

Numerical investigation elucidating effects of microstructure on the transient thermomechanical phenomena during laser impact welding

Glenn Gleason, Sumair Sunny, Ritin Mathews, Arif Malik^{*}

The University of Texas at Dallas, Department of Mechanical Engineering, 800 W. Campbell Road, Richardson, TX 75080, USA

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ABSTRACT

Transient thermomechanical phenomena such as extreme plastic strains and temperature spikes that occur during laser impact welding are impractical to experimentally observe given the sub-microsecond duration of the joining process. Thus, computational models are necessary to study in-situ behavior along the weld interface. While researchers have utilized computational models for such investigations, this work elucidates the specific influence of microstructure-level modeling that captures the associated inhomogeneity/anisotropic effects at smaller scales. An aluminum 1100-H19 flyer and a stainless steel 304-O target foil are modeled using an Eulerian framework to simulate cases with and without microstructure consideration during laser impact welding of dissimilar metallic foils. When considering microstructure modeling, variations in flow stress reveal intermittently elevated temperatures along the weld interface due to concentrations of shock pressure at relatively small grains; however, they are not found to be a significant source of instability initiating or influencing the joint formation. Grain refinement and material hardening are suggested within a 10 μm -thick zone of the flyer near the weld interface, while severe plastic deformation in the target indicates possible martensitic phase transformation. Grain boundary sliding driven by variations in yield surfaces among individual grains gives rise to relatively higher collision velocity. Consequently, higher plastic strain rates along with greater amounts of plastic heat dissipation at the interface result in increased material jetting at higher temperatures. Alternating transient shear stresses are predicted in each model, though the inhomogeneous model predicts the brief appearance of a concentrated shear zone in the rebound region which is not seen in the homogeneous model. This work illuminates correlations between microstructure and transient phenomena during laser impact welding of dissimilar metallic foils, thus demonstrating a numerical modeling approach extensible to numerous other impact welding processes that complete within a very short time span.

1. Introduction

Laser impact welding (LIW) is a technique for forming joints between solid surfaces, wherein a flyer is propelled at a high velocity towards a stationary target by confined, rapidly expanding plasma induced via pulsed laser irradiation, as illustrated in Fig. 1. This process resembles other impact welding methods in that there is no direct application of heat to form joints. LIW is notable for its utility at relatively smaller scales, however, allowing welds to be formed with greater precision and safety in certain applications. LIW has been successfully shown to join foils tens of micrometers thick of dissimilar metal alloys known to produce unfavorable weld characteristics in fusion processes [1,2], or between alloys that are infeasible to fusion weld due to mutual insolubility, even at high temperatures (e.g., magnesium and steel) [3]. Impact

techniques substantially increase the range of material combinations that may be joined, since fusion weldability is not of concern. This suggests their possible application in situations where designs must be considered according to other criteria, such as in microelectronics or biocompatible implants.

The use of laser-induced shock pressure to initiate the LIW process results in strain rates from 10^6 to 10^7 s^{-1} in a foil flyer [4]. Additionally, the velocities at which the collision point travels in an impact welding interface is on the order of the speed of sound in the materials (~ 0.2 to 1.5 km s^{-1}) [5]. Temperatures near at least one of the materials' melting points, severe plastic deformation, and high pressures occur in the narrow interfacial region, thus creating a weld absent intermetallic compounds [6]. Thin layers of oxides and other contaminants ablate from the surfaces in a jet of high-temperature particles, a phenomenon driven by extreme shear stresses near the collision point that oppose

^{*} Corresponding author.

E-mail address: arif.malik@utdallas.edu (A. Malik).

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Nomenclature			
A	Johnson-Cook reference yield strength	t	Time
a	Selective laser melting (SLM) parameter	t_p	Full-width half-maximum pulse width
B	Johnson-Cook strain hardening coefficient	U_i	Linear displacement ($i = \{X, Y, Z\}$)
b	SLM parameter	U_p	Particle velocity
C	Johnson-Cook strain rate hardening coefficient	U_s	Shock wave velocity
c_0	Bulk speed of sound	v	Scan speed
c_f	SLM parameter	v_x	Collision velocity
c_r	SLM parameter	$\dot{\mathbf{X}}$	Velocity vector
c_v	Specific heat (constant volume)	$\mathbf{X}$	Position vector
D_i	Major diameter of grain i	x_i	Center of laser spot (X-direction)
e_v	Internal energy per unit volume	α	Energy ratio
e_m	Internal energy per unit mass	Γ	Grüneisen material constant
f_f	SLM parameter	γ	Shock impedance (combined)
F_n	Nodal forces	γ_{Al}	Shock impedance (aluminum)
f_r	SLM parameter	γ_g	Shock impedance (borosilicate glass)
G	Elastic shear modulus	ϵ	Emissivity
h	Convective heat transfer coefficient	ϵ_{eq}	Equivalent plastic strain
I_0	Averaged laser pulse fluence	$\dot{\epsilon}_0$	Johnson-Cook reference strain rate
k	Thermal conductivity	ϵ_{el}	Deviatoric elastic strain
k_y	Strengthening coefficient	$\dot{\epsilon}_p$	Plastic strain rate
L	Plasma layer thickness	$\dot{\epsilon}_p$	Plastic strain rate tensor
L_e	Finite element edge length	ϵ_p	Plastic strain
m	Johnson-Cook thermal softening exponent	η	Ratio of particle velocity to shock velocity
n	Johnson-Cook strain hardening exponent	θ_i	Angular displacement ($i = \{X, Y, Z\}$)
n_l	Number of node layers	Λ	Absorptivity
$\hat{n}$	Unit normal vector	λ	Adiabatic constant
P	SLM laser power	ρ	Density
P	Laser-induced pressure	σ	Stress tensor
p	Shock wave pressure	σ_0	Dislocation movement stress threshold
Q	Volumetric heat input	σ_d	Deviatoric stress
R	Radial distance from spot center	σ_f	Flow stress
s	Ratio of ΔU_s to ΔU_p	σ_R	Standard deviation of intensity distribution
S	Source function (general)	$\sigma_{y, i}$	Yield strength of grain i
T	Temperature	τ_{XY}	In-plane (XY) shear stress
T^*	Homologous temperature	ϕ	Solution variable (general)
T_0	Ambient temperature	φ	SLM surface designation
T_m	Melting temperature	Ψ	Flux function
		ψ	Stefan-Boltzmann constant

direction in the flyer and target [7]. Transient phenomena such as these resolve on very short timescales, making in-situ observation of the process challenging; this is particularly notable in the case of in LIW (vs. other larger-scale types of impact welding), which resolves within approximately 1 μ s due to the small dimensions of the parts being welded. Complex patterns of shear stress, severe plastic deformation, and thermal dissipation emerge in an unstable manner during collision, and experimental methods are limited in the information that may be captured before the process is complete. Therefore, many computational investigations utilizing physics-based finite element (FE) techniques

have been performed to try to explain the mechanisms that influence joint formation; a summary of recent works may be found in Table 1.

