FDM SIMULATION OF LASER-INDUCED CRATER FORMATION

INTRODUCTION

Lasers are being used in more and more industries; the field of laser-material interactions has advanced significantly. The ablation of metals with nanosecond laser sources has become popular among the many processes that lasers provide. By absorbing pulsed laser light, material can be removed from a surface in a using laser ablation and is much cheaper as compared to fs or ps lasers. This process plays a important role in numerous applications, ranging from material processing to and scientific research. [3] The laser-material interaction studied in this report involves the application of a nanosecond (ns) laser source onto a thin SS316 plate. The primary processing mechanism in this interaction is thermal. The incident laser pulse is absorbed near the workpiece's surface, creating a volume heat source. This study takes the advantage of the explicit Finite Difference Method (FDM) to develop a two-dimensional numerical model, aiming to understand the thermal dynamics, material removal rate, and associated side effects (HAZ) during laser ablation. Laser ablation is a popular research topic, and a lot of research is being done on this topic currently. Few of the topics are cited in bibliography.

Aims and Objectives

Aim of the report is to develop a numerical model to simulate the interactions between a nanosecond laser source and metallic materials. And to simulate laser ablation of a single nano second laser pulse, in Matlab, resulting in formation of a crated that can be validated with provided experimental results. Find the HAZ of the interaction and approximating the temperature distribution across the workpiece.

METHODOLOGY

The model is based on conventional heat diffusion equation with heat source i.e. a single ns laser pulse with Gaussian temporal and spatial profiles. The relationship between temperature, energy density, and the state change of the material is considered in the model. Latent heat of evaporation is ignored because it is assumed that liquid to gas transition removes material, however latent heat of diffusion is considered.

The governing physics

The governing physics in the context of laser-material interaction involve the fundamental principles of heat transfer and phase change. The equations governing these physics are derived from principles in heat conduction, absorption of electromagnetic radiation, and phase change dynamics.

Heat Conduction

Using Heat Conduction Equation - a partial differential equation that describes heat distribution (or the temperature field) in a given body over time.

$$\rho C p \frac{\partial T}{\partial t} = K \nabla (\Delta T) + Q [1]$$

where ρ is the material density, Cp is the heat capacity, K is the thermal conductivity, T is the temperature, t is time, and ∇ is the del operator.

The general heat conduction equation in two dimensions:

$$\rho \ Cp \ \frac{\partial T(x,z,t)}{\partial t} = K \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial z^2} \right) + A(x,z,t)[1]$$

Absorption of Pulse Energy (electromagnetic radiation):

The absorption process is described by the Beer-Lambert law, considering the material's absorption characteristics. Here, A(x, z, t) is the volume heat source (the absorbed laser energy in a given unit of a material volume).

$$A(x,z,t) = \alpha I_0 p(t,x) e^{-\alpha z}$$

Here p(t, x) is spatial and temporal profile. The governing equation for the absorbed pulse energy accounting for the absorption coefficient α , laser intensity I_{θ} , and temporal and spatial profiles of the laser pulse p(t, x) is given as:

$$\rho \, Cp \, \frac{\partial T(x,z,t)}{\partial t} = K \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial z^2} \right) + \alpha I_0 p(t,x) e^{-\alpha z}$$

Rearranging,

$$\frac{\partial T(x,z,t)}{\partial t} = \frac{K}{\rho Cp} \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial z^2} \right) + \frac{1}{\rho Cp} \alpha I_0 p(t,x) e^{-\alpha z}$$

Finite Difference Method (FDM)

Now, discretize the governing equations using the explicit forward Finite Difference Method of derivatives, derived from the Taylor series, for numerical simulation. Let $T_{i,k}$ represents the temperature at grid point (i, k).

