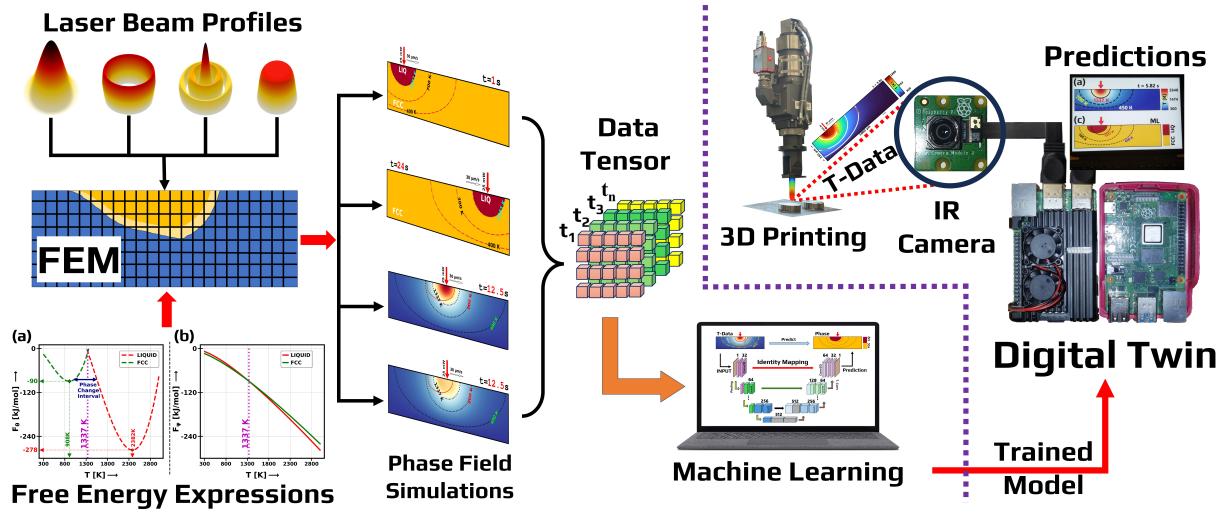


Graphical Abstract

A robust phase-field U-net framework to digitally identify the melt pools from different heat source models in real time.

Upadesh Subedi



Highlights

A robust phase-field U-net framework to digitally identify the melt pools from different heat source models in real time.

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- Phase field modelling of Laser heat source types
- Virtual DT deployable as physical DT
- PSI-U-Net enhances the deployability of PFM by 1.4E4 folds.
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- Digital Twin

A robust phase-field U-net framework to digitally identify the melt pools from different heat source models in real time.

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ABSTRACT

The uncertainties in the interaction between laser and microstructural interfaces pose a major hindrance to precision engineering in additive manufacturing. Proper assessment of the role of laser heat source types on microstructure evolution and phase transitions is crucial for understanding the process-property relationship of 3D-printed parts. To address this, we present a multiphysics computational study exploring thermal distribution, phase transformation, and meltpool-flow across different laser beam profiles and free energy expressions in an unary Au system. A detailed comparison of the microstructural pathways developed under four laser beam shapes (Gaussian, Flat-Top, Ring, and Bessel) along with two different mathematical expressions for free energy was conducted. Furthermore, **U-Net machine learning models** were trained on the simulation data to correlate temperature distribution with meltpool phase and its flow velocity, achieving training, validation, and test accuracies of 0.9992, 0.9989, and 0.9988, respectively. Additionally, we developed an interactive framework based on the trained model that can predict phase evolution from a user-supplied temperature distribution array. This framework provides a foundation for future work in constructing a Digital Twin model capable of real-time phase evolution prediction in experimental setups.

1. Introduction

[1]

This study presents a comprehensive computational analysis of how four different laser beam profiles affects the microstructure evolution in a unary Au-system during laser processing. Using Phase-Field (PF) simulations, we traced the meltpool geometry, its area, and the thermal history within the computational domain. A quantitative comparison between two different free energy expressions driving the phase transition was also carried out. The first approach used a parabolic free energy function fitted to thermodynamic data (fine-tuned expression), while the second relied on case equations extracted directly from a Thermodynamic Database (TDB) file using a Python script. Comparisons of free energy expressions in phase-field modeling are rare, as exact thermodynamic expressions are difficult to obtain, leading most studies to rely on polynomial fits [2]. Moreover, many such studies are often limited to free energy expressions defined at two fixed temperatures for two phases [3]. In this work, we have integrated thermodynamic expressions for free energies as a function of temperature, making the phase transition process inherently non-isothermal. Our study employs the MOOSE Framework as the multi-physics simulation environment [4, 5], where three coupled physical phenomena are solved: heat-transfer, phase-field and fluid-flow, using Finite Element Method (FEM).

As described in our previous work [6], most computational studies of laser processing treats thermal and phase

diffusion as identical. This assumption leads to the presumption that the LIQUID phase (meltpool) forms instantaneously upon reaching melting temperature, overlooking the real physical behavior in laser-based additive manufacturing where phase diffusion lags behind the thermal diffusion front [7]. In this study, we found that implementing the TDB-based free energy expression replicates the real-world behavior of the lead-lag dynamics between phase and thermal fronts. The main reason this distinction is often overlooked in contemporary research is likely computational cost and efficiency. However, ignoring it fails to capture the intricate interplay between the two diffusion fronts, which in turn influences other physical phenomena such as fluid flow, thermal conductivity, and phase densities. In addition to phase-field modeling, the FEM simulations generated data were used to train machine learning models capable of predicting the LIQUID phase, its shape, **areas** and its **velocity**, using the temperature distribution of the domain as input.

In the following section, we discuss in detail the types of laser heat sources, the expressions for thermodynamic driving forces, temperature-dependent material properties, and machine learning architectures. We also outline the conceptualization of physics informed virtual digital-twin for laser processing using the trained ML model. Finally in the Results and Discussion Section 8, we explore the effects on phase evolution, temperature distribution, and meltpool flow characteristics under different laser heat sources, and distinct free-energy expressions. For comparison of the laser beam profiles, the laser power (P), scan speed (v), and beam outer radius (r_x) were kept constant across all simulations.

2. Initial and Boundary Conditions

Simulations were carried out in a computational domain of $1000 \mu\text{m} \times 250 \mu\text{m}$ in the x-z plane, as shown in Figure

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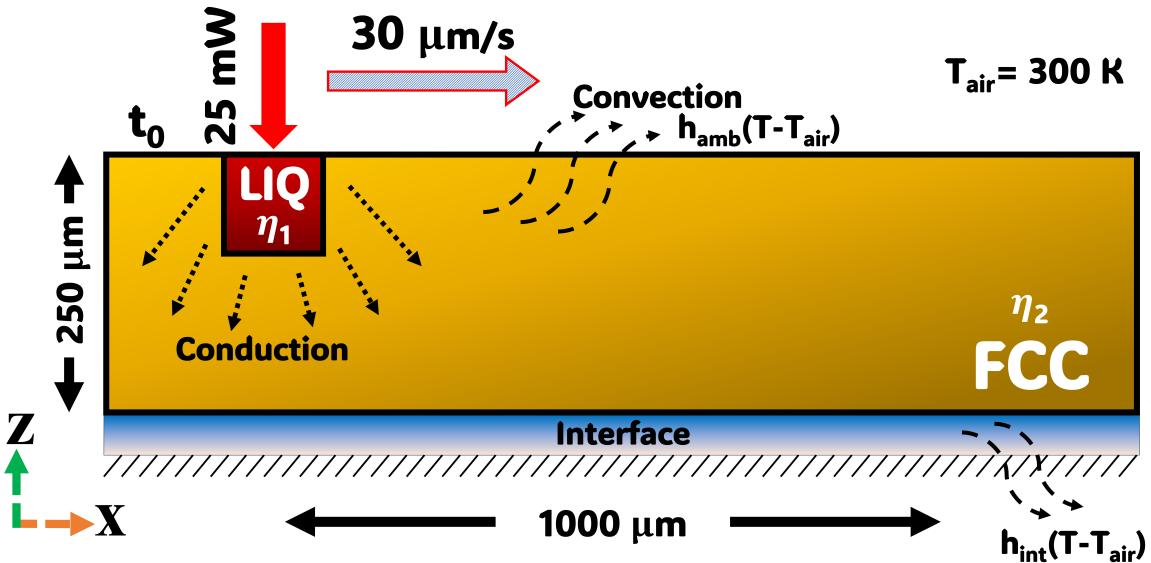


Figure 1: The schematic diagram of the computational domain setup illustrates the laser-induced phase evolution in Phase Field Modeling at time t_0 . A $1000 \mu\text{m} \times 250 \mu\text{m}$ section of a unary Au system in the x - z coordinate system represents the simulation's length scale. The computational system rests on an interface at the bottom, with ambient air surrounding it on the other three sides. Heat transfer into the system occurs through conduction, while radiative and convective heat transfer occurs out of the system through the air and interface, as shown in the figure. A laser heat source with a power of 25 mW was irradiated on the top surface of the domain, positioned $125 \mu\text{m}$ from the top-left corner, with a scan speed of $30 \mu\text{m/s}$, indicated by the red arrow just above the LIQUID phase. The initial LIQUID phase area, denoted by ' η_1 ' and representing the melt pool, is $2500 \mu\text{m}^2$, shown as a red-colored block, while the solid gold region is represented by the FCC phase, denoted by ' η_2 ' in the yellow-colored remaining area in the domain. The computational domain, phase structure, and initial areas, along with the laser processing parameters (power and scan speed), are kept identical across multiple simulations involving different laser beam profiles.

1. The system consists of two phases: LIQUID, representing molten gold, and FCC representing solid gold. At the initial time (t_0), a laser beam with power of 25 mW was irradiated on the top surface at a distance of $125 \mu\text{m}$ from the left, with a scan speed of $30 \mu\text{m/s}$. The initial area of melt pool was designed to be $2500 \mu\text{m}^2$. The computational domain is surrounded by an ambient environment at a temperature $T_{\text{air}} = 300 \text{ K}$ on three sides (left, right, and top), while the bottom rests on an interface with a heat transfer coefficient $h_{\text{int}} = 11500 \text{ W/m}^2\text{K}$ [8]. The convective heat transfer coefficient of the surrounding air is taken as $h_{\text{amb}} = 50 \text{ W/m}^2\text{K}$ [9], while the emissivity for radiative heat transfer is set to 0.3 [10]. To accurately assign the material properties of different phases, including densities, specific heat capacity, thermal conductivities, and melt pool viscosity, under non-isothermal conditions, these properties were defined as the function of temperature. The detailed formulations are provided in Section 6.

