

引用格式: 陈伊家, 马志远, 张天旭, 等. 非均质材料微观结构表征与重建研究进展[J]. 航空材料学报, 2025, 45(6): 13-32.
CHEN Yijia, MA Zhiyuan, ZHANG Tianxu, et al. Research progress in microstructure characterization and reconstruction of heterogeneous materials[J]. Journal of Aeronautical Materials, 2025, 45(6): 13-32.

非均质材料微观结构表征与重建研究进展

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摘要: 非均质材料广泛应用于航空航天、电子信息、国防等领域高端装备零部件, 其多相、多尺度、形貌复杂的微观结构特征决定材料宏观性能的优越性, 建立准确的微观结构模型对于深入理解结构-性能关系至关重要。然而当材料表现出强烈的非均质特性时, 该过程的复杂性显著提升且难度增大。近年来, 计算材料科学进步推动计算模拟方法发展, 材料微观结构表征与重建(microstructure characterization and reconstruction, MCR)技术作为计算模拟过程的关键环节, 为非均质材料的微观结构建模提供有力途径。目前, 非均质材料的 MCR 主要包括两类: (1)基于统计方法的建模技术; (2)基于机器学习方法及计算机视觉的建模技术。本工作总结并梳理这两类 MCR 技术, 阐释相关方法的特点及适用性, 并分析不同方法在非均质材料微观结构表征与重建方面的研究进展, 为如何选取 MCR 方法并将其应用于材料设计提供借鉴和指导。

关键词: 微观结构; 表征与重建; 非均质材料; 统计方法; 机器学习

doi: 10.11868/j.issn.1005-5053.2024.000195

CSTR: 32420.14.j.issn.1005-5053.2024.000195

中图分类号: TB303; V25

文献标识码: A

文章编号: 1005-5053(2025)06-0013-20

Research progress in microstructure characterization and reconstruction of heterogeneous materials

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Abstract: Heterogeneous materials are widely used in high-end equipment components of fields such as aerospace, electronic information and national defense, with the microstructure features of multi-phase, multi-scale and complex morphology, which determines the superior macroscopic properties of materials. Establishing an accurate microstructure model is crucial for deeply understanding the structure-property relationship. However, when the material exhibits strong heterogeneous characteristics, the complexity and difficulty of this process increase significantly. In recent years, advances in computational materials science promote the development of computational simulation methods. Microstructure characterization and reconstruction(MCR), as a key component of computational simulation process, provides a powerful approach for microstructure modeling of heterogeneous materials. Currently, MCR for heterogeneous materials mainly includes the following two categories: (1) modeling techniques based on statistical methods; (2) modeling techniques based on machine learning and computer vision. This work summarizes and organizes two categories of MCR techniques, explains the characteristics and applicability of the relevant methods, and analyzes the research progress of different methods in MCR of heterogeneous material. It aims to provide references and guidance for selecting MCR methods and applying them to material design.

Key words: microstructure; characterization and reconstruction; heterogeneous material; statistical method; machine learning

建立精准的加工-结构-性能 (processing-structure-property, PSP) 关系来理解材料行为是材料科学研究

的重要目标^[1], 微观结构作为 PSP 关系中的核心环节, 得到研究人员广泛关注, 大量研究借助扫描

电子显微镜(scanning electron microscope, SEM)^[2]、透射电子显微镜(transmission electron microscope, TEM)^[3]、电子背散射衍射(electron backscatter diffraction, EBSD)^[4-5]、CT成像^[6-7]等实验表征手段获得材料成分、形貌、晶体结构等信息,并结合相关物理及力学测试^[8],揭示微观结构与宏观性能之间关系。这种方法获取的微观结构局部统计结果准确,但试样制备过程费时低效,受限于仪器分辨率与试样尺寸的制约,大范围的精细观测往往需要耗费较多的试样和昂贵的设备资源^[9]。随着计算材料科学的发展,采用计算模拟的建模方法模拟材料在外场条件下呈现的物理和力学性能^[10-11],为实验表征方法提供有力支撑。在多种计算模拟方法中,第一性原理^[12-13]、分子动力学^[14]和蒙特卡洛^[15]方法主要用于解释材料在原子分子尺度的行为,相场^[16-17]和有限元法^[18-19]用于模拟材料微观及介观层面的特征,更适合解决多场耦合下具有复杂微观结构的问题,应用范围较广^[20],目前已有成熟应用的商业软件(如 ABAQUS、COMSOL 等)。以上两种方法的计算模拟过程通常需要以基于材料微观结构的模型为基础,通过设计和再现复杂结构并赋予各微观变量特定参数,获得准确的模拟结果。因此,对材料微观结构建立准确模型是模拟过程的重要基础。

早期,采用各向同性简化模型^[21-23]进行基于微观结构的建模,该方法计算成本低,便于工程应用,适用于结构简单的均质材料。近年来,随着高性能制造技术^[24-25]的飞速发展,很多零部件的材料结构趋于复杂化,其高性能是通过具有宏/微或微/纳等跨尺度的复杂结构特征实现的^[24]。其中,航空航天用纤维增强复合材料、热障涂层,以及电池电极用纳米颗粒增强复合材料、多孔陶瓷等通常具有多相、多尺度和形貌随机的非均质特征^[26-27],难以用各向同性简化模型对其进行描述,这些微观结构的非均质特征在一定程度上决定材料宏观性能优越性。You 等^[28]研究氧化物颗粒增强镍基涂层中不同尺度颗粒对涂层性能的影响,发现微米级颗粒可以提高涂层硬度,弥散分布的纳米级颗粒有利于提高涂层整体的耐腐蚀性,两种尺度颗粒协同优化使得涂层具有优异的综合性能。Zhu 等^[29]在 TC4 合金表面激光熔覆制备陶瓷增强的多相复合涂层,并通过纳米压痕法分析,这种多相复合涂层的耐磨性能比 TC4 基体提升约 5 倍。因此,准确建立非均质材料微观结构模型对深入理解其宏观性能至关重要。