The temporal and spatial derivatives can be approximated as follows: [1]

$$\frac{\partial T(x,z,t)}{\partial t} \approx \frac{T_{i,k}^{n+1} - T_{i,k}^{n}}{\Delta t}$$

$$\frac{\partial^{2} T}{\partial x^{2}} \approx \frac{T_{i+1,k}^{n} - 2T_{i,k}^{n} + T_{i-1,k}^{n}}{\Delta x^{2}}$$

$$\frac{\partial^{2} T}{\partial z^{2}} \approx \frac{T_{i,k+1}^{n} - 2T_{i,k}^{n} + T_{i,k-1}^{n}}{\Delta z^{2}}$$

Substituting the values of $\frac{\partial^2 T}{\partial x^2}$, $\frac{\partial^2 T}{\partial z^2}$ and $\frac{\partial T(x,z,t)}{\partial t^2}$ into the partial differential equation.

$$\frac{T_{i,k}^{n+1} - T_{i,k}^n}{\Delta t} = \frac{K}{\rho \ Cp} \left(\frac{T_{i+1,k}^n - 2T_{i,k}^n + T_{i-1,k}^n}{\Delta x^2} + \frac{T_{i,k+1}^n - 2T_{i,k}^n + T_{i,k-1}^n}{\Delta z^2} \right) + \frac{1}{\rho \ Cp} \ \alpha I_0 p(t,x) e^{-\alpha z}$$

Rearranging the explicit FDM equation for heat conduction is used to update the temperature field at each time step.

$$T_{i,k}^{n+1} = T_{i,k}^{n} + \frac{\Delta t K}{\rho Cp} \left(\frac{T_{i+1,k}^{n} - 2T_{i,k}^{n} + T_{i-1,k}^{n}}{\Delta x^{2}} + \frac{T_{i,k+1}^{n} - 2T_{i,k}^{n} + T_{i,k-1}^{n}}{\Delta z^{2}} \right) + \frac{\Delta t}{\rho Cp} \alpha I_{0} p(t,x) e^{-\alpha z}$$

Temporal and Spatial profiles of Beam

A beam with Gaussian temporal and spatial profiles is used for this laser-material interaction experiment. For beams with Gaussian temporal and spatial profiles p(t, x) is:

$$p(t,x) = \int e^{-\left(\frac{x}{R_0}\right)^2} \int e^{-\left(\frac{t}{\tau}\right)^2}$$

Here R_{θ} is beam radius at focus, τ is pulse duration, t is time.

Iterative equation:

$$T_{i,k}^{n+1} = T_{i,k}^{n} + \frac{\Delta t K}{\rho C p} \left(\frac{T_{i+1,k}^{n} - 2T_{i,k}^{n} + T_{i-1,k}^{n}}{\Delta x^{2}} + \frac{T_{i,k+1}^{n} - 2T_{i,k}^{n} + T_{i,k-1}^{n}}{\Delta z^{2}} \right) + \frac{\Delta t}{\rho C p} \alpha I_{0} e^{-\left(\frac{x}{R_{0}}\right)^{2}} e^{-\left(\frac{t}{\overline{t}}\right)^{2}} e^{-\alpha z}$$

The equation is explicit as the known temperature at the previous step in time determine unknown temperatures for the next time step i + 1. The next step in time is calculated by $\Delta t = \tau/10$ or the following formula whichever is smallest.

$$\Delta t \le 0.5 \times \frac{\rho C_p \Delta x^2 \Delta z^2}{K(\Delta x^2 + \Delta z^2)}$$

First row equation

The equation for estimating temperature in first row is obtained by substituting the term $T_{i-1,k}^n$ with ambient temperature.

$$\begin{split} T_{i,k}^{n+1} &= T_{i,k}^{n} + \frac{\Delta t \, K}{\rho \, Cp} \bigg(\frac{T_{i+1,k}^{n} - 2T_{i,k}^{n} + T_{0}^{n}}{\Delta x^{2}} + \frac{T_{i,k+1}^{n} - 2T_{i,k}^{n} + T_{i,k-1}^{n}}{\Delta z^{2}} \bigg) \\ &\quad + \frac{\Delta t}{\rho \, Cp} \alpha I_{0} e^{-\left(\frac{x}{R_{0}}\right)^{2}} e^{-\left(\frac{t}{\tau}\right)^{2}} e^{-\alpha z} \end{split}$$

Assumptions:

- Steady-state conditions are assumed.
- A rectangular grid with indices i, k representing spatial coordinates x, z respectively.
- The material properties (density ρ , heat capacity Cp, thermal conductivity K) are assumed to be constant.
- Ambient temperature is 20°C.

Phase Change:

The model also incorporates adjustments for latent heat of fusion during phase changes from solid to liquid. However, latent heat of evaporation is ignored because it is assumed that liquid to gas transition removes material. In simulation a mask is applied to store points where adjustment has already made to avoid making adjustment every time the loop runs.

$$T_{new} = T_{old} - \frac{L_m}{Cp} [2]$$

Simulation

The code starts with defining parameters such as material properties, laser parameters and simulation details. The metallic segment of $400\mu m$ in length and $80\mu m$ in depth is discretized in both spatial X, Z dimensions using the FDM. A grid to represent the plate is created as a Matrix.