3. Non-isothermal phase field model

The phase field model consists of two phases: LIQUID (melt pool) and FCC (solid), which are represented by the non-conserved order parameter ' η ' and ' $1 - \eta$ ' respectively. The value of ' η ' is set to 1 inside the LIQUID phase and 0 at the FCC phase. The conserved variable 'composition' remains constant throughout the domain as this work follows

the evolution of phases in a single-component system. Thus, this study focuses on the two phases and their transformation induced by laser heat deposition. For this setup, a swift transition of material properties between phases with thermodynamic consistency is required which is achieved using the interpolation function $h_i(\eta)$ introduced by Moelans [11], as presented in Equation 1.

$$h_i = \frac{\eta_i^2}{\sum_{k=1}^N \eta_k^2} \quad (1)$$

In the above equation, N and i represents total number of order parameters and specific phase in the system. The driving force dictating the morphological changes of microstructure in the domain is the total free energy of the system. With an external heat source, the total free energy (F_{total}) can be modeled as the combination of bulk free energy (F_{bulk}) and interfacial free energy (F_{int}), as given by Equation 2.

$$F_{\text{total}} = F_{\text{bulk}} + F_{\text{int}} = \int_V (f_{\text{bulk}} + f_{\text{int}}) dV \quad (2)$$

here, the bulk and interfacial energies are expressed in terms of free energy densities (energy per unit molar volume

of Au). The bulk free energy density (f_{bulk}) and interfacial free energy density (f_{int}) are further expressed in Equations 3 and 4 respectively.

$$f_{bulk} = \sum_i h_i f_{bulk}^i = \sum_i \frac{F_i(T)}{V_m} \quad (3)$$

In Equation 3, h_i represents the interpolation function, whereas f_{bulk}^i denotes the bulk free energy density of the i^{th} phase. V_m is the molar volume of gold, with a value of $10.21 \text{ cm}^3/\text{mol}$ [12], taken for both phases. Additionally, $F_i(T)$ represents the temperature-dependent Gibbs free energy of phase ' i '. The free energy expressions of individual phases, their formulation, and their temperature-dependent plots are presented in detail in Section 4.

$$f_{int} = m f_{barrier} + \frac{\kappa}{2} \sum_i (\nabla \eta_i)^2 \quad (4)$$

where, m and κ are the model parameters associated with interfacial energy ($\sigma [\text{J}/\text{m}^2]$) and diffused interface width ($\delta [\text{m}]$) as follows:

$$m = \frac{6\sigma}{\delta} \quad (5)$$

$$\kappa = \frac{3}{4} \delta \sigma \quad (6)$$

In this study, we have set the value of the interface width δ to be $10 \mu\text{m}$ and the interfacial energy to 0.5 J/m^2 . The term $f_{barrier}$ in Equation 4 is a fourth-order Landau polynomial of the phase field variable, expressed as follows:

$$f_{barrier} = \sum_i \left(\frac{(\eta_i)^4}{4} - \frac{(\eta_i)^2}{2} \right) + \gamma \sum_i \sum_{j \neq i} \eta_i^2 \eta_j^2 + \frac{1}{4} \quad (7)$$

During laser processing, the spatio-temporal tracking of non-conserved phase field variable, the order parameter (η), provides an accurate description of phase transformation. Equation 8 describes such evolution this variable as:

$$\frac{\partial \eta_i}{\partial t} = -L(\eta_1, \dots, \eta_N) \left(\frac{\partial f_{bulk}}{\partial \eta_i} - \nabla \cdot \frac{\partial f_{int}}{\partial \nabla \eta_i} \right) \quad (8)$$

where, $L(\eta_1, \dots, \eta_N) = L^i$ which is defined as follows:

$$L^i = \frac{\sum_{i=1}^N \sum_{j>1}^N L_{ij} \eta_i^2 \eta_j^2}{\sum_{i=1}^N \sum_{j>1}^N \eta_i^2 \eta_j^2} \quad (9)$$

The interfacial mobility in Equation 9 is further approximated as follows:

$$L_{ij} = \frac{4m}{3\kappa} \times \frac{M^i + M^j}{2} \quad (10)$$

here, M^i and M^j are the phase mobilities of the two adjacent phases. Similarly, for the heat deposited by the laser source, heat transfer follows the partial differential equation presented in Equation 11.

$$\rho^i C p^i \left(\frac{\partial T}{\partial t} + \vec{u} \cdot \nabla T \right) = k_{th}^i \nabla^2 T + Q_{laser} \quad (11)$$

In the above equation, temperature is denoted by T at time t . The density, specific heat capacity, and thermal conductivity of phase ' i ' are represented by ρ^i , $C p^i$, and k_{th}^i , respectively. The flow velocity inside the meltpool is given by \vec{u} , which contributes to convective heat transfer, while the external laser heat source is denoted by Q_{laser} . The viscosity, surface tension, and associated Marangoni effect inside the inside meltpool flow is further discussed in Section 6.

4. Thermodynamic Driving Force

For computational efficiency and faster numerical convergence, polynomial expressions of free energy are often preferred, especially parabolic expressions of second-order polynomials, which are widely used for modeling binary and ternary alloy systems [13, 14, 15]. Although, polynomial expressions with $n > 2$ generally offer more accurate descriptions, they are computationally expensive due to the compositional complexities they introduce into the diffusion equations. In this study on laser processing of pure element, the free energy depends solely on temperature (T), with constant composition and pressure. This condition allows for the flexibility to expand the polynomial expression beyond traditional parabolic forms to include logarithmic terms. Accordingly, the free energy for pure Au under temperature change is best described by the fine-tuned expression F_θ , as presented in Equation 12, derived in a manner similarly to [16, 17]. Being a continuous function for a given phase, this expression ensures numerical stability. In contrast, the TDB-extracted expressions (F_ψ) are piecewise continuous even within a single phase, as presented in Equation 12. These expressions are based on Thermodynamic Data Base file formulated by Khvan et al. [18]. From an engineering perspective, many applications, such as the development of digital-twins may prefer fitted/fine-tuned expressions when computational efficiency is the primary requirement.

In Equation 12, the coefficients $A, B, C, D, E, F, G, H, I, J$ and T_{th} , with subscripts ' θ ' and ' ψ ', represent the thermodynamic coefficients of the free energy function for the fine-tuned and TDB-based expressions, respectively. The coefficient values are listed in Table 1 for both the LIQUID and FCC phases. The variable ' T ' depicts the temperature dependence of the free energy in both expressions.

$$F_\theta = T_{th} \left[A_\theta - B_\theta - C_\theta(T-T_0) + D_\theta(T-T_0) \ln(E_\theta T) + F_\theta(T-T_0)^2 + G_\theta(T-T_0)^3 + H_\theta T^{-1} \right]$$

$$F_\psi = \begin{cases} LIQUID & : A_\psi T \ln \left[1 - \exp(-B_\psi T^{-1}) \right] - RT \ln \left[1 + \exp \left(C_\psi (D_\psi - E_\psi T) T^{-1} \right) \right] - F_\psi T^2 - G_\psi \\ FCC & : A_\psi T \ln \left(1 - \exp(-B_\psi T^{-1}) \right) - C_\psi + \begin{cases} T < 1337.33 & : D_\psi T^2 - E_\psi T^3 \\ T \geq 1337.33 & : F_\psi T^{-11} - G_\psi T^{-5} - H_\psi T \ln(T) + I_\psi T + J_\psi \end{cases} \end{cases}$$
(12)

Table 1

Coefficients of thermodynamic constants for the Free energy expressions.

Coeff.	LIQUID	FCC	Unit	Coeff.	LIQUID	Unit	FCC	Unit
A_θ	1337	300	J/mol	A_ψ	24.9435	J/mol K	24.9435	J/mol K
B_θ	24474	515	J/mol	B_ψ	126.6874	K	126.6874	K
C_θ	16.2	-46.2	J/mol K	C_ψ	-0.12027	–	6103.6566	J/mol
D_θ	24.5	-13.5	J/mol K	D_ψ	19700	K	-0.001281	J/mol K ²
E_θ	0.00214	0.1985	1/K	E_ψ	14.917	–	-4.02×10 ⁻⁷	J/mol K ³
F_θ	0.04512	-0.001	J/mol K ²	F_ψ	0.00067	J/mol K ²	1.55×10 ³⁶	JK ¹¹ /mol
G_θ	1.9×10 ⁻⁵	2.0×10 ⁻⁵	J/mol K ³	G_ψ	326.3861	J/mol	-2.27×10 ¹⁸	JK ⁵ /mol
H_θ	-17.4	-0.001	JK/mol	H_ψ	–	–	-2.0566	J/mol K
T_0	2662	121	K	I_ψ	–	–	9.8072	J/mol K
T_{th}	10.412	9.03	–	J_ψ	–	–	3898.778	J/mol

The two free-energy formulations were combined with four different laser beam profiles to analyze their effects on phase growth, while keeping other laser parameters constant. The expressions, and their temperature-dependent plots are presented in Equation 12 and Figure 2, respectively. As shown in Figure 2, the F_θ curves for the FCC and LIQUID phases display a distinct phase-change interval, while the F_ψ curves derived from the TDB expressions do not exhibit this feature.

A sharp or narrow phase-change interval, such as in pure metals, causes rapid phase transition during melting and solidification. This can result in residual stresses [19, 20], and may complicate numerical convergence [21]. In contrast, when modeling compositionally-complex alloys, a broader phase-change interval can play an important role in ensuring stability and convergence. Thus, a fine-tuned (fitted) free energy function can be effectively applied to multicomponent system, even with only limited energy-temperature thermodynamic data are available. On the other hand, when a thermodynamic database (.TDB) file is available, free energy expressions can be extracted directly and implemented into a FEM solver using a simple Python script, thereby formulating the required temperature-dependent expressions. This direct TDB-based approach not only ensures thermodynamic consistency but also enhances numerical accuracy. As observed in Figure 2(b), the near absence of a phase-change interval implies a very narrow temporal range over which multiple phases co-exist. This leads to rapid interpolation of material and phase-dependent properties, thereby improving the numerical stability of the model.

5. Laser Beam Heat Sources

The Gaussian laser beam is the most widely used profile for modeling laser-based melting and solidification in additive manufacturing, owing to its simple mathematical form. The beam peaks intensity at the center and decays outwards exponentially, creating steep thermal gradients that influences microstructure evolution [23, 24, 25]. However, uniform heating is often desired in practice to reduce thermal gradients, motivating alternative beam profiles such as the Flat-Top beam, which truncates the Gaussian peak to produce a uniform intensity region, and the Ring-shaped beam, which distributes heat in an annular pattern with maximum intensity at a specific radius [26]. The Bessel beam combines both characteristics, featuring a Gaussian-like center surrounded by concentric rings defined by the zeroth-order Bessel function [27]. Experimental studies confirm that beam shape strongly affects meltpool geometry and microstructure: Galbusera et al. [28] showed that varying beam shape alters meltpool aspect ratio and depth, while Wischeropp et al. [29] found that donut-shaped beams reduce defects in AlSi10Mg. Tumkur et al. [30] further demonstrated that Bessel beam improve control over meltpool dynamics, lowering porosity and keyhole defects. These findings highlight the critical role of beam profile in determining microstructural and mechanical properties, underscoring the value of computational modeling for deeper insights into phase transformation, heat flow and defect prediction, areas difficult to probe experimentally. In this work, we compare four laser beam profiles: Gaussian, Flat-Top, Ring and Bessel, under identical process parameters in laser-aided phase-field simulations of a pure Au system. The effects on meltpool shape, area, flow and temperature distribution are

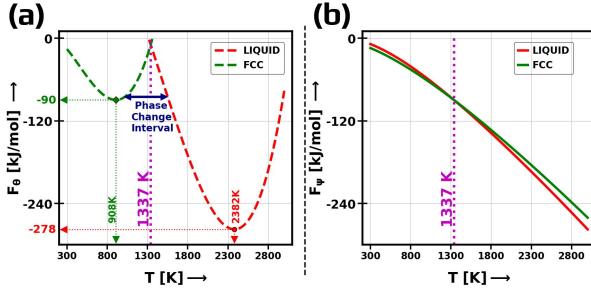


Figure 2: Plot depicting the graphical representation of two types of free energy expression used for the phase field simulation of laser processed unary Au system. In (a) the graph showcases the free energy expression based on higher order polynomial-logarithmic functions obtained from thermodynamic data fitting also referred as *fine-tuned expression* represented by $F\theta$ in Equation 12. The two curves in dashed green and red colors in (a) corresponds to FCC and LIQUID phases of unary Au system respectively. The curve indicates the FCC phase as more stable phase below the melting temperature of 1337 K with the global minima at around 908 K whereas, to the right of the 1337 K vertical line, LIQUID phase is highly stable with a global minima at around 2382 K. The gap between FCC and LIQUID curves at around 1337 K is recognised as Phase Change Interval where the phase transition is expected to occur. This gap also indicates the diffused zone between two phases where both phases can co-exists and is the result of fitting expressions. Whereas, in (b) the free energy expression extracted directed from the '.TDB' file is plotted with respect to Temperature, this expression $F\gamma$ is referred as TDB based expression in the paragraph sections represented by the Case Equation 12. Similar to (a) the red colored curve represents the LIQUID phase with lower free energy values in the temperature range above 1337 K while green curve indicates the FCC phase which is more stable than LIQUID phase below melting temperature. The intriguing aspect of TDB based free energy plot is the absence of phase change interval representing a rather small window of temperature where the phase transformation occurs near the melting temperature. Such presence and absence of phase change interval in (a) and (b) differentially dictates the rate of information relay of thermal history to the structural evolution making a striking difference in the overall simulation results.

analyzed, revealing a lead-lag dynamic between heat and mass diffusion fronts.

