

# A 3D model to predict explicit morphologies and volume fraction of lack-of-fusion pores generated in selective laser melting processes

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## Abstract

The performance of an additively manufactured (AM) component is dependent on the distribution of process-induced defects in addition to the complex microstructure of the material, surface roughness of the component and the process-induced residual stresses. For instance, it has been well demonstrated that lack-of-fusion (LoF) pores produced in the selective laser melting (SLM) AM process can significantly limit the fatigue performance of the material. Although two-dimensional (2D) models exist to predict the 2D profiles of LoF pores, the 2D pore profiles cannot be directly inserted into a three-dimensional (3D) microstructure domain that is output from several prevailing process simulation packages. A few commercial packages that simulate the SLM process can predict LoF pores in a 3D domain, but the morphologies of LoF pores are voxelated and hence do not capture sharp corners of the pores, thereby obviating their use in fatigue crack initiation studies.

In order to address the aforementioned gaps, a high-fidelity model that predicts not only the volume fraction, but also the explicit 3D morphologies and spatial distributions of LoF pores has been developed using a computer aided design-based environment. The model has been partially validated for Ti-6Al-4V alloy by comparing the predictions of the volume fraction of LoF pores predicted by the model with experimental data obtained from the literature. Absolute error in predicted volume fraction of LoF pores varied between 5.16% and 1.87% for energy density values between 13 J/mm<sup>3</sup> and 45 J/mm<sup>3</sup> where a significant amount (over 3% volume fraction) of LoF porosity was measured. The absolute error was within 1.87% for energy density values greater than 45 J/mm<sup>3</sup>.

## 1. Introduction

The selective laser melting (SLM) process produces multiple types of process-induced pores including: i) lack-of-fusion (LoF) pores [1-4], ii) keyhole pores [2,3], iii) entrapped gas pores [3], and iv) oxide-driven pores [5]. In addition to porosity, surface roughness and balling are the other types of defects, which, if present, can lead to the sub-optimal performance of SLM-built materials. The complex interplay between defects and microstructure control the mechanical behavior of parts produced through the SLM process.

Distinct process-specific mechanisms lead to the formation of the different types of defects in the SLM process. LoF pores are formed when a low power, high velocity laser is used that is unable to fully melt the powder particles. Using large hatch spacing also leads to the formation of LoF pores [4]. Additionally, spatter can increase the probability of the formation of LoF pores [6]. Keyhole pores are formed when a high energy laser moving with a low velocity creates deep melt pools that become unstable and lead to formation of bubbles that are unable to escape as they are trapped by the advancing solidification front [7]. Entrapped gas pores are the pores within the powder particles that get trapped in the part [3]. Oxides are formed from native oxide film on powder particles and from the oxidation of metal vapor during part manufacturing [8]. Oxide-driven porosity is caused by a thin oxide film surrounding the melt pool which inhibits fusion and sticking (i.e. wetting) to the surrounding solid [8,9].

The morphological attributes of defects and their spatial distribution within the bulk of the material influence its mechanical behavior [10-18]. Based on high resolution X-Ray computed tomography (CT) studies [2,3,19], it is evident that LoF pores have highly irregular geometry and are characterized by high aspect ratios and sharp corners that act as drivers for strain localizations that may initiate fatigue cracks [3,4,20]. Large LoF pores generate high stress-intensity factors and degrade the ductility of SLM-built components, while small LoF pores promote fatigue crack initiation [20]. Oxide-driven pores are also characterized by complex shapes of pores located in the vicinity of oxide particles [5,8]. On the other hand, keyhole and entrapped gas pores have smooth morphologies and are nearly spherical in nature, and consequently accumulate less strain in comparison to irregular LoF pores of similar size [21].