非均质材料微观结构特征主要包括组成相含量、数目、尺寸、形貌以及分布状态,基于微观结构建模的目标在于对这些特征进行统计表征并重建^[30]。2018 年, Bostanabad 等^[1]首次在 *Progress in Materials Science* 上发表基于计算的微观结构表征与重建(microstructure characterization and reconstruction, MCR)的综述文章,总结 20 世纪 90 年代以来 MCR 技术的发展,引起研究人员对其应用于非均质材料的广泛关注。自 2018 年以来,该领域的研究取得进一步发展, Seibert 等^[31]、Senthilnathan 等^[32]、Ma 等^[33]对多晶金属、复合材料、多孔岩石及陶瓷等复杂微观结构进行表征与重建,推动了 MCR 技术在非均质材料领域的深入应用。

MCR 技术旨在基于有限的显微图像样本,采用高通量计算方法建立统计等效的微观结构模型。其核心思想包括表征和重建两个过程^[34],表征是通过特征函数对目标微观结构进行量化表示,重建是根据已有的特征信息生成一组或多组统计等效的微观结构。Chen 等^[35]指出,一个好的 MCR 方法应具备以下特点:(1)能够体现目标材料微观结构突出的形态特征;(2)表征过程具有物理意义,易于映射 PSP 关系;(3)提供计算效率高的重建程序。目前很多研究采用统计方法实现 MCR,即预先提取并量化微观结构的统计特征,然后依据提取的量化特征实施重建,例如相关函数法^[36]、物理描述符^[37]、随机场^[38]等,这些方法可以灵活反映非均质材料的固有随机性,具备对微观结构的显式表达,利于构建 PSP 关系,应用广泛且日益成熟。近年来,人工智能技术的迅猛发展加速其在材料科学领域的应用^[39-40],基于神经网络的机器学习方法^[41]以及纹理合成等计算机视觉技术^[42]具有强大的复杂特征提取和拟合能力,通过学习目标图像像素分布的潜在特征,输出与之高相似度的重建图像^[43]。与统计方法不同的是,机器学习及纹理合成不需要预先提取微观结构的显示表征参数,其表征和重建过程一体化完成,这为非均质材料 MCR 提供新思路^[44-45]。

由于非均质材料类型多样,且微观结构特征千差万别,不同类型材料中 MCR 的应用效果存在差异, Li 等^[46]采用不同 MCR 方法对两相光学材料、多孔砂岩、金属合金、三相橡胶材料进行微观结构重建,发现相关函数、物理描述符、随机场方法适用于两相光学材料及多孔砂岩,机器学习方法在金属合金和三相橡胶材料中应用优势明显。随后利用适用于两相材料且计算效率高的随机场方法对

光学材料微观结构进行重建,通过数值模拟计算光吸收率这一性能,模拟结果的均方误差不超过0.1,精度较高。由此可见,依据目标材料微观结构特征选取合适的MCR方法,是研究材料结构-性能关系的重要基础。

本工作依据是否需要预先提取量化微观结构特征的显示表征参数,将MCR方法分为基于统计方法和基于机器学习及纹理合成方法两大类,分析不同方法的特点及适用性,并通过典型案例分析不同方法应用于非均质材料的研究进展,最后对材料MCR技术发展前景进行展望。

1 基于统计方法的微观结构表征与重建

基于统计方法的MCR基本思想在于首先采用某种统计函数提取微观结构中组分含量、颗粒尺寸、分布状态等描述性特征,再以这些特征为目标进行优化,获得与目标微观结构统计等效性最佳的重建模型。这种预先提取的描述性特征通常被表述为输入变量或评估标准^[47],表征过程作为输入变量,描述微观结构;重建过程作为多目标优化问题的评估标准,评估微观结构。

Cui等^[48]整理41种用于描述微观结构特征的统计函数,并分析其所描述特征量之间的差别和相关性。根据采用的统计函数及提取特征的不同,MCR方法主要包括相关函数法、物理描述符、随机场、Voronoi方法等,表1总结出这些典型方法描述的微观结构特征及应用^[36,49-87]。

1.1 相关函数法

常用相关函数包括两点相关函数 $S_2^i(x)$ ^[88]、两点聚类相关函数 $C_2^i(x)$ ^[56]、线性路径函数 $L^i(x)$ ^[58]等,其描述的物理意义可理解为在微观图像上随机抛出长度为 x 的线段, $S_2^i(x)$ 表示线段的两 endpoints 都位于组成相 i 内的概率,它是一种量化微观结构中各相按点分布的概率函数; $C_2^i(x)$ 表示线段的两 endpoints 都位于组成相 i 内且在同一团簇的概率,对具有颗粒簇状分布的结构更为敏感^[1],能够更好地体现聚集性; $L^i(x)$ 表示整个线段都落在组成相 i 内的概率,条件约束更强,量化了微观结构中沿直线的聚集数量,能够表征相与相之间的连通性^[89]。通过计算微观图像上述相关函数能够获取包含各组成相的成分、尺寸、分布状态等特征的统计信息。

Yeong和Torquato^[49]最先提出一种基于相关函数的MCR方法,称为YT方法。这种方法利用

模拟退火算法来随机交换像素并更新微观图像,通过不断迭代优化使生成图像与原始图像之间相关函数的误差最小,并对含有圆盘颗粒分布的两相介质、两相多孔砂岩等结构重建有很好的效果。Liu等^[56]基于相关函数法提出一种两相纳米颗粒/聚合物复合材料的微观结构表征与重建框架,其主要流程如图1所示,包括微观图像的获取及二值化处理、两点相关函数 S_2 及两点聚类相关函数 C_2 的表征、微观结构参数化、基于相关函数的重建、重建图像的有限元模拟。