5.1. Gaussian Beam

Among the four heat source types, the Gaussian beam serves as the reference case due to its simple formulation and well-understood thermal behavior [31, 32, 33]. It produces maximum irradiance at the center, decaying radially to form the characteristic Gaussian distribution. The irradiance (I_G) is defined in Equation 13 [27, 34], where r_G denotes the effective beam radius corresponding to $\frac{1}{e^2}$ of the peak intensity, P is the laser power, η_e is efficiency of laser power to heat conversion, and C_a and C_b are constants whose values are listed in Table 2. A representative Gaussian heat source is illustrated in Figure 3 with a 3D and cross-sectional view.

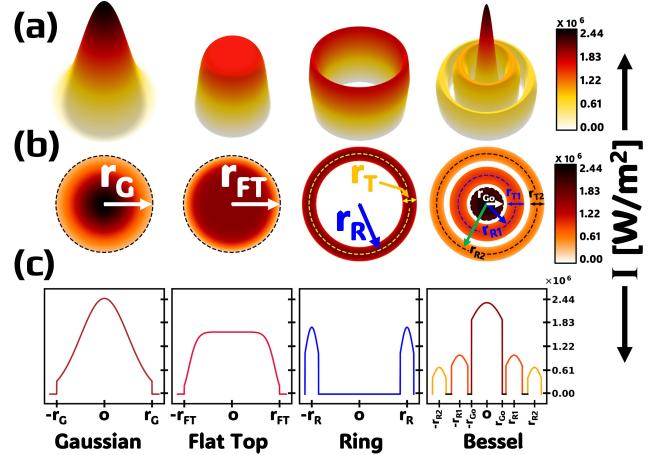


Figure 3: A visual demonstration of four different laser beam profiles: Gaussian, Flat-Top, Ring and Bessel used in the study for laser aided phase field simulation of unary Au system. (a) 3D visualization of laser intensity for four beam shapes with an equivalent outer radius of 70 μm [22]. The peak intensity at the centre of Gaussian beam is calculated to be $2.44 \times 10^6 \text{ W/m}^2$ whereas for Flat-Top, Ring and Bessel beams are $1.58 \times 10^6 \text{ W/m}^2$, $1.70 \times 10^6 \text{ W/m}^2$ and $2.33 \times 10^6 \text{ W/m}^2$ respectively as depicted by the colorbar. (b) Showcases the top view of the laser intensities for the four corresponding beams of (a). The Gaussian and Flat-Top beam radius is represented by r_G and r_{FT} similarly, r_R and r_T denotes the Ring beam radius and thickness of the ring. For the Bessel beam with one central beam with two outer ring beams, the central beam radius is denoted by r_{G_0} , whereas two ring beams radius are r_{R_1} and r_{R_2} with respective ring thickness of r_{T_1} and r_{T_2} as shown in the (b). The side view of the irradiance profile of laser sources showcasing the intensity radially outwards is presented in (c) with y-axis representing the irradiance level and x-axis representing the radial distance from the centre of the beam.

$$I_G = \frac{P}{\pi r_G^2} C_a \eta_e \exp \left[-C_b \left(\frac{r^2}{r_G^2} \right) \right] \quad (13)$$

5.2. Flat Top | Super Gaussian Beam

The Flat-Top or Super-Gaussian beam provides a near-uniform intensity across its radius with a sharp drop at the edges, enabling more homogeneous heating of the material [34, 35]. Its irradiance (I_{FT}) is defined in Equation 14 [27, 36, 34, 37], where r_{FT} is the effective beam radius. All other processing parameters P , η_e , C_a and C_b are kept identical for all four laser profiles, while the additional parameters k and $\Gamma(1/k)$ represents the super-Gaussian order, set to 4.2 in this study and gamma function respectively [27]. The Flat-Top beam profile is illustrated in the second column of Figure 3, with 3D, top and side views.

$$I_{FT} = \frac{P}{\pi r_{FT}^2} \frac{k}{\Gamma(1/k)} C_a^{1/k} \eta_e \exp \left[-C_b \left(\frac{r^2}{r_{FT}^2} \right)^k \right] \quad (14)$$

5.3. Ring Beam

The ring laser beam features a hollow circular profile with maximum intensity along its circumference and minimal intensity at the center. This configuration promotes outward-to-inward heat flow, helping achieve more uniform temperature distribution and reduced thermal defects [38, 39]. The beam introduces one additional process parameter, the ring width, which controls the energy spread across the domain [40, 41]. The irradiance (I_R) for the ring beam is defined in Equation 15 [25, 26, 42, 43]. All parameters (P , η_e , C_a , C_b) are identical to those used in Gaussian and Flat-Top sources, while r_R and r_T represents the ring radius and ring thickness respectively.

$$I_R = \frac{P}{\pi r_T^2 Y(r_R, r_T)} C_a \eta_e \exp \left[-C_b \left(\frac{(r - r_R)^2}{r_T^2} \right) \right] \quad (15)$$

The radial distribution function $Y(r_R, r_T)$, as described by Moore et al. [25], accounts for the combined influence of ring radius and thickness through an exponential decay and complementary error function expressed as:

$$Y(r_R, r_T) = \exp \left(\frac{-r_R^2}{2r_T^2} \right) + \frac{r_R}{r_T} \sqrt{\frac{\pi}{2}} \operatorname{erfc} \left(\frac{-r_R}{\sqrt{2}r_T} \right)$$

A visual representation of the ring beam is shown in the third column of Figure 3, including 3D, top and side views in (a), (b) and (c) respectively.

5.4. Bessel Beam

The Bessel beam profile consists of a core beam with concentric ring beams extending radially outward, with irradiance gradually decreasing along the radius. In this study, we consider a central Gaussian-type beam with two concentric ring beams, where each beam radius corresponds to the zeros of the zeroth-order Bessel function. In the literature, the radius of the central beam in a Bessel beam is often defined as the radial distance at which irradiance drops to $\frac{1}{e^2}$ of the beam spot's peak irradiance [44]. However, here we define the radius of the central beam as the location of the first zero of the Bessel function. For the radii of the two concentric ring beams, we use the second and third zeros of the Bessel function. The visualization of the Bessel beam is shown in the fourth column of Figure 3, with the 3D, top, and transverse profiles displayed in 3(a), (b), and (c), respectively. As this study aims to compare the effects of four laser beams under similar processing parameters, the total power of the Bessel beam is divided among the three beams, with attenuation coefficients a_0 , a_1 , and a_2 , as given in the mathematical expression in Equation 16 for the Irradiance (I_B) [27, 44].

Table 2
Laser processing parameters.

Coeff.	Gaussian	Flat-Top	Ring	Bessel	Unit
P	25	25	25	25	mW
C_a	2	2	2	2	–
C_b	2	2	2	2	–
α	0.75	0.75	0.75	0.75	–
r_G	70	–	–	–	μm
r_{FT}	–	70	–	–	μm
k	–	4.2	–	–	–
r_R	–	–	70	–	μm
r_T	–	–	20	–	μm
r_{G_0}	–	–	–	22.65	μm
r_{R_1}	–	–	–	40	μm
r_{T_1}	–	–	–	30	μm
r_{R_2}	–	–	–	70	μm
r_{T_2}	–	–	–	20	μm
a_0	–	–	–	0.1	–
a_1	–	–	–	0.5	–
a_2	–	–	–	0.4	–

$$I_B = \frac{C_a a_0 P \alpha}{\pi r_{G_0}^2} \exp \left[-C_b \left(\frac{r^2}{r_{G_0}^2} \right) \right] + \frac{C_a a_1 P \alpha}{\pi r_{T_1}^2 Y(r_{R_1}, r_{T_1})} \exp \left[-C_b \left(\frac{(r - r_{R_1})^2}{r_{T_1}^2} \right) \right] + \frac{C_a a_2 P \alpha}{\pi r_{T_2}^2 Y(r_{R_2}, r_{T_2})} \exp \left[-C_b \left(\frac{(r - r_{R_2})^2}{r_{T_2}^2} \right) \right] \quad (16)$$

here, C_a and C_b are the constant coefficients, P is the power of the laser, α is the absorptance. The radius of the central Gaussian beam is denoted by r_{G_0} , while the radii of the two concentric rings are represented as r_{R_1} and r_{R_2} , with their respective beam thicknesses given by r_{T_1} and r_{T_2} . The three attenuation coefficients, a_0 , a_1 , and a_2 , are unitless values that sum to 1, dividing the total supplied power P into P_{a_0} , P_{a_1} , and P_{a_2} , respectively. The numerical values of these process parameters are provided in Table 2.

6. Material Properties

In a phase-field simulation involving laser-induced phase transformations, the material properties of the different phases play an important role in phase evolution itself. Properties such as phase mobilities, thermal conductivities, densities, and specific heat capacity are highly influential in determining the overall microstructural evolution and the kinetics of the reaction. To accurately model the phase transformation phenomenon, these properties should be defined properly and precisely, as they themselves depend on temperature. Therefore, using constant values for thermo-physical properties in a non-isothermal laser processing simulation results in a highly inaccurate and unreliable model.

