the surface temperature has exceeded melting temperature during the calculation run.

After remeshing the movement of the free surface is calculated, based on the results on fluid flow from the preceding time step. Once the new free surface is given the beam propagation through the calculation domain can be calculated. Laser power that is absorbed in the vapor or in the work piece is handled as local heat source within the subsequent heat transfer module. From this module we get the temperature field and the latent heats due to phase changes. From this the mass flow due to possible evaporation is calculated and implemented as source term in the subsequent fluid flow calculation that takes mass conservation and surface tension into account. Solid material is fixed or keeps moving with a predefined working velocity during the calculation. Once the fluid flow is given the calculation loop starts again.

3. Results

In principle the developed model is capable for dealing with any kind of laser material processing that is governed by the physics already implemented. Namely one can simulate

- Laser beam welding
- Laser beam drilling and ablation with laser pulses > 1 ns
- Laser beam cutting

without modifying the model, only by means of adapting boundary conditions and defining appropriate laser parameters. As result of the simulations it is possible to trace the laser induced melt and vapor flow allowing us to thoroughly investigate the process dynamics. This again allows the identification of reasons for processing failures like e.g. holes in a weld seam. With some minor modification concerning the beam propagation and the absorption mechanisms the model has also been used for the simulation of electron beam material processing.

In the following examples of simulation results for laser beam welding, laser beam drilling and laser beam cutting are given.

3.1. Laser Beam Welding

Laser beam welding is a joining technology that has gained enormous importance for industrial production in the last two decades. The main advantages of this technology are the high flexibility of the process, the high possible welding speeds and the excellent joining qualities comprising low thermal impact and marginal distortion.

Though there are many applications, e.g. in automotive industry for joining metal sheets, the potential of laser beam welding for industrial production is not yet fully tapped. At diverse research institutions all over the world it is worked on methods to improve the reliability of laser beam welding processes. Prerequisite for the development of such methods is a thorough understanding of the beam material interaction and the resulting process dynamics. This thorough understanding can be best reached by means of a combined experimental and simulative approach. In this context simulations play an important role as they allow revealing the dynamic processes within the material. Furthermore phenomenological models derived from experimental observations can be tested by means of an implementation into the simulation model.

Figure 3 shows simulation results of the formation of the melt pool and the keyhole during a laser beam deep penetration welding process. The power of the laser is 3000 W, the focus radius of the Gaussian laser beam is 200 µm and the thickness of the sheet is 1 mm. The laser beam is fixed and the material moves with a velocity of 6m/min from the left to the right. One can see a cross section through the weld line and the interfaces between the solid, liquid and gas phase. The color corresponds to the temperature. The laser beam hits the material and heat conduction leads to the formation of a temperature field. The metal melts up and the vapour pressure leads to a deformation of the surface of the melt pool. After roughly 2.0 ms the keyhole has completely penetrated the sheet. Due to liquid melt flowing down the keyhole, it shows strong oscillations especially at the keyhole front. These waves running down the keyhole front have already been observed in high speed images and are often called keyhole humps [13, 14]. Hot liquid melt is transported to the end of the melt pool, which grows further and further and finally reaches a length of about 5.0 mm.