Recently, computational studies have been undertaken to study the effect of size, shape, and spatial distribution of pores on mechanical performance attributes of metallic materials. Using crystal plasticity finite element (CPFE) simulations, Prithivirajan et al. [22] showed that there exists a critical pore size beyond which fatigue crack initiation occurs near the vicinity of pores rather than at crystallographic features. Cunningham et al. [23], using a CPFE framework, showed that large pores accumulate higher strains compared to small pores. By embedding idealized (spherical) keyhole pores and idealized (super-ellipsoidal) LoF pores into the same microstructural volume, Yeratapally et al. [21] conducted CPFE analysis to quantitatively show that the LoF pores accumulate significantly more strain compared to an idealized keyhole pore of the same size. Kabir et al. [24], using a finite element framework, compared pores with convex and concave boundaries to investigate the von Mises stress profile in the vicinity of the pores. Pores with convex boundaries simulate the presence of keyhole or entrapped gas pores, whereas the pores with concave boundaries simulate the effect of LoF pores. It was shown that the pores with concave boundaries have highly inhomogeneous stress distribution with multiple, narrow plastic zones, unlike the stress profile surrounding pores with convex boundaries. Using an analytical model representing an isolated pore in a homogeneous elastic medium, Sobotka et al. [25] showed that maintaining a spherical pore geometry and reducing the pore size are desirable to promote higher fatigue lives.

Based on computational studies supported by experimental observations, it is evident that LoF pores with irregular morphologies play a role in considerably degrading the mechanical properties of SLM-built materials. This underscores the importance of the process parameters to eliminate the formation of LoF pores. Minimizing porosity by producing several specimens, each with a different combination of process parameters and characterizing porosities in each of the specimens using non-destructive evaluation techniques is a costly and time-consuming process. In order to overcome this barrier, a high-fidelity computational model that links process parameters to the explicit three-dimensional (3D) morphologies and distribution of LoF pores, which is the focus of the current study, is important. While oxide-driven pores have irregular morphologies, as well, simulating their formation is beyond the scope of the current study.

Over the past few years, considerable research has been dedicated to developing predictive models that link process parameters to the formation of LoF pores. Tang et al. [26,27] developed a two-dimensional (2D) model to predict the size, shape and distribution of LoF pores in a 2D simulation domain. Mukherjee et al. [28] used a heat transfer and fluid flow model to build a 2D model that solves for the 2D morphologies and area fraction of LoF pores. Further, he formulated a dimensionless number to help process engineers mitigate the formation of LoF pores. Two-dimensional descriptions, however, are somewhat limited given that the SLM process is inherently multi-dimensional. For example, 2D pore profiles from these 2D process models cannot be directly inserted into a 3D microstructure domain output from the prevailing process simulation packages. Incorporating these profiles would facilitate the study of the interplay between the complex heterogeneities of the microstructure and the LoF pores. Hence, prediction of explicit morphologies and spatial distribution of LoF pores in 3D is important to fully characterize the scatter in mechanical properties. Although there are commercial packages [29,30] that predict LoF pores in a 3D domain, their morphologies are voxelated and hence do not capture sharp corners of the pores, thereby obviating their use in fatigue crack initiation studies. The current work is aimed at addressing the aforementioned gaps that exist in modeling LoF pores. The LoF porosity model proposed in the current study is built on the foundation of the 2D model developed by Tang et al. [26,27] and extends it to 3D to extract explicit 3D computer aided design (CAD) geometries of LoF pores by taking the process parameters and thermal properties of materials as input.

A detailed overview of the 3D LoF porosity framework is provided in Section 2. Thereafter, a partial validation of the framework is given in Section 3. Conclusions of the study are presented in Section 4.

## 2. 3D lack-of-fusion model

The 3D LoF model discussed in this work is built using the framework of the 2D model developed by Tang et al. [8,26,27] as the baseline. CAD tools available in ABAQUS [31] are leveraged to build the 3D LoF model. Generation of 3D LoF pore geometries is accomplished in five steps: i) obtain the melt pool width from the Rosenthal equation, which takes into account both the process parameters and relevant material properties, ii) construction of a bi-elliptical melt pool cross-section, as discussed in Tang et al. [26,27], and extruding it into a single scan track, iii) produce multiple single tracks side-by-side (on the XY plane, as shown in Fig. 1) in such a way that each scan track is separated from the neighboring scan track by the hatch spacing,  $H$ , thereby achieving a single scan layer, iv) three dimensional arrangement of multiple scan layers in such a way that consecutive scan layers are separated vertically (in Z direction, as depicted in the schematic shown in Fig. 1) by the layer thickness,  $L$ , and is rotated from the preceding layer by the hatch rotation,  $\theta$ , and v) isolating non-overlapping regions, converting them into 3D CAD geometries. A schematic of the 3D CAD model with melt pool layers is shown in Fig. 1. It must be noted that there is no hatch rotation used for the example shown in Fig. 1. Each of the five steps are discussed in detail in the following sub-sections.