Table 3
Material Properties

Properties	Phase	Expression	Reference
Density (ρ^i)	LIQUID	$19325.28 - 1.44T$	[45]
	FCC	$19657.60 - 1.20T$	[45]
Specific Heat (C_p^i)	LIQUID	$158 + 5.08 \times 10^7 \exp(-0.0114T)$	[46]
	FCC	$132 + 2.5 \times 10^{-5}T^2 - 0.011T$	[46]
Thermal Conductivity (k_{th}^i)	LIQUID	$100 + 0.027397T$	[45]
	FCC	$338.91 - 0.0693T$	[45]
Phase Mobility (M^i)	LIQUID	$3.15 \times 10^{-15} \exp\left(\frac{-1073.15}{8.31T}\right)$	[?] unpublished
	FCC	$3.38 \times 10^{-17} \exp\left(\frac{-1165.84}{8.31T}\right)$	[?] unpublished
Viscosity (μ_{LIQ})	LIQUID	$\exp\left(-0.1990 + \frac{2669}{T}\right)$	[47]

To address this issue, we utilize thermodynamic expressions that define the values of material properties for a unary Au system as functions of temperature. Furthermore, these material properties are classified according to the individual phases under consideration. Using the interpolation function described in Equation 1 of Section 3, the FEM solver accurately adjusts the material properties for the respective phases at specified temperatures. Table 3 presents the mathematical expressions for the temperature dependence of material properties: density (ρ), specific heat capacity (C_p), thermal conductivity (k_{th}), phase mobilities (M), and melt pool viscosity (μ_{LIQ}) for the two distinct phases, LIQUID and FCC. It should be noted that this work assumes the thermal conductivity of both phases to be isotropic in nature. The driving force, or the free energy of the system governing phase evolution during laser processing, is another key material property that depends on the composition and temperature of individual phases. In a unary system, the composition is uniform across the entire computational domain, so the free energy depends solely on temperature. As discussed in Section 4, we consider two versions of free energy expressions: a fitted expression and an expression extracted from a thermodynamic database (TDB). These two temperature-dependent free energy expressions are listed in Equation 12. It is well known that phase field simulations are generally associated with a diffused interface model, so we introduce a mushy zone as an interface between the solid and melt pool regions, where the viscosity of this zone (μ_{adj}) is given by Equation 17. Similarly, in the study the absorption coefficient of gold is taken to be $8.5 \times 10^7 \text{ m}^{-1}$ [45].

$$\mu_{adj} = 10 \times \mu_{LIQ} \times [h_{LIQ} \times (1 - h_{LIQ})] \quad (17)$$

here, h_{LIQ} refers to the interpolation function that governs the switching action between the FCC and LIQUID phases at the interface, while μ_{LIQ} represents the temperature-dependent viscosity of the meltpool, with the expression provided in Table 3.

7. Machine Learning and Digital Twin

Further, we present a machine learning model capable of predicting the evolution of the meltpool (LIQUID phase)

in a 2D image format when provided with temperature distribution data as input. This trained model can be stored on a portable, lightweight mini-computing device, such as a *Raspberry Pi* [48], to predict phase evolution in real time during experiments, using input from an Infra-Red camera attachment that records the specimen surface's thermal history data. Additionally, we have developed a web application that allows users to input temperature distribution data in *numpy* array [49] format and predict the meltpool phase for the specified thermal data of a unary Au system. This web application can be extended to multiple alloy systems by training separate machine learning models for each alloy, enabling a Digital Twin that can be rapidly adapted to different applications and needs with multiple machine learning models.

U-NET [50]

7.1. Training Data and Model Architecture

The accuracy of any machine learning model depends on the volume of training data and on proper hyperparameter tuning of the model architecture. In this study, we utilize data generated from multiple FEM simulations, varying both the laser beam profile and the free energy function.

From eight distinct phase-field laser simulations, as described in Sections 4 and 5, a total of 3220 observations of temperature distribution and corresponding phase evolution were extracted from the exodus file generated by the FEM solver. The extracted data were converted into a Numpy 3D array in the format (x-coordinate, y-coordinate, time), containing numerical values for temperature and phase information at each coordinate and time step. The organized data array was randomly divided in an 80:10:10 ratio for training, testing, and validation purposes. For training and prediction, the input to the machine learning model, referred to as the Input Image, is an array of temperature distribution within the domain (x-coordinate, y-coordinate) at a specific time (e.g., t). The model's output, referred to as the Output Label, is an array containing information about the meltpool phase coordinates at the same time instance (t). As only two phases are considered: LIQUID and FCC, each can be represented by a single variable, η and $1 - \eta$, respectively.

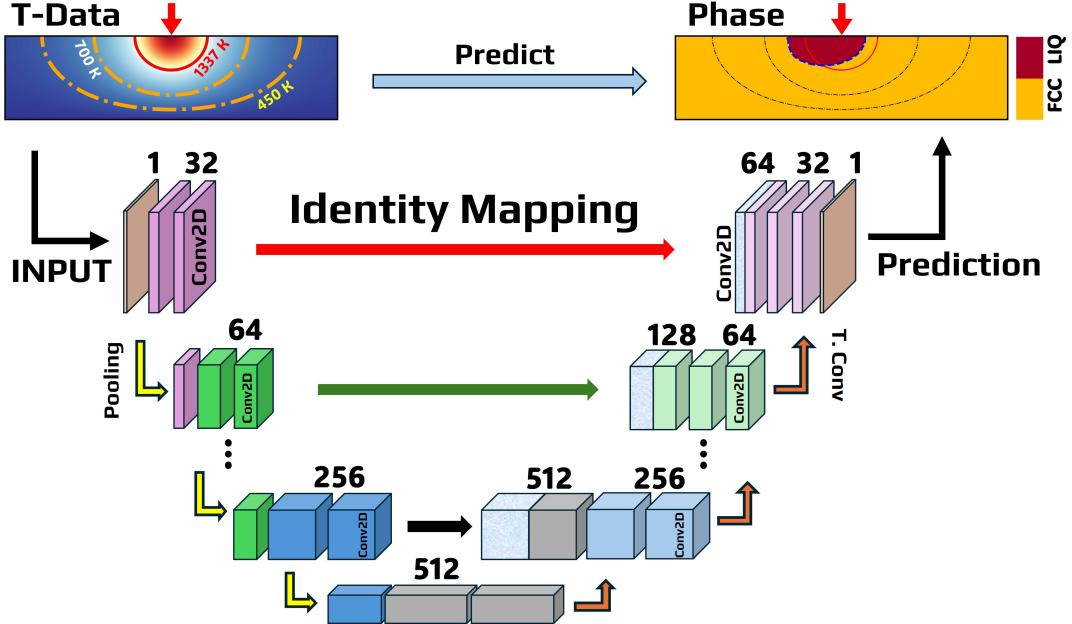


Figure 4: A schematics illustrating the tailored U-Net machine learning architecture to predict the phase dynamics based on the temperature distribution (T-Data) across the input domain. The model is intended to process the thermal data as an input going through multiple encoding and decoding blocks consisting of several convolutional layers and max-pooling inbetween to extract the features within the input data that is correlated with the phase profile for corresponding T-Data. The model architecture at the first half reduces the spatial dimension and increases the data channel at every encoding block as illustrated by 1, 32, 64, 124, 256, 512 channels. At the bottleneck, the end of encoding block and beginning of decoding block, the detailed features in input data is transferred to decoding blocks moving upwards. At every decoding block the channels are decreased from 512, 256, 124, 64, 32 to 1 whereas, the spatial dimension is increased by mapping the spatial identity from corresponding encoder to decoder block as shown by arrows pointing from left to right. Finally by the end of decoder block, the model predicts output segmenting the LIQUID and FCC phase in a equal spatial coordinate space with single channel data. During the training process thousands of T-Data observations are fed to the model and every prediction of phase is equated with actual phase evolution data from phase field simulation and the necessary training parameters (weights and bias vectors) are adjusted accordingly to minimize the differences between predicted result and ground truth generated phase data.

Table 4
Model Hyperparameters

Hyperparameter	Value
Batch Size	13
Learning Rate	1×10^{-4}
Number of Epochs	50
Input Channels	1
Output Channels	1
Loss Function	BCEWithLogitsLoss
Optimizer	Adam
Random State	69
Test Split	10%
Validation Split	10%

To enhance computational efficiency, the model output, representing LIQUID and FCC phases, is expressed as 1 or 0 at each spatio-temporal point. This unique system uses the temperature distribution as an input for predicting the spatio-temporal coordinates of the meltpool or FCC phase, thus presenting a binary classification problem.

For a binary classification problem to segment the LIQUID phase from FCC, we employed the U-Net architecture

[50], which is popularly used in image segmentation tasks. Here, the two phases, LIQUID and FCC, are processed as two segments within the computational domain at each time step, with the model trained to identify the LIQUID phase region. The U-Net architecture is a convolutional neural network with encoder and decoder blocks arranged in a symmetrical fashion. The schematic of the model architecture used in this study is presented in Figure 4, while the hyperparameters used in the machine learning process are listed in Table 4. A detailed model architecture, including fully functional code with encoder, bottleneck, and decoder blocks, along with the corresponding convolutional, max-pooling, upsampling layers, and individual channels, is available on the [GitHub](#) page further mentioned in Section 12. The accuracy, loss, and prediction results for training, testing, and validation are further discussed in Section 8.3.

8. Result and Discussion

In this section, we present extended insights into the results obtained from phase-field simulations and machine learning model predictions. In Section 8.1, we examine the

thermo-phase response to different energy models or expressions used during laser-induced phase-field simulations. The microstructural evolution of the melt pool, its area, temperature distribution across the simulation domain, and variations in the thermal profile under different laser beam profiles are discussed in Section 8.2. Finally, in Section 8.3, we discuss the predictions from a machine learning model trained on microstructure evolution data generated by phase-field simulations. Here, we elaborate on the model's capability to accurately predict laser-induced multiphase phenomena. Additionally, we provide insights on utilizing results from a simple, rapid, and effective heat transfer FEM simulation to predict phase transformations induced by heat input using the trained ML model, with a visual demonstration.

8.1. Phase Response to Energy Models/Expressions

Phase evolution is a complex phenomenon primarily driven by the free energy of the system, a phase with minimum free energy at a given temperature dictates the stability moving forward temporally. This study attempts to compare the response of phases, their stabilities and transitions in addition to the thermal history, for two sets of driving force expressions in a laser aided phase field simulation. Looking at the Graph 2, we can notice that for fitted expression of 2(a) the free energy curves for two phases are distinct parabolic in nature intersecting near the melting point of Au creating a phase change gap between them, whereas for TDB based free energy curves in 2(b) cross each other at same temperature without any gap between the LIQUID and FCC curves.

The evolution of LIQUID phase with fine-tuned free energy expression (F_θ) in the phase field simulation is visually distinct from that of TDB based expression which can be observed in Figure 5. The initial LIQUID phase of area $2500 \mu\text{m}^2$ grows to a semi-circular shape exactly matching the contour of 1337 K temperature on the domain at around 1s into the simulation as shown in Figure 5(a). As the simulation progresses, the LIQUID (meltpool) follows the temperature contour of 1337 K refer Figure 5(b) until the heat source is turned off. Whereas the result of simulation with TDB extracted expression (F_ψ) depicted in Figure 5(c), it can be seen that the meltpool is not fully developed at time $t = 1\text{s}$ as compared (a). The visible distinction in meltpool geometry between the (a) and (b) is that for F_θ meltpool front and meltpool shape exactly lines up with the contour of melting temperature (1337 K) whereas for F_ψ the thermal front of 1337 K leads the LIQUID phase front. While the Figure 5 shows the phase evolution on application of Gaussian laser beam profile, similar result and distinction is observed in LIQUID phase evolution for all other three laser beams. The result from other three beams is presented in Appendix A.

