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基于机器学习的激光粉末床熔融工艺参数优化、 过程监测和服役寿命预测的方法论

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摘 要: 激光粉末床熔融工艺(LPBF)因成形精度较高、制造周期短,成为增材制造的主流方法之一,但其制造工艺的可重复性、生产过程的可解释性和成形构件的可靠性仍面临重大挑战。LPBF 成形过程涉及的参数众多,不同工艺参数的选择会导致构件内部产生不同类型的微观/宏观缺陷,进而影响构件的服役性能。因此明确工艺参数、缺陷和性能三者之间的联系是当前激光粉末床熔融制造的热点与难点。作为大数据与人工智能发展到一定阶段的必然产物,机器学习方法为有效处理高维物理量之间的复杂非线性关系提供了契机,在增材制造过程中工艺参数优化、缺陷监测和性能预测等方面得到持续关注。本文介绍了常用的机器学习(ML)模型,总结了 LPBF 中 ML 的输入信息,重点分析了数据驱动和物理驱动 ML 模型在 LPBF 各领域的应用,最后指出当前 ML 的局限性,并探讨了其发展趋势和技术前景。

关键词: 参数优化;缺陷监测;服役寿命预测;数据驱动;物理驱动

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Methodological Approach to Optimizing Process Parameters, Monitoring, and Predicting Fatigue Life in Laser Powder Bed Fusion via Machine Learning

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Abstract: Laser powder-bed fusion (LPBF) is recognized as a predominant method within additive manufacturing because of its high precision and shortened manufacturing cycle. However, the process still faces significant challenges regarding the repeatability of its manufacturing techniques, the interpretability of the production process, and the reliability of the formed components. The LPBF formation process involves a multitude of parameters, and the selection of different process parameters can lead to various types of micro/macroscale defects within the components, thereby affecting their service performance. Therefore, clarifying the interconnections among process parameters, defects, and performance represents a current hot topic and a formidable challenge in laser powder bed fusion manufacturing. As an inevitable product of the evolution of big data and artificial intelligence, machine learning (ML) methods offer opportunities to address the complex nonlinear relationships between high-dimensional physical quantities effectively. In the realm of additive manufacturing, ML has garnered sustained interest for its applications in process parameter optimization, defect monitoring, and performance prediction. This article reviews common ML models, summarizes the input information for ML in the LPBF, and focuses on analysing the applications of data-driven and physics-driven ML models in various domains of the LPBF. Finally, it highlights the current limitations of ML and explores its development trends and technical prospects.

Key words: parameter optimization; defect monitoring; fatigue life prediction; data-driven; physics-driven

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激光粉末床熔融(laser powder-bed fusion, LPBF)是一种采用移动激光热源逐层熔化成形金属粉末的自动成形技术,具有复杂形状构件一体化成形,原材料利用率高的独特优势,被广泛用于不锈钢、钛基、铁基、镍基和铝合金等金属构件的制造^[1-3]。但 LPBF 制造工艺的可重复性、生产过程的可解释性和构件的可靠性仍面临巨大挑战^[4]。由于 LPBF 成形过程中涉及的参数众多,激光-粉末-熔池间相互作用复杂,容易导致气孔、未熔合、球化、开裂等微观/宏观冶金缺陷的产生,从而影响构件的成形质量及服役性能^[5]。因此厘清多流程、多因素耦合的增材制造过程与增材构件服役性能的内在联系,建立工艺参数、缺陷和性能的关联模型,有利于增材制造工艺优化与构件服役性能预测。但基于实验分析、理论建模、数值求解等传统方法构建的预测模型,计算成本高昂、计算效率及计算精度较低,限制了其广泛应用^[6]。机器学习(machine learning, ML)是一种从数据中学习决策规则的计算机算法^[7],其基于高通量数据驱动,可以有效发掘空间尺度或时间尺度数据集间的相关性,克服数据规模差距,实现各种输入参数之间高度非线性关系的多维度预测^[8],成为建立 LPBF 参数优化-过程监测-服役性能预测模型的有效方法之一,ML 统筹多参量实现非线性多维度预测的过程如图 1 所示。

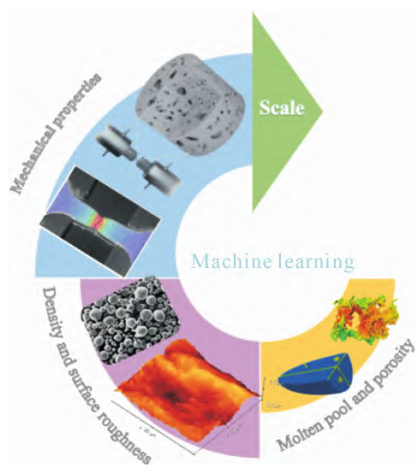


图 1 ML 实现多参数间非线性多维度预测

Fig.1 ML realizes nonlinear multidimensional prediction among multiple parameters

目前用于 LPBF 中的 ML 存在一定局限性：①模型忽略了输入数据与响应参量之间的物理的关系,只能判断二者之间的统计相关性,导致该模型的可解释性差,即通常所说的“黑箱”模型。②过程控制不容易执行,材料的动态演变数据易丢失。③模型的开发、训练和验证需要原位数据。为了解决上述限制,使用先进的过程传感器实时收集

LPBF 制造过程中的原位信息,并将收集的数据集作为数据驱动和物理驱动 ML 的信息输入,实现 LPBF 领域的工艺参数-缺陷-性能关系准确分析^[9-11]。本文从 LPBF 的打印流程中提取工艺参数信息、打印过程信息和构件服役过程信息用作 ML 数据输入,总结了用于优化工艺参数^[12-13]、实现原位缺陷检测^[14-16]和预测增材构件疲劳性能^[17]的 ML 算法。同时,对物理定律在 ML 模型开发中的约束作用进行了总结,并探讨了 ML 在增材制造(additive manufacturing, AM)领域面临的机遇与挑战。

1 机器学习的基本概念

ML 是人工智能(artificial intelligence)的一个分支,旨在为系统提供从经验中学习和改进的能力而无需明确编程。根据数据集对人工参与类别划分或标签标识的需求程度,可将 ML 模型划分为如图 2 所示的 4 种范式:监督学习(supervised learning)、无监督学习(unsupervised learning)、半监督学习(semi-supervised learning)和强化学习(reinforcement learning)。其中,监督学习是 LPBF 领域使用最广泛的 ML 范式,其训练的数据集需要使用输入值和相应的输出值进行标记。监督学习的目的是减少预测值与实际值之间的差异,因此该方法适用于工艺参数优化、缺陷监测和服役性能预测。目前,增材制造领域监督学习可基于数据或物理驱动,下面将详述两者之间的区别。

1.1 数据驱动的 ML

近年来,以 ML 为代表的“数据科学”强调因素之间的相关性,已成为发展数据驱动研究范式的基础。该范式是从数据出发,提取数据的特征,抽象出数据的模型,发现数据的知识,又回到对数据的分析与预测中,其通用过程如图 3 所示。常见由数据驱动的模式有以下几种。

线性回归(linear regression, LR)是一种经典的 ML 模型,它建立了自变量和因变量之间的线性关系,通过最小化残差平方和来求解最优参数,适用于连续变量的预测和拟合。其建模速度快,但只适用于存在线性关系的数据。支持向量机(support vector machine, SVM)是一种二分类模型,它的基本模型是定义在特征空间上的间隔最大的线性分类器。可以通过核函数进行非线性分类,泛化错误率低,但对参数调节和核函数的选择敏感,原始分类器仅适用于处理二类问题。决策树(decision tree, DT)是一种模拟人类决策过程的树形结构模型,广泛应用于分类和回归分析。该模型通过递归选择最优特征并对数据集进行分割,构建出由内部节点、分支和叶节点组成

