Modelling and simulation of equilibrium and non-equilibrium solidification in laser spot welding

Pradeep Reddy\textsuperscript{1}, Virendra Patel\textsuperscript{2}, Anshul Yadav\textsuperscript{3}, Sushil Patel\textsuperscript{4} and Arvind Kumar\textsuperscript{5}

Department of Mechanical Engineering, Indian Institute of Technology Kanpur, Kanpur - 208016, India
\textbf{E-mail:} ypradeep@iitk.ac.in\textsuperscript{1}, vpatel@iitk.ac.in\textsuperscript{2}, anshuly@iitk.ac.in\textsuperscript{3}, psushil@iitk.ac.in\textsuperscript{4}, arvindkr@iitk.ac.in\textsuperscript{5}

Abstract. In this work, rapid solidification in laser welding is studied by solving transient, coupled, governing equations of mass, momentum and energy conservation using a fixed-grid, finite volume methodology. The solidification process in laser welding occurs with high cooling rates involving rapid solidification kinetics. The non-equilibrium phase change is accounted at the solid-liquid interface of the weld pool and it is assumed that heterogeneous nucleation occurs instantaneously when the temperature in the melt pool reaches the nucleation temperature. Simulation results of laser welding with undercooling and without undercooling are compared. It is found that the melt pool width is larger in the case of undercooling case, however, the maximum temperature in the weld pool is higher in the case of without undercooling case.

1. Introduction
Laser welding has a wide range of applications in the field of aerospace, ship building, energy, electronics and medical industries, because of being precise beam control, high energy density, high productivity, good accessibility and high welding speed. The principle of laser welding is to heat the material by irradiating the laser beam onto the substrate, the joining of two metal plates is obtained by a local fusion and solidification, forming the weld bead. The solidification process usually takes in a few tens of milliseconds, producing metastable microstructure. Final mechanical, chemical properties are strongly affected by cooling rate. Because of very high cooling rates lie in non-equilibrium kinetics during solidification which makes the improved microstructure and properties of the surface having advantage of high wear and corrosion resistance\cite{1}.

There is a profound difference between laser spot welding and moving laser welding in terms of temperature and cooling rates. It is observed that the temperature in spot welding will never reach the quasi-steady state and the rate of heating and cooling are high compared to moving laser welding \cite{2}. Small weld pool size, rapid change of temperature and short process duration characterize the laser spot welding. Because of being a short duration process, measurement of temperature and velocity fields is very difficult. Heating and cooling rates and convection in the weld pool influence the final weld pool dimensions and weld microstructure. Microstructural study is important for estimating the shape of the heat input and the quality of the weld. By placing thermocouples temperature can be measured, however it is very expensive and time consuming. Due to small fusion zone, high temperature gradients are present and accurate prediction of temperature is difficult. Therefore, it suggests the need of developing numerical model for predicting temperature, weld pool dimensions and velocity field \cite{3}.
Recently, notable studies have been carried out on the process of rapid solidification [4,5]. In general, solidification is the sequence in which liquid metal is first cooled to its phase-change temperature, and followed by solidification while releasing its latent heat. The release of latent heat and the heat transfer from the weld pool keep the process at a constant temperature. In the presence of undercooling, solidification does not take place at the phase-change temperature. Rather, the liquid phase continues to cool below the phase-change freezing temperature. There it becomes thermodynamically unstable and thus a small amount of energy withdrawal can initiate the solidification process, with a sharp increase in the temperature due to spontaneously released latent heat. This stage is known as the kinetic solidification. Very high cooling rates involve in the non-equilibrium kinetics during solidification. The difference between the nominal solidification temperature and the nucleation temperature is called the degree of sub-cooling [5]. All materials do not solidify at their nominal phase change temperature. Rather, nucleation occurs in them at a lower temperature. This phenomenon is usually termed as sub-cooling. Wang et al., [6] developed an effective interface tracking numerical scheme based on the integration of control volumes for predicting temperature field and modeling phase change during rapid solidification.

Subcooled solidification consists of four stages. (a) Subcooling of the liquid metal from its initial temperature \( T_i \), to its nucleation temperature \( T_N \). The primary crystallization takes place under non-equilibrium conditions during the recalescence period, the rapid release of the heat of fusion during rapid crystal growth. The released latent heat is entirely or partly, consumed by the emulsion of solid-in-liquid, depending on the rate of heat removal, raising the temperature to \( T_m \). The process along this path is rapidly completed, without heat removal to the surroundings. (c) Once it reaches the melting temperature, solidification occurs at constant phase change temperature till solidification ends. (d) Further the solid-state cooling takes place.

