Effect of Thermocapillary Flow on the Surface Profile in Pulsed Laser Micro Polishing

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\section*{ABSTRACT}

The objective of this paper is to understand and predict how surface profiles produced by thermocapillary flow change with material properties and process parameters during pulsed laser micro polishing (PLµP). Thermocapillary flow is driven by surface tension gradient which is induced by temperature gradient in a melt pool. Experimental work has shown that great reductions in surface roughness can be achieved by manipulating thermocapillary flow (thermocapillary regime). The existing surface prediction model only works for PLµP through damping of stationary capillary waves (capillary regime) where thermocapillary flow is negligible. It is desirable to develop a predictive capability for the thermocapillary regime to offer guidance for parameter selection and optimization. Analytical heat transfer and fluid flow models are derived for laser induced thermocapillary flow. A dimensionless number, normalized average displacement (NAD) of a liquid particle during thermocapillary flow, is proposed and calculated directly from material properties and laser process parameters. NAD is found to be strongly correlated with the surface profile introduced by thermocapillary flow and successfully used to predict polishing achievable in thermocapillary regime. Combining this model with the existing surface prediction model will enable prediction of the outcome of PLµP over a wide range of parameters.

\section*{INTRODUCTION}

Pulsed laser micro polishing (PLµP) is an emerging surface smoothing process suitable for micro/meso metallic parts. In PLµP, short laser pulses are used to melt small spots on the surface of the part such that surface asperities can be smoothed out by the melt pool flow. The PLµP that is described in this work does not involve any ablation as melt temperatures are maintained below the boiling point. PLµP is advantageous over traditional polishing methods in many aspects such as selectivity, reliability, productivity and ease of automation [1-6]. Extensive experimental work has shown significant surface roughness reduction (up to 90\%) through PLµP [3-9]. Recently, two regimes for PLµP with distinct results have been discovered, capillary regime and thermocapillary regime, depending on whether thermocapillary flow (also known as Marangoni flow) dominates melt pool flow [6, 9].

For most liquid metals, surface tension is a function of temperature. The dependence of surface tension on temperature is described by the surface tension coefficient (STC, $\frac{dy}{dT}$). A temperature gradient along the surface of a melt pool results in a surface tension gradient. The surface tension gradient will induce a surface flow toward regions of higher surface tension: so-called thermocapillary flow. The direction of thermocapillary flow is determined by the sign of STC. For example, the STC of Ti6Al4V is negative, which means that surface tension is greater in the cooler regions at the outer perimeter of the melt pool, hence flow is outward. At the boundary of the melt pool, the liquid metal resolidifies, piles up and forms a ridge as shown in Fig. 1a. The radial thermocapillary flow smooths the surface of the melt pool. Overlapping laser spots (melt pools) that are used to polish an area result in processing features introduced by the ridges formed from the thermocapillary flow. Fig. 2a shows a generic surface height profile of PLµPed sample in thermocapillary regime. The process parameters were 21.2 µm laser beam radius, 4.20 µs pulse duration and 25.0 W laser power.

The intensity of the thermocapillary flow depends on material properties and laser process parameters. For a given material, the magnitude of thermocapillary flow decreases as the laser power and pulse duration decrease and the beam radius increases. In case of negligible thermocapillary flow (capillary regime), the molten surface features oscillate as stationary waves driven by surface tension and damped because of viscosity as shown in Fig. 1b. The features with higher frequency are more significantly damped. A smoother surface results from viscous damping without leaving significant processing marks as shown in Fig 2b. The process parameters were 21.2 µm laser beam radius, 4.20 µs pulse duration and 25.0 W laser power.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{Schematics of line profile by PLµP in thermocapillary a) and capillary b) regimes}
\end{figure}
Previous work was mostly focused on the PLµP in capillary regime [1-3]. The capillary regime surface prediction model can accurately predict the polished surface topography given initial surface profile, material properties and process parameters [2]. Recent research suggests that PLµP in the thermocapillary regime can produce smoother surfaces than capillary regime polishing. However, new surface features that are related to the laser spot overlap and step-over are produced. If the thermocapillary flow is significant, it can wipe out almost all of the original surface features and thus the final surface roughness is determined only by the introduced features. Therefore, it is of great interest to determine the geometry and dimension of the features.