相关函数方法的稳定性好,但随机交换像素生成大量中间路径图像的方式非常耗时,迭代次数通常需要上万甚至百万次^[57],计算成本高。针对计算效率低的问题,后续研究中改进模拟退火算法^[51,53]、优化像素交换规则^[52]等策略可用于加快算法的收敛速度。例如,Tang等^[90]采用基于不同相邻域的像素交换规则进行优化,使其收敛的迭代次数由百万次降低一个数量级。目前相关函数法主要适用于结构简单的两相随机介质,该方法是从概率分布角度对微观结构各组成相的特征提供统计描述,可能会遗漏一些微观结构的形态学信息而产生误差。

1.2 物理描述符

早期物理描述符用于对微观结构的量化表征^[91],主要包括粒子含量、尺寸、数目、分布位置等具体特征参数。与相关函数相比,物理描述符具有低维度和明确的物理意义,可以直观地体现单个粒子的形态学信息,更有利于构建PSP关系,越来越多研究人员逐渐以物理描述符作为优化参数对材料微观结构进行重建。

Xu等^[37,58-60]提出基于物理描述符的微观结构表征与重建方法,并将其用于两相纳米颗粒/聚合物复合材料,其基本思想如图2所示^[59]。根据描述的微观结构信息将物理描述符分为3个层次^[37],由高到低为成分、几何形状和分布状态,低层次的描述符分配给单个粒子特征,高层次的描述符用于表征整体微观结构。其中,分布状态描述符描述第二相粒子的空间关系及邻域状态,包括最近邻距离 d 和粒子数量 N ;几何形状描述符提供第二相粒子的形状和尺寸信息,例如面积 S 、宽高比 α 等;成分描述符用于表示第二相的体积分数。基于“分层重建”思想依次对低层次到高层次描述符进行重建:首先采用优化算法调整第二相粒子的质心位置,再以椭圆拟合的方式在每个粒子质心位置赋予其几何形状,最后依据体积分数进行成分调整。

表1 基于统计方法的MCR技术提取的微观结构特征及应用
Table 1 Features and applications of microstructure extracted by MCR technique based on statistical method

Technique	Features of microstructure	Material	Reference	
Correlation function	Two-point correlation function	Pb-Sn alloy	[36]	
	Two-point clustering correlation function	Debye random media	[49]	
	Linear path function		Fontainebleau sandstone	
			Boron-carbide/aluminum composite	[50]
			Two-phase and three-phase porous sandstone	[51]
			Polymer electrolyte fuel cell (PEFC) catalyst layer	[52]
			Solid oxide fuel cell	[53]
			Porous transducer material	[54]
			Porous sandstone	[55]
			Polymer nanocomposite	[56]
Ceramic foam	[57]			
Physical descriptor	Particle size	Polymer nanocomposite	[37, 58-60]	
	Area	Rubber composite containing carbon black nano-fillers	[61]	
	Number	Epoxy resin/SiO ₂ nanocomposite	[62]	
	Aspect ratio	Particulate composites	[63]	
	Orientation angle	Nanoporous gold	[64]	
	Nearest neighbor distance		Porous rocks	[65]
			Expansive porous soil	[66]
Random field	Spectral density function	Nanoporous gold	[67]	
	Autocorrelation function	Two-phase and multi-phase random media	[68]	
		Cancellous bone material	[69]	
		Three-dimensional braided C/C-ZrC composites	[70]	
		Carbon fiber reinforced polymer	[71-72]	
		YSZ thermal barrier coating	[73]	
		AlSi-PHB seal coating	[74]	
		Aging pipeline material	[38]	
		Polymer/SiO ₂ nanocomposite	[75]	
		Quasi-random nanophotonic structures	[76]	
Voronoi	Grain size	Nickel-base superalloy IN100	[77-78]	
	Number	Aluminum alloy AA6061	[79]	
	Orientation angle	Polycrystalline Al ₂ O ₃	[80]	
	Nearest neighbor distance		Ag/SnO ₂ alloy	[81]
			Titanium alloy	[82]
			Polycrystalline ceramic materials	[83]
			Polymer bonded explosive	[84]
			Pearlitic steel	[85]
	Bone trabecular structure	[86]		
Trabecular-like Ti-6Al-4V scaffold	[87]			