The absorbed pulse energy is calculated at each grid point using the absorption coefficient, laser intensity, and the temporal-spatial profile of the laser pulse. This accounts for how much energy is being deposited into the material. The heat conduction equation is discretized and solved at each time step.

At each time step, the code checks if the temperature at any point has reached the melting point. If so, it adjusts the temperature to account for the latent heat of melting. A mask is applied to store points where adjustment has already made to avoid making adjustment every time the loop runs.

The simulation begins at the start of pulse and maximum laser intensity occurs at $t = 0.5 \tau$ (pulse duration), aligning with the pulse duration τ for simplicity. The simulation iterates through multiple time steps, updating the temperature distribution based on the absorbed pulse energy, heat conduction, and any adjustments for phase change.

RESULTS

The detailed contour plots showing the evolving temperature distribution and crater depth in the Z direction is obtained as a result of simulation. These plots are generated at regular intervals, specifically every step Δt in the pulse duration. The visualization provides a comprehensive understanding of how the material responds to the single laser pulse over time (0ns - 140ns).

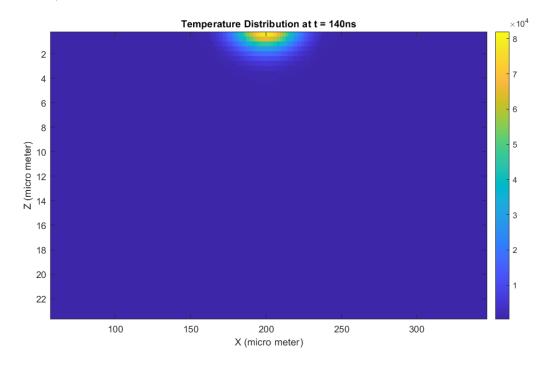


Figure 1: Temperature Distribution at time 140ns

Material Properties

The table below summarizes the physical, optical, and thermal properties of SS 316.

Table 1: Material Properties

Properties	Symbol	Value	Unit
Melting Point	Tm	1670	K
Boiling Point	Tb	3173	K
Density	Rho	8238	Kg/m^3
Specific-heat capacity	μm	468	J/kg K
Thermal conductivity	K	13.4	W/m K
Latent heat of melting	Lf	3.0+5	J/K
Absorption coefficient	alpha	5.45e+7	1/m

Model Validation

To validate the model against the available experimental results. The data is exported in excel to find the exact point in material where the temperature has raised above the boiling point.

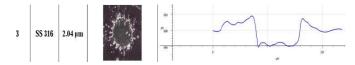


Figure 2: Provided Experimental data



Figure 3: Temperature data of the area of interest of workpiece

Crater Depth = Number of rows above the boiling point $\times \Delta z$

Crater Depth =
$$6 \times 0.4 \mu m = 2.4 \mu m$$

The crater depth provided in the experimental data is $2.04 \mu m$. Whereas results obtained from simulation is $2.4 \mu m$. The difference among them is 15%. The depth obtained from simulation is 15% more than the experiment. Which is close enough to be used for our results.

Crater Depth at Δt steps in time.

Table 2: Crater Depth at different time steps

t	Number of rows above T _b	Crater depth	Crater depth
0ns	0	0×0.4μm	0µm
14ns	1	1×0.4μm	0.4µm
28ns	2	2×0.4µm	0.8µm
42ns	3	3×0.4μm	1.2µm
56n	3	3×0.4µm	1.2µm
70ns	4	4×0.4μm	1.6µm
84ns	4	4×0.4μm	1.6µm
98ns	4	4×0.4μm	1.6µm
112ns	5	5×0.4μm	2.0µm
126ns	5	5×0.4μm	2.0µm
140ns	6	6×0.4μm	2.4µm

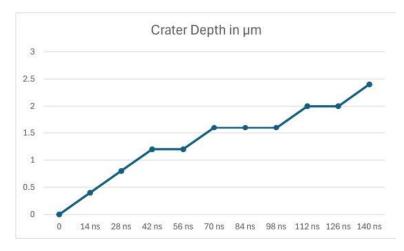


Figure 4: Crater depth in μm

Crater Diameter = Number of columns above the boiling point $\times \Delta x$

Crater Depth =
$$35 \times 2\mu m = 70\mu m$$

Material Removal Rate (MRR)

To calculate the material removal rate following formula can be used. Since volume is not modelled in simulation and it deals with area only. Material removal rate can't be estimated exactly.