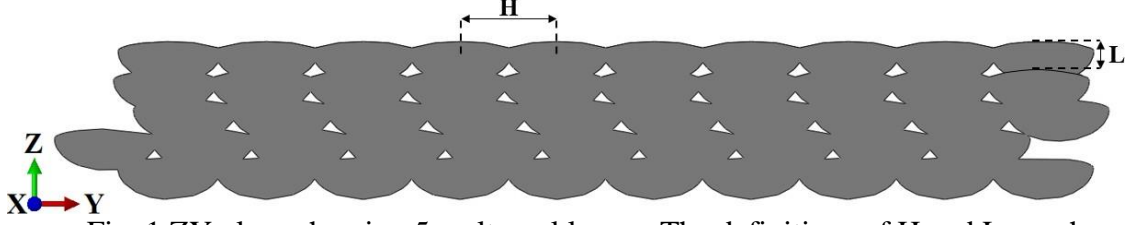


Fig. 1 ZY plane showing 5 melt pool layers. The definitions of H and L are shown.

## 2.1 Obtaining melt pool width using Rosenthal equation

For the purpose of the current study, the cross-section of a melt pool scan track is assumed to be bi-elliptical, as shown in Fig. 2, based on the work of Tang et al. [26,27]. The width, depth, and bead height of the melt pool are represented by  $W$ ,  $D$  and  $R$ , respectively. Given the power ( $Q$ ) and velocity ( $V$ ) of the laser, the melt pool width,  $W$ , is obtained by analytically solving the Rosenthal equation for a special case where  $D$  is assumed to be half of  $W$ . For this special case ( $D=W/2$ ), the relation between  $Q$ ,  $V$ ,  $W$ , and other material-specific parameters like the melting temperature ( $T_f$ ), absorptivity ( $\alpha$ ), thermal conductivity ( $k$ ), ambient temperature ( $T_o$ ), density ( $\rho$ ), and heat capacity ( $C$ ) is given by Eq. 1, adapted from the work of Tang [8].  $W$  was obtained by solving Eq. 1.

$$\alpha Q = \pi k(T_f - T_o)W + 0.125\epsilon\pi\rho C(T_f - T_o)VW^2 \quad (1)$$

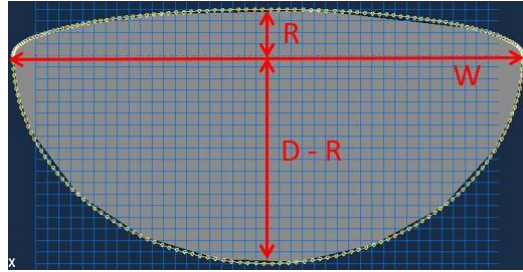


Fig. 2. Schematic of an idealized bi-elliptical cross-section of a melt pool scan track.

For the purpose of the current study, Ti-6Al-4V alloy has been chosen. Although the Rosenthal equation has been rigorously validated for the conduction mode, a customary validation effort is undertaken in the current work to verify that the melt pool widths obtained from Eq. 1 are comparable to experimental values. Experimental melt pool widths for various process parameter combinations are obtained from the values furnished in the literature for Ti-6Al-4V alloy [32]. Figure 3 shows the comparison between the model predictions and experimental data as a function of laser power for various velocities. From this data, it is evident that the model is predicting the melt pool widths reasonably well. Table 1 shows the values of the material properties used in Eq. 1 to solve for the melt pool widths. The value for absorptivity ( $\alpha$ ) was chosen based on the work of Yang et al. [33], while the values for the rest of the parameters were borrowed from the work of Tanget al. [5,8]. It must be noted that there would be a certain level of uncertainty in the values of parameters,  $\alpha$ ,  $k$ ,  $C$  and  $\rho$  at temperature  $T_f$ . Since the purpose of the current work is to demonstrate the framework of the 3D LoF model, the uncertainties in the aforementioned parameters will be ignored.