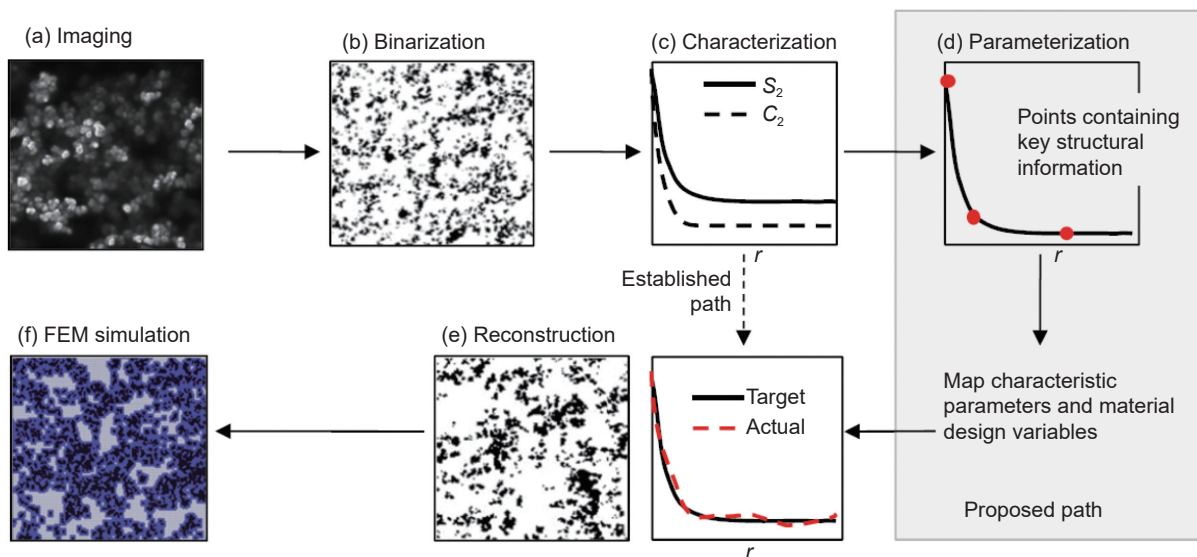


图 1 基于相关函数法的两相随机介质微观结构表征与重建^[56] (a)微结构图像技术(扫描电子显微镜、透射电子显微镜等); (b)通过图像处理算法将图像二值化; (c)通过相关函数法表征; (d)微结构参数化; (e)通过相关函数法重建; (f)通过有限元方法预测材料性质

Fig. 1 MCR of two-phase random media based on correlation functions^[56] (a)microstructure imaging techniques(SEM, TEM and so on); (b)image binarization via image processing algorithm; (c)characterization via correlation functions; (d)microstructure parameterization; (e)reconstruction via correlation functions; (f)predicting material properties via finite element method(FEM)

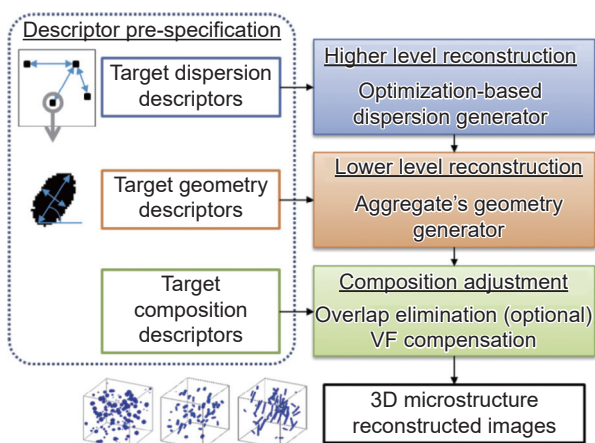


图 2 基于物理描述符的两相聚合物/纳米复合材料微观结构表征与重建^[59]

Fig. 2 MCR of two-phase polymer/nanocomposites based on physical descriptors^[59]

物理描述符方法的优化过程通常是针对粒子的质心位置或识别粒子边缘像素来调整,不涉及大量像素随机交换,计算成本比相关函数法低,通常需要几分钟到几小时不等^[1]。该方法优势在于能够提供单一粒子大小、形状等清晰的物理含义,适用于第二相为低含量、小尺度和颗粒状的两相结构。当第二相形貌复杂且颗粒边缘杂乱交错难以识别时,物理描述符的重建结果会偏离真实形貌。为了更好地表征颗粒的复杂形状特征, You 等^[63]提出基于一系列组成相形态描述符的微结构重建算法,通过 CT 图像获取粒子单元模型,建立形态

存储库,计算粒子表面积、形状指数等形态描述符并与存储库匹配采样,重建结果更好地保留两相颗粒增强复合材料中第二相粒子的真实形态。

2022 年以来, Seibert 等^[31,92-93]指出,针对不同材料的微观结构特征选择合适的描述符。进而将多种类型描述符以及相关函数等统计特征进行整合,开发一个可扩展的模块化开源工具 MCRpy,利用该平台方便基于任意描述符进行微观结构表征和重建。

1.3 随机场方法

随机场方法最初应用于地球物理探测中地质模拟^[94-95],将地质模型视为由大、小两种尺度介质组成的随机介质,大尺度组成描述介质的平均特性,用一阶统计量-均值表示;小尺度组成用于描述施加于平均特性上的随机扰动^[96],这种随机扰动特征用二阶统计量-空间自相关函数 $R(x, z)$ 表示,常用的高斯-指数混合型椭圆自相关函数定义见式(1)^[34]:

$$R(x, z) = \exp \left\{ - \left[\frac{(x \cos \theta + z \sin \theta)^2}{a^2} + \frac{(x \sin \theta + z \cos \theta)^2}{b^2} \right]^{\frac{1}{1+r}} \right\} \quad (1)$$

式中: a 和 b 分别为随机介质的自相关长度,描述随机扰动的平均尺度; θ 为取向角,表示自相关椭圆的长轴方向与坐标轴的夹角; r 为粗糙度因子,决定随机介质边界的粗糙程度。

由于随机介质的功率谱与其自相关函数互为傅里叶变换, 因此对图像功率谱进行傅里叶逆变换, 即可提取自相关函数中表征随机介质特征的特征参数。将微观结构视为高斯或指数型随机场, 通过水平切削随机场来重建所需目标图像, 该方法适用于随机多孔结构的重建, 对于颗粒结构效果不佳^[1]。为改善这一问题, 发展了模拟退火优化与随机场结合的方法^[75], 以及采用滤波泊松随机场进行水平切削^[97]等策略。