Material Removal Rate (MRR) = Volume Removed/Pulse Duration

DISCUSSION

The discussion interprets the simulation results, emphasizing the influence of laser material interaction parameters such as power, pulse duration, and material absorptivity on temperature distribution and crater depth. The spatial and temporal profiles of the laser pulse are analysed for their impact on the heat affected zone and crated depth in the material. The effects of latent heat during phase transitions are scrutinized, highlighting their importance in accurately predicting material behaviour that validates with the experimental results.

Crater Formation

To find the crater depth, the data of temperature distribution is subtracted from evaporation point of material resulting in formation of a mask which is then plotted to make the crater. In this picture formation of crater can be seen clearly.

Exact crater depth calculation is made on excel at Δt steps in time and graph of area of interest is plotted on xz plane.

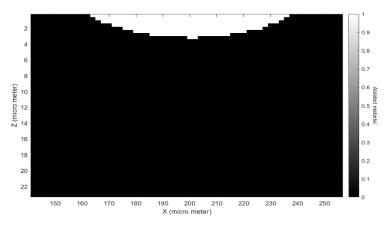


Figure 5: Formation of Crater

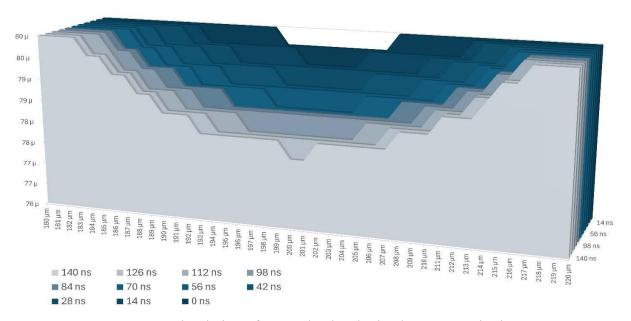


Figure 6: Simulation of crater depths obtained at Δt steps in time

Heat Affected Zone

The heat-affected zone (HAZ) in laser ablation is typically defined as the region in the material where the temperature rises significantly but doesn't reach the threshold for material removal or vaporization. t is the region that experiences thermal changes without undergoing significant physical changes. Localized thermal load and heat affected zone can be calculated given the temperature threshold. In simulation it can be modelled the similar way crater formation is modelled. If threshold is assumed 0.7Tm the Heat Affected Cells are given as yellow-coloured

cells in the picture of excel sheet below. Multiply the number of affected cells with dx and dz, one can calculate exact dimensions of HAZ.



Figure 7: Heat Affected Zone marked as Yellow Cells

CONCLUSIONS

In conclusion, the Explicit Finite Difference Method (FDM) is used to simulate nanosecond laser ablation of metals, and the results have provided understandings of the thermal aspects of the process. The majority of the material is removed by ablation when the laser is at peak intensity. The intensity exhibits a bell-shaped curve of a Gaussian temporal profile, peaking at the middle of the pulse duration. This suggests that this central period is where the critical material removal and thermal effects are concentrated.

The temperature distribution of the metallic plate affects greatly by introducing Latent heat of fusion. Spatial and temporal profile also play an important role in deciding when the maximum material is removed during the pulse duration and position of pulse. Depth decay is directly proportional to the depth of the material. It also changes with material and depends on the absorption coefficient of material.

A comprehensive understanding of the heat distribution across a thin metallic plate, allowing for predictions of crated depth and assessments of thermal effects such as heat affected zone and layer development. The crater depth of the simulated example is $2.4\mu m$ and crater diameter is $70\mu m$. Which is very close to the provided experimental results. The simulation closely estimates the heat distribution across the thin metallic plate.