The continued application of computational methods to the problem of impact welding has yielded useful knowledge on the process. However, the effects of metallic microstructure when incorporated into numerical models have been minimally explored. Table 1 lists recent research that utilizes continuum-scale FE models, employing homogeneous material properties for the welded specimens. It is important to note that none of the previous studies have captured the effects of microstructure modeling. Given that previous works on impact welding

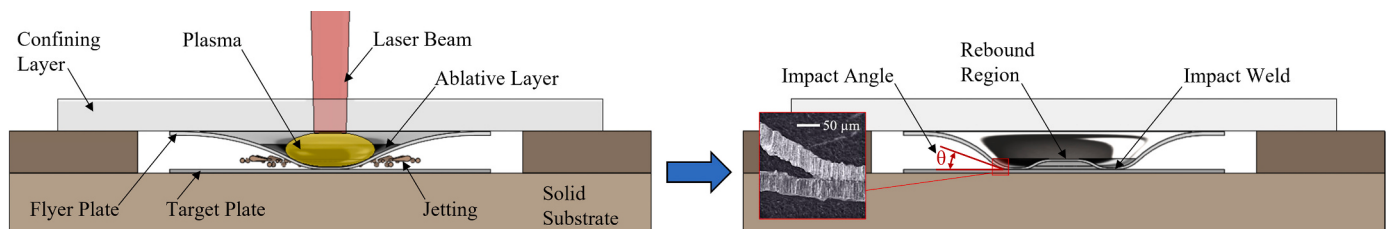


Fig. 1. (Left) Schematic of a laser impact welding process illustrating the expanding plasma that propels the flyer towards the stationary target. Upon impact, material jetting phenomena is observed. (Right) The resulting impact weld, featuring a rebound region that may develop [8]. (Inset) Optical micrograph featuring a cross section of an Al 1100 – SS 304 laser impact weld, adapted from an earlier publication by the authors [9].

Table 1

Summary of recent works pertaining to numerical modeling of transient phenomena in impact welding. Note, effects of grain structure were not captured.

Author (year)	Process & materials (specification)	FE model formulation	Investigated quantities	Notable findings
Nassiri et al. (2017) [10]	Vaporizing foil actuator welding (VFAW); Ti-Cu (110)	Arbitrary Lagrangian Eulerian (ALE), smoothed particle hydrodynamics (SPH)	- Pressure - Temperature - Plastic strain - Velocity (collision point)	- Simple wavy weld morphologies were successfully captured using ALE and SPH. - Only SPH provided insights into waveforms with vortex shedding phenomena and jetting. - Transient molten zones were predicted near vortices. - Emergence of jet indentation mechanism predicted in EXW. - Qualitative similarities found between vortex shedding zones in model and experiment.
Zhang et al. (2018) [11]	Explosive welding (EXW); Al (2024)-steel (4340)	SPH	- Temperature - Pressure - Weld interface - Jetting	- Various impact velocities simulated to determine relationship between weld interface morphology and collision point velocity (compared to sound speeds in material). - Impact angle found to increase with distance from spot center. - Significant shear stresses found in flyer prior to impact. - Transient alternating shear stresses due to elastic interactions found to trail the weld front.
Gupta et al. (2019) [12]	VFAW; Cu-Ti, Al (6061-T6)-Steel (4130)	Eulerian	- Temperature - Velocity - Weld Interface - Temperature - Plastic strain - Velocity - Shear stress	- Impact angle found to increase with distance from spot center. - Significant shear stresses found in flyer prior to impact. - Transient alternating shear stresses due to elastic interactions found to trail the weld front. - Rapid changes in plastic strain and temperature result in an impact affected zone at impact weld interface, distinct from the heat affected zones found in fusion welds.
Gleason et al. (2020) [7]	LIW; Al (1100-H19)-stainless steel (304-O)	Eulerian	- Temperature - Plastic strain - Velocity - Shear stress - Pressure - Temperature - Plastic strain - Velocity (collision point)	- Molten zones must be brief and discontinuous to prevent brittle intermetallic formation. - Simulation based on SPH framework predicted jetting of mostly Al composition preceding nearly flat weld interface formation. - Johnson-Holmquist ceramics model applied to brittle BMG substrate. - Plastic strain profiles of near-surface elements (particles) show severe plastic deformation of both materials, including the BMG.
Lee et al. (2020) [13]	VFAW; Cu-Cu	SPH	- Plastic strain - Weld interface - Jet composition	- Simulation based on SPH framework predicted jetting of mostly Al composition preceding nearly flat weld interface formation. - Johnson-Holmquist ceramics model applied to brittle BMG substrate. - Plastic strain profiles of near-surface elements (particles) show severe plastic deformation of both materials, including the BMG.
Liang et al. (2020) [14]	Underwater EXW, Al (1060)-BMG (Zr-based)	SPH	- Temperature - Velocity - Weld interface - Plastic strain - Velocity - Stress (von Mises, shear)	- Modification of simulation parameters revealed a dependence of waveform dimensions on density ratio, impact velocity/angle, and other parameters. - Shear stress temporal profile at traveling collision point used to confirm weld formation time. - Equivalent plastic strain thresholds used to predict geometry of welds.
Meng et al. (2020) [15]	VFAW; Cu-Ti	SPH	- Temperature - Plastic strain - Velocity - Weld interface	- Wavy interface morphology is shown to form via repeated deformations of flyer and target surfaces during weld, not in a simultaneous surface distortion. - Localized high-temperature zones predicted by FE model in good agreement with intermetallic compound zones found in experiment.
Hosseinizadeh et al. (2021) [16]	Gas mixture detonation impact welding, Al (6061-T6)-Cu (OFHC)	Lagrangian	- Temperature - Plastic strain - Velocity - Weld interface	- High jet temperature predictions partly caused by isolation of ablated material from substrate. - Tracking thermal history of individual nodes allows characterization of weld interface due to transient temperature effects.
Li et al. (2021) [17]	Magnetic pulse welding (MPW); Al (6060-T6)-Cu	Eulerian (for interface mechanics)	- Pressure - Temperature - Plastic strain - Shear stress - LIW cross-sectional morphology	- Transient oscillations in jet ejection direction modeled in SPH used to show transition in weld interface morphology at increasing values of laser energy used for welding. - Jet indentation mechanism shown to include participation from both specimens' materials, as opposed to only the lower-density material (Ti flyer) considered in other analyses [1,20].
Li et al. (2021) [18]	LIW; Ti (TA1)-Ni	Coupled SPH-Lagrangian, SPH, Eulerian	- Pressure - Temperature - Plastic strain - Shear stress - LIW cross-sectional morphology	- Conditions at impact weld analyzed via FE model to explain porosity and cracks at interlayer between Mg-Steel interface. - Fe found to be diffused/mixed into a deposit layer formed by local melting of Mg, contributing to a metallurgical bond without a wavy interface/interlocking.
Lu et al. (2021) [19]	LIW; Ti (TA1)-brass (H62)	SPH	- Velocity - Temperature - Plastic strain	- Extreme shock pressures concentrate at small, hard grains of SS 304, resulting in local thermal spikes at weld - Equivalent plastic strains crossing an exothermic phase transformation range are achieved in the SS 304 target during weld
Xiong et al. (2021) [3]	VFAW; Mg (AZ31)-steel (DP590)	Eulerian (impact phase), Meshed Lagrangian (cooling phase)	- Pressure - Temperature	
Gleason et al. (2022) [21]	LIW; Al (1100-H19)-Stainless steel (304-O)	Eulerian	- Velocity - Temperature - Plastic strain	

have noted the role of dynamic instability in the initiation and development of impact weld interfaces [22], this work seeks to provide further novel insights into the effects an inhomogeneous grain structure may have as the joining process proceeds. Variations in grain structures are known to arise for fabrications by additive manufacturing (AM) (e. g., selective laser melting (SLM)), resulting in inhomogeneity and anisotropy in the material properties, and thus presents challenges in

predicting the response of parts during subsequent processing. Indeed, continued investigations of the corresponding inhomogeneous thermo-mechanical behavior in such parts present opportunities to tailor AM microstructures to realize improved LIW strength.