本课题组^[71-73]将随机场方法引入碳纤维增强树脂基复合材料和热障涂层微观结构表征与重建, 建立描述孔隙复杂形貌和随机分布特性的固-气两

相随机孔隙模型(random void model, RVM), 该模型既保留孔隙含量、平均尺寸、取向等统计学特征, 又充分体现孔隙的不规则形貌和分布随机性。在此基础上通过双相峰谷搜索法控制各组成相的面积分数, 将两相 RVM 扩展为三相, 进一步提出随机多相介质模型(random multi-phase medium model, RMMM)^[74], 并将其应用于 AISi-PHB 封严涂层三相微观结构的表征与重建, 如图 3 所示, 其重建结果再现 PHB 复杂的形貌以及孔隙的弥散分布特性。近年来, He 等^[69]基于三维高斯随机场对具有各向异性特征的松质骨三维微观结构进行表征与重建, 并通过界面曲率分布等几何参数验证随机场

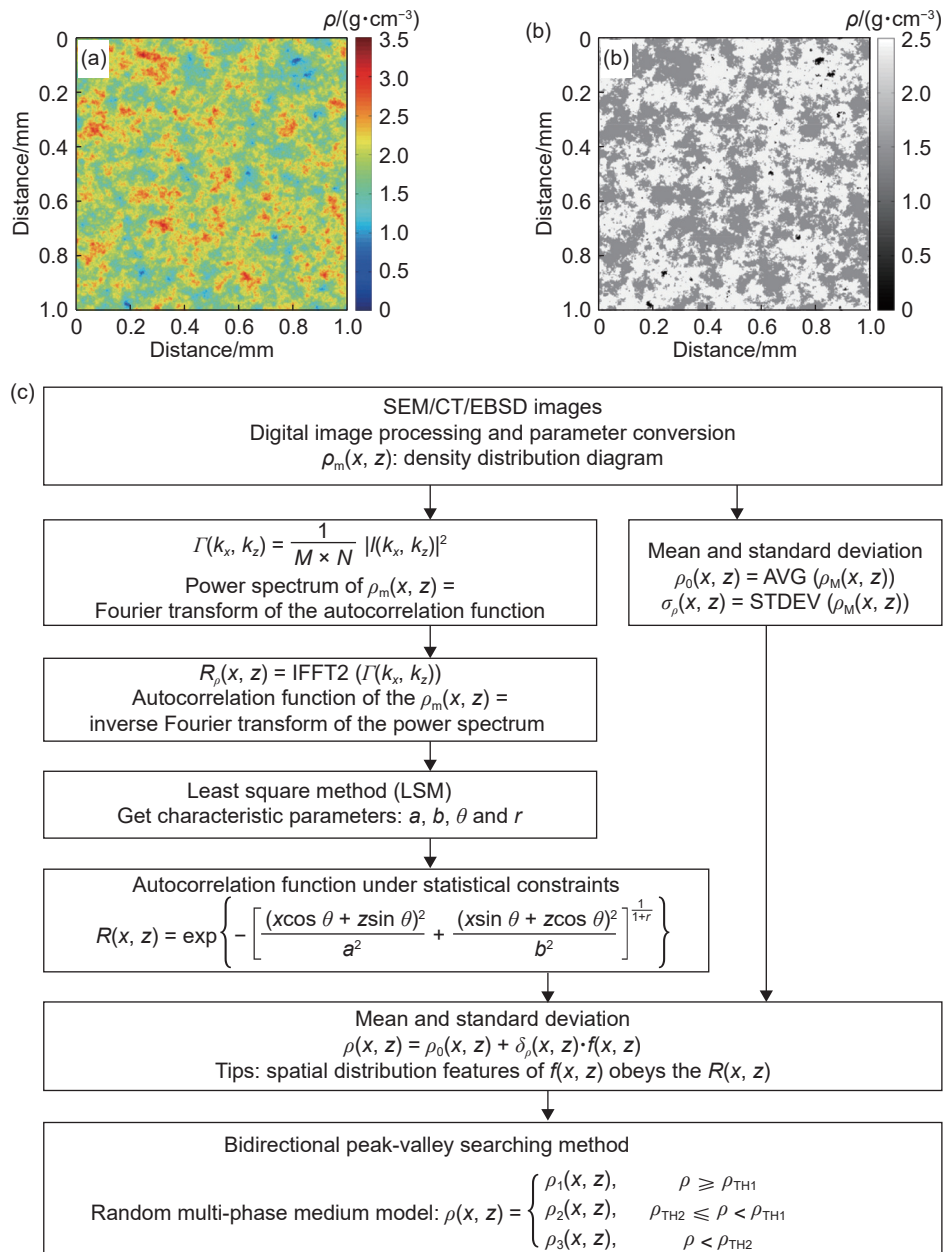


图 3 基于随机场方法的三相 AISi-PHB 封严涂层微观结构表征与重建^[74] (a) 随机介质; (b) 随机多相介质模型; (c) 流程图
 Fig. 3 MCR of three-phase AISi-PHB seal coatings based on random field method^[74] (a) random medium; (b) RMMM; (c) flow chart

重建的骨结构与 CT 图像具有相似的柱状形态特征。

总的来说,随机场 MCR 方法能够完整地保留整体材料微观结构的统计特征,具备描述微观结构特征的显示表达式,适用于形貌随机的两相或多相复杂结构。与同样依据微观结构统计特征重建的相关函数法相比,随机场方法的计算效率更高,Jiang 等^[75]比较基于模拟退火优化的相关函数法与随机场方法的重建效率,发现随机场方法的计算复杂度不受图像大小的影响,相关函数法计算的迭代次数随目标图像像素数目的增加呈指数增长,当像素数增加至 10240 时,相关函数法的迭代次数比随机场方法增加约一个数量级。