Another aspect where a significantly different observation can be made between simulations with F_θ and F_ψ is in the range of maximum temperature measured inside the domain. Plot 6 depicts the bar graph showcasing the range

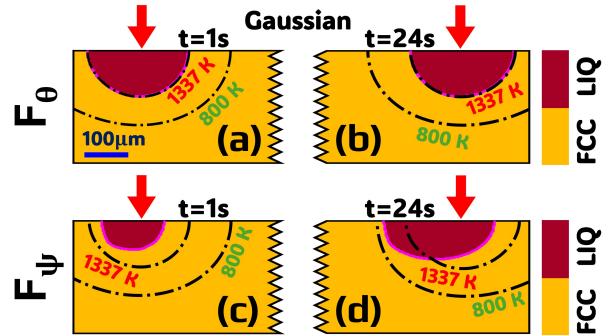


Figure 5: The illustration of phase evolution in unary Au system on being irradiated by the Gaussian laser beam profile with power of 25 mW at a scan speed of $30 \mu\text{m}/\text{s}$ from top left of the computation domain to top right. The subplots (a) and (b) represents the simulation at two time stamps at $t=1\text{s}$ and $t=24\text{s}$ respectively for the phase field simulation with fine-tuned free energy expression (F_θ). It can be noted at both time stamps the LIQUID phase represented by dark red color aligns perfectly with the melting temperature contour line of 1337 K. Whereas (c) and (d) represents the phase evolution resulted from simulation with TDB-file based free energy expression (F_ψ). The key difference in phase evolution with fine-tuned free energy expression and TDB-file extracted expression is on the gap that is present in second between the leading melting temperature contour line of 1337 K and LIQUID phase front. The positional time lag between these two fronts can be attributed to the difference in phase diffusion and thermal diffusion with thermal diffusion leading the phase. Other key difference in LIQUID phase evolution with two free energy considerations is that at time $t=1\text{s}$, the melt pool is fully developed with an area of $18484.18 \mu\text{m}^2$ for F_θ compared to an area of $7575.42 \mu\text{m}^2$ for F_ψ . The difference in melt pool area evens out reaching a mean of $\approx 17800 \mu\text{m}^2$ near the end of simulation as depicted in (b) and (d) respectively although the actual shape of melt pool is drastically different between two simulation results. The phase evolution simulation results from Flat-Top, Ring and Bessel beams are presented in Appendix A

of peak temperatures at the top surface of the computational domain, over the simulation duration for fine-tuned free energy 6(a) and TDB extracted free energy 6(b). It can be noted that for any given laser beam profile, the greater temperature in the domain is observed for simulation with fine-tuned free energy (F_θ) compared to TDB based expression (F_ψ). In Figure 6(a), Gaussian beam profile produces an average peak temperature of 2958 K over the total computational time, whereas in 6(b) the mean peak temperature for Gaussian beam is 2880 K. Another noticeable difference in the plot is the range of maximum temperature that the domain attains over time. For simulation with F_ψ the range of highest temperature attained by the domain is bigger compared to the simulation with F_θ indicated by the wider error-bars for all four laser beam profiles in Figure 6(a) and (b).

On analysing, it is observed that the free energy expression plays another crucial role in the melt pool / LIQUID phase i.e. on its flow velocity. Figure 7(a) and (b) shows the flow velocity for two different laser beam profiles Bessel

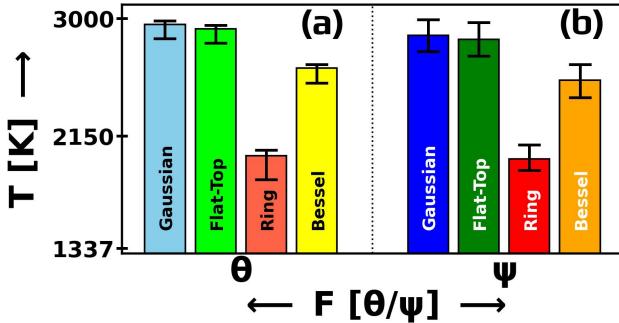


Figure 6: A bar graph comparing the average peak temperature measured at the top surface of the computational domain when the laser transverses from left to right during the phase field simulation. In (a), the mean peak temperature from phase field simulation involving the fine-tuned free energy (F_θ) expression. From the plot it is observed that the Gaussian beam profile increased the temperature of the domain to a maximum peak of 3061.58 K followed by Flat-Top, Bessel and Ring beam shapes at 3028.92 K, 2748.94 K and 2180.13 K respectively. Similarly, in (b) the plot showcases the peak temperature during the simulation with free energy expression extracted from the TDB file (F_ψ). The trend is similar to that of (a) with highest temperature reached during the Gaussian laser beam simulation followed by Flat-Top, Bessel and Ring beam shape with the peak temperature during the whole simulation time measure at 2996.36 K, 2966.37 K, 2680.17 K and 2069.10 K respectively. The key differentiation between (a) and (b) with the use of free energy expression F_θ and F_ψ is that for simulation with fine-tuned free energy expression compounded to an average higher temperature values for all four laser beam profiles to the simulation conducted with free energy expression from a TDB file.

and Ring at mid-simulation (time $t = 12.5$ s) for the fine-tuned energy expression ($F\theta$). Whereas, Figure 7(c) and (d) relates to simulation with TDB based expression ($F\psi$) for same beam profiles (Bessel and Ring) at the same time. From the figure, it can be noted that for $F\theta$, the peak flow velocity is $81 \mu\text{m/s}$ for Bessel heat source and $18.90 \mu\text{m/s}$ for Ring beam. Similarly, for $F\psi$ based simulation, the peak velocity incase of Bessel beam profile is about $56.29 \mu\text{m/s}$ whereas for Ring heat source it is $23.71 \mu\text{m/s}$ respectively. We found that the Ring laser beam acts as an exception to other beam studied, as for it the peak flow velocity during the simulation is higher for TDB based expression F_ψ compared to fine-tuned (F_θ) one. This phenomenon is further discussed in Section 8.2.

In the case of temperature distribution and peak temperature reached by the computational domain, the role of different the free energy expressions becomes quite distinct. First of all, the major noticeable distinction in temperature-meltpool profile as a result of different free energy expressions is, for F_ψ , there exists the physical gap between leading thermal front of melting temperature (1337 K) and actual meltpool front as shown in Figure 8(c) and (d) indicated by red contour line for meltpool and black dotted contour lines for temperature. The positional lag between thermal

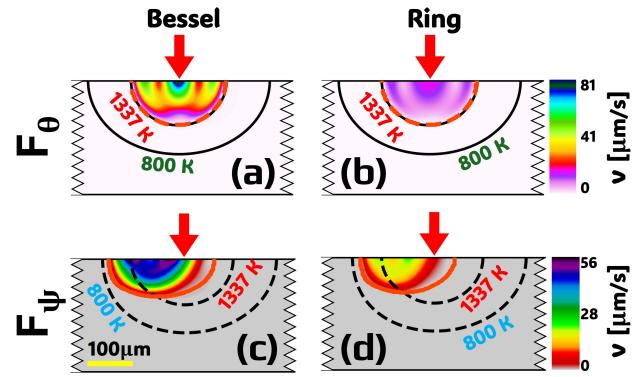


Figure 7: The subplots illustrating the velocity profile of meltpool when the laser beam reaches the domain mid point ($500 \mu\text{m}$ from top left corner) at time $t=12.5$ s into the simulation for two different laser beam profile with two free energy expressions considered for the study. In (a) and (b) the plots depicts the meltpool flow velocity for Bessel and Ring laser beam with simulation conducted with fine-tuned free energy expression (F_θ). Similarly in (c) and (d) the LIQUID phase velocity profile is presented for Bessel and Ring laser irradiation for the free energy expression (F_ψ) implemented directed from the TDB file. The noticeable difference in flow velocity due to the application of Bessel and Ring beam profile is the range of velocity inside the meltpool is comparatively higher for simulation with Bessel beam to that of Ring beam for both free energy expression. For F_θ expression, the maximum velocity inside the LIQUID phase for Bessel type laser beam is calculated to be around $81 \mu\text{m/s}$ to that of $18.90 \mu\text{m/s}$ for Ring beam whereas for simulation with F_ψ expression, the respective maximum flow velocity are $56 \mu\text{m/s}$ and $23.71 \mu\text{m/s}$ for Bessel and Ring beam respectively. In case of the difference seen in velocity profile with respect to free energy expression type, it can be observed that for Bessel beam fine-tuned free energy expression results in an overall higher flow velocity in-contrast for Ring beam the TDB based free energy produced a greater flow inside the meltpool compared to fine-tuned expression.

and phase diffusion can be observed only in simulations with TDB extracted free energy (F_ψ) while there is no such gap for F_θ indicated by red dotted contour lines for melt pool overlapping the white dotted thermal contour line at 1337 K in Figure 8(a) and (b) respectively.

Another exciting phenomenon observed in simulations with F_ψ is that the temperature distribution at the leading front of the domain (to the right of the laser moving from left to right) is wider than that in lagging part (to the left of the laser). This can be clearly visualized in Figure 8(c) and (d) where the spatial difference between thermal front of 1337 K and 800 K at the top right surface (β_ψ and β'_ψ) is larger than that in top left surface (α_ψ and α'_ψ) for same temperature fronts. Whereas, for simulation with fine-tuned free energy expression (F_θ), there is no significant difference in thermal contour at leading and lagging fronts i.e. $\alpha_\theta \approx \beta_\theta$ and $\alpha'_\theta \approx \beta'_\theta$ in Figure 8(a) and (b) respectively.

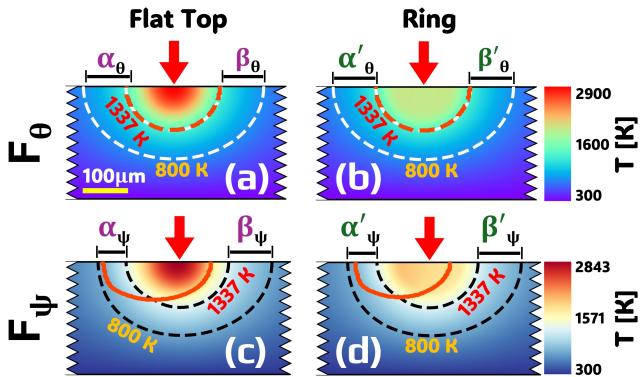


Figure 8: A comparative illustration of temperature distribution for Flat-Top and Ring laser beam profile mid simulation at time $t=12.5\text{s}$ when the laser reaches the exact midpoint of the top surface of computational domain. Subplot (a) and (c) refer to Flat-Top beam profile for simulation conducted under fine-tuned free energy expression F_θ and TDB extracted free energy expression F_ψ respectively where as figure (b) and (d) corresponds to Ring laser beam for F_θ and F_ψ correspondingly. Starting with (a) for the Flat-Top laser beam shape with F_θ free energy, the temperature distribution is symmetrical in both leading and trailing edges of temperature contour i.e. $\alpha_\theta \approx \beta_\theta \approx 97.76\text{ }\mu\text{m}$ with a peak of around 2900 K at the beam centre. Similar is the case for (b) although the temperature distribution across the Ring radius appears uniform with a peak of 1967.28 K, the leading and lagging edges of temperature contours are near symmetrical with values of $\alpha'_\theta \approx \beta'_\theta \approx 92.27\text{ }\mu\text{m}$. One of the noticeable visual clue in both (a) and (b) is that the temperature contour line of 1337 K perfectly aligns with the melt pool phase boundary represented by dashed red line which suggest that there is no any lag between phase diffusion front and thermal diffusion front on implementing fine-tuned free energy expression for the phase field simulation. Whereas, in case of free energy expression extracted from TDB file and implemented directly into FEM solver script, there is a noticeable gap between temperature front and phase front depicted by the red contour line for melt pool phase and dashed black line for 1337 K in (c) and (d). In addition, it is observable that there is an asymmetry in thermal contour lines at the leading and trailing fronts in F_ψ based simulations. In (c) for Flat-Top laser profile, the gap between two selected temperature contour values of 1337 K and 800 K at the leading front β_ψ ($94.76\text{ }\mu\text{m}$) is greater than trailing front α_ψ ($62.34\text{ }\mu\text{m}$) which is the case for (d) as well with values of β'_ψ and α'_ψ as $94.76\text{ }\mu\text{m}$ and $64.83\text{ }\mu\text{m}$ respectively. The key difference between Flat-Top and Ring beam on imparting heat energy to the computational domain and temperature distribution across is that Flat-Top heat source raises temperature of the domain significantly higher compared to that of Ring laser heat source for any free energy expressions.