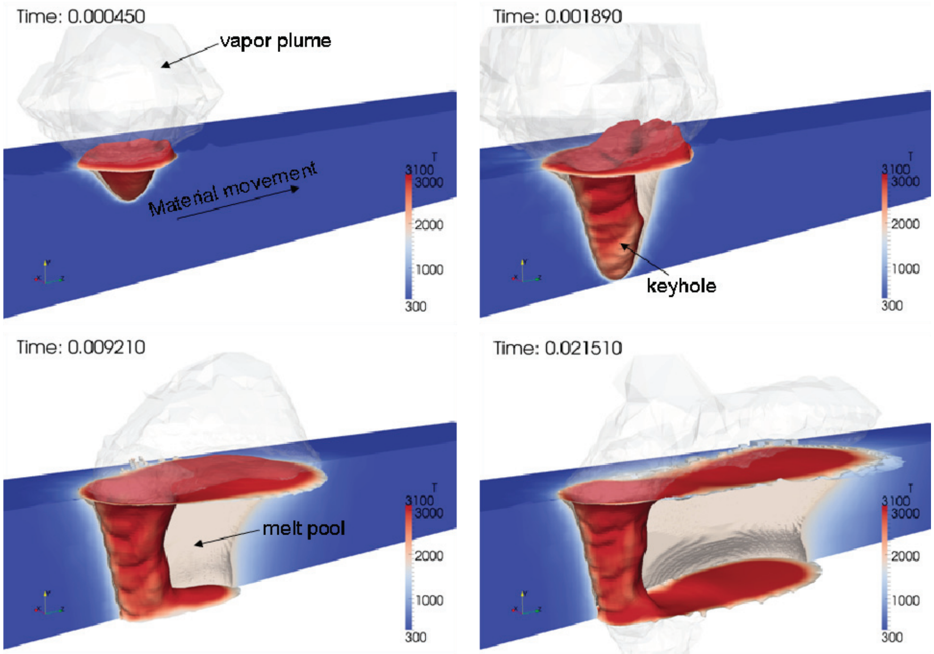

Figure 3: Simulation results for keyhole and melt pool formation during laser beam deep penetration welding of 1mm thick stainless steel sheet. Laser power: 3 kW; wavelength: 1.06 µm; beam radius: 200 µm; profile: Gaussian; feed rate: 6 m/min.

The simulation model allows a look into the fluid dynamics of the welding process. In figure 4 vertical and horizontal views of the streamline distribution within the melt pool can be seen [15]. The velocity field shows waves of liquid melt running down the front of the keyhole. These waves lead to a periodical change of the keyhole diameter and are causal for keyhole oscillations. The liquid melt is accelerated around the keyhole. At about two-thirds the length of the melt pool, the melt flow hits the backflow from the back of the melt pool and turbulences can be observed in the lower rear part. In the upper part of the melt pool, the flow pattern is more laminar. The melt flow changes the direction and recloses the keyhole. Furthermore, in simulations with higher feed rates the formation of pores in the weld seam can be observed (see figure 5) [16]. Wavelength dependent effects on the process dynamics are analyzed in [17].

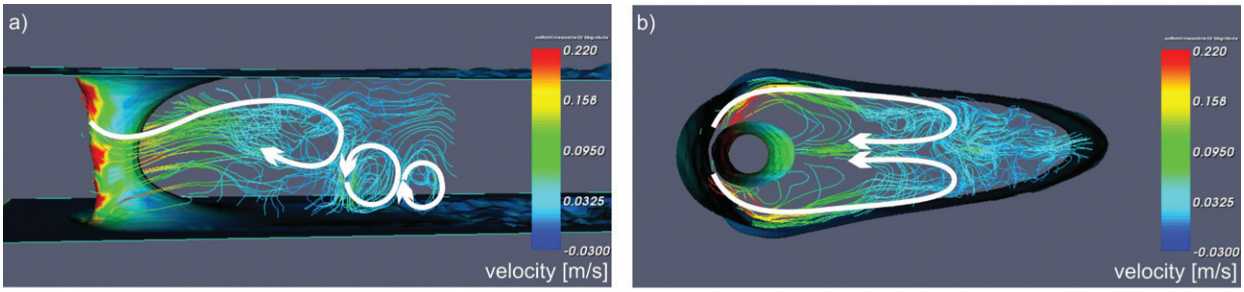

Figure 4: Fluid dynamics of the melt pool during laser beam deep penetration welding of stainless steel: a) vertical view; b) horizontal view. Laser power: 3 kW; wavelength: 10.6 µm; beam radius: 200 µm; profile: Gaussian; feed rate: 6 m/min. [15, 16]