1.4 Voronoi 方法

Voronoi 方法最初由 Aurenhammer^[98]提出,它实质上是基于邻近原则生成一个点集,对应点集中的每个点镶嵌多边形(即 Voronoi 元胞),这些多边形构成集合称为 Voronoi 图。Voronoi 方法与物理描述符类似,都是依据颗粒质心位置赋予颗粒形状,其重建效率与物理描述符方法相当。二者不同之处在于,物理描述符是在基体介质中随机填充第二相,Voronoi 图则是基于多边形轮廓对空间结构进行剖分,这种方式更适合于具有晶体结构或骨架结构的材料。

1997 年,Ghosh 等^[99]开发了一种 Voronoi 元胞有限元模型(Voronoi cell finite element model,

VCFEM),应用于金属基复合材料的结构建模并进行力学有限元模拟,这为 Voronoi 方法在材料 MCR 领域应用奠定良好基础。经过 20 余年研究,Groerber 等^[77-78]将 Voronoi 镶嵌方法与 EBSD 图谱相结合,通过获取晶粒尺寸、数量、取向等参数特征,利用 Voronoi 镶嵌生成对应晶体学参数等效的微观结构,实现对镍基高温合金等金属的微观结构表征与重建。

在采用 Voronoi 方法镶嵌过程中,由于多边形元胞的形状、尺寸等是表征晶体结构的重要参数,大量研究通过控制多边形的镶嵌方式以及相邻元胞之间边界的确定方法,对 Voronoi 方法进行改进,使其更好地应用于非等轴晶粒^[79]、热处理态的尺寸不均匀晶粒^[80]、多尺度双相钢^[85]等复杂晶体结构。例如,2020 年,Schneider 等^[81]在获取 EBSD 晶体学信息的基础上,通过控制各相体积分数,提出一种基于分层 Voronoi 的重建算法,建立了两相 Ag/SnO₂ 多晶材料的二维及三维微观结构模型,如图 4 所示。可以看出,重建结果再现 Ag 晶粒结构以及晶粒内部和沿晶界分布的第二相 SnO₂ 颗粒。

此外,Groerber 等^[100]进一步集成微观结构的处理、量化、表征、重建等一系列程序,开发了 DREAM 3D 软件平台,目前已逐渐成为多晶金属材料 MCR 领域的有效工具^[101]。

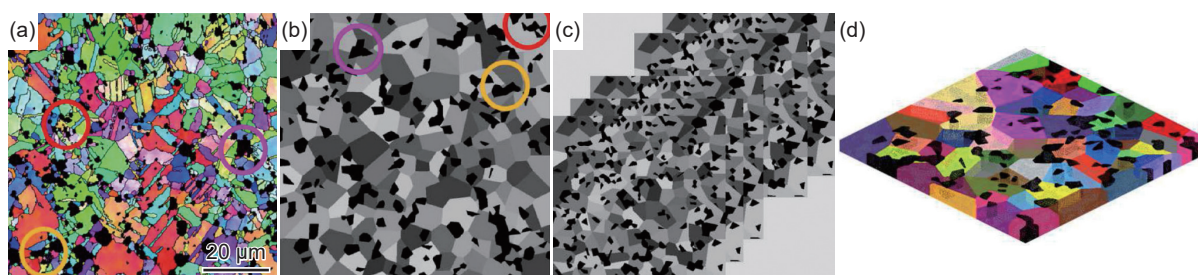


图 4 基于 Voronoi 镶嵌法的两相 Ag/SnO₂ 多晶微观结构表征与重建^[81] (a)EBSD 图像;(b)Voronoi 图;
(c)Voronoi 二维切片;(d)Voronoi 三维模型

Fig. 4 MCR of Ag/SnO₂ polycrystalline material based on Voronoi inplay technique^[81] (a)EBSD image;(b)Voronoi diagram;
(c)Voronoi 2D slice;(d)Voronoi 3D model

除金属晶体外,Voronoi 方法也用于骨架结构的表征与重建,例如,Gómez 等^[86]采用 Voronoi 镶嵌法建立骨小梁结构的多孔支架模型,该模型与骨小梁实际微观组织的形态学指标(包括骨小梁厚度、间距、数量、骨体积、总体积比等)匹配性一致。同时,该方法易于与 CAD 等计算机辅助设计软件结合使用,为仿生骨支架的设计提供优良的模型基础。

2 基于机器学习及纹理合成的微观结构表征与重建

机器学习技术的发展加速材料科学研究的新进程,目前已越来越多地应用于材料微观结构的量化表征、重建等^[102]领域。由于微观结构通常以 2D/3D 图像形式表示,针对本工作关注的 MCR 问题,一些基于图像的神经网络等机器学习方法展现

出强大潜力,引起广泛关注^[103-104]。此外,以计算机视觉为代表的图像识别技术也能够通过搜索微观图像的像素分布生成与之相似的新图像,很多研究人员逐渐将其用于加速改进材料微观结构的表征与重建^[105],其中纹理合成方法的应用较为广泛。表2总结了机器学习和纹理合成MCR方法的特点及应用^[42,44,46,104,106-132]。

与基于统计方法的MCR不同,机器学习与纹理合成方法不需要预先获得目标微观结构特征的统计参数,其表征过程通常是隐式的^[103,109]。例如,Cang等^[133]提出基于编码器和解码器的机器学习MCR方法,其中编码器可将输入的微观图像转换为潜在特征空间中的像素数据分布,解码器根据潜在特征向量输出微观图像的像素。这种图像数字化拟合重构的过程能够生成接近样本真实形貌的微观结构,最大限度地减少预先提取微观结构统计特征时的形态学信息损失。