First, a prediction of the inhomogeneous grain structures for AM aluminum and stainless steel foils are established via a Dynamic Kinetic Monte Carlo (KMC) model, described further in Section 2.1. Section 2.2

outlines the Eulerian numerical formulation used for the FE model. Following this, Section 2.3 details the model layout and boundary conditions, while Section 2.4 describes the material modeling. A discussion of the results from the inhomogeneous material model is provided in Section 3, with comparisons made to a homogeneous LIW model to better elucidate the importance of microstructure modeling on prediction of transient phenomena. Finally, key findings and concluding remarks are summarized in Section 4.

2. Numerical modeling

To obtain a 3D microstructure model that can be implemented in the numerical framework for each foil, the foils are considered to be AM via SLM, as discussed by [23]. This process would give rise to variations in microstructure, i.e., a mix of columnar (or elongated) grains that grow towards the direction of maximum thermal gradient, and finer, equiaxed grains that form along the path of the scan lines. Such variations are hypothesized to influence the transient, anisotropic thermomechanical responses during LIW. In this section, the SLM model is first discussed, from which the thermal history is used as input for a Dynamic KMC simulation [24] for grain structure prediction. The predicted microstructure is subsequently spatially mapped into an Eulerian grid, wherein an LIW experiment by the authors [9] is emulated. The influence of variation in grain size during the highly dynamic process, for both the flyer and target foils, is captured by implementing a Johnson-Cook Hall-Petch (J-C H-P) material model [27], along with a linearized Hugoniot Equation of State [28].

2.1. Selective laser melting model

An SLM numerical model to predict the thermal history is depicted in Fig. 2. A 4 mm × 5 mm patch on the top surface of a 50 μm thick layer of powder, atop a 25.4 mm square × 3.2 mm deep substrate is scanned in a raster pattern as illustrated. The thermal history of the process is governed by Eq. (1) which represents the 3D heat conduction in the model. Temperature-dependent material parameters such as thermal conductivity, k , specific heat (constant volume), c_v , and density, ρ , are adopted from literature for both metals [29,30]. The transient, volumetric heat energy input, Q , is modeled using a double ellipsoid Gaussian heat source described by Eq. (2), introduced by Goldak et al. [26], which captures the influence of scan speed, v , laser power, P , and absorptivity, Λ . The heat input process parameters adopted in this work, for both the aluminum 1100-H19 (Al 1100) flyer and stainless steel 304-O (SS 304) target, are summarized in Table 2.

$$\nabla \cdot (k \nabla T) + Q = c_v \rho \frac{\partial T}{\partial t}, \quad \text{for } t \geq 0 \quad (1)$$

Table 2
SLM process parameters and calibration constants [23,34–36].

Parameter	Al 1100	SS 304
<i>SLM process model</i>		
P (W)	175	200
v (m s ⁻¹)	0.195	0.8
Scan pattern	Raster	Raster
Layer thickness (μm)	50	50
Hatch spacing (μm)	50	50
Λ	0.35	0.4
ϵ	0.32	0.56
h (W m ⁻² K ⁻¹)	10	10
<i>Heat source model</i>		
a (μm)	160	180
b (μm)	160	180
c_f (μm)	276	180
c_r (μm)	1520	540
f_f	1.4	1.4
f_r	0.6	0.6

$$Q = \begin{cases} \frac{6\sqrt{3} f_r P \Lambda}{abc\pi\sqrt{\pi}} e^{-\frac{3z^2}{a^2}} e^{-\frac{3y^2}{b^2}} e^{-\frac{3(x-x_i)^2}{c_r^2}}, & X \geq x_i \\ \frac{6\sqrt{3} f_f P \Lambda}{abc\pi\sqrt{\pi}} e^{-\frac{3z^2}{a^2}} e^{-\frac{3y^2}{b^2}} e^{-\frac{3(x+x_i)^2}{c_f^2}}, & X < x_i \end{cases} \quad t > 0 \quad (2)$$

A *DFLUX* user subroutine is scripted herein to continually update the position of the scanning laser and is recomputed during every increment of the thermal solution. Eq. (2) represents a piecewise-continuous function moving linearly along the X direction. For all $X \geq x_i$, the frontal heat distribution fraction is computed, and for all $X < x_i$, the aft heat distribution fraction is computed. Calibration constants for the heat source model are provided in Table 2 and details regarding calibration of the heat input model can be referenced from [24].

Since pre-heating of the substrate is not considered in this work, as an initial condition, the entire model is set to ambient temperature, T_0 , as given by Eq. (3).

$$T(\mathbf{X}, 0) = T_0 \quad (3)$$

As heat is added, during scans, internal heat transfer via conduction, convection and radiation on surface φ is modeled per Eq. (4), which describes the surface energy balance of the system. In Eq. (4), ϵ is the emissivity, h is the convective heat transfer coefficient, and ψ is the Stefan-Boltzmann constant (5.6704×10^{-8} W m⁻² K⁻⁴).

$$-k \nabla T \cdot \hat{n} + h(T - T_0) + \psi \epsilon (T^4 - T_0^4) = 0 \text{ on surface } \varphi \quad (4)$$

The thermal history, once predicted, is used as input for the Dynamic

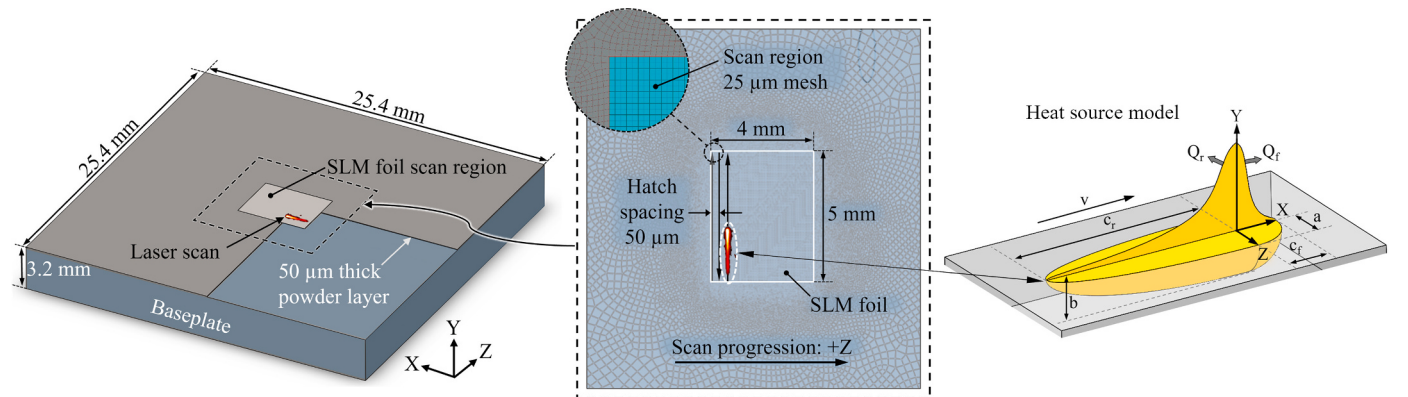


Fig. 2. (Left) Schematic of the SLM model to manufacture metal foils (having inhomogeneous microstructure). All dimensions are adapted from thermography experiments conducted by NIST [25]. A geometrically identical model is used for Al 1100 and SS 304, with only the temperature-dependent material properties, SLM & heat source parameters, and thermal calibration differing. (Right) Double ellipsoid heat source model [26] used to model the scanning laser.