Most of the previous numerical models on laser welding have considered only the temperature dependent liquid fraction \([7,8]\). It is important to consider the amount of deviation from the local equilibrium conditions which affects the interface kinetics. Liu et al. [7] studied rapid solidification of a pure metal under non-equilibrium conditions. They found that for rapid solidification with high undercooling, the interface velocity will be high and there is significant impact of non-equilibrium effects. Probability of nucleation of sub-cooled water in cylindrical containers was experimentally carried out by Chen et al. [8]. They concluded that nucleation probability is high when the coolant temperature was lower.

Many researchers \([1,2,4,6,9]\) have studied heat and fluid flow in the melt pool. Most of the models employ two-dimensional or axisymmetric models, to predict the behaviour of melt pools subjected to various process parameters. During welding, as the heat source interacts with the work piece, melting, solidification and various other physical processes take place, which influence the structure and properties of the welded joints. The results of modeling can be used to explain physical phenomena in welding process and for optimizing the welding parameters.

Rapid solidification process has a large undercooling at the solid-liquid interface. In order to consider this, it is important to predict accurate interface temperature and velocity field coupled with the non-equilibrium kinetics. The aim of the present work is to develop a computational model for simulating the rapid solidification process in spot laser welding that can predict recalescence characteristic and transport phenomena in the weld pool. Gaussian laser pulse is applied on the top surface of the workpiece, and temperature variation and melt pool behavior are studied considering rapid solidification. Surface tension and buoyancy forces were taken into account for the calculation of weld pool convection. The numerical model predicts the evolution of melt pool shape, interface temperature and interface velocity and sub-cooling behavior. The results for equilibrium as well as non-equilibrium solidification have been compared.

2. Model description
The schematic diagram of the computational domain for laser spot welding process is shown in Figure 1. The process parameters and physical properties of the material are tabulated in Table 1. The domain for simulation is of length 0.8 mm and height 0.4 mm.
The following assumptions are made in the model.

1. The flow in the weld pool is considered laminar and incompressible.
2. Boussinesq approximation is applied to simulate buoyancy-induced convection in the melt pool.
3. The weld pool surface is assumed to be flat.
4. Gaussian distribution is used to describe the laser heat flux.

**Figure 1.** Schematic of the computational domain showing boundary conditions.

| Table 1. Process parameters and material properties. |
|------------------------------------------------------|
| Ambient temperature (K) | 323          |
| Melting temperature (K) | 1727         |
| Nucleation temperature (K) | 1627       |
| Latent heat of phase change (J/kg) | $1.2 \times 10^6$ |
| Specific heat capacity (J/kg-K) | 714          |
| Density (kg/m$^3$) | 7200         |
| Thermal conductivity (W/m-K) | 40           |
| Dynamic viscosity (N-s/m$^2$) | 0.1          |
| Surface tension coefficient (N/m-K) | -0.00043 |
| Thermal expansion coefficient (1/K) | 0.00012 |
| Laser spot size (mm) | 0.159        |
| Laser power (W) | 1000         |
| Laser efficiency | 15 %         |
| Convective heat transfer coefficient(W/m$^2$-K) | 10           |

**3. Mathematical modelling**

The present model is 2D axi-symmetric. The weld pool dynamics is modeled using the continuum equations of mass, momentum, and energy conservation. The radiative and convective heat losses on the top and convective heat losses on side surfaces have been taken into account [10, 11]. During spot welding, melting continues till the laser is on, once the laser is switched off solidification of the melt pool starts.
3.1. Weld pool thermo-fluid modeling

Conservation of mass

The continuity equation during the laser welding is given by

$$\nabla \cdot \mathbf{u} = 0$$  \hspace{1cm} (1)

Conservation of momentum

The fluid flow in the melt pool can be represented by the following equation.