Table 1. Ti-6Al-4V alloy material properties used in Rosenthal equation

Parameter (units)	Value
$\alpha$	0.38
$T_f$ (K)	1913
$T_o$ (K)	303
$k \left( \frac{W}{m K} \right)$	6.7
$C \left( \frac{J}{kg K} \right)$	526
$\rho \left( \frac{kg}{m^3} \right)$	4430

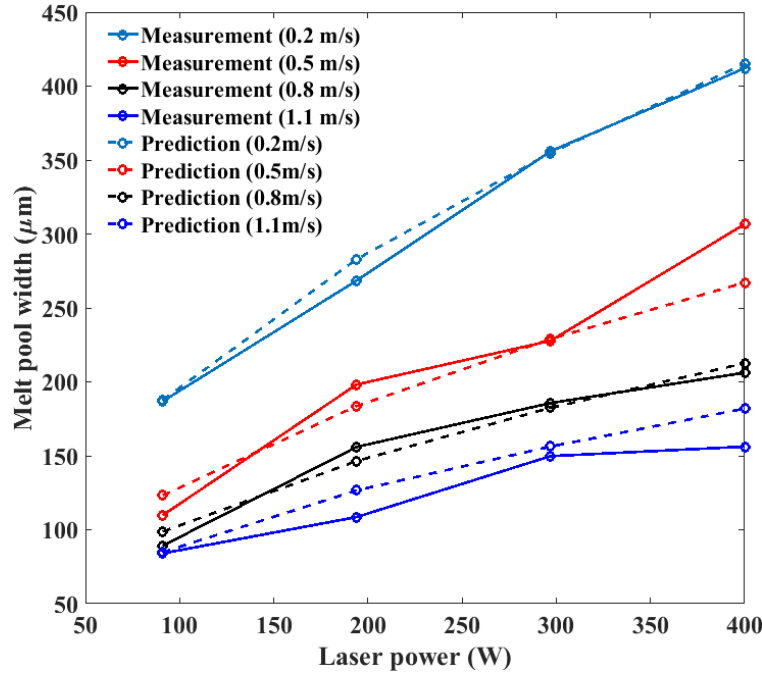


Fig. 3. Comparison of experimental measurements of melt pool width (for varying laser power and scan velocity) of SLM built Ti-6Al-4V material with predictions from the Rosenthal equation.

## 2.2 Constructing an idealized scan track with bi-elliptical melt pool cross-section

It is assumed that the cross-section of the melt pool remains constant throughout the scan path. Hence, the scan track was modeled by simply extruding the bi-elliptical melt pool cross section. The length of the scan track is arbitrarily chosen by the user. In choosing the length of the scan track for this study, measures were taken to ensure that it was not too small to render no LoF pores and not too large to overburden ABAQUS' CAD package. For the build in Fig. 4, W, D and R were taken to be 99.4  $\mu m$ , 49.7  $\mu m$ , and 10  $\mu m$ , respectively. A scan track modeled using the aforementioned parameters is shown in Fig. 4(a). A 3D scan track with varying cross-section can be readily generated in a CAD framework, for example, using the LOFT functionality in AUTOCAD [32], but modeling a scan track with varying cross section is beyond the scope of the current work.