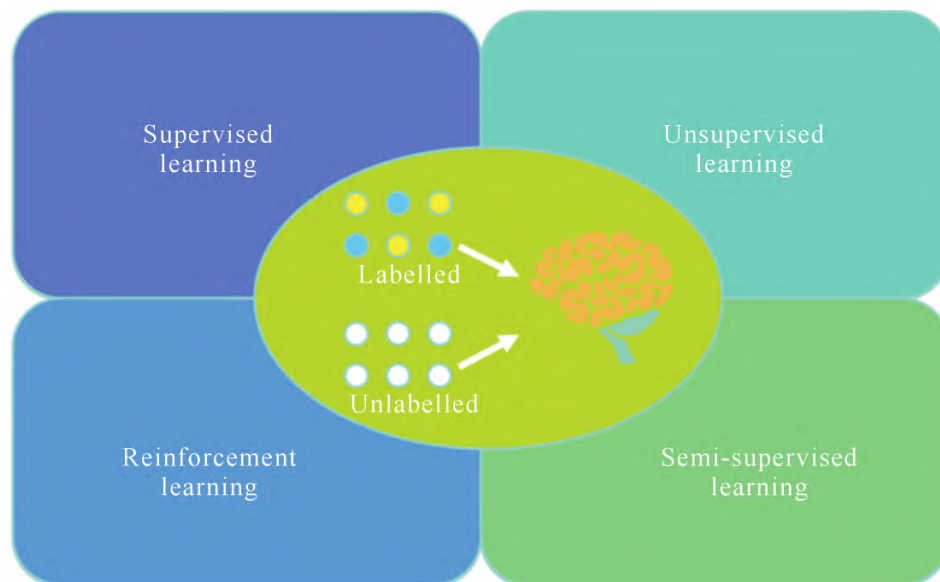


图2 ML分类
Fig.2 Classification of ML

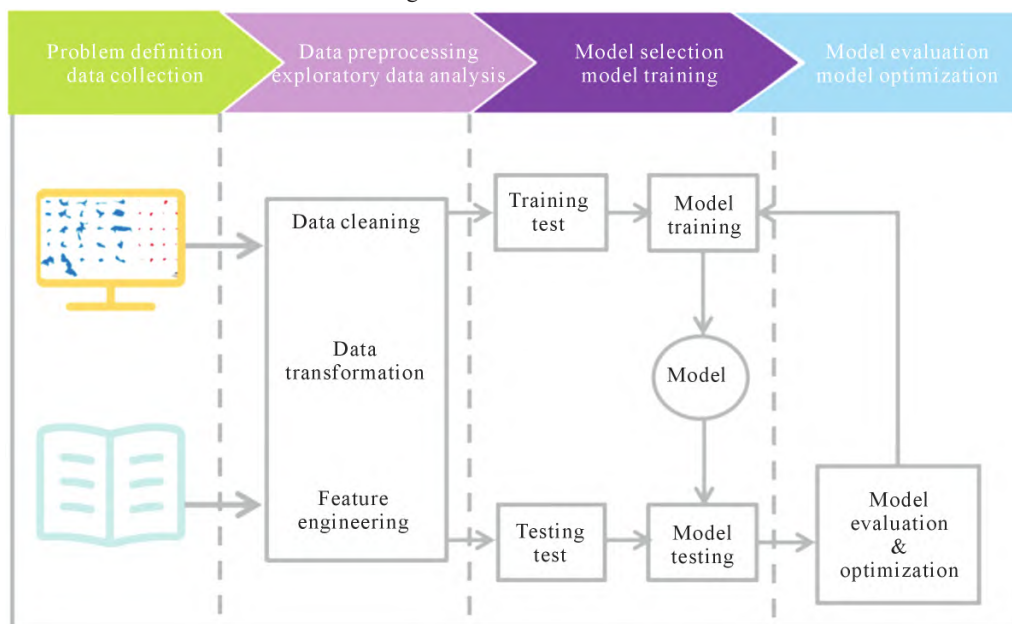


图3 数据驱动的 ML 流程
Fig.3 Data-based ML process

的树状图。内部节点表示属性的决策点,分支代表决策结果的流向,而叶节点则代表最终的决策结果或输出值。决策树的构建涉及特征选择、树的生长和剪枝策略,旨在优化模型的预测准确性。该模型的主要优势在于其高度的可解释性和直观性,但其易受到噪声和异常值的影响,导致过拟合。随机森林(random forest, RF)是通过集成学习的装袋(bagging)思想将多棵决策树集成的一种算法,能够处理大数据集的回归和分类问题。但其在某些噪声较大的分类或回归问题上会过拟合且牺牲了决策树的可解释性。朴素贝叶斯(naive Bayes classifier, NBC)是一种基于贝叶斯定理的概率推断方法,它在分类过程中对特征之间的条件独立性做出了简化假设。

该算法通过评估样本在各个类别下的后验概率,并选择概率最大的类别作为样本的预测分类。主要局限性源于其对特征条件独立性的简化假设。 K -近邻算法(K nearest neighbor, KNN)是一种基于距离的学习技术,用于分类和回归任务。在分类中,它通过测量新样本与训练集中样本之间的距离,选取距离最近的 K 个邻居,并依据这些邻居的类别通过多数投票确定新样本的类别。在回归中,它则基于 K 个最近邻居的平均值进行预测。KNN算法简单直观,但计算效率受数据规模和维度的影响,且对特征缩放敏感。神经网络(neural network, NN)是一种模拟人脑神经元连接的计算模型,通过多层结构处理信息,用于识别数据中的复杂模式。典型的神经网络包括

多层感知器(multilayer perceptron, MLP)、卷积神经网络(convolutional neural networks, CNN)、循环神经网络(recurrent neural network, RNN)、长短期记忆网络(long short-term memory, LSTM)和生成对抗网络(generative adversarial networks, GAN)。由于其出色的非线性拟合能力和良好的泛化性,能有效处理大规模数据。其不足之处在于训练复杂度高、易过拟合、模型解释性差,以及对参数和初始权重设置敏感。

包括但不限于上述模型的应用涵盖了从材料属性预测、缺陷检测与分类、大规模数据分析,到设计和工艺参数的优化等多个方面。具体而言,LR 模型能够揭示打印参数与材料性能之间的线性关系,SVM 则在缺陷分类和产品质量评估方面展现出其独特优势,DT 和 RF 通过模拟决策过程和集成方法增强了对制造现象的预测和分析能力,KNN 和 NBC 可以对打印过程中的缺陷进行快速而有效的分类,而神经网络,特别是深度神经网络(deep neural network, DNN)模型,通过其强大的非线性拟合能力,能够识别和预测制造过程中的微观结构和复杂模式。

但现有用于增材制造领域的驱动 ML 面临着对数据的过度需求,可靠实验数据的收集成本高,有限数据训练得到的 ML 模型泛化能力差的挑战。此外,依靠数据驱动的 ML 模型,只能通过发现输

入和输出之间的统计相关性来对下一次的输入进行结果预测,缺乏物理可解释性,易受到噪声、缺失或错误数据标签等引起的数据污染,且从不同传感系统收集的数据集无法完全代表完整的增材制造过程物理场。如何增强 ML 模型对底层过程物理场的认识,以实现完整的模型可解释性是目前的难题。

1.2 物理驱动的 ML

为了提高 ML 模型的可解释性、透明度和分析能力,近年来大量学者将数据驱动的 ML 模型和物理知识联系起来,得到融合物理信息的物理驱动 ML 方法(physics-informed machine learning, PIML) 以便及时准确分析制造构件的工艺结构特性。PIML 是在数据驱动 ML 模型的基础上通过偏微分方程描述增材制造过程中条件和响应之间的潜在物理关系,旨在利用物理知识指导 ML 的建模和训练过程,其核心思想是通过将物理方程或物理约束嵌入到 ML 的结构或损失函数中来提高神经网络的建模能力和预测性能^[18]。PIML 与数据驱动 ML 模型的对比如图 4 所示。

通过推断物理知识与 ML 模型之间的集成机制,可将当前 PIML 分为 3 种不同的类别^[19],如图 5 所示。其中物理信息引导(physics-informed domain knowledge, PIDK)的 ML 模型通过傅立叶变换和时间序列分析等理论手段对原位生产数据进行分析,

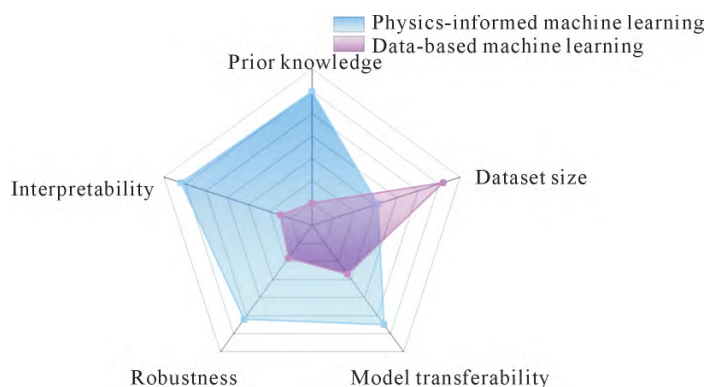


图 4 数据驱动和物理驱动模型的比较

Fig.4 Comparison of data-based models and physics-informed models

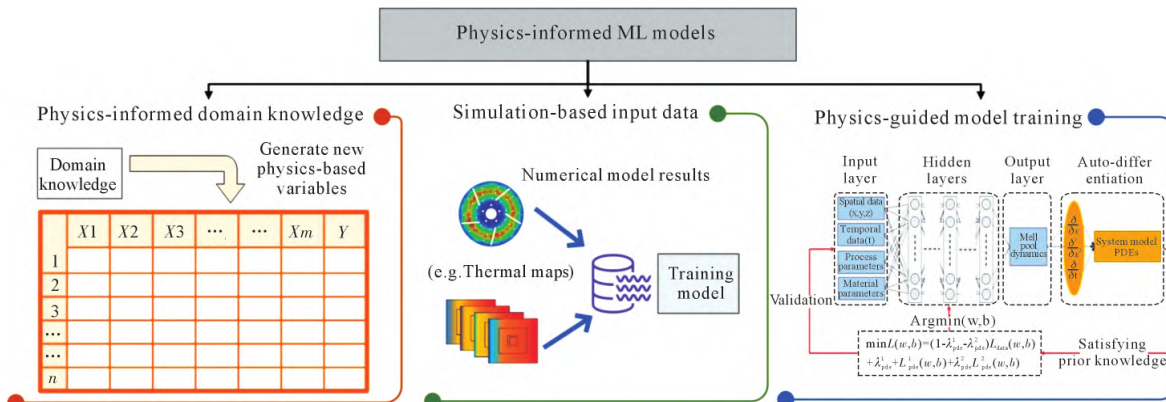


图 5 PIML 方法概述^[19]