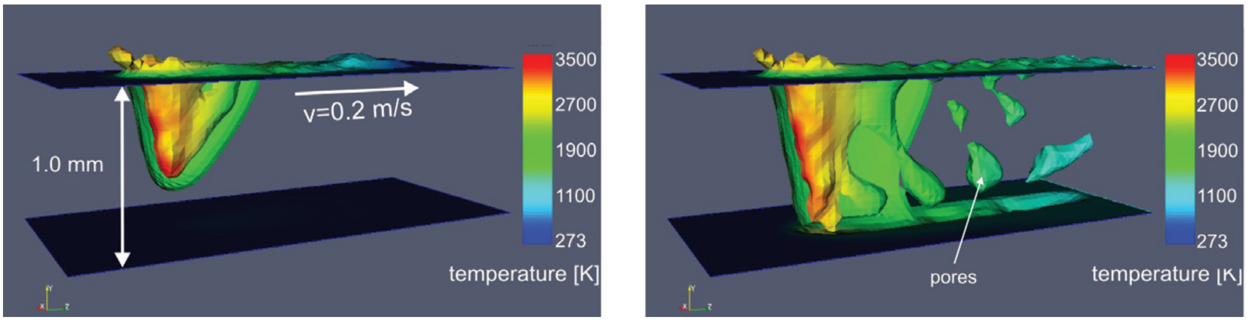

Figure 5: Pore formation during laser beam deep penetration welding of stainless steel at higher feed rates. Laser power: 6 kW; wavelength: 10.6 µm; beam radius: 200 µm; profile: Gaussian; feed rate: 12 m/min. [16]

In order to compare the simulation results with experimental data, the integrated evaporation rate was compared with the process emissions detected with an on-axis Si-photodiode looking at the optical process emissions in a spectral range form 300 to 900 nm (see Figure 7). The process emissions and therefore the detected signals correlate with the integrated evaporation rate inside the keyhole and mirror its dynamic behavior [18]. The signals of simulation and experiment show a similar shape in time domain. By a closer look, a certain periodicity, reflecting oscillations of keyhole and melt pool, can be recognized in both signals. This gets more evident in the frequency domain. Although the two spectra acquired by a numerical fast Fourier transformation are far from being identical, they at least show a similar global structure. Both spectra include a band of peaks at lower frequencies, corresponding to melt pool oscillations. The peaks at about 3,000 Hz correspond to the oscillation of the keyhole [18-20]. The similar structure of the spectra shows that the simulation quite realistically predicts process dynamics.