8.2. Laser Profiles and Phase Dynamics

In this section, we present the discussion about results obtained from phase field simulation coupled with heat transfer physics which initiates the phase transformation. Specifically, here we elaborate on how the different laser beam profiles changes the phase dynamics. As mentioned

in Section 5 the four beam profiles considered for the study are: Gaussian, Flat-Top, Ring and Bessel. And the effect of each of them on phase dynamics is carried out on equal laser processing parameters i.e. laser power, scan speed and effective outer beam radius. In our investigation, we found that among four beam shapes, Ring beam profile behaves uniquely in context of heat distribution and temperature profile. This results in a different trend of melt pool area evolution, LIQUID phase flow velocity and peak temperature attained by the system.

Starting with the temperature distribution and thermal history along inside the simulation domain it is observed that with Gaussian beam, the peak domain temperature is maximum compared to all other three beams. Following the Gaussian beam, Flat-Top laser source with equal beam radius of $70\text{ }\mu\text{m}$ generates second highest peak temperature. For Gaussian beam, the domain reached a peak of 3061.58 K and 2996.36 K for F_θ and F_ψ respectively, whereas for Flat-Top, the peak temperatures are 3028.92 K and 2966.37 K for F_θ and F_ψ as shown in Figure 6(a) and (b) in shades of blue and green bars. Similarly, for Bessel beam, the maximum temperature attained by the domain over the simulation are: 2748.94 K and 2680.17 K for F_θ and F_ψ represented by yellow shades of bars in Figure 6. For these three beam profiles, the peak temperature of the domain are in similar range (over 2500 K) but for the Ring laser beam, the drastic difference can be observed. The red shades of bar in Figure 6 represents the maximum temperature inside the computational model, for simulation with fine-tuned free energy expression F_θ , the peak temperature is around 2180.13 K and for TDB free energy expression F_ψ it is measured to be the lowest of all i.e. 2069.10 K . The low temperature for Ring beam profile can be associated with the way heat energy is distributed inside the system. For Gaussian, Flat-Top and Bessel beam, the presence of central beam makes the energy transfer radially outwards from the centre with a concentrated high irradiance at the centre, but for a Ring beam, the centre of the beam gets near-zero direct irradiance from the source. The heat energy deposited is focused on a circular ring away from the centre hence the heat transfer occurs both inwards to the centre of the beam and outwards of the ring creating a uniform heat distribution which inturns does not let temperature to abruptly rise to peak as compared to other three beam profiles. This can be further noticed in Figure 8(b) and (d) where we can see that the temperature profile is rather uniform and distributed radially around the top surface equally compared to Flat-Top beam in Figure 8(a) and (c) with maximum temperature directly at the centre of the beam.

The temperature profile for other two laser beams (Gaussian and Bessel) at $t = 12.5\text{s}$ into the simulation i.e., when the laser beam spot reaches middle of the domain, is presented in Figure A2 at Appendix A. For Gaussian and Bessel beam, the thermal distribution profile is near similar to one another with a single main difference being the peak temperature attained by the computational system. The Gaussian beam imparts dense irradiation at the centre of the beam which

exponentially decays radially whereas for the Bessel beam, the centre beam and two outer ring beams share the total power supplied in a ratio of attenuation coefficients: a_0 , a_1 , and a_2 , as expressed in Equation 16 with $a_0+a_1+a_2=1$. From the mathematical formulation it can be said that the Bessel beam gets benefits of both Ring and Gaussian profile by varying the values of attenuation coefficients.

Another key insight regarding the difference in laser beam profiles can be understood with the effects beam shape on governing the microstructure and evolution of the phases. For meltpool phase the evolution studied by measuring its area throughout the simulation time. The area of meltpool is tracked at every time iteration during the simulation and a comprehensive overview is prepared. Plot 9 demonstrates the LIQUID phase area growth from the start of the simulation till the end for four types of laser heat sources including the variation of two free energy expression in the phase field setup. From the graph, it can be deduced that for all four heat source with fine-tuned free energy expression (F_θ) the meltpool grows in a similar trend during the simulation with an average area of around $\approx 16,500 \mu\text{m}^2$ denoted by green, yellow, navy and brown coloured lines in Figure 9(a), (b), (c) and (d) respectively. Whereas, for the simulation with TDB based free energy, the three beam profiles of Gaussian, Flat Top and Bessel represented by red, blue, and purple lines in Figure 9(a), (b) and (d) respectively results in similar meltpool area evolution with an average area of $\approx 15,500 \mu\text{m}^2$. But for the Ring laser beam denoted by magenta line in Figure 9(c), the meltpool area is quite lower with an average of $\approx 12967 \mu\text{m}^2$.

With the meltpool area versus time plot, we can suggest which beam profile to choose during an additive manufacturing process, for example: for process requiring bigger meltpool and heat affected zone, Flat Top heat source can be utilized which produced the biggest average meltpool size in our simulation ($16545.82 \mu\text{m}^2$ for F_θ and $15839.72 \mu\text{m}^2$ for F_ψ). The relevance of TDB based free energy is more suitable for real experimental comparison as there exists a certain gap between phase and thermal diffusion in real nature which is emulated by the simulation with TDB extracted free energy. Similarly, from the simulations we can infer that for a 3D printing job requiring uniform heating of the material but with a smaller heat affected zone, Ring laser beam profile is more suitable. This analysis paves a way that can help decide the selection of proper laser heat source for specific additive manufacturing task from an equivalent laser processing parameters choices.

An analysis of temperature distribution for four laser beam profile is performed at computational domain's horizontal mid point i.e. $500 \mu\text{m}$ from left-top edge as marked by a red arrow in a inset picture in Figure 10. The four subplots of Figure 10 shows the thermal history for the entirety of the simulations. In all subplots it can be noticed that the temperature gradually rises, reaches peak when laser source reach the mid-point and then drops afterwards. From Figure 10(a) it is observed that the Gaussian beam produces a higher temperature (2873.29 K) when the beam centre

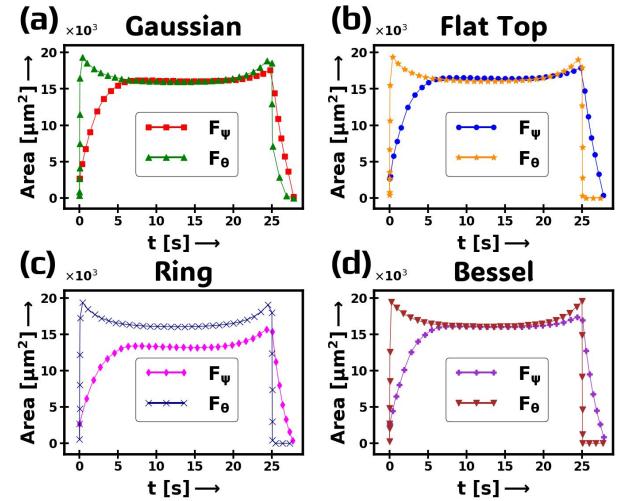


Figure 9: The graphs in subplot illustrates the area evolution of meltpool (LIQUID) phase over the simulation duration for four different laser heat source profiles and two types of free energy expressions influencing the meltpool growth for each beam shapes. In (a) the meltpool area growth for simulation performed with Gaussian beam is plotted where it can be observed that for fine-tuned free energy F_θ sharply causes the meltpool to rise sharply to a value of $19422.59 \mu\text{m}^2$ within seconds of simulation and balances out at around $16497.74 \mu\text{m}^2$ on average till the end as depicted by the green colored line with triangular marker. Whereas, for the simulation with TDB file driven free energy expression $F-\psi$, the meltpool area gradually grows without a sudden peaking and settles at around similar area of $15551.55 \mu\text{m}^2$ throughout the end till the laser is turned off after 25s into the simulation as denoted by the red line with square markers. The similar trend can be observed for Flat-Top in (b) and Bessel beam in (d) with sudden rise in meltpool area for fine-tuned energy expression and gradual increase in LIQUID phase for TDB based expression both averaging around $16500 \mu\text{m}^2$. The exception in this trend is visible for Ring laser beam as shown in (c) where, the fine-tuned fitted free energy expression produced an average meltpool area of $16549.60 \mu\text{m}^2$ (blue colored line with cross symbols) from the beginning of the simulation till the laser is turned off where as for TDB extracted free energy simulation, the meltpool area is drastically low with an average of $12967.09 \mu\text{m}^2$ gradually peaking to $16338.35 \mu\text{m}^2$ depicted by magenta line with diamond markers. A unique difference in evolution of LIQUID phase area between simulations involving fine-tuned free energy F_θ and TDB based free energy F_ψ is that the a small delay is noticed in meltpool to fully develop when the laser is irradiated at the beginning of the simulation and when the laser is turned off at $t = 25\text{s}$ there exists a lag in solidification of meltpool phase back to FCC for F_ψ compared to sharp rise and plummeting of LIQUID phase at the beginning and when laser is turned off for F_θ .

is just above the domain's midpoint whereas for the Ring beam the system reaches a maximum of 1975.98 K when the beam centre move past the midpoint with receding edge of ring shines directly above it at time $t = 14.46 \text{ s}$ into the simulation. In Figure 10(b) the comparison between temperature distribution from Gaussian and Bessel beam profile is

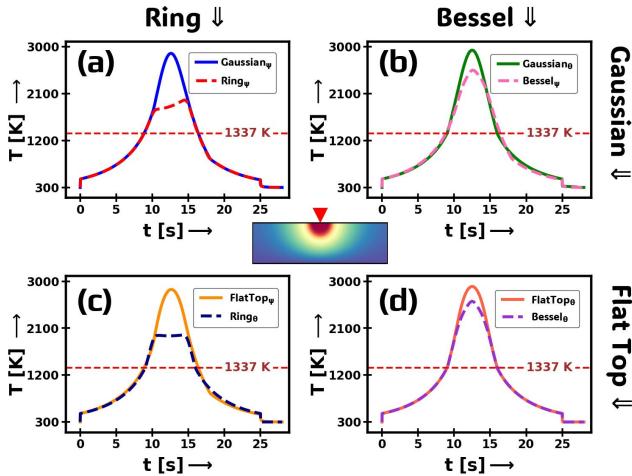


Figure 10: The figure illustrates time-temperature plot for a spatial point at the mid-top surface as shown in the inset. The subplot (a) presents the temperature profile for Gaussian and Ring heat sources with F_ψ denoted by blue solid line and red dashed line respectively. The key observation to be made here is that when the laser passes through the selected point, a bell shaped temperature curve is formed for Gaussian beam with peak reaching to 2873.29 K whereas a flat T-profile is seen for Ring beam peaking around 1975.98 K. In (b) a comparative plot is shown for temperature evolution for Gaussian beam with F_θ (green solid line) and Bessel beam with F_ψ (pink dashed line), it is observed that the Gaussian beam causes the highest temperature rise compared to Bessel beam with a maximum of 2933.98 K compared to 2550.24 K. Similarly, (c) showcases the time-temperature profile for Flat-Top heat source with F_ψ (yellow solid line) and Ring beam with F_θ (dashed blue line). From the plot, it is to be inferred that Ring beam provides an uniform heating where Flat-Top makes the temperature to increase gradually and drop slowly as laser traverses. The peak temperature attained by the point of study for Ring beam with F_θ is 1967.24 K and that for Flat-Top with F_ψ is 2873.02 K. Finally, in (d) the plot showcases the time-temperature profile for Flat-Top laser beam with F_θ and Bessel beam with F_ψ driving force expressions. Both of them generated a similar time-temperature profile with a bell shaped curve reaching to a peak of 2900.08 K and 2614.45 K for Flat-Top and Bessel beam respectively. From the four subplots, it can be noted that to achieve an uniform heating, Ring laser beam is to be preferred compared to other three whereas with a same power and scan speed. Whereas, for processing materials with higher melting point Gaussian or Flat-Top beam is suggested as they produce highly localized and concentrated heating at the beam centre.