A line profile of polished surface in thermocapillary regime is shown in Fig. 3, which is taken along the center line of polished surface as shown in Fig. 2a. As a first approximation the line profile can be modeled as a periodic triangle function, which is described by two parameters: the wavelength and the slope. The wavelength is the laser scanning velocity divided by pulsing frequency. The objective of this paper is to correlate the introduced feature slope (IFS) with material properties and process parameters through analytical heat transfer and fluid flow models. Using the wavelength and predicted slope of introduced features, the surface roughness produced by PLµP in the thermocapillary regime can be determined.

### MODELING APPROACH

The sample is heated by laser pulses one after another in PLµP. The laser is generally pulsed at a short duty cycle (≤20%), thereby allowing longer time for cooling than heating. Therefore, it is assumed that the material cools down to its initial temperature (e.g., room temperature) before being heated by the next laser pulse. Hence, modeling surface melting induced by a single laser pulse and subsequent solidification is sufficient to represent the process. Both the fluid flow and heat transfer models will estimate what happens due to a single pulse. To simplify the model, the material is assumed homogeneous and isotropic. The material properties are assumed constant (temperature independent). Chemical reaction is assumed not to occur since high-purity argon is flowing over the surface of the sample during PLµP. Ablation is not modeled because PLµP is conducted below the boiling temperature. The following sections will present the two separate analytical models for fluid flow (thermocapillary flow) and heat transfer. In this first attempt to predict the surface roughness these models are not coupled.

### FLUID FLOW MODEL

A large overlap (~80%) between two adjacent laser pulses has historically been applied in PLµP, therefore, only the surface features around the melt pool boundary are retained and contribute to the final surface roughness after PLµP as shown in Fig. 2a. For materials with a negative surface tension coefficient there is an outward flow of material that results in a ridge around the boundary. The IFS is expected to be directly related to the average displacement of a liquid particle divided by the melt pool radius because this value is indicative of the amount of liquid particles that reach the boundary. This normalized average displacement (NAD) will be estimated through analytical heat transfer and fluid flow models and compared with the IFS that is measured from polished surfaces in order to obtain the correlation between them.

Normalized average displacement (NAD) is defined as:

\[ l_n = \frac{\bar{v}_s \bar{t}_m}{\bar{r}_m} \]  

where, \( \bar{v}_s \) is the average surface velocity, \( \bar{t}_m \) is the average melt duration, and \( \bar{r}_m \) is the average melt pool radius. \( \bar{v}_s \) can be approximately estimated based on the force balance that governs thermocapillary flow. Assuming a flat surface,

\[ -\frac{\partial \gamma}{\partial T} \frac{\partial T}{\partial r} = \mu \frac{\partial v_s}{\partial z} \]  

where, \( \gamma \) is surface tension, \( T \) is temperature, \( r \) and \( z \) are position, \( \mu \) is the dynamic viscosity, and \( v_s \) is the surface ve-
locity in the radial direction. The left side of the equation is the surface tension gradient, the diving force of thermocapillary flow, while the right side is viscous stress, the resistant force. The derivative terms in Eqn. (2) can be approximated with the corresponding average values.

\[
\frac{\partial v}{\partial z} \approx \frac{v}{\bar{d}_m} \tag{3}
\]

\[
\frac{\partial T}{\partial r} \approx \frac{\Delta T}{\bar{r}_m} \tag{4}
\]

where, \(\bar{d}_m\) is the average melt depth, and \(\Delta T\) is the average surface temperature difference between the center and the boundary of the melt pool. Combining Eqns. (1) – (4), NAD is expressed as:

\[
l_n = -\frac{\partial v}{\partial T} \frac{\Delta T \bar{d}_m \bar{r}_m}{\mu \bar{r}_m^2} \tag{5}
\]

To estimate \(l_n\) with Eqn. (5), the values of \(\Delta T\), \(\bar{d}_m\), \(\bar{r}_m\) and \(\bar{r}_m\) will be determined from the analytical heat transfer model.