2.1 机器学习

机器学习应用于材料MCR的主要思想在于将微观结构特征的隐式提取过程拟合到一个适当的模型中,拟合模型类似于编码过程,重建过程相当于解码。目前主要的模型包括分类树、人工神经网络(artificial neural network, ANN)、卷积神经网络(convolutional neural network, CNN)、递归神经网络(recurrent neural network, RNN),以及近些年发展的生成式对抗网络(generative adversarial network, GAN)、基于扩散的深度生成模型等,这些模型多应用于金属晶体和多孔介质材料^[134]。机器学习方法通常需要建立样本图像数量庞大的数据库,其特征学习过程只需一次,重建过程需要几秒到几分钟^[115],具有灵活性和高效性。

Bostanabad等^[107]首次采用基于分类树的机器学习模型对材料微观结构进行表征与重建,该拟合模型提供图像中所有像素分布的隐式表征,用于簇状各向异性材料、聚合物/纳米复合材料、多孔介质等材料的微观结构重建,并通过计算两点相关函数、两点聚类相关函数及线性路径函数,验证了重建图像与样本图像的统计等效性。在后续研究中,一些基于神经网络的机器学习算法在图像识别领域展现出强大的能力,研究人员对此类算法在材料MCR领域的应用进行大量尝试。例如,Fu等^[108-109]从二维图像中收集像素的条件分布概率,将其输入包含两层隐藏层的人工神经网络进行训练,利用经训练的ANN模型对多孔介质的微观结构进行重建,得到结果如图5所示^[108]。其中,图5(a)~(c)

为各向同性结构的重建结果,通过计算两点相关函数证明该方法的有效性;图5(d)~(f)为各向异性结构的重建结果,可以看出,重建图像与样本图像中的颗粒取向分布曲线具有一致性。

Fernandez-Zelaia等^[112]开发深度卷积神经网络框架以重建增材制造马氏体合金的晶粒结构,由于制造过程中工艺条件变化使合金中奥氏体转化为马氏体,该方法的优越性在于通过学习包含晶体学信息的EBSD图像,在基于给定子相马氏体结构的条件下重建其母相奥氏体结构,这对于描述相与相之间转变的晶体学关系以及研究加工-结构-性能关系具有重要意义。

近年来,基于博弈论的生成式对抗网络在生成高分辨率图像能力方面显现出优势,其基本思想是利用生成器和鉴别器两个神经网络模型^[135],其中生成器用于生成虚假的图像,判别器用于鉴别生成图像的真伪,二者相互交替训练直至达到平衡。该方法已应用于材料MCR领域,Zhang等^[114-117]深入研究在以岩石为例的多孔介质微观结构表征与重建,主要包括以下3个方面:(1)基于GAN模型从有限的局部小尺寸图像重建更大尺寸范围的图像;(2)开发两阶段的深度生成对抗质量增强网络,由二维切片重建模块和三维融合模块组成,增强重建三维微观图像的质量;(3)长短期记忆(long short term memory, LSTM)网络和生成式对抗网络相结合,实现由二维到三维的重建,如图6所示^[114]。该混合网络模型可以通过一系列二维切片学习相邻切片层之间的空间关系,有助于构建多孔介质的三维结构。

2.2 纹理合成

纹理合成起源于计算机图形学,通常假定样本图像服从马尔可夫随机场纹理模型,它具有平稳性和局部性两个特性。平稳性表示纹理图像的任意两个空间区域都是相似的,或理解成纹理在平移过程中保持不变;局部性表示图像中任意一个像素可由与其空间相邻的一小组像素表征,而与图像中其他像素值无关^[132]。基于上述假设,纹理合成的目标是生成一个新的纹理图像,使其每个局部区域与输入纹理图像中的局部区域相似。新的纹理图像通常是按照特定顺序逐个像素生成的,首先初始化一个随机噪声图像,通过反复搜索样本图像学习像素邻域特征,并将其与生成图像的邻域匹配,搜索到邻域匹配性最佳的像素作为重建图像的像素值。

与机器学习方法类似,纹理合成同样不需要预先获取微观结构的显示表征;不同的是,纹理合成

表2 基于机器学习及纹理合成的MCR技术特点及应用
Table 2 Features and applications of MCR techniques based on machine learning and texture synthesis

Technique	Theory	Material	Reference	
Machine learning	Classification trees	Rubber/SiO ₂ nanocomposite	[106]	
		Porous ceramics		
		Rubber/SiO ₂ nanocomposite	[107]	
		Perfectly geometric inclusions Fontainebleau sandstone		
	Artificial neural network(ANN)		Rubber/SiO ₂ nanocomposite	[108]
			Leopard sandstone	
			Fontainebleau sandstone	
			Synthetic silica with high porosity	
			Multiphase porous electrode	
			Porous ceramic	[109]
			Mesoporous silica	
	Convolutional neural network(CNN)		Pearlitic steel	[44]
			Martensitic steel	
			Aluminium alloy	
			Dielectric materials with silicon particles	
			Porous ceramics	
			Polycrystalline microstructures	
			Carbonate	[46]
			Polymer composites	
			Sandstone	
			Ceramics	
			Block copolymer	
			Metallic alloy	
Recurrent neural network(RNN)		Three-phase rubber composites		
		Ti-6Al-4V alloy	[110]	
		Pb63-Sn37 alloy		
		Fontainebleau sandstone		
		2D suspension of spherical colloids		
		Low-carbon-steel	[111]	
		Martensitic alloy AF9628	[112]	
		Isotropic and anisotropic porous sandstone	[113]	
Homogeneous sandstone	[114]			
		Heterogeneous carbonate rock		

表2 (续)
Table 2 (Continued)