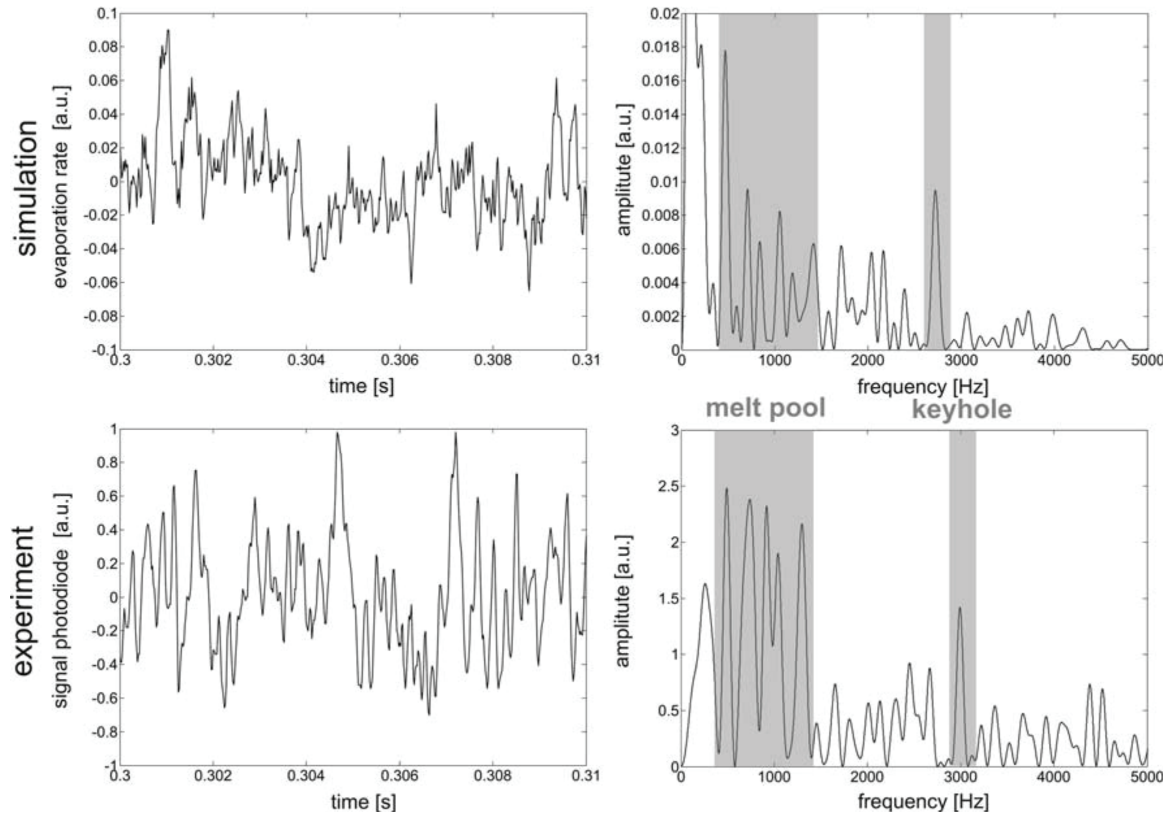

Figure 6: Evaporation rates and spectra of a simulated and an experimental welding process on stainless steel [16]. Laser power: 2.5 kW; wavelength: 10.6 µm; material thickness: 1 mm; beam radius: 200 µm; profile: Gaussian; feed rate: 6 m/min.

4. Ablative Processes

Laser beam drilling, structuring or cutting are ablative processes where material is removed from the work piece. The group of ablative processes can be subdivided into processes, where an external gas jet is applied to blow out the molten material like in conventional laser beam cutting, and processes, where the expanding vapor itself expulses the material like in laser beam drilling. The latter process group can again be subdivided into processes, where most of the material leaves the work piece in form of vapor (e.g. drilling with short pulsed lasers), and processes, where the recoil pressure produced by vapor expansion expulses liquid material in form of droplets (e.g. drilling with longer pulses or ablative remote cutting). The developed model for laser material processing is in principle capable for modeling all these different processes as long as there are no nonlinear beam-material interaction mechanisms like in ultra-short pulsed laser processing. As the relevant mechanisms like momentum conservation and phase transitions are taken into account in a self consistent way all these processes can be simulated just by adapting the machining parameters within the model.

Actually we just do one quite severe simplification that should also be avoided in the future: As the model is right now only capable for modeling incompressible fluid flow, effects that origin from the compressibility of e.g. the vapor flow cannot be simulated. To phenomenological take shock waves in the expanding vapor into account we apply a decelerating counter force on the expanding vapor if sonic speed is reached. Thus we avoid too high velocities in the expanding vapor plume. Figure 7 shows results from a simulation of a drilling process with a 15 ns laser pulse. The material removal is dominated by the expanding vapor, droplet blowout cannot be observed. Further results on laser beam drilling can be found in [21].