KMC. The advantage of the Dynamic KMC over the conventional KMC technique [31] is that it captures the influences of intra- and interlayer heat accumulation on grain growth and nucleation prediction. After calibration the method can predict grains in FCC and BCC structures. Given that both metals used herein, for the flyer and target foils, have FCC crystal structures [32,33], the Dynamic KMC approach is applicable. An advantage of 3D microstructure prediction over electron backscatter diffraction (EBSD) imaging is that the experimental approach only offers 2D data and suitable assumptions must be made for out-of-plane grain dimensions. This can introduce errors in the framework. Nevertheless, EBSD imaging has been used to help verify the model calibration; for details on the Dynamic KMC framework and its calibration the reader is referred to [24].

The microstructure, once predicted, is mapped as a volume fraction into an Eulerian grid, discussed next, via a Python script. Each grain being mapped will accordingly also have its very own material definition, based on the respective grain's major diameter, D_i , obtained using a spherical fit to circumscribe the grain.

2.2. Eulerian numerical formulation

Eulerian models are useful for modeling fluid transport and severe solid deformation problems, thus making them appropriate for LIW considering the extreme strain (>20%) and strain rates involved in the laser-based manufacturing process. The Eulerian approach uses a spatially fixed mesh that is entirely remapped during every solution increment, avoiding mesh distortion errors that would occur in the case of a Lagrangian approach. Additionally, in contrast to a smoothed particle hydrodynamics framework, the Eulerian frame allows the laser-induced plasma pressure load described in the next subsection to be applied to the flyer.

The governing Eqs. (5)–(7) describe conservation of mass, momentum, and energy within the Eulerian domain, respectively. In Eqs. (5)–(7), $\dot{\mathbf{X}}$, $\boldsymbol{\sigma}$, $\dot{\epsilon}_p$, t , and e_v , represent the velocity vector, stress tensor, plastic strain rate tensor, time, and internal energy per unit volume, respectively.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \dot{\mathbf{X}}) = 0 \quad (5)$$

$$\frac{\partial \rho \dot{\mathbf{X}}}{\partial t} + \nabla \cdot (\rho \dot{\mathbf{X}} \otimes \dot{\mathbf{X}}) = \nabla \cdot \boldsymbol{\sigma} \quad (6)$$

$$\frac{\partial e_v}{\partial t} + \nabla \cdot (e_v \dot{\mathbf{X}}) = \boldsymbol{\sigma} : \dot{\epsilon}_p \quad (7)$$

Eq. (8) represents the generalized form of Eqs. (5)–(7), where Ψ is a flux function, S is a source function, $\mathbf{X}$ is the position vector, and ϕ is a solution variable.

$$\frac{\partial \phi}{\partial t} + \nabla \cdot \Psi(\phi, \dot{\mathbf{X}}, \mathbf{X}, t) = S \quad (8)$$

Eqs. (9) and (10) are obtained via operator splitting in Eq. (8) and are solved in separate steps during each Eulerian solution increment.

$$\frac{\partial \phi}{\partial t} = S \quad (9)$$

$$\frac{\partial \phi}{\partial t} + \nabla \cdot \Psi(\phi, \dot{\mathbf{X}}, \mathbf{X}, t) = 0 \quad (10)$$

Eq. (9) takes the form of a Lagrangian governing equation with the only exception being the terms on the left side where a material time derivative is used in place of the spatial time derivative. To avoid displacement across more than one element length, solution variables are calculated within a sufficiently small time increment on a temporary Lagrangian mesh. This Lagrangian mesh is then remapped to the stationary Eulerian grid and the solutions to Eq. (10) account for changes in solution variables on the fixed mesh due to advection. This process

allows for equivalent plastic strain, internal energy, and mass to be tracked throughout the LIW process.

2.3. Laser impact welding process model

An LIW experiment documented in previous work by the authors is emulated by the model illustrated in Fig. 3; the general approach used, except without microstructure, has shown good overall agreement with experimental observation [9]. The thermomechanical model assumes a plastic heat dissipation fraction, $\sigma : \dot{\epsilon}_p$ (ref. Eq. (7)) of 90%. The FE model features a linear hexahedral Eulerian mesh having thermal and translational degrees of freedom. The cubic elements have an edge length, L_e , of 2 μm and hence reduced integration is implemented to decrease computational time. The transparent borosilicate glass overlay and stainless steel substrate are modeled as Lagrangian discrete rigid bodies; they are not involved in the weld formation which occurs entirely within the Eulerian domain. Both rigid bodies are constrained in translation ($U_x = U_y = U_z = 0$) to emulate the experiment conditions. The 50 μm thick Al 1100 flyer foil and SS 304 target foil are both modeled within the Eulerian domain and are separated only by a 260 μm standoff distance that has been experimentally found to offer successful welds.

As described earlier, for both flyer and target, the predicted volume fractions with corresponding material assignments comprise the entire foil volume being modeled. As a simplification, the standoff region is treated as a void, i.e., no material (e.g., gas medium) assignment. Since the transient phenomena should manifest radially outward from the laser shot center, a symmetry condition ($U_x = \theta_y = \theta_z = 0$) is applied on plane $X = 0$ to further reduce the computational cost and the out-of-plane thickness is limited to 6 μm . Since the out-of-plane characteristics are not being studied, a displacement boundary condition ($U_z = 0$) restricting motion along the Z direction is imposed throughout. This enforces a simplifying plane strain condition, validated by experimental observations by Lee et al., who noted less impact weld morphology variation in the direction normal to the weld cross section [37]. Furthermore, based on experimental observation since the annulus of the weld does not exceed 600 μm , the radial length (X direction) of the modeled foils is limited to 600 μm . A no-slip, isotropic Coulomb friction condition is implemented to capture the shear interaction between the colliding foil surfaces. Correspondingly, the coefficient of dry friction is estimated to be 0.6 [38]. This is found to be appropriate as per observations by Raelison et al. [39], wherein impact welds were formed without slip or debonding.