**HEAT TRANSFER MODEL**

The analytical heat transfer model of laser induced surface melting accounts for phase change using the equivalent heat capacity method. The equivalent volumetric heat capacity \(c_v'\) is defined as:

\[
c_v' = \rho(c_p + \frac{L}{T_b - T_0}) \tag{6}
\]

where, \(\rho\) is density, \(c_p\) is specific heat capacity, \(L\) is specific latent heat, \(T_b\) is boiling temperature, and \(T_0\) is initial temperature. The estimation assumes that latent heat is evenly distributed from the initial temperature to boiling temperature. The equivalent heat capacity would be a fairer estimate if the maximum temperature was used instead of boiling temperature in Eqn. (6). The present method underestimates the heat capacity in the liquid phase because the maximum temperature is less than the boiling temperature in PLµP. But it overestimates the heat capacity in the solid phase cause \(c_v' = \rho c_p\) for solid. These two effects will cancel each other to some extent.

The heat conduction is assumed to be one-dimensional, which is valid if

\[
\alpha t \ll \frac{r_b^2}{\tau} \tag{7}
\]

where, \(\alpha\) is the thermal diffusivity, \(\tau\) is the pulse duration, and \(r_b\) is the laser beam radius. It is satisfied for most materials if \(\tau < 10 \mu s\) and \(r_b > 10 \mu m\), which are common operational conditions for PLµP. The advection heat transfer in the liquid phase and the heat losses from convection and radiation on the surface are neglected since they are not significant compared with heat conduction into the bulk of the workpiece. Laser irradiation is considered as a surface heat source, which is valid for PLµP of metal alloys.

Based on the assumptions, the transient temperature field is governed by the one-dimensional conduction equation:

\[
\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial z^2} \tag{8}
\]

where, \(t\) is the time, \(z = 0\) is at the surface, and the \(z\)-axis points into the workpiece. The boundary conditions are surface heating given by Fourier’s law and constant temperature at infinite depth:

\[
-k \frac{\partial T}{\partial z} (z = 0, t) = \alpha_A q''(t) \tag{9}
\]

\[
T(z = \infty, t) = T_0 \tag{10}
\]

where, \(k\) is thermal conductivity, \(\alpha_A\) is laser absorptivity, and \(q''\) is laser-induced heat flux. Assuming laser power is constant during a laser pulse, \(q''(t)\) is expressed as:

\[
q''(t) = \left\{ \begin{array}{ll}
q_m', & 0 \leq t \leq \tau \\
0, & t > \tau
\end{array} \right. \tag{11}
\]

where, \(q_m'\) is laser heat flux while laser pulse is on. For a Gaussian laser intensity distribution with a beam radius \(r_b\) at 1/e², laser heat flux at the center of the beam is:

\[
q_m' = \frac{2P}{\pi r_b^2} \tag{12}
\]

where, \(P\) is laser power. The initial condition defines the temperature of the entire part when the laser pulse starts,

\[
T(z, t = 0) = T_0 \tag{13}
\]

By solving Eqns. (8) – (12), while the laser pulse is on (\(0 \leq t \leq \tau\)), the temperature field is given by:

\[
T = \frac{4\alpha_A P \sqrt{\tau} f \left( \frac{z}{2\sqrt{\alpha\tau}} \right)}{\pi r_b^2 c_v' \sqrt{\alpha}} + T_0 \tag{14}
\]

where, \(f(x)\) is the integral of the complementary error function. Numerical values of \(f(x)\) are tabulated [Abramovitz 1970 and Carlslaw 1988]. After the laser pulse ends (\(t > \tau\)), the temperature field is given by superposition of a power input starting at \(t = 0\) and the same but negative power input starting at \(t = \tau\):

\[
T = \frac{4\alpha_A P \sqrt{\tau} f \left( \frac{z}{2\sqrt{\alpha(t - \tau)}} \right) - \sqrt{\tau - \tau} f \left( \frac{z}{2\sqrt{\alpha(t - \tau)}} \right)}{\pi r_b^2 c_v' \sqrt{\alpha}} + T_0 \tag{15}
\]

Knowing the transient temperature field from Eqns. (14) and (15), the values of \(\Delta T\), \(\bar{d}_m\), \(\bar{r}_m\) and \(\bar{r}_m\) can be determined.