REFERENCE

- [1] I. (2009, July 1). Fundamentals Of Heat And Mass Transfer, 5Th Ed. John Wiley & Sons.
- [2] Dobrev, T., Dimov, S. S., & Thomas, A. J. (2006, November 1). Laser milling: Modelling crater and surface formation. Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science, 220(11), 1685–1696. https://doi.org/10.1243/09544062jmes221
- [3] Dutta Majumdar, J., & Manna, I. (2011, November). Laser material processing. International Materials Reviews, 56(5–6), 341–388. https://doi.org/10.1179/1743280411y.0000000003
- [4] M.H. Mahdieh, M. Nikbakht, Z. Eghlimi Moghadam, M. Sobhani. "Crater geometry characterization of Al targets irradiated by single pulse and pulse trains of Nd:YAG laser in ambient air and water", Applied Surface Science, 2010

APPENDIX

MATLAB Code of the simulation is attached below

```
% Parameters
clear all;
melting_mask = false(200,200); % Mask to apply temperature adjustment
melting_mask1 = false(200,200); % Mask to store last applied adjustment
                 % Radius of the laser beam spot at the focus [m]
I0 = Pav / (f * tau * pi * R0^2); % Peak on-line laser intensity [W/m^2]
% Spatial and temporal discretization
% Discretization along z axis [m]
dz = 4e-7;
dt1 = 0.5*(rho*Cp*dx^2*dz^2)/(Kappa*(dx^2+dz^2)); % Time step (s)
dt2 = tau/10;
dt = min([dt1 dt2]);
Lx = 4e-4;
                   % Length of the material in x [m]
Lz = 8e-5;
                  % Length of the material in z [m]
                          % Number of spatial grid points in X
Nx = round(Lx / dx);
                       % Number of spatial grid points in Z
% Number of time steps
Nz = round(Lz / dz);
Nt = round(tau / dt);
% Boundry Conditions
T0 = 293.15; % Initial Temperature [K]
Tx = 293.15; % Temperature Left and Right [K]
Tz = 293.15; % Temperature Bottom [K]
% Initialize temperature field
T = T0 * ones(Nz, Nx);
% Transformation Variables
   x pulse = Lx / 2;
    t pulse = Nt*dt*0.55;
% Simulation loop
for n = 0:Nt
% Calculate heat source term (pulse at the center)
    A = alpha * I0 * exp(-((((1:Nx) * dx) - x_pulse) / R0) .^2)...
        * exp(-(((n * dt) - t_pulse) / tau)^2);
    for i = 1:Nz-1
        depth_decay = exp(-alpha*(i-1)*dz);
        for k = 2:Nx-1
            if i==1
               T(i, k) = T(i, k)...
```

```
+ (((dt * Kappa) / (rho * Cp)) * ((T(i+1, k) - 2 * T(i, k)))
k) + T0) / (dz ^ 2) + (T(i, k+1) - 2 * T(i, k) + T(i, k-1)) / <math>(dx ^ 2)))...
                    + (dt / (rho * Cp)) * A(1, k) * depth_decay;
            else
                T(i, k) = T(i, k)...
                    + (((dt * Kappa) / (rho * Cp)) * ((T(i+1, k) - 2 * T(i,
k) + T(i-1, k) / (dz^2) + (T(i, k+1) - 2 * T(i, k) + T(i, k-1)) / (dx^2)
2)))...
                    + (dt / (rho * Cp)) * A(1, k) * depth_decay;
            end
        end
    end
% Boundary conditions (fixed temperature at boundaries)
    T(end, :) = Tz;
    T(:, 1) = Tx;
    T(:, end) = Tx;
% Adjust temperature for melting
    melting_mask = T > Tm;
    melting mask =logical(melting mask-melting mask1);
    T = T - melting_mask * (Lf / Cp);
    melting mask1 = logical(melting mask1 + melting mask);
% Plot temperature distribution every time step
        figure;
        imagesc((1:Nx)*dx/1e-6, (1:Nx)*dz/1e-6, T)
        title(['Temperature Distribution at t = ' num2str(n*dt/1e-9) 'ns']);
        xlabel('X (micro meter)');
        ylabel('Z (micro meter)');
        colormap(gca, "default");
        colorbar;
        clim([290 82000]);
        cb = colorbar();
        ylabel(cb, 'Temperature (K)', 'Rotation', 270)
        drawnow;
end
% Crater
evaporatedMask = T>Tb;
colorbar;
figure;
imagesc((1:Nx)*2, (1:Nx)*0.4, evaporatedMask)
xlabel('X (micro meter)');
ylabel('Z (micro meter)');
colormap(gca, "gray");
colorbar;
clim([0 1]);
cb = colorbar();
ylabel(cb, 'Ablated material', 'Rotation', 270)
drawnow;
```