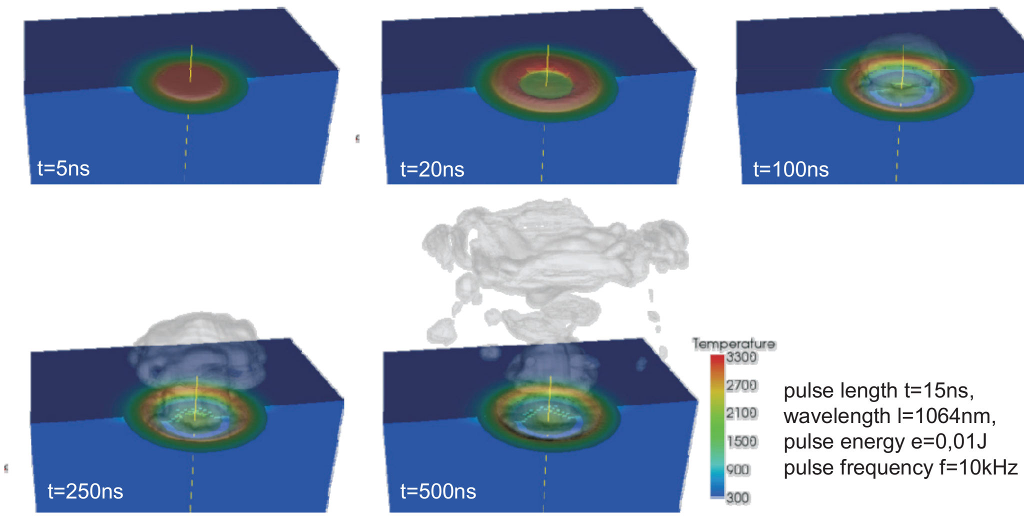

Figure 7: Simulation of laser beam drilling with short pulsed lasers

Gas-free remote cutting of sheet metal with highly brilliant laser beams is a quite newly developed laser technology [22, 23]. For this process one uses a laser beam with a high beam quality and sufficient power thus intensity exceeds around 10^8 W/cm^2. Due to the high intensity combined with high laser power the illuminated material evaporates and expands very rapidly. The strong recoil pressure squeezes the molten material out of the work piece resulting in a large amount of droplets leaving the work piece. Figure 8 shows results from a first simulation run on remote cutting of stainless steel. One can see a more or less periodic detachment of droplets from the work piece resulting in a groove with a depth of around 80 µm.

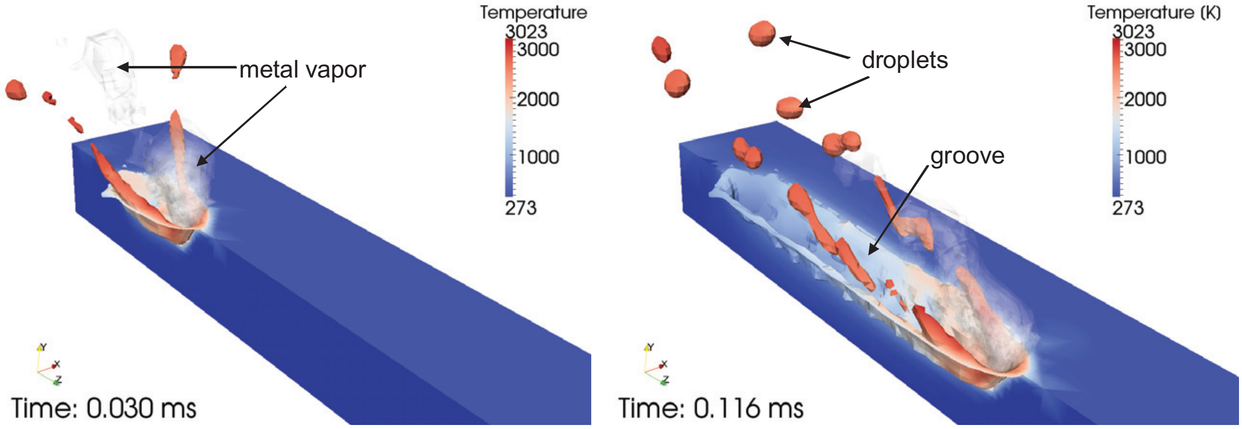

Figure 8: Gas-free remote cutting. Laser power: 1 kW; wavelength: 1.06 µm; beam radius: 25 µm; profile: Gaussian; feed rate: 420 m/min; material: stainless steel, s = 200 µm.