Fig.5 An overview of different PIML approaches^[19]

提取隐含的物理信息作为模型的输入,从而增强机器学习模型的预测能力和物理解释性。目前已经探索的物理信息之一是 LPBF 打印过程中信号发射的顺序性质,从而产生了时间序列 ML 模型。不同于 PIDK 使用物理相关特征补充数据结构,基于仿真输入(simulation-based input data, SBID)的 ML 模型提供了一种替代方法,通过使用数值仿真的结果在各种场景下训练 ML 模型来减少昂贵的实验设置。此外,利用多尺度多物理场模型的计算数据,对 AM 过程中的不确定性进行了量化分析,深化了对工艺参数不确定性影响材料性能的理解,其输出和输入数据都有助于 ML 模型训练。此外,物理法则引导模型训练(physics-guided model training, PGMT)框架下的机器学习模型通过将物理法则整合至模型训练的正则化过程中,确保了在数据有限情形下预测结果的物理一致性。在此框架下,形成了物理信息知情网络(physics-informed neural network, PINN)。PINN 基于 DNN 来实现函数逼近,解决了 AM 过程中的正向问题(设计指导制造)和反向问题(从需求推导设计)。在正向问题中,PINN 在无监督学习模式下运行,通过迭代调整 DNN 的参数,确保 DNN 的输出满足域内特定点的控制偏微分方程,从而预测温度场^[20]或熔池尺寸^[21]等 LPBF 过程的关键行为。另一方面,反向问题涉及监督学习方法,PINN 在训练期间集成数据与物理知识,将代表系统固有物理特性的控制偏微分方程与神经网络的损失函数耦合,降低了预测值与观测值之间的差异。因此,PINN 可以生成以数据为导向、符合已知物理原理的预测结果。

与理论建模和数值求解相比,PIML 具有对动态系统的实时响应、数据驱动的决策逻辑以及量化不确定性的能力等优势,且与纯数据驱动的方法相比,PIML 具有与生俱来的物理一致性,在金属增材制造领域原位监测和质量检测方面展现出了广泛的应用潜力^[15, 22-23]。

1.3 ML 性能评价指标

监督学习是通过分析标记的训练数据集,建立输入特征与输出标签之间的映射模型,来进行性能评价。该映射模型能够实现两种主要的预测任务:回归和分类^[24]。对于回归任务,ML 模型致力于揭示输入特征与连续参数输出之间的关联,如预测孔隙率、熔池深度及机械性能等。分类任务则关注于从输入特征中识别离散的类别标签,例如缺陷类型或质量评估等级。ML 模型通过学习训练集中的分类模式,能够对新的输入数据进行准确的类别划分。

在 LPBF 领域,回归模型主要应用于工艺参数优化和服役性能预测,旨在生成精确的工艺图,以指导生产过程,分类模型可用于区分零件的多种质量状态,如缺陷与非缺陷、不同质量等级等,为质量控制和评估提供支持。

上述任务的完成情况有以下评价标准。分类任务的评估通常借助图 6 所示的混淆矩阵,采用式(1)~(4)的精度(precision, Pr)、召回率(recall, Re)、准确性(accuracy, Ac)和 F_1 分数(F_1 score)指标。回归任务主要通过比较模型预测值与观测值之间的差异来评价,常见的评估指标有均方根误差(root mean squared error, RMSE)、平均绝对百分比误差(mean absolute percentage error, MAPE)和决定系数(coefficient of determination, R^2),如式(5)~(7)所示。

$$Pr = \frac{TP}{TP + FP} \quad (1)$$

$$Re = \frac{TP}{TP + FN} \quad (2)$$

$$Ac = \frac{TP + TN}{TP + FN + FP + TN} \quad (3)$$

$$F_1 = 2 \cdot \frac{Pr \cdot Re}{Pr + Re} \quad (4)$$

		Prediction	
		Positive	Negative
Actual	True	TP	FN
	False	FP	TN

图 6 混淆矩阵

Fig.6 Confusion matrix

图 6 与式(1)~(4)中,TP(true positive)为真正例,即模型正确预测为正例的次数;FN (false negative)为假反例,模型错误地将正例预测为反例的次数;FP(false positive)为假正例,模型错误地将反例预测为正例的次数;TN(true negative)为真反例,即模型正确预测为反例的次数。

$$RMSE = \sqrt{\frac{\sum_{i=1}^N (\hat{y}_i - y_i)^2}{N}} \quad (5)$$

$$MAPE = \frac{100\%}{N} \sum_{i=1}^N \frac{|\hat{y}_i - y_i|}{y_i} \quad (6)$$

$$R^2=1-\frac{\sum_i(\hat{y}_i-y_i)^2}{\sum_i(\hat{y}_i-\bar{y})^2} \quad (7)$$

式中, N 为样本的数量; y_i 为第 i 个样本的观测值; $\hat{y}_i$ 为第 i 个样本的预测值; $\bar{y}$ 为所有观测值的平均值。

2 基于 ML 的工艺参数优化

LPBF 制造中加工参数与零件质量之间关系的不确定性导致了最终打印前需通过成本高昂、耗时的样品打印与性能测试来验证实验设计。实验和模拟虽有助于建立参数与质量的关联,但在多变量情形下寻找最优参数组合却显得不切实际。ML 提供了一种高效的解决方案,可辅助工艺参数优化,在实现减少时间成本和制造成本的同时,确保了零件质量。

2.1 工艺参数类别

LPBF 制造过程中涉及激光功率、扫描速度、扫描间距、扫描策略、铺粉厚度和激光束有效直径等众多参数,不同参数的选择会造成组织、性能的差异,实际生产中常常通过不同的参数组合来获得目标构件。

此外,激光对原料粉体的加工效果还受到粉体的激光吸收率/反射率、颗粒形状和尺寸及堆积密度等物理性质和状态的影响。粉体对于特定波长激光的吸收率直接影响它在激光加工过程中的实际输入能量密度。为整体性调控激光加工效果并体现各种主要加工参数的影响,提出了激光能量密度的概念,下式为其经验计算公式^[25]:

$$E=\frac{\alpha P}{v \cdot h \cdot t} \quad (8)$$

式中, E 为激光能量密度, J/mm^3 ; α 为粉体激光吸收率; P 为激光功率, W ; v 为扫描速度, mm/s ; h 为扫描间距, mm ; t 为铺粉厚度, mm 。

LPBF 制造过程中高动态熔池、超高凝固/冷却速率和高温度梯度等工艺特性不可避免地会影响增材构件的微观结构特征,并导致不同类型工艺诱导缺陷的产生,包括球化、未熔合和匙孔等。这些缺陷是循环载荷下限制寿命的主要因素之一,也是构件疲劳裂纹萌生的热点^[26-30]。尽管后处理能适当减少缺陷,但并不能达到理想的效果。因此从前端工艺出发,选择合适的工艺参数来尽量避免大尺寸缺陷的产生。

工艺图是选取最佳工艺参数以提高构件质量的有效工具之一,如图 7 所示。该技术由 Beuth 和

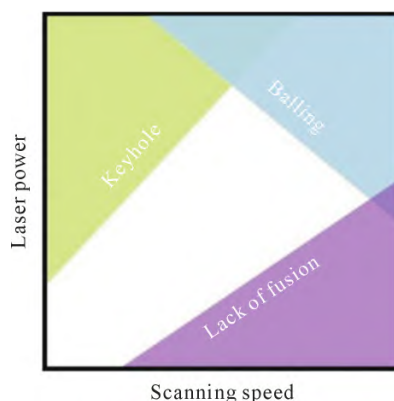


图 7 LPBF 工艺的 PV 加工图中 3 种不同的孔隙缺陷:匙孔、球化和未熔合

Fig.7 PV processing map for the LPBF process showing three distinct porosity defects: keyhole, balling, and lack of fusion

Klingbeil^[31]于 2001 年首次开发使用,用于总结激光束功率和扫描速度对熔池大小的影响,并描绘某些缺陷状态。

工艺图本质上是保证构件属性的加工窗口。其工作原理为基于不同的工艺参数打印构件,测量结果并生成过程图,旨在获得各种工艺参数的最佳组合^[32-35]。因此,工艺图对于精确指导激光粉末床熔化过程中的实验设计及工艺参数选择具有关键性作用,其确保了材料合成与性能表征的迭代优化^[36],但依赖重复实验获得的工艺图既昂贵又耗时。ML 是一种简化寻找最优 LPBF 参数、避免高成本实验和测试的方法。其绕过了与运行多物理场和多尺度仿真相关的计算负担,又具备识别增材制造大型数据集中内在关联的能力^[37]。

2.2 数据驱动 ML 工艺参数优化

基于数据驱动的 ML 回归模型的本质是通过发现输入与输出参数之间的统计相关性来预测新的变量。基于实验结果建立数据集可以提高数据驱动的 ML 模型的准确性。

目前已实现了将工艺参数作为主要数据输入的多维度预测。Akbari 等^[12]提出了名为 MeltpoolNet 的方法,该方法利用收集的工艺参数、熔池尺寸和缺陷类型数据作为 RF 模型的输入,以表征熔池行为并预测其几何形态及缺陷类别。Tridello 等^[38]开发了两种基于监督前馈神经网络(feed-forward neural network, FFNN)的算法:概率机器学习和最大极端值分布(largest extreme value distribution, LEVD)机器学习,用以评估增材制造构件中的缺陷。通过输入 LPBF 工艺参数(激光功率、扫描速度、粉末床厚度和建造方向)和构件体积,上述模型可预测特定尺寸缺陷的发生概率以及缺陷尺寸的统计分布参数。在 TC4 材料的 LEVD 算法验证中,模型的 R^2 高达