A spatial and temporally varying laser-driven plasma pressure pulse is modeled based on experimental characterization documented by Hatamleh et al. [40]. Fabbro et al.'s 1D hydrodynamic model is used to develop a piece-wise continuous plasma pressure temporal profile given by Eq. (11) [41]. As depicted in Fig. 3, there is a heating phase, $t < t_p$, followed by an adiabatic cooling phase, $t \geq t_p$, at the confined ablation interface.

$$P(t) = \begin{cases} \frac{1}{10} \left\{ \left[\frac{\alpha \gamma I_0}{2\alpha + 3} \right] \left[1 - \left(\frac{L(0)}{L(t)} \right)^2 \right] \right\}^{\frac{1}{2}}, & \text{for } t < t_p \\ P(t_p) \left[\frac{L(t_p)}{L(t)} \right]^{\lambda}, & \text{for } t \geq t_p \end{cases} \quad (11)$$

The initial plasma thickness $L(0)$, is estimated to be 10 μm and the combined shock impedance, γ , at the confined ablation interface is calculated by Eq. (12), where γ_{Al} and γ_g represent the aluminum foil and borosilicate glass impedances, respectively.

$$\gamma = \frac{\gamma_{Al} \gamma_g}{2(\gamma_{Al} + \gamma_g)} \quad (12)$$

A peak pressure of 2.7 GPa, calculated at time t_p during the LIW simulation, is used to scale a normalized spatial pressure profile. This

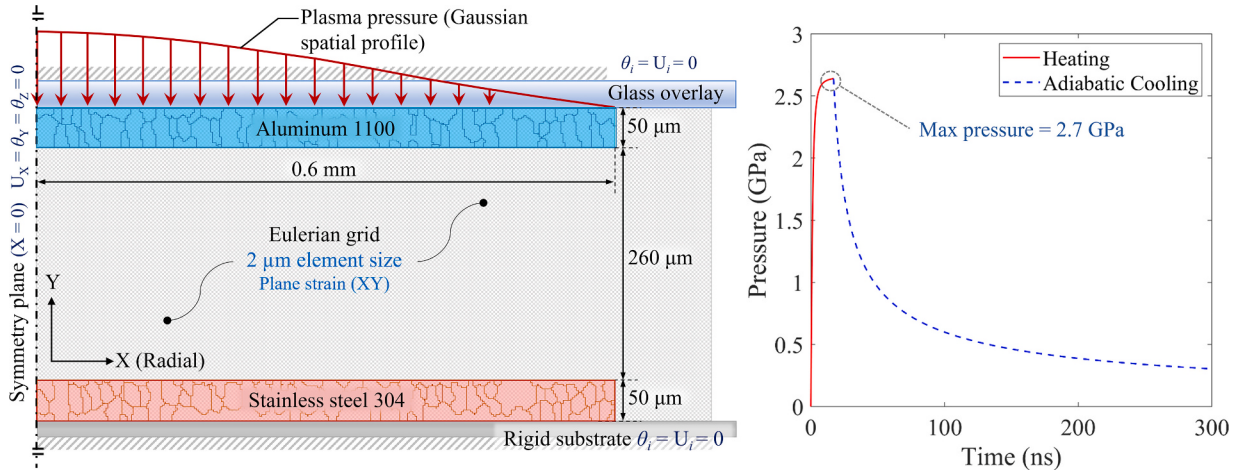


Fig. 3. (Left) A schematic of the laser impact welding process model used to emulate experiments documented in [9], showing the Gaussian spatial plasma pressure profile used to replicate realistic loading conditions. (Right) Experimentally characterized plasma pressure temporal profile.

profile is obtained from experimentally acquired spatial laser pulse intensity data in the form a 3D point cloud [40]. The 3D point cloud is scaled from pixels to radial distance, R , from the spot center ($X = 0$), and undulating noise is filtered before a Gaussian profile, $P(R)$, described by Eq. (13), is fit to the data. This simplification facilitates modeling of the load in the Eulerian plane strain configuration and provides to the flyer foil a more realistic velocity profile and deformed shape prior to impact [7]. In Eq. (13), the standard deviation, σ_R , describes the dispersion of the 3D point cloud data from the laser spot center. The peak plasma pressure, $P(t_p)$, (ref. Eq. (11)), obtained from the 1D hydrodynamic model, is used to scale the normalized spatial pressure distribution. A summary of the hydrodynamic model parameters used to compute the peak pressure temporal pressure profile are given in Table 3.

$$P(R) = \frac{1}{\sigma_R \sqrt{2\pi}} e^{-\frac{1}{2} \left(\frac{R}{\sigma_R} \right)^2} \quad R \geq 0 \quad (13)$$

The Gaussian plasma pressure profile, $P(R)$, is represented by an equivalent distribution of concentrated nodal forces, $F_n(R)$, apportioned equally among all the nodes, n_i , that span the 50 μm thick flyer (Y direction), as described by Eq. (14). During the confined ablation induced loading phase a peak nodal force magnitude of 3.24×10^{-4} N is predicted.

$$F_n(R) = \frac{L_e^2 P(R)}{n_i} \quad (14)$$

2.4. Material model for laser impact welding

Since the Dynamic KMC method used to predict the 3D microstructure does not provide information about crystal lattice orientation, approaches such as crystal plasticity finite element techniques cannot be implemented. A more rudimentary approach is adopted herein, where the Hall Petch (H-P) relation given by Eq. (15), is used as the yield strength parameter in the Johnson Cook (J-C) plasticity model given by

Eq. (16) [43–45]. Individual grains are assigned unique yield strengths, $\sigma_{y,i}$, per Eq. (15), calculated based on their individual major diameters, $D_{i,j}$, which can be rationalized given that the major diameter of non-spherical grains corresponds to the lowest strength direction in a polycrystalline alloy [46]. In Eq. (15), σ_0 is the threshold stress beyond which dislocations will move, and k_y is the strengthening coefficient.

$$\sigma_{y,i} = \sigma_0 + \frac{k_y}{\sqrt{D_{i,j}}} \quad (15)$$

In conjunction with grain size dependency, a strain-rate dependent and temperature dependent J-C plasticity model, per Eqs. (16)–(17), is implemented for its ability to capture the dynamic responses that occur during the high strain rates and elevated temperatures from plastic heat dissipation experienced in LIW [47].

$$\sigma_f = [A + B(\epsilon_p)^n] \left[1 + C \ln \left(\frac{\dot{\epsilon}_p}{\dot{\epsilon}_0} \right) \right] [1 - (T^*)^m] \quad (16)$$

$$T^* = \begin{cases} 0 & \text{for } T < T_0 \\ \left(\frac{T - T_0}{T_m - T_0} \right) & \text{for } T_0 \leq T \leq T_m \\ 1 & \text{for } T > T_m \end{cases} \quad (17)$$

As the laser induced shock waves propagate through the surface of the metal, a small increase in entropy occurs given the large bulk moduli and adiabatic index at ambient conditions [48]. The Mie-Grüneisen equation of state, given by Eqs. (18)–(19), describes the resulting volumetric stress-strain response, associated to changes in pressure, p , and volume, during the LIW process. The presented model implements a Hugoniot form featuring a linearized relation between shock wave velocity U_s and particle velocity U_p , where c_0 is the bulk speed of sound within the dissimilar foil materials, η is the ratio of U_p to U_s , s is the ratio of change in U_s to change in U_p , e_m is the internal energy per unit mass, and Γ is a dimensionless Grüneisen parameter capturing thermodynamic material response.

$$p = \frac{\eta \rho c_0^2}{(1 - \eta)^2} \left(1 - \frac{\eta \Gamma}{2} \right) + \Gamma \rho e_m \quad (18)$$

$$U_s = c_0 + s U_p \quad (19)$$

Additionally, Eq. (20) captures the deviatoric stress-strain response of each foil, where σ_d is the deviatoric stress, G is the elastic shear modulus, and ϵ_{el} is the deviatoric elastic strain. All the LIW material constitutive model parameters are given in Table 4.