Another interesting remote cutting technique recently developed is the so called vapor pressure fusion cutting technique [24, 25]. Within this technology the melt is blown out at the bottom side of the sheet metal. The driving force is again the recoil pressure of the evaporating vapor. The process itself has a lot of similarities with laser deep penetration welding. In the relevant section 3.1 of this paper it has already been mentioned that there are so called keyhole humps that run down the keyhole front. At certain machining parameters the momentum of these humps is high enough to exceed the forces due to surface tension at the outlet of the keyhole. Thus droplets can detach from the work piece (see figure 9 on the right). Remarkably the process experimentally obtained process parameters suitable for vapor pressure fusion cutting correspond very well with simulation parameters that lead to the blow out of droplets at the keyhole outlet.

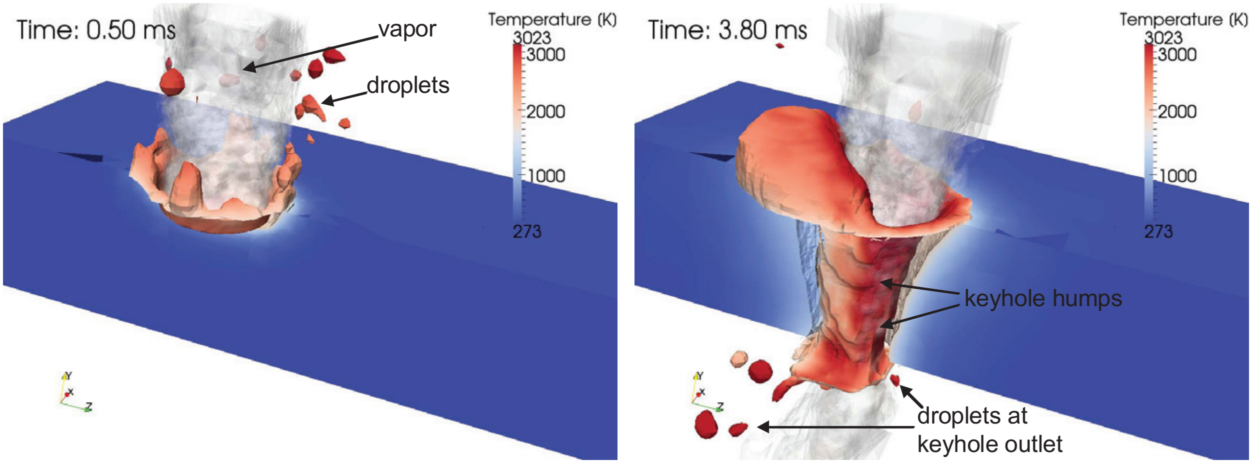

Figure 9: Early stage of vapor pressure fusion cutting. Laser power: 3 kW; wavelength: 1.06 µm; beam radius: 300 µm; profile: Gaussian; feed rate: 4.2 m/min; material: stainless steel.

Of course also conventional laser beam cutting processes using an external gas jet to blow out the molten material can be simulated. However the simulation of the external gas jet is quite challenging as it is necessary to model the compressible gas flow through the cutting nozzle to get satisfactory results comparable with experimental observations.

5. Summary and Future Perspectives

Building up a model for analyzing dynamics of laser material processing is a challenging task as one has to take into account many different physical phenomena that are coupled with each other. Aiming at such a model we built up a framework of modules within OpenFOAM® that enables for the simulation of thermal and fluid dynamical effects for several laser processes like e.g. laser beam welding, remote cutting or drilling. Further results covering also processes like laser beam droplet welding or laser beam brazing are given in [26]. First comparisons between simulation results and experimentally obtained data show quite sufficient correlations.

Though many physical aspects of laser beam material processing like melting and evaporation are already implemented within the model, there are still a lot of challenges ahead. One very important task especially with respect to industrial applications of the model is the coupling of fluid dynamics with thermo-mechanics. While stand alone simulations of thermo-mechanical and metallurgical processes in laser material processing are already state of the art, their coupling with fluid dynamics, e.g. in a transient weld pool, has not yet been established. Such a coupling is planned as one of our future development tasks.

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