0.93。此外通过测量不同工艺参数下的机械性能,建立实验数据库,可直接预测构件的致密度、表面粗糙度和力学性能^[39-41]。基于上述研究的预测数据,可构建工艺参数图,达到优化工艺参数的目的。

目前可通过正向、反向和双向建模来实现工艺参数的优化,表1总结了ML在工艺参数优化中的应用^[13,40-48]。在正向建模中,高斯过程回归(Gaussian process regression, GPR)和MLP等ML模型常用于给定工艺参数下熔池形貌、致密度与表面粗糙度和力学性能的预测,以此筛选理想的工艺窗口。而反向模型则根据所需的结果(结构或性能)精确定位最佳参数输入,其效率显著优于前者。相比正向模型迭代识别,反向模型将成为未来优化工艺参数的主要研究手段。此外,也可通过交换输入输出,实现双向建模。

2.3 物理驱动 ML 工艺参数优化

不同于上述数据驱动ML模型只能通过发现输入和输出之间的统计相关性来对下一轮的输入进行结果预测,物理驱动的ML模型是以数据为导向,生成符合已知物理原理的预测结果。

物理信息引导的LSTM模型通过将高温计采集的热反射数据按图8a所示的时间序列分析方法

处理为具有热特性(传热速率、热梯度)的序列数据,耦合工艺参数作为输入,以达到监测熔池是否过热的目的,实现单层打印后的参数调整^[49]。为了更好地对比PIDK模型与数据驱动模型的区别,将与能量密度和压力有关的物理效应作为信息输入,定义了机器设定和机器设定-物理效应组合的基准模型。前者的输入是与板材、构件、激光和层相关的空间和几何参数,后者的输入为其和物理效应特征的组合。结果表明,机器设定-物理效应组合的基准模型能够在不依赖于特定机器设置的情况下,对孔隙率进行有效的预测和分析^[50]。

此外,为了量化LPBF的快速非平衡过程和补充数据集^[51],可基于质量守恒、动量守恒和热能守恒方程,以及边界条件构建多尺度多物理场模型。基于SBID的ML模型可将多物理场模拟得到的低保真(low-fidelity, LF)数据耦合高保真(high-fidelity, HF)的实验数据作为输入,满足在参数空间内密集采样。多尺度建模方法克服了实验测量的挑战,其不仅量化了LPBF过程中的热历史和熔池动力学,还促进了设计、预测和参数优化的循环,具有实时监控数值模型和实验验证的潜力^[52]。

表1 ML在工艺参数优化中的应用
Tab.1 Application of ML in process parameter optimization

ML model	Input	Output	Evaluation indicator
MLP ^[42]	Process parameters	Molten pool morphology	$R^2=0.97$
CNN+ANN ^[13]	Molten pool images	Process parameters	Ac=96%
PINN ^[43]	Process parameters, temperature of molten pool	Molten pool morphology	Er=5.9%
GPR ^[44]	Process parameters	Density and surface roughness	MAPE=1%
ANN+DT ^[45]	Process parameters and surface topography	Surface topography and process parameters	$R^2=0.813$
GPR ^[40]	Process parameters	Density and surface roughness	Er=1.49%
DT ^[46]	Process parameters	Density	$R^2=0.93$
GPR ^[47]	Process parameters, molten pool morphology	Mechanical property	Er=5.39%
LVGP ^[48]	Process parameters	Mechanical property	RMSE=0.69

Note: artificial neural network, ANN; physics-informed neural network, PINN; latent variable gaussian process, LVGP.

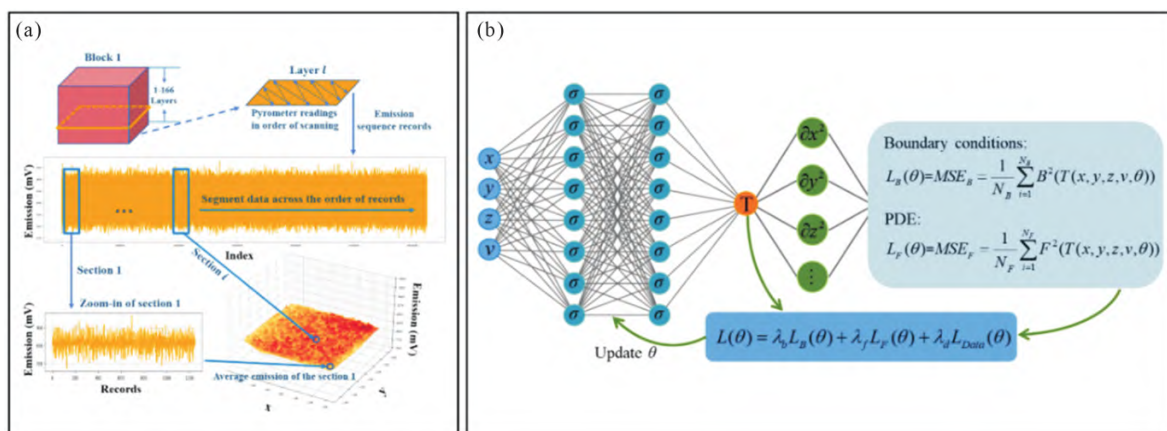


图8 物理信息场的集成:(a)提取热反射数据的物理特性;(b)将物理约束引入损失函数,构件物理信息知情网络^[49,53]
Fig.8 Integration of physical information fields: (a) extracting physical information from the thermal reflection data; (b) introducing physical constraints into the loss function to construct the PINN^[49,53]

Jiang 等^[53]将边界条件的残差(L_B)、控制方程的残差(L_F)和数据约束(L_{Data})作为损失函数,构建了物理法则引导模型训练(physics-guided model training, PGMT)框架下,以扫描速率为输入的 PINN 模型,如图 8b 所示。该模型在训练过程中考虑了物理定律,在使用少量标记数据的情况下准确预测金属增材制造过程中熔池温度和熔池尺寸。此外,Zhu 等^[43]基于金属增材制造过程的物理原理,建立了动量、质量、能量守恒的控制偏微分方程(partial differential equations, PDEs),将控制方程约束(LPDE)和实验数据约束(LData)集成为损失函数。通过最小化损失函数来训练 PINN 模型,并利用自动微分和 Adam 优化算法进行网络训练,减少了对大规模标记数据的依赖,提高了预测精度。

3 基于 ML 的 LPBF 制造过程原位监测

得益于过程传感技术的不断进步,目前已实现了从 LPBF 打印过程中收集原位信息,用于训练新的 ML 模型或为预训练的 ML 模型提供信息,以便快速、自动地做出决策。

3.1 过程信息的采集

LPBF 制造过程是一个耦合光、热、声等多物理场的复杂过程,原位信号的异常与打印过程中缺陷的产生直接相关,因此利用先进的传感手段采集动

态数据,是实现 LPBF 制造过程原位监测的前提^[54]。

3.1.1 孔隙

孔隙是增材构件中的常见缺陷,其会不同程度降低构件的使用性能,具体表现为表面质量下降、强度/延展性降低、耐久性减弱,甚至过早失效^[55]。阿基米德法可以根据成分密度估算孔隙率体积百分比,是测量孔隙率的最简单的非破坏性方法。但阿基米德法无法确定孔隙的形状、大小和分布细节^[56]。金相法弥补了这一不足,但其具有破坏性且无法准确测量孔隙的体积。此外,这种方法仅对大于 $50\text{ }\mu\text{m}$ 的孔隙有效^[57],如图 9a 所示。超声波检测可以以非破坏性的方式诊断样品内部数米的孔隙大小、形状,但仅对大于 $100\text{ }\mu\text{m}$ 的孔隙有效^[58]。X 射线计算机断层扫描^[59-60]根据不同相之间的密度差异来表征孔隙缺陷,能够重建孔隙大小、形状、分布等详细信息。然而,X 射线计算机断层扫描在高密度材料中的应用仍然具有挑战性。基于同步加速器(X 射线)的显微断层扫描具有功率密度大、稳定性高、纯度高、脉冲间隔短(从 $10^{-8}\sim 10^{-11}\text{ s}$)及可预测、可控等优点^[61]。其分辨率小于 $1\text{ }\mu\text{m}$,这使得被检试样尺寸可达毫米级,可以检测到 $1.5\text{ }\mu\text{m}$ 左右的孔隙^[62]。同步加速器(X 射线)的显微断层扫描提供了一种实时、无损的方法,可以在高空间和时间分辨率下直观地阐明孔隙的起源和演变,极大地方便了构件中孔隙缺陷的检测^[63-64]。