Table 3
1D hydrodynamic model parameters [40–42].

Hydrodynamic model parameter	Value
FWHM pulse width, t_p	~17 ns
Averaged laser pulse fluence, I_0	1.8 GW cm ⁻²
Energy ratio, α	0.25
Adiabatic constant, λ	1.4
Glass shock impedance, γ_g	1.14×10^6 g cm ⁻² s ⁻¹
Al shock impedance, γ_{Al}	2.75×10^6 g cm ⁻² s ⁻¹

Table 4
Laser impact welding material model parameters [1,20,28,49–51].

Parameters	Al 1100	SS 304
<i>Hall-Petch parameters</i>		
σ_0 (MPa)	9.7	147.4
k_y (MPa $\mu\text{m}^{-0.5}$)	41	551.67
<i>Johnson-Cook plasticity</i>		
A (MPa) ref. Eq. (15)	$\sigma_{y,i}$	$\sigma_{y,i}$
B (MPa)	345.5	1500
C	0.001	0.014
$\dot{\epsilon}_0$ (s^{-1})	1	1
n	0.183	0.36
m	0.895	1
T_0 (K)	293	293
T_m (K)	916	1673
<i>Equation of state</i>		
ρ (kg m^{-3})	2712	7905
c_0 (m s^{-1})	5451.8	4722
s	1.2592	1.441
Γ	2.14	1.93
G (GPa)	27.4	78

$$\sigma_d = 2G\epsilon_{el} \quad (20)$$

By modeling individual grains as unique volume fractions and assigning to them distinct plasticity behavior, the foils can be considered as having inhomogeneous microstructures. As mentioned earlier, to illuminate the anisotropic effects on transient phenomena such as shear stress and temperature spikes associated to the distribution of plastic strain during impact as a result of the inhomogeneous model, an identical simulation is executed featuring homogeneous Al 1100 flyer and homogeneous SS 304 target. All material parameters listed in Table 4 are applied, however the J-C yield strength remains constant throughout the volume of the foils, i.e., 148.4 MPa and 110 MPa, respectively, for the Al 1100 flyer and SS 304 target [1]. Results of the LIW simulation, which

focus on transient interfacial material behavior when comparing the inhomogeneous and homogeneous models, are discussed next.

3. Results and discussion

To study the changes in the transient phenomena during the impact weld formation, three sub-microsecond time frames, at 475, 575, and 675 ns, respectively, are examined, as depicted in Fig. 4. Additionally, Fig. 4 includes a 400 ns frame, to reveal the shape of the grains in both foils just prior to impact. As the weld forms, observations radially outward from the weld center ($X = 0$ mm) show that the impact angle increases and grains become more elongated; this agrees with experimental observations where more elongated grains suggest a greater degree of dynamic shear strain and the likelihood of adiabatic shear bands (ASB) [52]. ASB results when thermal softening in the material reaches a point beyond which strain hardening is no longer possible, such that any plastic heat dissipation causes an adiabatic rise in temperature, thereby inducing plastic flow instability [53]. The presence of ASB indicates work hardening given that the high shear deformation can increase dislocation density [54]. ASB is often observed alongside dynamic recrystallization (DRX) [55], however it should be noted that prediction of DRX is a limitation of the implemented Dynamic KMC microstructure prediction tool. As seen in Fig. 4, the aluminum grains (blue) reveal relatively more elongation in comparison to the stainless-steel grains (red). Since H-P strengthening is implemented in the material constitutive modeling, AM process-parameter dependent grain sizes have direct influence the range of yield strength, as depicted by the colormap. Considering the high strain rates associated with LIW, differences in the stacking fault energy (SFE) for both metals influence the choice of H-P coefficients [56]. Furthermore, the alloy composition for steel will also influence the choice of H-P coefficients, given its low SFE. Beyond changes in impact angle, differences in yield strengths, SFE for the two dissimilar metals, and differences in velocity during collision, the effect of grain-boundary sliding (GBS), i.e., shear movement at the boundary shared among neighboring grains, should also be noted.

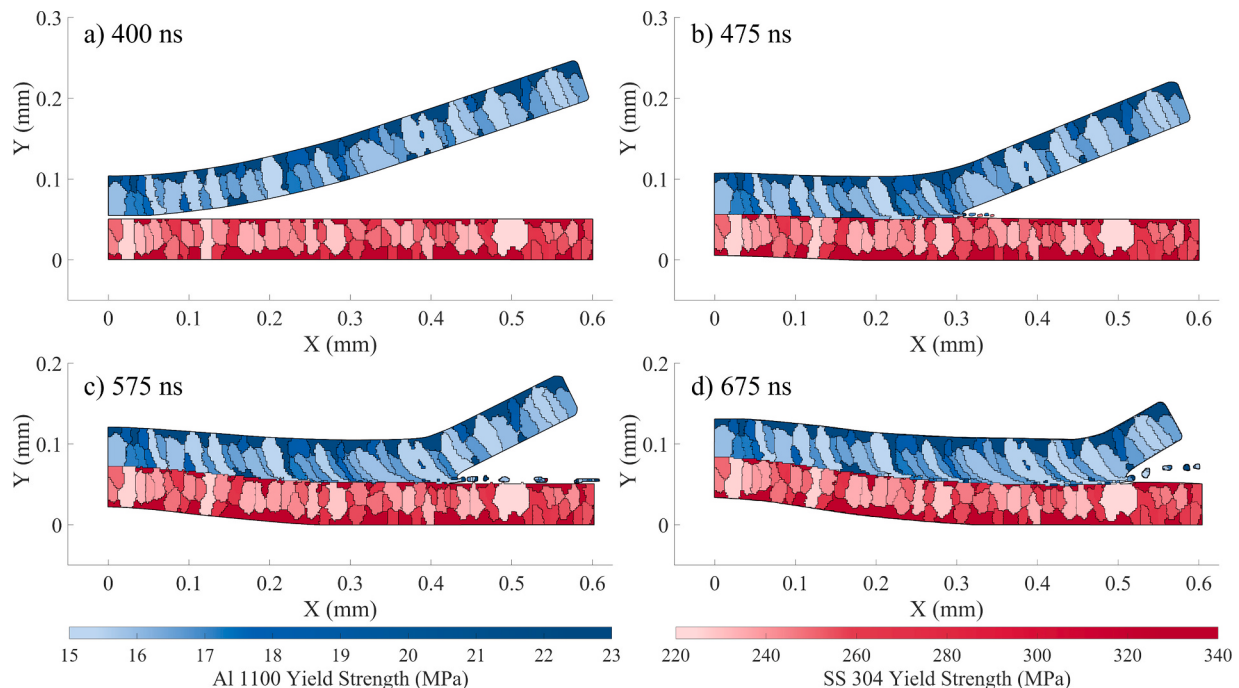


Fig. 4. Microstructure in the aluminum (blue) and steel (red) foils at different stages of the laser impact weld process: (a) $t = 400$ ns, just prior to impact, (b) $t = 475$ ns, just after formation of the impact weld, (c) $t = 575$ ns, during weld formation, increased jetting and an increasing impact angle, and finally (d) $t = 675$ ns, towards the end of weld formation, when aluminum grains near the mouth of the weld show the greatest elongation. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

GBS is more prominent when deformation occurs at temperatures exceeding 45% of the respective metal's melting point.