**AVERAGE SURFACE TEMPERATURE DIFFERENCE**

\(\Delta T\) is the average surface temperature difference between the center and the boundary of the melt pool. The temperature at the melt pool boundary remains constant and is equal to the melting temperature \(T_m\). The surface temperature at the center of the melt pool increases from \(T_m\) to a maximum \(T_{max}\) and then decreases from \(T_{max}\) to \(T_m\). If the average boundary temperature is \(T_m\) and the average center temperature is assumed to be the arithmetic average between \(T_m\) and \(T_{max}\), \(\Delta T\) is given by:

\[
\Delta T = \frac{T_{max} - T_m}{2} \tag{16}
\]

The maximum temperature occurs on the surface (\(z = 0\)) and the center (\(r = 0\)) of the melt pool at the end of a laser pulse. Substituting \(r = 0, z = 0, t = \tau\) and \(T = T_{max}\) in Eqn. (14),
\[ T_{\text{max}} = \frac{4\alpha_A P}{\pi^{1.5}r_b^2 c_v'\sqrt{\alpha}} + T_0 \]  

For simplicity, temperature is normalized in the following way:

\[ \theta = \frac{T - T_0}{T_n} = \frac{T - T_0}{T_{\text{max}} - T_0} \]

where, \( \theta \) is normalized temperature and \( T_n \) is normalizing temperature.

\[ T_n = T_{\text{max}} - T_0 = \frac{4\alpha_A P}{\pi^{1.5}r_b^2 c_v'\sqrt{\alpha}} \]

In this manner, \( \Delta T \) can be expressed as:

\[ \Delta T = \frac{(1 - \theta_m) T_n}{2} \]

where, \( \theta_m \) is normalized melting temperature as following:

\[ \theta_m = \frac{T_m - T_0}{T_n} \]

B. AVERAGE MELT POOL RADIUS

In a period around a single laser pulse, the melt pool radius increases from zero to a maximum \( r_m \), and then decreases to zero again. As a first approximation, \( r_m \) is assumed same as the laser beam radius.

\[ r_m = r_b \]

The average melt pool radius is assumed half of the maximum:

\[ \bar{r}_m = \frac{r_b}{2} \]

C. AVERAGE MELT DEPTH AND MELT DURATION

As with the average melt pool radius, the average melt depth is taken as half of the maximum value. The average melt depth is defined as full width at half maximum [1]. Unfortunately, explicit solutions to melt depth and duration are not available because the complementary error function is present. However, the dimensionless average melt depth \( \bar{d}_m \) and melt duration \( \bar{t}_m \) only depend on \( \theta_m \) if they are normalized in the following ways:

\[ \bar{d}_m = \frac{\bar{d}_m}{\sqrt{\alpha \tau}} \]

\[ \bar{t}_m = \frac{\bar{t}_m}{\tau} \]

\( \bar{d}_m \) and \( \bar{t}_m \) are obtained for various \( \theta_m \) and fitted by exponential functions (Fig. 4). The coefficients of determination \( R^2 \) are 0.98 and 0.99 for \( \bar{d}_m \) and \( \bar{t}_m \), respectively. The fitting functions are:

\[ \bar{d}_m = 2.28\exp(-3.78\theta_m) \]

\[ \bar{t}_m = 11.30\exp(-5.02\theta_m) \]

Combining Eqs. (24) – (27), the complete analytical solutions for average melt depth and melt duration can be obtained.
Table 1: Material properties of TiAl4V used in this study