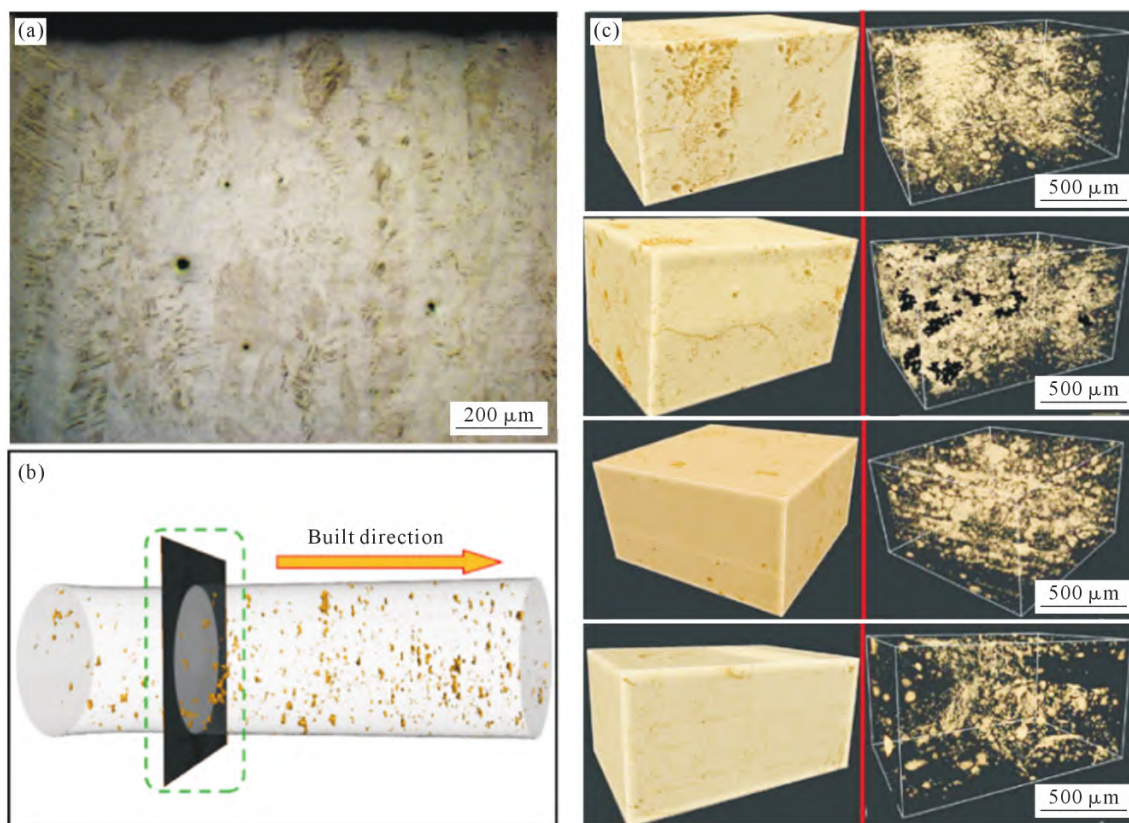


图 9 孔隙的表征手段:(a) 光学显微镜;(b) X 射线计算机断层扫描;(c) 同步辐射 X 射线断层扫描^[57,64-65]

Fig.9 Measurements of porosity defects: (a) optical microscopy; (b) X- CT; (c) SR- μ CT^[57,64-65]

3.1.2 熔池

孔隙的产生通常与能量输入密度和熔池不稳定性有关。不同能量输入下,熔池的形状和大小截然不同,分为浅碗状、半球形及匙孔状。马兰戈尼力、重力和反冲压力之间的动态平衡决定了熔池流动的稳定性^[66]。

熔池的状态直接影响凝固条件、孔隙特性及微观结构特征等,但受限于材料的不透明性,SEM等传统的离位表征方法仅限于凝固后熔池组织结构及缺陷二维特征的评定^[67]。制造过程中涉及的诸多高动态、瞬态的热力耦合现象无法实时追踪,导致熔池的热力学条件和动力学行为无法得到明确的阐释。近年来,基于搭建的传感器和传感系统,大量学者开展了有关熔池温度和形貌原位监测的研究^[16, 68-69]

熔池的温度分布信息与构件的成型质量密切相关^[70],产生缺陷或残余应力较大的熔池会呈现出异常的温度分布,可以通过与熔池中温度场相关的光谱信息来识别^[71]。因此快速准确地获取熔池中的温度场对于缺陷的在线检测至关重要。高温计可以将探测器收集的信号与温度分布相关联,用来测量和监测熔池周围的温度场^[72],但高温计的空间分辨率较低^[73]。通过红外相机能够提供高空间分辨率的图像且可捕捉熔池的瞬态热响应,从而提供熔池的实时信息,但实际温度受视场辐射温度、发射率、透射率和大气透射率等因素的影响,红外相机仅提供基于材料发射率信息的辐射温度,而不是真实的温度测量结果^[74-75]。为了追踪熔池的实际温度,Feng等^[76]设计了单相机双波长熔池在线测温系统,针对熔池温度和熔池边界特点,提出了温度分布相似性(temperature distribution similarity detection, TDSD)的缺陷检测方法,能够实时获取高分辨率的熔池温度分布和演变图像,实现了对打印过程中熔池温度场的同步监测。

为了使监测结果更直观,更多的研究集中在追踪熔池形貌上,如表2所示^[15-16, 77-81]。大量学者依托原位过程信息,探究熔池传热模式的转变^[16, 82-83]、熔池

动力学行为^[84-86]。

3.1.3 声信号

在激光照射粉末床的过程中,会产生携带熔池动力学和激光质量的声信号^[87-88]。提取信号特征可用于区分不同缺陷,并用作ML模型的输入。与成像(2D数据)或扫描(3D数据)相比,声学传感器能在提供高时间分辨率的同时,保证数据处理速度,同时声学传感器的灵敏度高且成本更低。目前,基于声学的超声波测试和声发射光谱学^[89]已广泛应用于LPBF工艺。

超声波检测是一种广泛用于确定内部缺陷的无损监测方法,将其安装在构建平台下方可以实现对打印过程中具有简单几何形状孔隙的原位监测。通过原位超声监测,可以观测到由于激光功率变化诱导产生的多孔层,这种方法能够及时发现打印过程中的缺陷并修正^[90-91]。

通过记录LPBF过程中的声发射,可以检测开裂、分层、表面粗糙度过高或气孔形成等缺陷。传声器和空间分辨声发射光谱可以提供关于构件打印过程中的实时孔隙率和质量的定性数据^[92-93]。通过小波包变换和卷积神经网络等先进的信号处理方法,能够提取声信号的关键物理特征并进行质量等级分类^[94]。此外,X射线成像技术关联声学信号可以进一步精细化缺陷的特征向量提取^[95]。通过声学 and 光电二极管信号的融合分析,证明了量化动态熔池特征的可行性,为提高LPBF打印部件的可靠性和性能提供了有力的技术支持^[15]。

3.2 数据驱动ML过程监测

在LPBF领域,ML通过整合多源信号和跨尺度特征,已被有效应用于检测多种制造缺陷,实现了过程的原位监测和参数的反馈控制。

光信号的采集和应用较为成熟,基于高速摄像机采集的打印过程中的熔池形貌,DNN可识别羽流、飞溅等缺陷^[77, 96-97],LSTM可预测熔池的面积,实现层级的原位监测和反馈控制^[98]。此外,从熔池形貌提取多维视觉特征,用作SVM的输入,可实现熔池的分类^[79]。Zhang等^[99]结合高温计和离轴高速摄像机

表2 熔池形貌表征
Tab.2 Means of sensing molten pool morphology

Sensor equipment	Monitoring object	Feature
High-speed camera ^[77-79]	Process defects, melt pool morphology, dynamic behavior of the melt pool	Superior dynamic performance, real-time, high cost, complex data processing
Photodiode ^[15, 80]	Melt pool morphology, melt pool light intensity and distribution, laser power variation	Fast response, low cost, high robustness, missing details, difficult to calibrate
High-speed X-ray ^[16, 81]	Internal defects (porosity, unfused, high density inclusions, cracks, etc.), quality information (dimensional deviations, density distribution)	Non-contact, high precision, microscopic defects, high cost

原位提取熔池的面积和温度,作为 LSTM 的输入,精确预测了构件的表面拓扑参数,实现了介观-宏观的连接。为了降低数据的传输、存储和处理难度,可使用光电二极管捕捉熔池的光信号,以此来预测构件的相对密度、加工硬化指数和断裂伸长率^[100]。随着传感手段的进步,同步辐射 X 射线成像因具有高时空分辨率,结合 ANN 可以实现原位高精度的体积缺陷分类^[101]。

红外相机常用于热信号的采集,基于采集的热信号,DNN 和深度信念网络(deep belief networks, DBN)可实现对熔池状态的原位监测和缺陷分类(如层间剥离和溅射物)^[102-103]。将熔池的热图像输入残差-循环卷积神经网络(residual-recurrent convolutional neural networks, Res-RCNN)可对构件孔隙率精确预测^[104]。

目前,DNN 因采用堆叠和层化的全连接网络结构在图像数据的回归和分类方面表现出优异的性能,显示出比传统 ML 模型更好的预测性和准确率,如表 3 所示^[77-79,96-97,99-106]。

3.3 物理驱动 ML 过程监测

由于 LPBF 的非线性、强耦合和多参数等特性,不同的因素会影响竣工构件的内部缺陷。依靠单一的传感信息监测熔池内局部和瞬时的变化并不可靠,因此开发多传感器系统的多信息融合算法或模型,对于在缺陷监测中实现更高的精度是必要的。