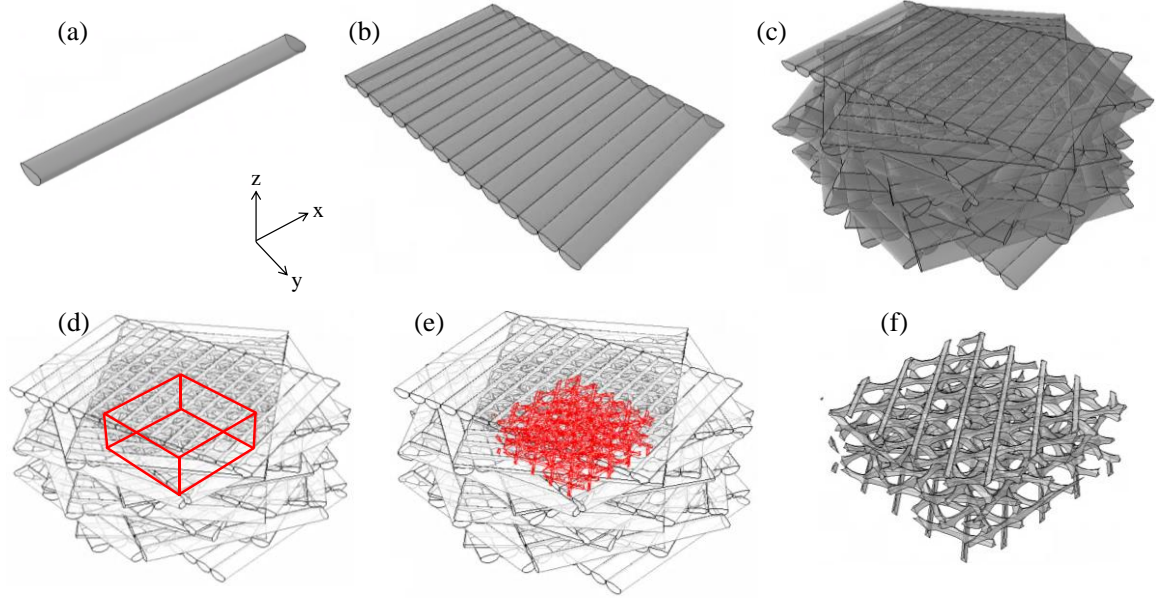


Fig. 4. (a) An idealized scan track with a constant bi-elliptical cross section. (b) A scan layer built by laying the scan tracks side-by-side. (c) Multiple scan layers arranged on top of each other, separated by a specified layer thickness, in such a way that each consecutive layer is rotated by a specified hatch rotation. (d) Box used for LoF pore extraction. The scan tracks cut this box, and the resulting fragments within the box are the desired LoF pore morphologies. (e) LoF pore morphologies highlighted among scan tracks. (f) Explicit morphologies of LoF pores.

### 2.3 Constructing scan layers

An idealized scan layer is modeled by placing a scan track alongside another (as shown in Fig. 4(b)) in such a way that any two consecutive scan tracks are offset by  $H$ . In order to achieve this, multiple instances of the idealized scan track are created in the assembly module in ABAQUS. Based on the work of Dilip et al. [35],  $H$  was chosen to be  $100\text{ }\mu\text{m}$ . Non-overlapping melt pools ( $W < H$ ) result in an enormous amount of LoF porosity and should always be avoided. For the purpose of demonstrating the framework, the value of  $W$  was kept  $99.4\text{ }\mu\text{m}$  (as discussed in Section 2.2) to achieve non-overlapping melt pools that would result in clearly distinguishable morphologies of LoF pores. Based on the aforementioned values of  $W$ ,  $D$ ,  $R$  and  $H$ , the CAD drawing shown in Fig. 4(b) depicts a single scan layer that constitutes consecutive scan tracks that do not overlap with one another. Further, in order to replicate a simple build, multiple scan layers, like the one shown in Fig. 4(b), are stacked on top of each other. Figure 4(c) shows twenty such scan layers. In the build shown in Fig 4(c),  $L$  and  $\theta$  are taken to be  $30\text{ }\mu\text{m}$  and  $67^\circ$ , respectively, based on the work of Tang et al. [5,8].

### 2.4 Extracting LoF pores

Extracting LoF pores is the most computationally expensive step of the entire process. First, a solid box is fit inside multiple scan layers such that it is fully enveloped by the tracks, Fig 4(d). Next, using a subtract boolean operation in ABAQUS, the scan

layers are used to cut the solid box. The uncut regions of the box, effectively regions where no scan track traversed, are the desired LoF pore geometries. The regions shown in red in Fig. 4(e) are the LoF pore regions. The explicit morphologies of the LoF pores formed in the build are shown in Fig. 4(f).