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \mathbf{u} \cdot \nabla (\rho \mathbf{u}) = -\nabla p + \nabla \cdot \left( \mu \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \right) + \mathbf{F}_n + \mathbf{F}_s$$  \hspace{1cm} (2)

The buoyant flow in this model is applied with the help of Boussinesq approximation. The buoyancy source term \( \mathbf{F}_N \) is given as

$$\mathbf{F}_N = \rho g \beta_T (T-T_{ref})$$ \hspace{1cm} (3)

where \( \mathbf{F}_N \) is the natural buoyancy source term, \( \rho \), \( \beta_T \) and \( T_{ref} \) are density of liquid, coefficient of thermal expansion and reference temperature, respectively.

$$\mathbf{F}_s = \left(1 - f_l\right)^2 \frac{C}{f_l^3 + \varepsilon}$$ \hspace{1cm} (4)

The constant \( C \) in above equation represents morphological constant having a large value (150,000 kg m\(^{-3}\) s\(^{-1}\)) to make the velocity zero in unmelted portion of the domain [12]. The term \( \varepsilon \) is a constant with small value to prevent division by zero [12].

Energy conservation

$$\frac{\partial (\rho C_p T)}{\partial t} + \mathbf{u} \cdot \nabla (\rho C_p T) = \nabla \cdot (K \nabla T) - \rho \frac{\partial (\Delta H)}{\partial t}$$ \hspace{1cm} (5)

3.2. Liquid fraction calculation

Liquid fraction values are required in the governing equations for fluid flow, heat transport and interface velocity. Its calculation should be consistent with the non-equilibrium rapid solidification kinetics as well as the equilibrium solidification. The calculation of liquid fraction is described in the subsequent sub-sections.

3.2.1. Equilibrium solidification

In equilibrium solidification, enthalpy porosity method is used to calculate liquid fraction \( f_l \). Enthalpy porosity method is an iterative method described below.

$$f_l = \frac{\Delta H}{L}$$ \hspace{1cm} (6)

Latent heat content of each cell needs to be updated as per the temperature values predicted in each iteration within a time step. The iterative updating scheme [12,13] is given by

$$\left[ \Delta H_p \right]_{n+1} = \left[ \Delta H_p \right]_n + \frac{\alpha_p}{a_p} \lambda \cdot \left[ h_p \right]_n - G^{-1} \left[ \Delta H_p \right]_n$$ \hspace{1cm} (7)

where \( \lambda \) is the relaxation factor, \( a_p \), \( \alpha_p \) are coefficients of nodal temperature in the discretized energy equation and \( G^{-1} \) is inverse of suitable latent heat function. For solidification of pure substance it is given as

$$G^{-1} \left[ \Delta H \right]_n = c_p T_m$$ \hspace{1cm} (8)
3.2.2. Non-equilibrium solidification model

To consider the kinetic effect during rapid solidification, a linear correlation between the undercooling and interface velocity is usually adopted [14-17]. The relation between crystal growth velocity and undercooling is modelled by power law [16].

\[ V_i = a \Delta T^b \]

where \( V_i \) is the interface velocity, and \( \Delta T \) is the interface undercooling, \( a = 2.8 \times 10^{-3} \) and \( b = 1.8 \).

\[ \Delta T = T_m - T \]

Using solid-liquid interface growth speed solid fraction is updated as [16]

\[ f_{s}^{n+1} = f_{s}^{n} + \frac{V_{ix} \Delta T}{\Delta X} + \frac{V_{iy} \Delta T}{\Delta Y} \]

where \( f_{s} \) is the solid fraction, \( \Delta T \) is the time step, \( V_{ix} \) is the \( x \) component of interface growth speed, \( V_{iy} \) is the \( y \) component of interface growth speed, \( \Delta X \) and \( \Delta Y \) are the cell widths in \( x \) and \( y \) directions, respectively.

3.3. Boundary conditions

Thermal boundary condition on the top surface is given by

\[ k \frac{\partial T}{\partial n} = q - h_c (T - T_\infty) - \alpha \sigma (T^4 - T_\infty^4) \]

where \( q \) is the laser heat flux given by

\[ q = \frac{P}{\pi R^2} \exp \left( -\frac{r^2}{R^2} \right) \]

In Eq. (13) \( r \) is the distance from the center of beam and \( P \) is the power of the laser beam and \( R \) is the beam radius.

Bottom surface is considered as insulated, and on the side walls only convective heat loss is considered [10]. Therefore, energy balance at the side surfaces is given by

\[ k \frac{\partial T}{\partial n} = -h_c (T - T_\infty) \]

The shear force as a result of surface tension gradient (Marangoni effect) is considered at the free surface of melt pool, and is expressed as

\[ \tau_{xy} = -\mu \left( \frac{\partial u}{\partial y} \right) = \left( \frac{\partial y}{\partial T} \right) \left( \frac{\partial T}{\partial x} \right) \]

The governing equations in the present model are solved using a pressure-based finite volume method according to the SIMPLE algorithm. The resultant system of algebraic equations is solved by a line-by-line tri-diagonal matrix algorithm (TDMA).