按时间顺序提取 LPBF 过程的声信号和热信号,可作为物理信息引入 ML 模型,从而构建 PIDK 模型。Mahato 等^[22]讨论了热发射传感器数据的顺序时间序列性质,并探索了基于 KNN 分类的初步性

能。随后,有研究通过红外相机、光电二极管和声学传感器等捕捉了过程中一维的声信号和二维的热图像,提取信号的时间序列,并基于小波变换处理上述具有固定时间跨度的信息,将其转变为标度图,标记缺陷的生成,实现了多信息的压缩与融合^[14-15],如图 10b 和 c 所示。结合同步加速器 X 射线和热成像, Ren 等^[6]发现在 LPBF 的快速非平衡过程中存在两种匙孔振荡模式,通过热成像提取两种振荡模式下熔池的时间序列信号,进行小波分析转换为标度图,根据 X 射线成像结果标记孔隙的生成,将其输入到 CNN 模型中,实现了高保真度和高分辨率检测熔池内部缺陷的生成。

不同于数据驱动的 ML 直接利用收集的多维视觉特征进行熔池的原位监测和缺陷识别(羽流、飞溅等),基于声学 and 热学得到的一维时间序列信号有助于识别与熔池动力学相关的频率特征,而标度图可揭示时间序列的特征振荡,其与熔池的异常、缺陷的生成直接关联,具备物理可解释性。标记异常现象的特征振荡,将其作为 PIDK 模型的输入信息,结合同步加速器 X 射线实现了熔池的原位监测和实现熔池内部缺陷(球化、未熔合、传导模式和匙孔气孔)的精确分类。此外,除了通过信号处理技术实现信息的融合,也可利用传感系统易于解释、基于统计的特征,保留底层物理现象的可解释性,将信号分层输入模型中^[107],实现在决策层的融合^[108]。

与传统 ML 方法相比,NN 在图像识别等方面表现优异,适用于多传感器图像数据。目前有研究表明可将训练好的 NN 模型迁移至异质材料,并呈现较好的预测率,这或将成为过程监测新的发展方向^[23]。

表 3 基于不同传感信号的 ML 在过程监测中的应用
Tab.3 Application of machine learning based on different sensing signals in process monitoring

Sensor equipment	ML model	Output	Evaluation indicator
High speed camera	CNN ^[77]	Defects classification	Ac=92.7%
	SVM ^[105]	Defects classification	Ac=85%
	SVM ^[79]	Molten pool classification	Ac=85.1%
	DCNN ^[96]	Defects classification	Ac=99.4%
	DNN ^[97]	Molten pool classification	Fr=1.1%
	GPC ^[78]	Melting state identification	$F_1=86.86\%$
	LSTM ^[99]	Surface topography prediction	Ac=99.4%
Photodiode	CNN+LSTM ^[106]	Molten pool classification	Ac=98%
	SVR ^[100]	Mechanical property prediction	$R^2=0.8$
High-resolution X-ray	ANN ^[101]	Defects classification	Ac=99.2%
	DBN ^[102]	Melting state identification	Ac=83.40
IR camera	DNN ^[103]	Defects classification	Ac=96.8%
	Res-RCNN ^[104]	Porosity prediction	Ac=99.49%

Note: support vector regression, SVR; gaussian process classification, GPC; deep convolutional neural network, DCNN.

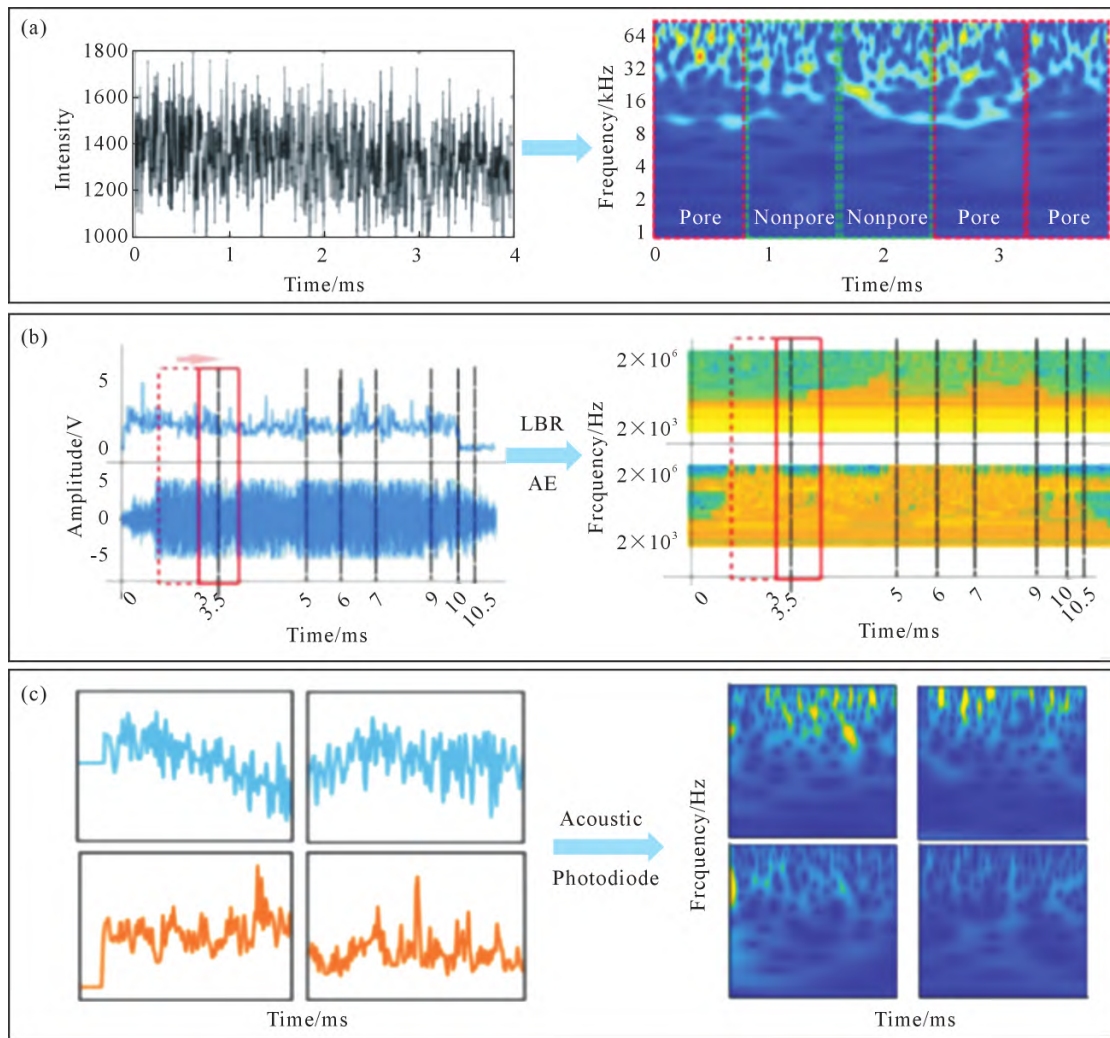


图 10 对时间序列信号进行小波分析:(a)对匙孔区域平均发射强度的时间序列信号进行小波分析;(b)对 LBR 和 AE 的时间序列信号进行小波分析;(c)对声学 and 光电二极管的时间序列信号进行小波分析^[14-16]

Fig.10 Wavelet analysis performed over the time-series signals: (a) wavelet analysis of time-series signals of mean emission intensity in the keyhole region; (b) wavelet analysis of LBR and AE time-series signals; (c) wavelet analysis of acoustic and photodiode time-series signals^[14-16]

4 基于 ML 的构件寿命预测

研究表明,打印过程中形成的体积缺陷是影响增材构件疲劳性能的重要因素^[55,109-111],因此采用 ML 结合监测手段,预测增材构件在循环载荷下的疲劳失效对延长构件寿命至关重要。

4.1 服役信息的采集

目前,用于预测结构材料失效行为和寿命的模型已被广泛研究。主要包括基于力学的有限元方法与 Gurson-Tvergaard-Needleman 模型、Gunawardena 模型和连续介质损伤力学(continuum damage mechanics, CDM)模型^[112-115]相结合。有限元可根据重复载荷循环下屈服轨迹的变化和相应的应力-寿命(S-N)曲线等输入进行疲劳寿命预测。此外,材料的几何形状、载荷和边界条件没有输入限制^[115-118]。然而,基于力学的模拟在表示缺陷的微观结构能力方面存在局限。传统的离线表征手段(TEM、EBSD 或

SEM)可以揭示详细的微观结构^[119-120],但其具有破坏性且涉及漫长的样品制备阶段,故上述方法均不适用于机械载荷下的实时监测。

作为监测增材制造构件早期裂纹形成的无损技术,中子成像观测到样品断裂前断口处晶体结构的变化,但并未给裂纹形成提供直接证据^[121]。X-CT 是目前用于分析缺陷特征的先进无损技术之一。通过 X-CT 对疲劳试样进行原位疲劳试验可以在高空间和时间分辨率下直观地阐明孔隙的起源和演变,探究缺陷诱发疲劳裂纹加速扩展的原因^[65,122]。