plotted, here we can see that the Gaussian laser beam heats up the domain to a higher temperature than Bessel beam. Similarly, in Figure 10(c), the plot of time-temperature is presented for Ring laser beam versus Flat Top laser beam. In the figure, it can be observed that Flat Top beam profiles causes the domain's top midpoint to heat up to a temperature of 2843.02 K at time $t = 12.5$ s into the simulation where as an unique flat temperature profile (1958.09 K) can be seen for Ring laser beam at the midpoint from time $t = 10.61$ s to 14.39s. The flattened temperature profile for Ring beam

can be associated with an uniform heating of the domain causing a steady temperature profile when the beam passes through an specific spatial point in the domain with leading and trailing ring edges contributing to the rise in temperature with no irradiance at the beam centre. In case of Figure 10(d), the comparison of temperature distribution due to Flat Top and Bessel laser beam is presented, where it is observed that Flat Top beam imparts more heat energy to the domain with peak temperature greater than that obtained with Bessel beam. In overall, Gaussian, Flat Top and Bessel beam leads to a similar bell shaped temperature profile at a coordinate point on the top surface of the domain whereas for the Ring beam, an uniform heating scene with flatter peak is observed making it an unique case among four beam shapes studied.

For simulation with fine-tuned free energy expression (F_θ), the effect of laser beam profile on meltpool flow velocity resembles the temperature profile with Gaussian beam inducing the highest flow velocity with an average of $123.75 \mu\text{m/s}$ denoted by magenta line in Figure 11(a). Whereas, Flat Top laser beam nearly matches the Gaussian beam producing the time-averaged peak flow velocity of $119.94 \mu\text{m/s}$ depicted by green line in Figure 11(b). For the Bessel beam, the aggregate maximum flow velocity over the simulation duration is about $84.65 \mu\text{m/s}$ represented by purple line in Figure 11(d) and finally, for the Ring beam, the domain-averaged peak flow velocity over time is recorded to be $20.37 \mu\text{m/s}$, the lowest among other three beam profiles as presented by cyan coloured line in Figure 11(c). Similarly, for the simulation with TDB based free-energy, the time-averaged maximum flow velocity throughout the simulation period is highest for Flat Top beam followed by Gaussian and Bessel beam and lowest for Ring beam with the values: $76.86 \mu\text{m/s}$, $71.76 \mu\text{m/s}$, $52.39 \mu\text{m/s}$ and $22.65 \mu\text{m/s}$ respectively represented by red, blue, brown and orange curves in Figure 11(b), (a), (d) and (c). In a similar fashion to that of temperature profile, for Ring laser beam shape, the peak average velocity is higher for simulation with free energy expression extracted from TDB file (F_ψ) compared to that of simulation with fine-tuned free energy expression F_θ . The values of which are: $22.65 \mu\text{m/s}$ and $20.37 \mu\text{m/s}$ respectively denoted by cyan and orange lines in Figure 11(c).

8.3. Machine Learned Meltpool Profiling

The U-Net machine learning architecture model as described in Section 7 was trained for 50 iterations on the dataset generated form the FEM simulations of laser processing. During the 50 epochs, the model peaked an impressive training accuracy of 0.9992 and validation accuracy of 0.9989 by the last iteration. Similarly, the training and validation loss (Binary Cross-Entropy with Logits Loss) were recorded to be 0.0016 and 0.0024 respectively. The training and validation accuracy versus loss plot is presented in Figure 12.

The trained model is then used to predict the phase for the test-dataset which contained randomly selected 10% of the simulation generated data, these test-dataset were unseen to the model during its training period. The trained model

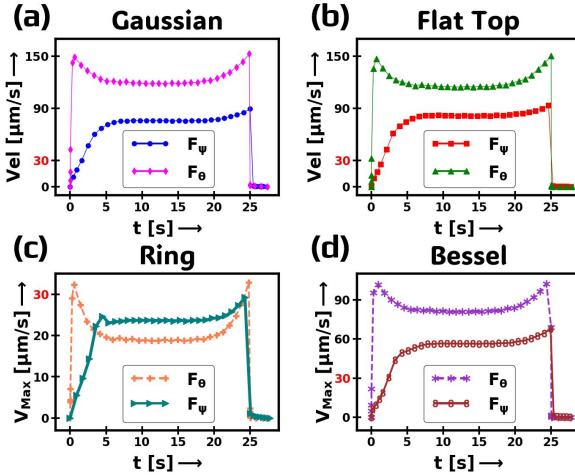


Figure 11: Subplots demonstrating maximum flow velocity inside the meltpool over the total duration of simulation with varying laser beam profile and driving free energy expressions. Firstly, in (a) the plot showcases the peak velocity during simulation for both driving force expressions F_θ and F_ψ for Gaussian laser beam. For fine-tuned free energy expression, the peak velocity measured inside the LIQUID phase is higher (magenta line with diamond markers) in-comparison to that with TDB based expression (blue line with circular markers). The average peak velocity in the meltpool over the total duration of simulation for F_θ and F_ψ are $123.75 \mu\text{m/s}$ and $71.76 \mu\text{m/s}$ respectively. In a similar trend for Flat-Top laser beam in (b) the velocity inside LIQUID phase in simulation with fine-tuned free energy expression (green line with triangular marker) is higher than F_ψ (red line with square marker) with an average peak velocity of $119.94 \mu\text{m/s}$ and $76.86 \mu\text{m/s}$ respectively. Meanwhile a unique twist is observed for Ring laser heat source results in (c) where the simulation with F_ψ produced in average a higher flow velocity (cyan line with triangular marker) than that with F_θ (orange dashed line with plus marker). The flow inside meltpool over the total simulation duration accounts to an average of $20.37 \mu\text{m/s}$ for F_θ compared to $22.65 \mu\text{m/s}$ for that of F_ψ . And for the flow profile with Bessel heat source, the trend follows to that of (a) and (b) but the peak velocity value is relatively lower with an average peak of just $84.65 \mu\text{m/s}$ (purple dashed line with star marker) and $52.39 \mu\text{m/s}$ (brown line) for simulations with free energies F_θ and F_ψ respectively. It is to be noted that the y-axis ticks values are different in subplots (c) and (d) to accommodate the range difference, a marker of $30 \mu\text{m/s}$ is colored in red in all four subplots to make the comparison easier.

predicted with an average accuracy of 0.9988 for the test-dataset.

$$h_T = \frac{1}{1 + e^{-10(\frac{T}{1337} - 1)}} \quad (18)$$

To test the actual prediction capabilities of the trained machine learning model, we setup a FEM simulation in MOOSE Framework with just the heat transfer module solving for temperature distribution across the domain under the

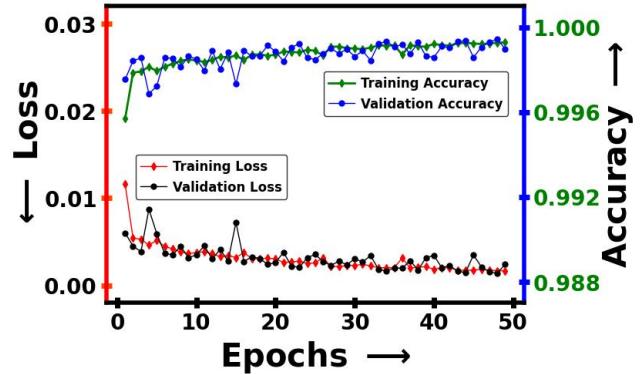


Figure 12: The illustration of machine learning model training metrics over the iterations. The model trained for 50 epochs starts with a training and validation loss of around 0.01 at the beginning and gradually the loss metrics is reduced to a minimum of 1.67×10^{-3} and 2.41×10^{-3} represented by red and black lines respectively, corresponding to y-axis at left side of the plot. Whereas, the training and validation accuracy of the model during the training process gradually increased to 0.9993 and 0.9990 by the end of the 50 epoch as shown by green and blue colored lines respectively to the right y-axis in the plot. Following the training and validation metrics, it can be inferred that the model learned absolutely at its best on predicting the phase evolution with input of temperature distribution across the domain.

Bessel laser beam profile with same laser power and scan-speed to the base phase-field simulations. We proceed to introduce an interpolation function as Expressed in Equation 18 that can smoothly switch the material properties such as thermal conductivity, specific heat and density over the domain in relation to the melting temperature of gold (1337 K). The result of FEM simulation without phase field and fluid flow physics was converted to the torch tensor format and was feed to the trained model as an input. The prediction of spatial coordinate of meltpool phase from temperature history data with the trained model was then compared with the phase evolution data generated from phase-field simulation at each time steps of the simulation. Figure 13(a) presents a snapshot of temperature distribution across the domain resulting from the simulation with only heat transfer module active. Whereas, Figure 13(b) shows the phase evolution at the same time point as (a) obtained from the phase-field simulation. Figure 13(c) depicts the phase evolution predicted by the trained machine learning model with the input as temperature distribution of (a) and the error in machine learning model predicted meltpool phase compared to that of phase-field simulation generated result is presented in Figure 13(d). In Figure 13(d) the green color represents the *False Positive* which is the region inside the domain where the ML model predicted the presence of meltpool phase but phase-field simulation result denies any existence of meltpool. Whereas the FN (False Negative) region in red color means the ML model could not predict the LIQUID phase at those spatial points where the phase-field simulation