4. Results and discussion

4.1. Thermal and flow field

When the high intensity of beam irradiates on top surface, molten pool starts to form and it will continue until the power source is turned off. Figures 2(a) and 2(b) show the temperature distribution and flow field during melting at \( t = 1 \) ms and \( t = 2 \) ms, respectively. Due to high energy of the beam, larger temperature gradients are present on the top surface. Marangoni convection has a significant influence on the temperature distribution in the weld pool [11]. The laser pulse was on till 3 ms and Fig. 2(c) shows the thermal and flow filed in weld pool at this instance.

Figures 3(a)-(f) shows the evolution of temperature in the melt pool with superimposing of melt pool contour at various time instants after the laser is switched off for both equilibrium and non-equilibrium solidification. When solidification starts at \( t = 3 \) ms, rapid cooling takes place in the melt pool due to high temperature gradients and the temperature starts to fall in the melt pool. At the top surface due to
heat losses, temperature contours will start to shrink in radially inward direction. The temperature continues to fall till the weld pool is fully solidified. From the simulation results, it can be seen that in the case of equilibrium solidification, the solidification takes place at the equilibrium melting temperature and the interface temperature is fixed at melting temperature during the entire phase change. In case of non-equilibrium solidification, initially temperature of the melt pool is decreased to nucleation temperature, solidification starts at the nucleation temperature and there is a significant temperature increase at the solid-liquid interface compared to the initial temperature. This is due to recalescence. Recalescence is the increase in temperature of an undercooled liquid metal as a result of the latent heat evolution during nucleation. After some time, the interface temperature is constant for a while then it will continue to decrease. Figures 3(b)-(e) shows the sharp increase in the temperature due to the spontaneous release of the latent heat.

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure2.png}
\caption{Temperature map and flow filed in the melt pool during the melting stage (Power = 1000 W)}
\end{figure}

4.2. Melt pool evolution

When the heat source is applied at the top surface, a strong thermal gradient develops from top to bottom of the melt pool. As a result, solidification starts from the solid-liquid interface at the bottom and propagates towards the top surface of weld plate [11]. Marangoni convection occurs, which develops a velocity loop just below the surface of the melt pool. The flow of molten metal in the melt pool is driven by combined surface tension or Marangoni force and thermal buoyancy. The flow is directed radially outwards from the center to the exterior of the pool.

Figures 4 (a)-(f) show the comparison of the melt pool evolution for equilibrium and non-equilibrium solidification. The melt pool evolution is same in both cases upto 3 ms. It can be seen from figure 4 that as the solidification continues, weld pool size is large in the case of non-equilibrium solidification compared to the case of equilibrium solidification. Equilibrium solidification starts at
freezing temperature, whereas in non-equilibrium solidification, it first cools down to nucleation temperature then solidification starts. From figure 4(e), it can be seen that two symmetrical vortices are formed in the weld pool due the temperature rise at solid-liquid interface by the latent heat is released during nucleation (recalescence). The thermal gradient set by this release drives this flow loops by buoyancy. Weld pool solidifies completely at time $t = 5.5$ ms in the case of equilibrium solidification and at $t = 5.76$ ms in the case of non-equilibrium solidification.

![Figure 3. Temperature map in the melt pool during solidification stage (Power = 1000 W)](image-url)
Equilibrium Solidification

Non-equilibrium Solidification

(a) $t = 2$ ms

(b) $t = 3$ ms

(c) $t = 3.4$ ms

(d) $t = 4$ ms

(e) $t = 4.4$ ms

(f) $t = 5.4$ ms

Figure 4. Evolution of the melt pool (Power = 1000 W)

4.3. Rapid solidification with undercooling

Figure 5 compares the temperature-time variation for equilibrium and non-equilibrium solidification at a position T1 (shown in figure 1). It can be seen that liquid metal first cools down to nucleation temperature which is below the freezing temperature then starts rapidly solidifying. This is due to release of latent heat which causes the increase in the local temperature. As the temperature reaches freezing temperature solidification rate decreases. The solidification temperature remains constant further until the liquid metal gets solidified. After that, the temperature falls down due to solid sensible cooling.
5. Conclusions

Transport phenomena and recalescence characteristic in the weld pool during laser spot welding was investigated using numerical simulations. A transient model was developed incorporating heat transfer, convective and radiative losses, rapid solidification kinetics and natural and Marangoni convection driven fluid flow in the melt pool. Marangoni convection is the dominant factor influencing the melt pool geometry and the maximum temperature in the melt pool. It was found that the melt pool is larger in the case of solidification with undercooling compared to solidification without undercooling, because the time needed to cool down to the nucleation temperature is longer in the case of solidification with undercooling. The solidification starts only after reaching to the nucleation temperature, which is below the freezing temperature and this phenomenon affects the final shape and size of the weld pool. The model well captures the recalescence phenomenon that is the local temperature rise at the solid-liquid interface during solidification due to the latent heat evolution.