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Surface Tension Coefficient (N/m-K)</td>
<td>-0.26×10^{-3}</td>
<td>[10]</td>
</tr>
<tr>
<td>Dynamic Viscosity (Pa·s)</td>
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<td>[11]</td>
</tr>
<tr>
<td>Thermal Conductivity (W/m-K)</td>
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<td>[12]</td>
</tr>
<tr>
<td>Equivalent Volumetric Heat (J/m^3·K)</td>
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<td>[12]</td>
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<tr>
<td>Thermal Diffusivity (m^2/s)</td>
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<td>[12]</td>
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<td>Laser Absorptivity</td>
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<td>[13]</td>
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<td>Initial Temperature (K)</td>
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<tr>
<td>Melting Temperature (K)</td>
<td>1928</td>
<td>[11]</td>
</tr>
</tbody>
</table>

EXPERIMENTAL METHOD

To determine the correlation between NAD and IFS, IFS was measured for various process parameters and compared with the predicted NAD. PLµP experiments on Ti6Al4V were carried out. Initial surfaces on the Ti6Al4V samples were produced using micro end milling with a 2-flute, 1-mm-diameter, tungsten-carbide (WC) tool at a spindle speed of 40,000 rpm and 800 mm/min feed rate. The basic experimental setup for PLµP is illustrated in Fig. 6. A 1070 nm fiber laser (SPI Lasers, Model: SP-200C-W-S6-A-B) was used for experimentation. The laser was directed into a scan head (ScanLab HurryScan 14 mm) to allow for high-speed, two-dimensional scanning at a beam velocity of up to 1.5 m/s. The scan head was controlled by a ForeSight control card (LasX Industries) and furnished with an f-theta objective (Linos f-theta-Ronar, Model: 4401-302-000-20/21) with a focal length of 100 mm. A z-axis manual stage was used to adjust the laser spot size and accommodate samples of various thicknesses.

Surface profiles were measured using a white-light interferometer (Zygo NewView 6300). The interferometry technique also captures the surface curvature. The mean plane was computed with a least squared error method and removed. IFS was calculated along the center line of a polishing path based on the frequency spectrum of the line profile. The roughness of the surface was characterized using linear average surface roughness, $R_a$, after filtering the waviness of the surface using a high pass Gaussian spatial filter with a waviness cut-off frequency of 12.5 mm^{-1} (0.08 mm cut-off wavelength) [14, 15].

RESULTS

Note that the normalized average displacement (NAD) is predicted from the analytical model in Eqn. (28) and the introduced feature slope (IFS) is measured after PLµP experiments. Fig. 7 shows both NAD and IFS as functions of beam radius at the same pulse duration (1.56 µs) and laser power (48.6 W). NAD and IFS decrease rapidly following the same curve as the laser beam radius increases. Fig. 8 shows NAD and IFS as functions of pulse duration at the same beam radius (21.2 µm) and laser power (25.0 W). Both NAD and IFS increase in parallel as pulse duration increases and follow a similar trend. Fig. 9 shows both NAD and IFS as functions of laser power at the same beam radius (21.2 µm) and pulse duration (1.56 µs). Both NAD and IFS increase nearly linearly as laser power increases.
Fig. 9: Normalized average displacement (NAD) and introduced feature slope (IFS) as functions of laser power (21.2 µm laser beam radius and 1.56 µs laser pulse duration)

NAD and IFS appear to be closely correlated since they follow very similar trends as a function of all three laser parameters (Figs. 7–9). Fig. 10 plots IFS as a function of NAD and a linear curve fit. The coefficient of determination $R^2$ is 0.80, which indicates a successful regression. The fitting function is given by:

$$\delta_f = 0.00445 l_n$$

(29)

The high quality of fitting confirms that NAD is a great indicator for IFS. The deviation from a perfect fit could be mostly due to the variation in original unpolished surface.