Weld formation between the two colliding dissimilar foils does not occur at the moment of initial contact, $t = 425$ ns, but is confirmed once the initial jetting of material is seen at $t = 475$ ns, as shown in Fig. 5 (top). During the initial few nanoseconds of interfacial contact, the relatively small impact angle inhibits initiation of the shear instability necessary to ablate the colliding foil surfaces under high pressure and bring them into interatomic-scale contact. Between $t = 450$ ns to 475 ns, v_x peaks at ~ 4050 m s $^{-1}$ and 3850 m s $^{-1}$ for the homogeneous and inhomogeneous models, respectively. Around $t = 475$ ns, reflected pressure waves cause internal spallation and rebound, as was experimentally observed by [1]. A build-up of compressive stress predicted between the target and the

rigid substrate drives a transient rise in temperature at the bottom of the target. Note, this is effect is only prominent in the inhomogeneous model and not the homogeneous one. By this stage of the LIW process, both models already exhibit subtle differences in peak equivalent plastic strain, ϵ_{eq} , and distribution of temperature, T , along the weld interface as seen in Fig. 5 (top left). Moreover, the localized peaks do not overlap between the models, illuminating the effect that inclusion of micro-structure modeling has in the numerical framework.

At $t = 575$ ns (ref. Fig. 5 middle), both models exhibit jetting, which reveals that the respective welds are underway, albeit the inhomogeneous model predicts a greater volume of ejecta as compared to the homogeneous model. Other noteworthy observations when comparing the inhomogeneous model with the homogeneous one include: (1) GBS

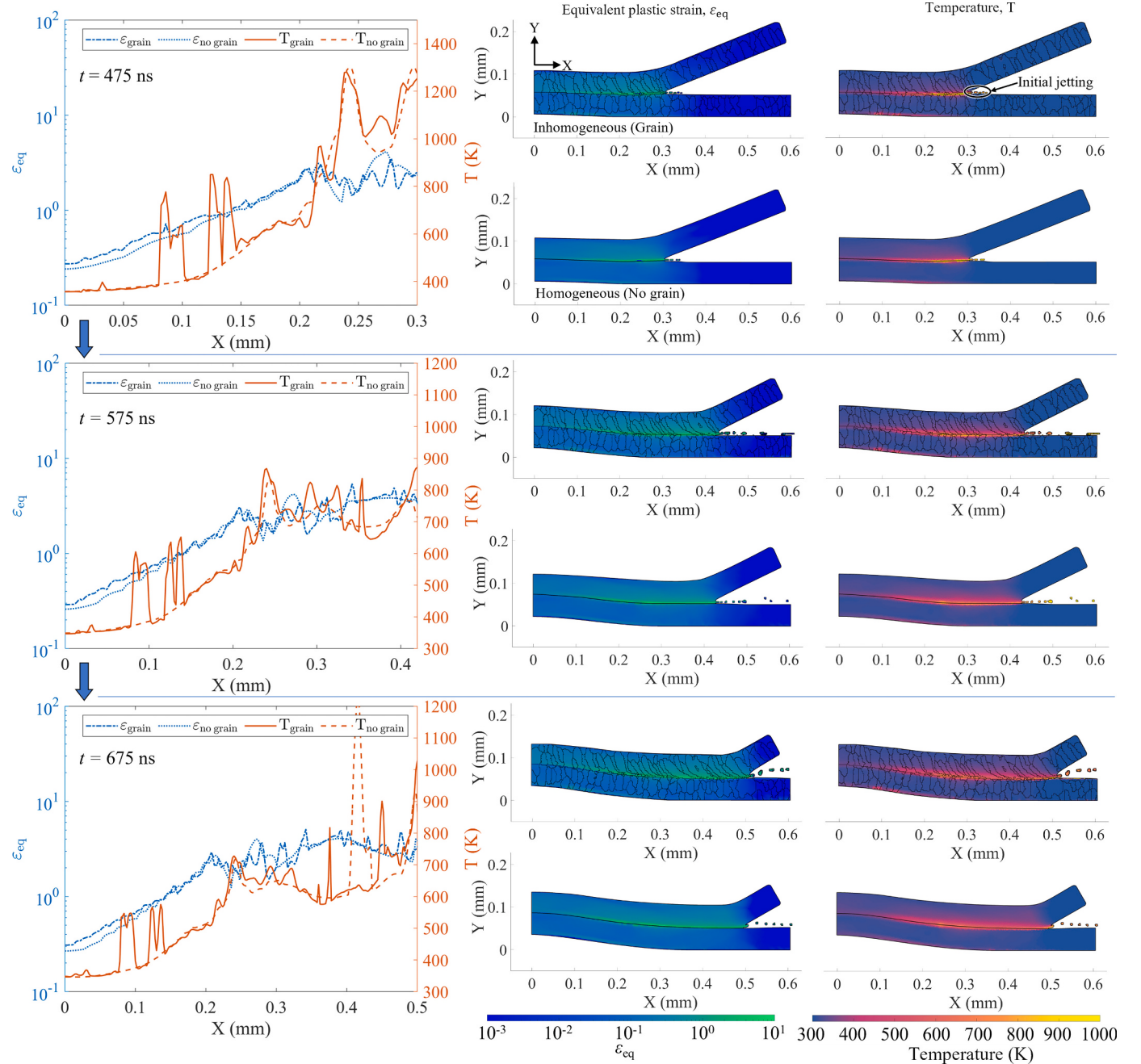


Fig. 5. Material response at $t = 475$ ns (Top), 575 ns (middle), and 675 ns (bottom). (Left) Quantitative comparison of the localized temperature (T) and equivalent plastic strain (ϵ_{eq}) sampled along the contact interface in both inhomogeneous (grain) and homogeneous (no grain) models. (Right) Qualitative comparison of distribution of equivalent plastic strain (ϵ_{eq}) and temperature (T) for inhomogeneous and homogeneous models. (For interpretation of the reference to color in the figure, the reader is referred to the online version of this article.)

within the respective foils, as driven by variations in yield surfaces among individual grains, gives rise to relatively higher collision velocity, v_{xs} of 1540 m s^{-1} , contrasted with the homogeneous model's 1420 m s^{-1} . The consequent increase in plastic strain rates at the interface, along with greater amounts of plastic heat dissipation, offers an explanation for the increased volume of ejecta at higher jet temperatures. (2) Variations in flow stress also promote intergranular shear instabilities that spur more fluctuations (or peaks) in equivalent plastic strain ϵ_{eq} , as seen in the corresponding plot. Accordingly, there are also more localized peaks in temperature T predicted along the collision interface. Given the extreme temperatures that have been observed at metallic material interfaces in impact welding experiments [57] and the unstable, concentrated stresses at impact welding collision points, significant variations in temperatures are likely to present at the interface. With the inclusion of an equation of state, the effects of varying deformation among grains of varying hardness are seen in the increased occurrence of thermal spikes among the inhomogeneous temperature data (Fig. 5 left).