4.2 数据驱动 ML 寿命预测

LPBF 工艺产生的体积缺陷随机分散在构件中,加剧了疲劳裂纹萌生和扩展的风险,导致疲劳寿命明显降低。传统的疲劳寿命模型难以满足高精度、高可靠性的寿命预测。而 ML 以其在处理复杂影响因素和降低计算成本方面的优势,已成为预测复杂问题中不可或缺的关键技术。该技术能够有效地建

立数据之间的相关性,为解决多变量和高维度问题提供了一种高效且精确的解决方案。

基于非原位的扫描电子显微镜获得疲劳断口的显微形貌,可以作为 DNN 和梯度提升树(extreme gradient boosting, XGBoost)的数据输入。ML 能够实现离线高精度评估后处理^[123]、体积缺陷^[124-125]对疲劳寿命的影响,但受限于是传感技术,无法对裂纹扩展机理进行原位分析。

原位预测构件在随机载荷下的疲劳失效时间及探索缺陷的位置、大小和形态对疲劳寿命的影响依赖于失效过程的原位传感,即利用声发射、数字图像相关技术追踪损伤累积过程^[126]和结合 SR- μ CT 精确提取构件缺陷原位变形的信息^[127],如图 11 所示,将采集的数据输入到 ANN 和 SVR 中以预测疲劳寿命。结果表明,ML 能精确预测疲劳寿命,但受限于是相对较小的数据集,模型的泛化能力不足。针对实验数据不足的情况,有学者采用蒙特卡罗模拟和立方样条插值等数学方法扩大数据集^[128-129],并基于 Levenberg-Marquardt 算法建立了考虑缺陷和构建方向

影响的反向传播神经网络(backpropagation neural network, BPNN)预测模型,实现了高精度的疲劳寿命预测^[129]。

4.3 物理驱动 ML 寿命预测

数据驱动的 ML 实现了较高精度的疲劳寿命预测,但其易与基本的物理规律产生矛盾或决策过程不够透明,限制了模型在工业上的应用。通过修改网络模型或损失函数的结构,将先验知识或物理约束整合至模型训练的正则化过程中,构建 PGMT 模型可减少模型训练期间所需的样本量,降低过拟合,并增强训练模型的可解释性和鲁棒性。

为了提升 ML 对材料疲劳行为的理解和预测的泛化能力,可建立实验与仿真数据集,作为 SBID 模型的输入。基于晶体塑性有限元和扩展有限元生成大量裂纹扩展传播的数据,结合衍射和相位对比断层扫描采集高保真实验数据,作为贝叶斯网络(Bayesian neural networks, BNN)和 BPNN 的数据输入,用以预测疲劳裂纹扩展方向、速率^[130]和寿命^[131],如图 12 所示。此外,通过求解 CDM 模型可获得大

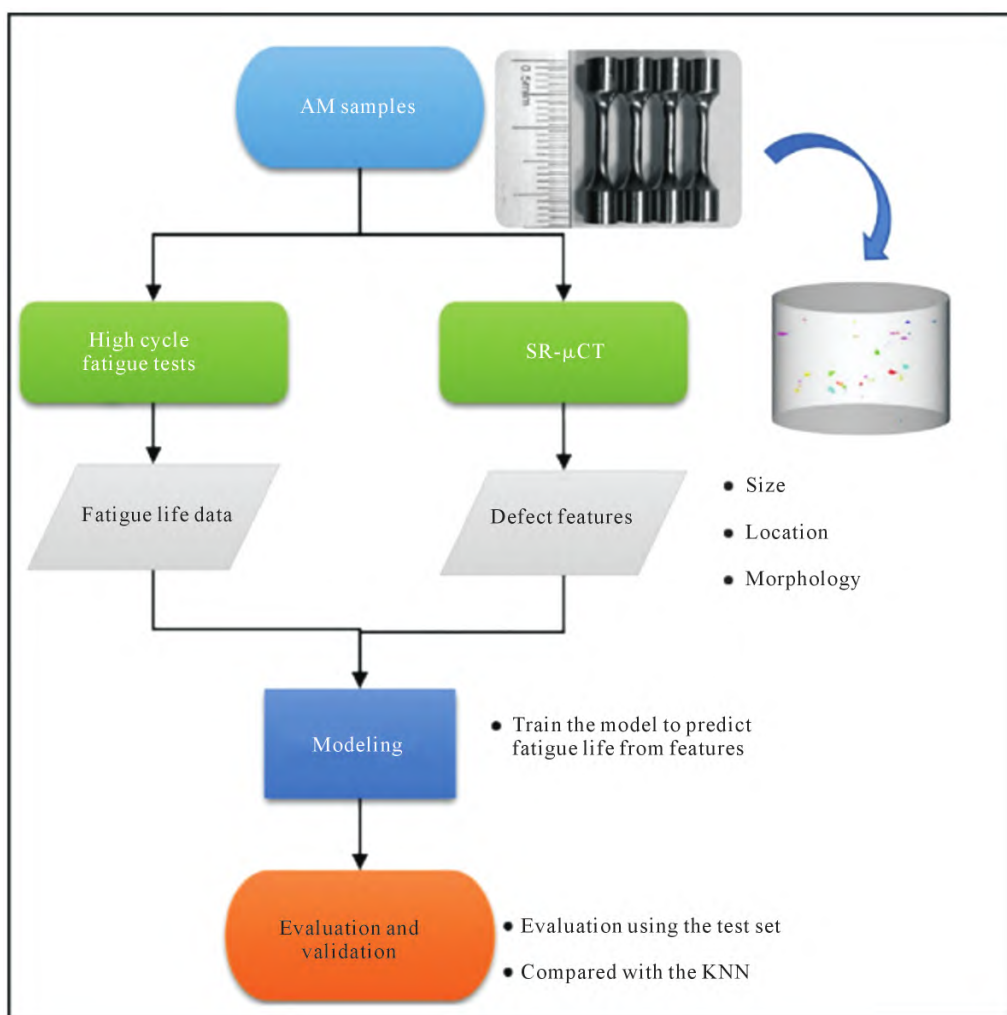


图 11 基于 SVR 模型的疲劳寿命预测流程^[127]

Fig.11 Overview of the fatigue life prediction procedure based on the SVR model^[127]

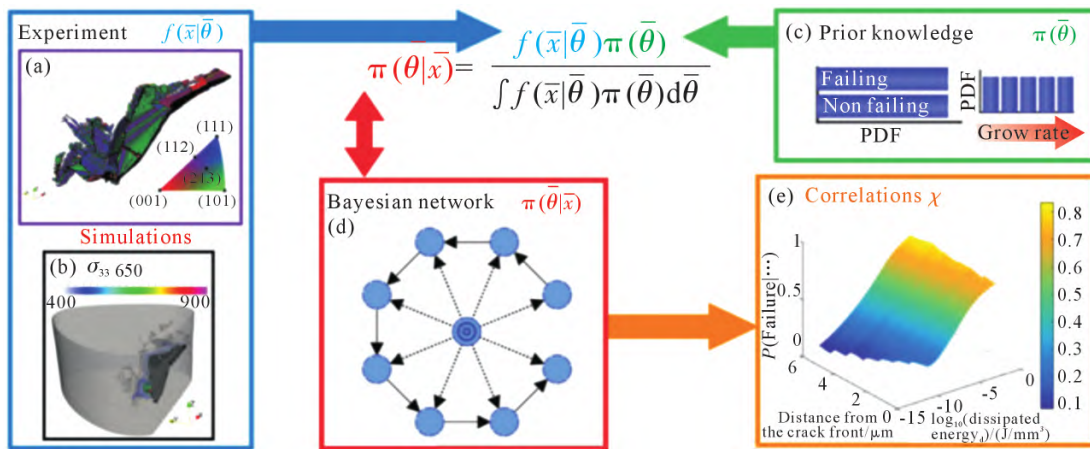


图 12 非原位数据驱动的概率裂纹传播框架示意图:(a) 实验结果数据集;(b) 仿真数据集;(c) 均匀的先验分布;(d) 贝叶斯定理计算得到的后验概率;(e) 数据中嵌入的相关性^[130]

Fig.12 Schematic representation of the non-local, data-driven probabilistic crack propagation framework: (a) experimental dataset; (b) simulation dataset; (c) uniform prior distributions; (d) posterior probability via Bayes' theorem; (e) correlations embedded in the data^[130]

量在不同工艺参数和疲劳载荷条件下的寿命数据,用于 ANN、RF 和 SVM 的输入^[132-133],解决了数据集体量小的问题。

以工艺参数作为数据输入的 PGMT 模型,通过将损失函数定制为似然函数的负对数,并将物理知识转化为如式(9)~(11)所示的数学公式作为约束,克服了数据驱动模型在疲劳数据分析中的局限性,得到具有物理一致性曲率和非奇异方差的概率疲劳寿命(P - S - N)关系,有效解决了利用缺失数据集预测疲劳寿命的问题^[134-135]。Ciampaglia 等^[136]为了实现从工艺参数和热处理方法来准确预测构件的 S - N 关系,将 Frobenius 范数作为损失函数,物理约束为代表缺陷和微观结构效应的潜在变量,并设计网络输出层来预测不同循环次数下的疲劳强度,确保了预测的 AlSi10Mg 合金试样 S - N 曲线遵循单调递减的物理规律。此外,也有研究基于 Basquin 公式构建损失函数,将与应力水平相关的物理公式作为约束整合到神经网络的架构中,用于预测构件的疲劳寿命^[137]。

$$\frac{\partial \sigma}{\partial S} \leq 0 \quad (9)$$

$$\frac{\partial^2 \mu}{\partial S^2} \geq 0 \quad (10)$$

$$\frac{\partial \mu}{\partial R} \geq 0 \quad (11)$$

式中, S 为应力水平; σ 为疲劳寿命的标准差; R 为应力比; μ 为疲劳寿命的平均值。

上述研究分别定义了损失函数和约束中的物理规律,为了简化模型结构,可将疲劳寿命与应变幅度、应变率和温度的关系等物理约束以偏导数的形式嵌入损失函数,确保模型遵循已知的物理原理。结果表明,融合了 S - N 物理知识的模型,对于小规模数