Fig. 10: Introduced feature slope (IFS) as a function of normalized average displacement (NAD)

Since Eqn. (29) directly relates IFS to NAD, it can be used to predict the average surface roughness contribution from the introduced features during thermocapillary flow in PLµP. Assuming the introduced features produce a periodic triangular function, the linear average surface roughness $R_a$ is given by:

$$R_{a,f} = \frac{\delta_f \lambda_f}{8}$$

(30)

where $\lambda_f$ is the wavelength of the features, which is simply the laser scanning velocity $v_{sc}$ divided by the pulsing frequency $f_p$:

$$\lambda_f = \frac{v_{sc}}{f_p}$$

(31)

Combining Eqns. (29) – (31), the contribution of the introduced features to surface roughness is:

$$R_{a,f} = \frac{0.000556 l_n v_{sc}}{f_p}$$

(32)

Since this estimation only considers introduced features and ignores features remaining from the original surface, it should be considered a lower bound to the average surface roughness achievable in the thermocapillary regime. Fig. 11 shows that the measured surface roughness is almost always greater than the predicted roughness (Eqn. 32). As NAD increases, two effects increase simultaneously and compete with each other: smoothing of the original surface and roughing by introduced features. With increasing NAD, the smoothing effect becomes less and less significant and finally saturates, and the roughing effect dominates. It is thus seen that the measured surface roughness decreases, reaches a minima and then increases again as NAD increases. The difference between the measured $R_a$ and the predicted $R_{a,f}$ decreases, and the measured $R_a$ asymptotically approaches the predicted $R_{a,f}$, as NAD increases. This shows that the predicted $R_{a,f}$ becomes more accurate as NAD, hence thermocapillary flows, increase.

Fig. 11: Measured $R_a$ and the predicted $R_{a,f}$ as a function of normalized average displacement (NAD) for PLµP of Ti6Al4V

CONCLUSIONS

Analytical heat transfer and fluid flow models are derived for a single laser pulse induced melting. The normalized average displacement (NAD) of a molten metal particle is introduced as a parameter for estimating the shape of the resolidified melt pool when thermocapillary flows are present. The normalized average displacement increases with increasing laser power and pulse duration and decreasing beam radius. The normalized average displacement and the introduced feature slope (IFS) by thermocapillary flow were found to be strongly correlated. The introduced feature slope represents new surface features that are a result of thermocapillary flows moving material to the outer edges of the melt pool.
and the subsequent overlapping of multiple laser spots. For PLµP of Ti6Al4V a strong correlation between the estimated NAD and measured IFS is found. The correlation is used to predict the lower bound of the average surface roughness produced by PLµP in the thermocapillary regime, i.e., the best polishing achievable in this regime. The predictions match well with experimentally measured values when stronger thermocapillary flows are present. As the thermocapillary flows decrease, and the capillary regime is approached, the predictions underestimate the actual surface roughness. This method will be useful tool to guide PLµP parameter selection and process optimization. Combining this model with the existing model for predicting average surface roughness in the capillary regime will enable better prediction of the outcome of PLµP over a wide range of operating conditions.

ACKNOWLEDGMENT

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NOMENCLATURE

<table>
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<tr>
<th>Symbols</th>
<th>Description</th>
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<td>c_p</td>
<td>Specific heat</td>
<td>J/kg-K</td>
</tr>
<tr>
<td>c_v'</td>
<td>Equivalent volumetric heat</td>
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<td>d_m</td>
<td>Average melt depth</td>
<td>µm</td>
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<tr>
<td>d_n</td>
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<td>k</td>
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Greek symbols

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<th>Symbol</th>
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<tr>
<td>α</td>
<td>Thermal diffusivity</td>
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<td>α_l</td>
<td>Laser absorptivity</td>
<td>-</td>
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<td>γ</td>
<td>Surface tension</td>
<td>N/m</td>
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<tr>
<td>δ_f</td>
<td>Introduced feature slope = IFS</td>
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</tr>
<tr>
<td>λ</td>
<td>Feature wavelength</td>
<td>µm</td>
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<tr>
<td>μ</td>
<td>Dynamic viscosity</td>
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<tr>
<td>ρ</td>
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<tr>
<td>τ</td>
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<td>s</td>
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<tr>
<td>ΔT</td>
<td>Average temperature difference</td>
<td>K</td>
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<tr>
<td>θ</td>
<td>Normalized temperature</td>
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</tr>
<tr>
<td>θ_m</td>
<td>Normalized melting temperature</td>
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</table>

Acronyms

IFS = Introduced feature slope = \( \delta_f \)

NAD = Normalized average displacement = \( l_n \)

REFERENCES