It is noteworthy that Steps 1-5 are automated in a Python-based macro which can be executed within ABAQUS CAE. The macro accepts eight inputs: (1) desired number of scan tracks in the x-y plane, (2) scan length, (3) number of layers, (4) hatch rotation -  $\theta$ , (5) hatch spacing - H, (6) layer thickness - L, (7) melt pool width - W (from Rosenthal equation), and (8) melt pool depth - D. When considering approximately 300 scan tracks, the macro runs in a couple of minutes on a desktop workstation with a 3<sup>rd</sup> generation Intel Core i7 processor and 24 GB of RAM.

### 3. Validation of the model

The predictions made by the 3D LoF porosity model have been validated against experimental data published in the literature. Specifically, the volume fraction of LoF porosity,  $v$ , measured for various combinations of process parameters has been used as a validation metric in the current study. The variation of  $v$  with respect to the energy density, E (defined as  $\frac{P}{VHL}$ ), has been obtained from the work of Dilip et al. [35] for Ti-6Al-4V alloy, and this data will be compared to the predictions from the model for the purpose of validation. It must be noted that this is considered only a partial validation since only volume fraction of LoF pores are being compared to experimental measurements, and not the explicit morphologies and spatial distributions of the pores. The parameters of H, L and  $\theta$  have been assigned fixed values 100  $\mu\text{m}$ , 30  $\mu\text{m}$  and 67°, respectively, throughout the validation study. Table 2 shows various combinations of process parameters that have been chosen to study the variation of  $v$  with respect to E.

Table 2. Process parameters used in the validation study. Values have been chosen based on the experimental studies of Dilip et al. [35]

P (W)	$V \left( \frac{\text{mm}}{\text{s}} \right)$	$E = \frac{P}{VHL} \left( \frac{\text{J}}{\text{mm}^3} \right)$
50	500	33.33
50	750	22.22
50	1000	16.67
50	1200	13.89
100	750	44.44
100	1200	27.78
150	500	100
150	750	66.00
150	1000	50.00

Figure 5 compares the predictions of the 3D LoF model with experimental data. Absolute error in the prediction of volume fraction of LoF porosity is shown in Fig. 6. The absolute

error is between 5.16% and 1.87% for energy density values between 13 J/mm<sup>3</sup> and 45 J/mm<sup>3</sup> where a significant amount (over 3% volume fraction) of LoF porosity was measured. The absolute error is within 1.87% for energy density values greater than 45 J/mm<sup>3</sup>. Beyond the energy density value of 66 J/mm<sup>3</sup> the formation of keyhole pores is favored, and hence the LoF porosity prediction model is not applicable in this domain.

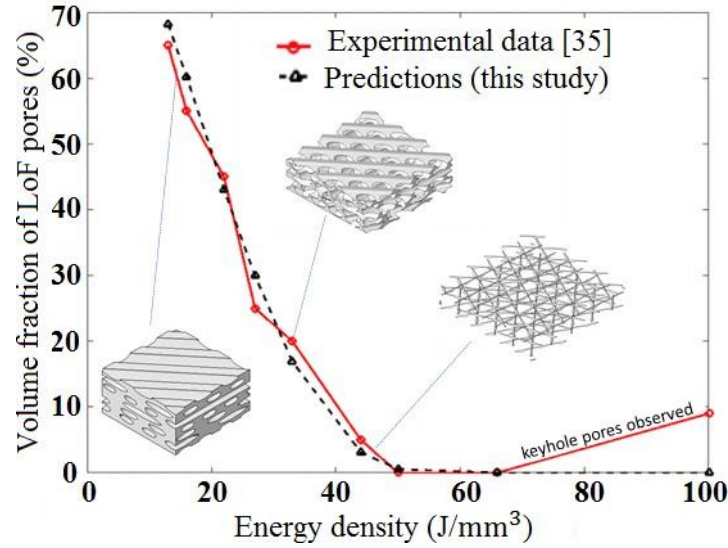


Fig. 5. Variation of LoF porosity with laser energy density (E) for Ti-6Al-4V alloy, as predicted by the 3D LoF model and that obtained from experiments [35]. Pore morphologies are shown for select energy densities.