Near the end of the joining process ($t = 675 \text{ ns}$, ref. Fig. 5 bottom) peak values of ϵ_{eq} exceed 1 in a region approximately $10 \mu\text{m}$ thick at the interface, with this threshold surpassed in both the flyer and target materials in both cases. The inhomogeneous model shows the elongation of Al grains at the emerging interface, and ϵ_{eq} values reach 5.06 in the grained flyer. More notable, however, is the peak value of 3.96 that appears in the grained SS target at the weld, where the local reference yield strength, A_1 is 327.8 MPa (ref. Eq. (16)), which is among the highest 10% for this material property in the inhomogeneous model. The severe plastic deformation may result in a partial martensitic phase transformation of the SS 304 material within this distance from the interface, with the shear bands acting as new nucleation sites [58]. When examining the thermal profiles, an extreme peak T of 1261 K occurs in the homogeneous model at $X = 0.42 \text{ mm}$, while the inhomogeneous model reaches 1027 K at the weld front ($X = 0.5 \text{ mm}$). The thermal peak of the homogeneous model is coincident with an extreme compressive stress, and without the modeling of the latent heat of fusion, the equation of state predicts a temperature spike that reflects what is most likely to be a negligible localized melt region. The inhomogeneous model's temperature peak is coincident with the still-advancing collision point, where the plastic dissipation is still the dominant thermal effect responsible for the elevated temperatures throughout the weld region ($0.15 < X < 0.5 \text{ mm}$).

While the presented framework does not directly capture DRX, the

propensity for grain refinement is suggested along the $10 \mu\text{m}$ thick band near the weld interface ($X > 0.15 \text{ mm}$) where $\epsilon_{eq} > 1$ for the aluminum flyer. At the interface, a peak ϵ_{eq} of 5.06 is predicted, far exceeding the refinement threshold; and during processes involving severe plastic deformation, fine equiaxed grains ranging from 0.1 to $1 \mu\text{m}$ in diameter have been observed to arise in aluminum [59], along with an associated increase in the alloy's hardness [60]. However, the occurrence of DRX cannot be confirmed, due to the very short timeframe of the LIW process ($< 1 \mu\text{s}$).

During the early stages of jet formation shown in Fig. 6, a pronounced concentration of shear stress is found in the target foil, with peak values of 634 MPa and 733 MPa at the weld front ($X \sim 0.3 \text{ mm}$) for the homogeneous and inhomogeneous models at $t = 475 \text{ ns}$, respectively. Given the significantly higher yield strengths and elastic moduli of stainless steel versus aluminum in both cases, greater magnitudes for both maximum and minimum shear stresses are expected due to the elastic response. However, the -555 MPa minimum found in the inhomogeneous target is located in the rebound region at $X \sim 0.1 \text{ mm}$, whereas the homogeneous target's -399 MPa minimum is found trailing the weld front in the shear wake ($X \sim 0.175 \text{ mm}$), consistent with the homogeneous model in a previous work [7]. Finally, shear stress minima return to the shear wake loci immediately trailing the weld front at $(X, t) = (0.375 \text{ mm}, 575 \text{ ns})$ and $(0.45 \text{ mm}, 675 \text{ ns})$ in both models.

4. Conclusions

The computational framework presented investigates changes in transient phenomena such as temperature, equivalent plastic strain, and shear stress during a laser impact welding process involving two dissimilar metal foils. The influence of microstructure modeling on the anisotropic material response during collision of the foils is also examined and reveals the following key findings:

- The imposition of a variable flow stress according to a J-C H-P model causes temperatures to be intermittently further elevated along the weld interface due to concentrations of shock pressure at relatively small grains.
- Grain boundary sliding, driven by variations in yield surfaces among individual grains, gives rise to relatively higher collision velocity during the weld. Consequently, higher plastic strain rates along with

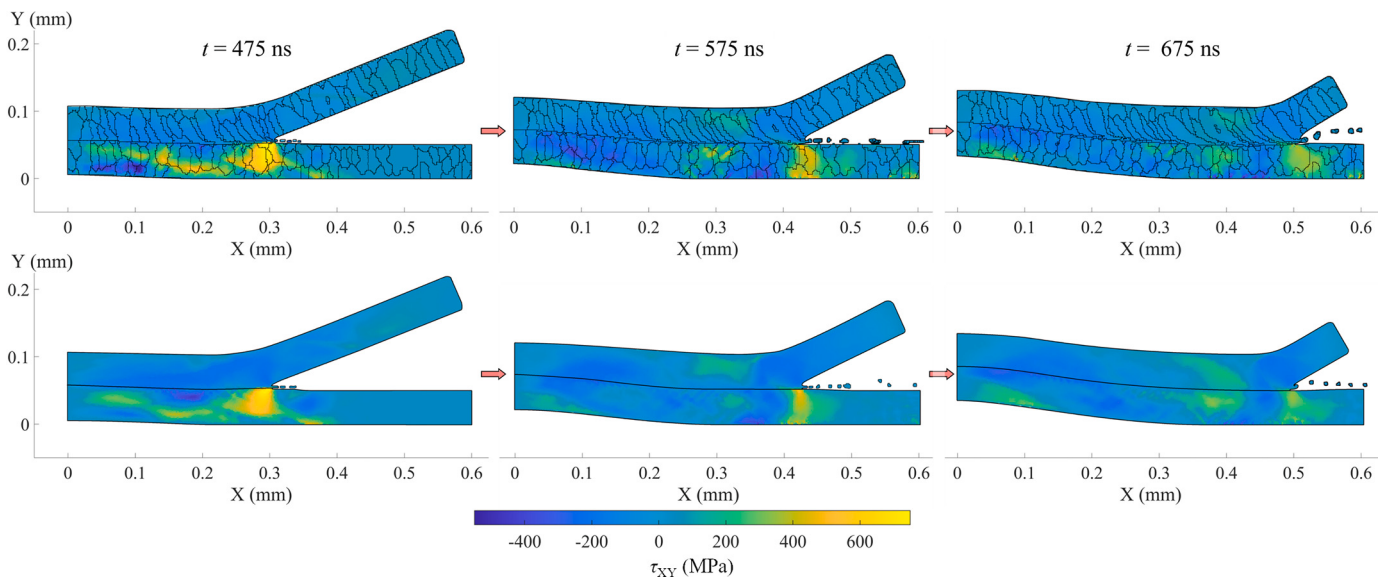


Fig. 6. Distribution of shear stress, τ_{XY} , at $t = 475 \text{ ns}$ (left), 575 ns (center), and 675 ns (right), for the inhomogeneous (grain) model (top) and the homogeneous (no grain) model (bottom).

greater amounts of plastic heat dissipation at the interface result in increased material jetting that occurs at higher jet temperatures.

- The patterns of alternating shear stresses emerging during weld formation vary not just in terms of their peak values according to whether grained structures are modeled, but also in terms of distribution—with a significant difference found in the magnitude of shear stress in the rebound region that persists only for a short time, indicating transient internal stress concentrations in the target that are not indicated in the homogeneous model.
- Severe plastic deformation occurs in a narrow region at the interface, suggesting grain refinement, material hardening, and phase change; however, the differences in the plastic deformation are less pronounced than those of temperature and shear stress. Moreover, the variation of flow stresses in the inhomogeneous model is not deemed to be a significant source of instability to initiate or otherwise affect the formation of the joint.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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