据集,展现出了较高的预测精度和泛化能力^[138-139]。

如图 13 所示为 PGMT 模型的框架,通过将物理约束和富含物理信息的损失函数引入架构,使得输入和输出具有物理一致性。通过对比表 4 两种驱动的 ML 模^[123-124,128,131,133,136,138,141-142],发现物理信息引导的 ML 模型具有更稳定的性能。此外,物理信息引导的 ML 模型提供了数据空间的先验知识,从而降低了 ML 训练的复杂性和对大量训练数据的需求,从而节省了训练时间和成本。ML 对训练数据的依赖性降低,使其能够获得更广义的模式和规律。

表4 数据驱动和物理驱动模型性能对比

Tab.4 Performance comparison of the data-based and physics-informed ML models

ML type	ML model	Evaluation indicator	Publication
Data-based	DNN	$R^2=0.983$	Makeki ^[123]
	XGBoost	$R^2=0.95$	Peng ^[124]
	ANN+GPR	$Ac=83.30\%$	Farid ^[128]
	SVM	$R^2=0.927$	Wang ^[133]
	DNN	$R^2=0.934$	Zhang ^[141]
Physics-informed	RF	$R^2=0.942$	Zhan ^[142]
	PINN	$R^2=0.9$	Jiang ^[138]
	BPNN	MAPE=1.49%	Feng ^[131]
	PINN	MAPE=4%	Ciampaglia

5 总结与展望

LPBF 过程中涉及诸多高动态、瞬态的热力耦合现象,基于传统的实验分析、理论建模、数值求解难以简便、快捷和低成本地探究工艺、缺陷和服役性能之间的联系。随着计算机算力的发展和原位传感技术的进步,ML 方法为有效处理先进制造高维物理量之间的复杂非线性关系提供了契机。为此,本文重点论述了 ML 在 LPBF 中的应用进展。首先,简述

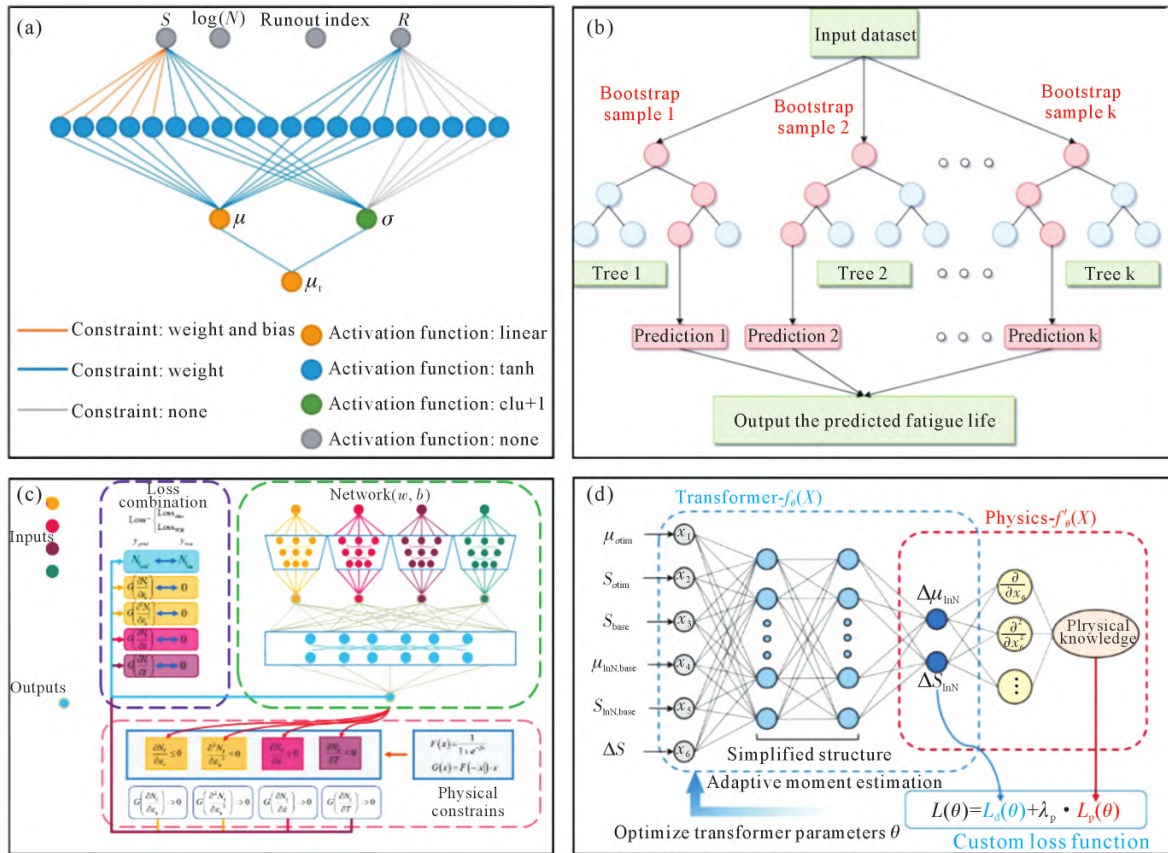


图 13 物理模型的网络架构:(a)用于预测疲劳 P - S - N 曲线的概率物理引导神经网络;(b)具有 k 个决策树的射频模型示意图;

(c)用于预测低循环疲劳寿命的物理驱动模型;(d)物理信息引导 ML 模型的框架^[135,138-140]
Fig.13 Schematic diagram of physics-informed ML models: (a) probabilistic physics-guided neural network for fatigue P - S - N curve estimation; (b) schematic diagram of the RF model with k decision trees; (c) physically informed low-cycle fatigue life prediction method; (d) framework of physics-informed transformer^[135,138-140]

了常见的 ML 算法和通用的 ML 流程,由于传统的数据驱动 ML 模型在可解释性和泛化能力方面具有很大的局限性,进一步提出了融合物理信息的物理驱动 ML。物理驱动 ML 主要分为物理信息引导的模型、基于仿真输入的模型和物理法则引导训练的模型三种。上述物理驱动模型现已逐渐运用在工艺参数优化领域,弥补了该领域数据驱动数据集和物理可解释性的不足。过程监测领域主要依赖于 PIDK 模型,借助于先进的传感手段和数据预处理手段,可提取与缺陷对应的物理特征信号,提高了 ML 模型的可解释性和预测准确率,实现了熔池的原位监控。PGMT 模型则服役寿命的预测中广泛应用,通过将经典的力学损伤模型作为偏微分方程作为约束,确保模型的输出结果遵循已知的物理原理。总体上看,已经实现了工艺-缺陷、工艺-性能、缺陷-寿命的 ML 建模,DNN 模型逐渐成为主要的研究手段。相较于数据驱动的 ML,物理驱动 ML 的泛化能力强。尽管如此,ML 与增材制造的融合仍存在机遇。

(1)ML 建模方式的转变 目前通过正向模型来实现优化工艺参数的任务,以此筛选理想的工艺窗口。相比正向模型反复的迭代识别,反向模型则根据所

需的结果(结构或性能)精确定位最佳参数输入,展现出更高的优化效率,预示着未来研究方向。此外,也可通过交换输入输出,实现双向建模,进一步增强模型的灵活性和全面性。这些方法不仅推动了工艺参数优化,也为过程监控、质量保证及疲劳性能预测提供了新的视角。

(2)ML 范式的革新 近年来迁移学习逐渐在增材制造领域兴起,如图 14 所示,迁移学习作为一种强大的机器学习范式,通过将源域中获得的知识迁移到目标域,源域中预训练的模型能够为解决目标

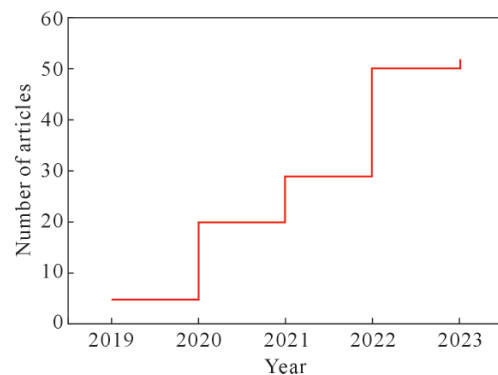


图 14 2019—2023 年发表有关迁移学习的论文数量
Fig.14 Number of papers published on transfer learning from 2019 to 2023

域中的任务提供有价值的先验知识, 迁移学习有效解决了增材制造领域因数据稀缺而导致的学习性能问题, 将进一步推动 ML 在增材制造领域的发展和应用。

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