References

[1] B. Basu, A.W. Date 1992 Rapid solidification following laser melting of pure metals-I Study of flow field and role of convection. *International Journal of Heat and Mass Transfer* **35** pp 1049–1058.

[2] X. He, P.W. Fuerschbach, T. DebRoy 2003 Heat transfer and fluid flow during laser spot welding of 304 stainless steel *Journal of Physics D: Applied Physics* **36** pp 1388.

[3] R. Rohit 2008 Modeling of heat transfer and fluid flow in keyhole mode welding *The Pennsylvania State University*
[4] P. Galenko, S. Sobolev 1997 Local nonequilibrium effect on undercooling in rapid solidification of alloys *Physical Review E* **55** pp 343–352.

[5] A. Yosef, Y. Kozak, Y. Korin, I. Harary, H. Mehling, G. Ziskind 2017 A novel multi-dimensional model for solidification process with supercooling *International Journal of Heat and Mass Transfer* **106** pp 91–102.

[6] G.X. Wang, E. Matthys 1992 Numerical modeling of phase change and heat transfer during rapid solidification process: use of control volume integral with element sub division *International Journal of Heat and Mass Transfer* **35** p141.

[7] H. Liu, M. Bussmann, J. Mostaghimi 2009 A comparison of hyperbolic and parabolic models of phase change of a pure metal *International Journal of Heat and Mass Transfer* **52** pp 1177–1184

[8] S.L. Chen, P.P. Wang, T.S.D. Lee 1998 An experimental investigation of nucleation probability of supercooled water inside cylindrical capsules *Experimental Thermal and Fluid Science* **18** pp 299–306.

[9] G.X. Wang, E.F. Matthys 1991 Modelling of heat transfer and solidification during splat cooling: effect of splat thickness and splat/substrate thermal contact *International Journal of Rapid Solidification* **6** pp 141–174.

[10] A. Ghosh, A. Yadav, A. Kumar 2017 Modelling and experimental validation of moving tilted volumetric heat source in gas metal arc welding process *Journal of Material Processing and Technology* **239** pp 52–65.

[11] A. Yadav, A. Ghosh, A. Kumar 2017 Experimental and numerical study of thermal field and weld bead characteristics in submerged arc welded plate. *Journal of Materials Processing Technology* **248** pp 262–274.

[12] A.D. Brent, V.R. Voller, K.J. Reid 1998 Enthalpy-porosity technique for modeling convection-diffusion phase change: application to the melting of a pure metal *Numerical Heat Transfer, Part A Applications* **13** pp 297–318.

[13] V. Arghode, A. Kumar, S. Sundarraj, P. Dutta 2008 Computational modeling of GMAW process for joining dissimilar aluminum alloys *Numerical Heat Transfer, Part A: Applications*, **53** pp 432–455.

[14] T. Clyne 1984 Numerical treatment of rapid solidification *Metallurgical Transactions B* **15** pp 369–381.

[15] W. Zhang, J.W. Elmer, T. DebRoy 2003 Modeling of heat transfer and fluid flow during gas tungsten arc spot welding of low carbon steel *Journal of Applied Physics* **93** pp 3022–3033.

[16] H. Zhang, X.Y. Wang, L.L. Zheng, S. Sampath 2004 Numerical simulation of nucleation, solidification, and microstructure formation in thermal spraying *International Journal of Heat and Mass Transfer* **47** pp 2191–2203.

[17] Y. Lahmar-Mebdoua, A. Vardelle, P. Fauchais, D. Gobin 2010 Modelling the nucleation process in alumina lamellae deposited on a steel substrate *International Journal of Thermal Sciences* **49** pp 522–528.

[18] G. Mi, X. Zhan, Y. Wei, W. Ou, C. Gu, F. Yu 2015 A thermal–metallurgical model of laser beam welding simulation for carbon steels *Modelling and Simulation in Materials Science and Engineering* **23** 035010