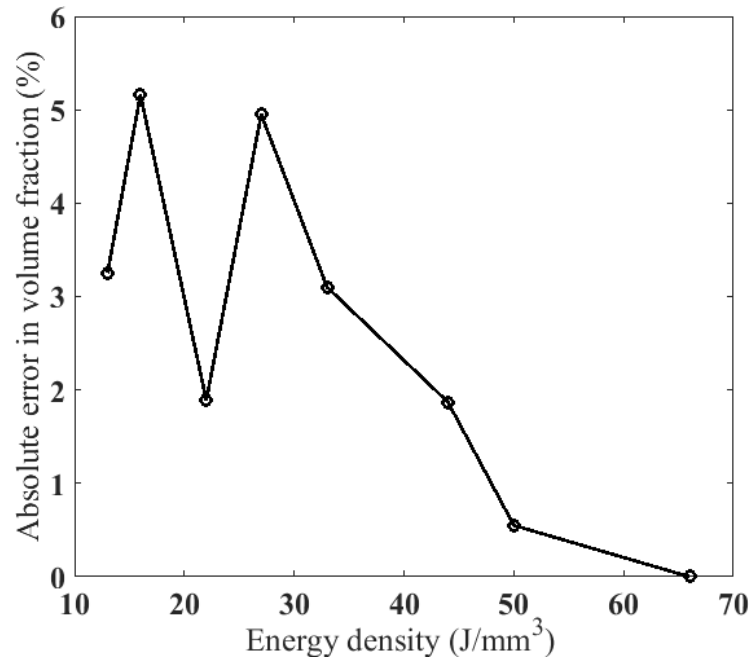


Fig. 6. Absolute error in predicted volume fraction of LoF pores for various energy densities.

## 4. Conclusions

This report details the extension of a pre-existing two-dimensional (2D) lack of fusion (LoF) porosity model [26,27] to three dimensions and the resulting CAD-based implementation. LoF porosity is caused by non-overlapping melt pools, a phenomenon dictated by melt pool geometries and scan path strategies. The model presented herein incorporates these two factors to create an assembly of three-dimensional (3D) scan tracks and subsequently generates geometries of non-overlapping (viz. not-melted) regions. This report includes partial validation of the model—its ability to predict pore volume fractions is demonstrated, but the resulting morphologies (which are crack-like and qualitatively mimic LoF pores) have yet to be experimentally validated.

The model was designed to be incorporated into multiscale simulation workflows wherein process-induced defects (such as the LoF species) are considered explicitly in life estimation. For example, the 3D LoF pore morphologies produced by this model could be incorporated directly into a process-informed 3D microstructural model (such as from SPPARKS [36]) for crystal-plasticity finite-element analysis with a high-performance FE driver like ScIFEN. Given the CAD-based model's relatively short run times (on the order of a couple of minutes), uncertainty quantification is possible. For example, stochastic reduced order models [37,38] could be used to propagate uncertainty through this crystal plasticity finite element framework to assess the influence of a particular process parameter (e.g. laser power) on lifing capability.

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<b>14. ABSTRACT</b> The performance of an additively manufactured (AM) component is dependent on the distribution of process-induced defects in addition to the complex microstructure of the material, surface roughness of the component and the process-induced residual stresses. For instance, it has been well demonstrated that lack-of-fusion (LoF) pores produced in the selective laser melting (SLM) AM process can significantly limit the fatigue performance of the material. Although two-dimensional (2D) models exist to predict the 2D profiles of LoF pores, the 2D pore profiles cannot be directly inserted into a three-dimensional (3D) microstructure domain that is output from several prevailing process simulation packages. A few commercial packages that simulate the SLM process can predict LoF pores in a 3D domain, but the morphologies of LoF pores are voxelated and hence do not capture sharp corners of the pores, thereby obviating their use in fatigue crack initiation studies. In order to address the aforementioned gaps, a high-fidelity model that predicts not only the volume fraction, but also the explicit 3D morphologies and spatial distributions of LoF pores has been developed using a computer aided design-based environment. The model has been partially validated for Ti-6Al-4V alloy by comparing the predictions of the volume fraction of LoF pores predicted by the model with experimental data obtained from the literature.						
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