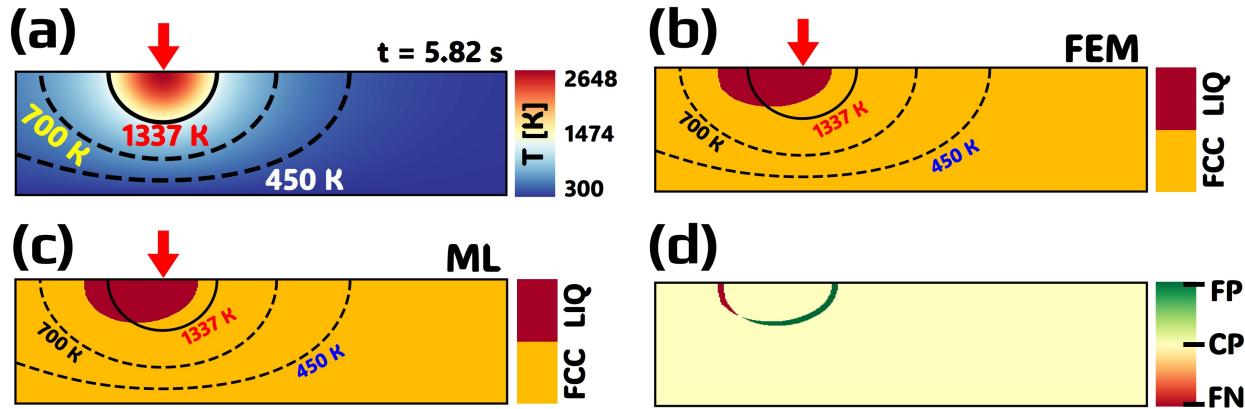


Figure 13: A snapshot of test demo for the result of prediction made by the trained machine learning model compared to the phase evolution computed from FEM simulation with the error and accuracy in predicted phase. **(a)** The input supplied to the trained ML model with the data of temperature distribution across the domain, the temperature history is computed via a laser heat transfer simulation without phase field module. In a real-time Digital Twin model prediction scenario, the temperature distribution as an input to the ML model is supplied from the IR camera with a post-processing performed to match the model input shape in micro-computer as *Raspberry Pi*. **(b)** The phase evolution data computed from the phase field modelling of laser processing simulated via FEM with the exactly same laser processing parameters to that of **(a)** presented at the same time instance of $t=5.82\text{ s}$ into the simulation. In **(c)**, the predicted result of two phases LIQUID and FCC from the trained ML model with an input of temperature distribution **(a)**. Finally in **(d)**, the comparison between phase field simulation computed result of phase evolution in **(b)** and machine learning model predicted of phase evolution of **(c)** with just the thermal distribution data of **(a)**. The three colors inside the domain represent three different regions comparing the results of **(b)** and **(c)** with light yellow color denoted by CP meaning the *Correct Prediction* from ML model with respect to phase field generated result, green color region represented by FP denote to the *False Positive* indicating that the presence of phase was predicted by the ML model but phase field simulation suggests that there is actually absence of the respective phase. Finally the red colored region marked by FN stands for *False Negative* suggesting that the machine learning model failed to predict the presence of a phase which is calculated via phase field simulation. Overall, it can be noted that the majority of the region inside the domain is correctly predicted by the ML model with irregularities at the interface of LIQUID and FCC phase, and the prediction accuracy can be further increased in those interfaces with a stronger ML model trained with multiple more simulation data for a longer training iterations in further work.

result suggests there should be LIQUID phase. The coordinate space where both the phase-field simulation result and ML model predicted result align with each other is marked as Correctly Predicted (CP) region shown in light-yellow color. A video animation comparing the of results phase evolution generated from phase-field simulation and ML predicted at every time step of laser simulation is provided in Section 12 as well as in Appendix B.

9. Conclusion

In this study we presented the result of computational modelling of laser induced phase transformation and microstructural evolution in unary Au system. Multiple simulations were performed by varying laser beam profiles of Gaussian, Flat-Top, Ring and Bessel types, along with multiple different free energy expressions driving the phase transition phenomenon. The free energy expression in consideration were higher order logarithmic-polynomial fitted expression and expression extracted from Thermodynamic Data Base file. The phase transformation due to heat deposition from different laser types were typically similar in nature for Gaussian, Flat-Top and Bessel beam with maximum temperature measured at the beam centre and radially

distributed outwards, similar is the case for flow velocity inside meltpool where the maximum velocity profile is observed at the centre of beam. A drastic different result was noticed for Ring beam profile where the thermal distribution was observed to be uniform inside the ring beam radius. The most intriguing distinction was found in phase evolution with the variation of driving force expressions. For the fine-tuned (fitted) expression, it was observed that the melting point of Au dictated the LIQUID phase exactly matching the temperature contour of 1337 K as the interface of FCC and LIQUID phases whereas a unique phenomenon of thermal front leading the phase front was noticed in simulations conducted under TDB extracted free energy expressions. For the TDB based driving force, the lead-lag dynamics of phase and thermal front was concluded to be linked with the thermal and phase diffusion rates differing with each other making it more realistic according to the thermodynamics. Finally, a U-Net machine learning model architecture was trained on the simulation dataset of thermal history correlating with the meltpool phase evolution. With the trained model a prediction framework is developed where user can interact with the model by uploading the T-data not only from simulation but also from experimental results in a 2D array format. This framework can be regarded as a first

step towards the construction of a Digital Twin capable of predicting phase evolution in real time experiments with input data taken from infrared cameras onsite. Currently, the model is limited to a single component Au system which will be expanded to multi-component alloy system in a multitude of laser processing parameters in future studies. The development of multimodal Digital Twin is expected to expedite the real-time prediction of phase transformation, and details related to evolving phases making it as milestone in precision engineering in Additive Manufacturing sector.

10. Declarations

The authors declare to have no conflicts of interest that are relevant to the content of this article.

11. Acknowledgment

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12. Data Availability

Codes and data used for this work is available at https://github.com/subediupadeth/Digital_Additive_Manufacturing.

CRedit authorship contribution statement

Upadeth Subedi: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Data Curation, Writing - Original Draft, Visualization.

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Appendix A:

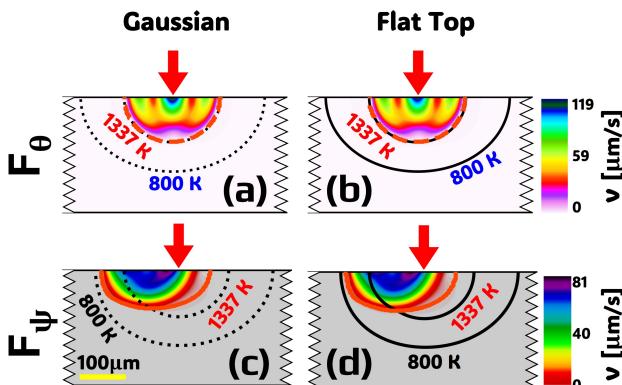


Figure A1: The illustration of velocity profile inside the melt pool when the laser heat source traverses to the domain midpoint at 12.5s into the simulation. Subplot (a) and (c) are associated with simulation under the Gaussian heat source for free energy expression of F_θ and F_ψ respectively. The peak flow velocity for in the LIQUID phase for (a) and (c) are $119 \mu\text{m}/\text{s}$ and $75.61 \mu\text{m}/\text{s}$ respectively. In (b) and (d), the flow profile for simulation conducted under the Flat-Top heat source for F_θ and F_ψ is presented. Although visually the velocity profile between results from Gaussian and Flat-Top laser beam look alike there exists a smaller difference in numerical value of peak melt pool flow velocity reached at the illustrated time stamp with $114.47 \mu\text{m}/\text{s}$ and $81 \mu\text{m}/\text{s}$ for Flat-Top laser induced flow for F_θ and F_ψ respectively.

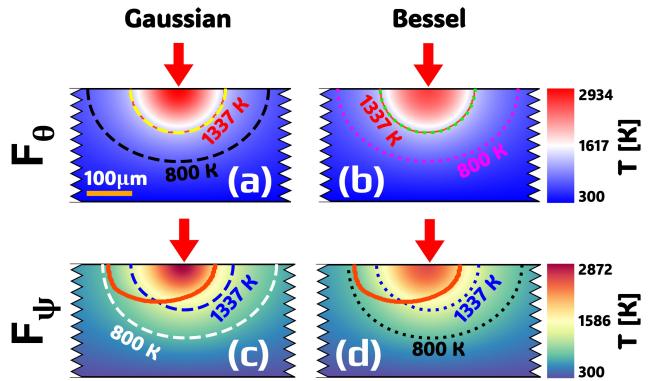


Figure A2: Visualization of thermal distribution across a cutout of simulation domain for Gaussian and Bessel laser sources. Plot (a) and (c) showcases the temperature profile for Gaussian heat source with driving force expression of F_θ and F_ψ respectively. Similarly, (b) and (d) represents the temperature inside the computational domain with Bessel heat source for F_θ and F_ψ correspondingly. A subtle difference in temperature profile can be noticed between Gaussian and Bessel based simulation results with a higher concentration of temperature distribution at the beam centre for Gaussian beam, the peak temperature reached by the domain under Bessel beam are found to be 2613.11 K in (b) and 2548.95 K in (d).

Appendix B:

Video Animations:

Video Animation of Phase-evolution comparison between ML predicted and phase-field generated:

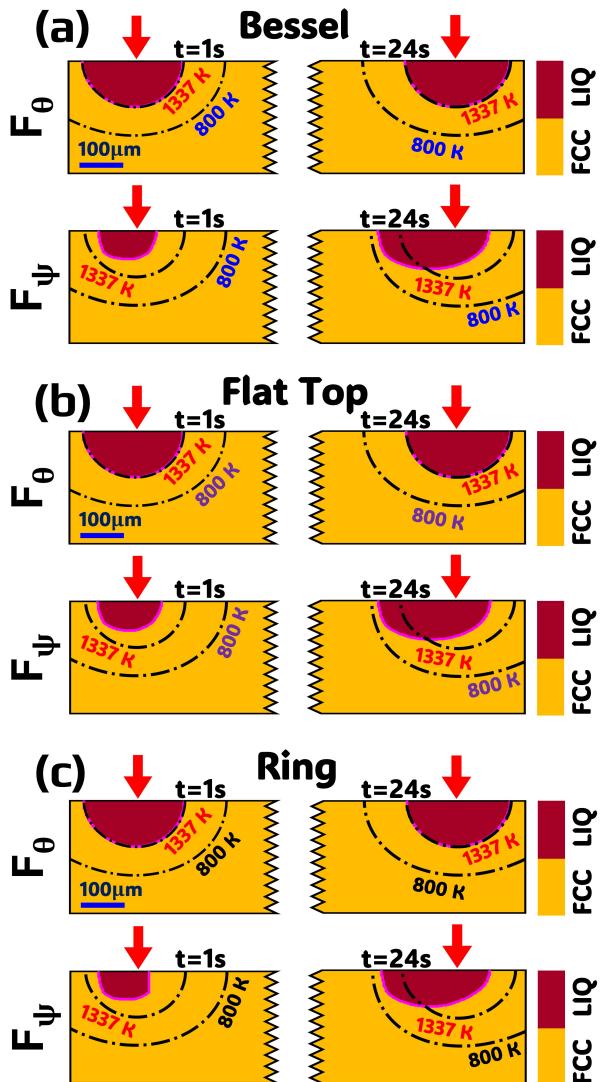


Figure A3: Visual illustration of laser induced phase evolution during the phase field simulation in unary Au system with different heat source profiles with different free energy expressions. (a) The four subplots depicts the growth of meltpool at time $t=1\text{s}$ and $t=24\text{s}$ under the Bessel beam with top row corresponding to fine-tuned free energy expression F_θ and bottom row with F_Ψ . Similarly, in (b) the LIQUID phase status is presented for Flat-Top laser profile with F_θ and F_Ψ as driving force for phase transformation in top and bottom row subplots. Finally (c) represents the meltpool phase growth similar to that of (a) and (b) but for the simulation with Ring laser beam under two free energy expressions. Although the different laser beam profile resulted in drastic temperature history and velocity profile inside the domain, the overall phase growth is in near similar fashion and is possible difficult to distinguish on a visual basis.