Technique	Theory	Material	Reference
	Generative adversarial network(GAN)	Fiber reinforced ceramic matrix composites	[104]
		Porous sandstone	[115-117]
		Berea sandstone, estailades carbonate	[118]
		Micrometer-scale solid-void porous media	[119]
		Nanoporous metal	[120]
		Additively manufactured Ti-6Al-4V	[121]
		Fontainebleau sandstone	[122]
		Soft soils	
Texture synthesis	Markov random field(MRF)	Ti-7Al alloy	[42]
		Metal	[123]
		Fabric	
		Tile	
		Stone	
		Flowers	
		Leaves	
		Disperse spheres	[124]
		Anisotropic lamellar microstructure	
		Polycrystalline microstructure	
		Berea sandstone	[125]
		Two-phase W-Ag composite	[126]
		Aluminum alloy AA3002	
		Polycrystalline copper	[127]
		Ivory	[128]
Macadamia nutshells			
Al-Li alloy	[129]		
Additively manufactured 316L stainless steel	[130]		
AlSi-PHB seal coating	[131-132]		

是将微观图像视为纹理,通过穷尽搜索样本图像中的相似邻域来完成重建,不涉及拟合训练模型输出结果。这种穷尽搜索的方式增加纹理合成的计算成本,其重建效率取决于目标图像分辨率和选取邻域的大小^[125],随着邻域尺寸以及目标图像像素数增加,重建时间由数分钟到数小时不等。

Sundararaghavan^[124]首次将纹理合成算法应用于材料MCR领域,重建各向同性分散球体、各向异性片层结构、多晶结构3种微观图像,通过比较

重建图像与原始图像的两点相关函数统计特征,验证该方法的有效性。在后续研究中,该研究团队进一步针对纹理合成算法的优化以及在不同情况微观结构重建的应用进行探索,主要包括:

(1)以纹理合成的平稳性原理为基础,由小尺寸样本图像合成更大尺寸范围的图像,用于模拟二维微观结构演变,如图7所示^[127]。与基于静止图像的微观结构重建问题不同,该方法能够很好地预测晶粒生长等随时间演化的微观结构,降低全尺寸

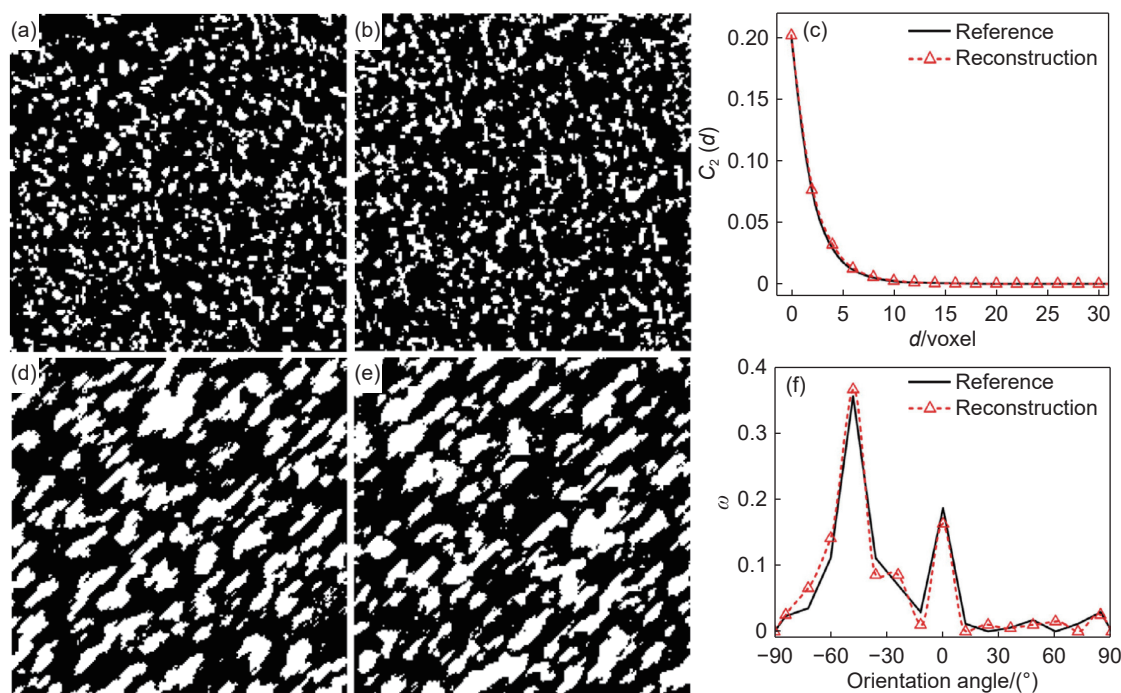


图5 基于神经网络的多孔介质微观结构表征与重建^[108] (a)各向同性结构样本图像;(b)各向同性结构重建图像;(c)各向同性结构样本图像与重建图像两点相关函数;(d)各向异性结构样本图像;(e)各向异性结构重建图像;(f)各向异性结构样本图像与重建图像的颗粒取向分布

Fig. 5 Microstructure characterization and reconstruction of porous media based on ANN^[108] (a)sample image of isotropic structure;(b)reconstructed image of isotropic structure;(c)two-point correlation functions of sample and reconstructed image in the isotropic structure;(d)sample image of anisotropic structure;(e)reconstructed image of anisotropic structure;(f)particle orientation distribution of sample and reconstructed image in the anisotropic structure

微观结构重建的成本^[126-127]。

(2)二维像素采样扩展到三维像素,由3个正交平面上的二维切片重建三维纹理图像,结合RGB光谱的直方图匹配原则实现彩色图像的合成^[129],该方法在基于EBSD图像的多晶微观结构表征与重建中展现出优势,能够保留晶粒尺寸、取向性、邻域分布等重要特征。

(3)近年来,Javaheri等^[130]逐渐将纹理合成算法应用于增材制造316L不锈钢微观结构的重建,通过获取二维正交平面上局部切片的EBSD图像,重建三维全尺寸微观结构,该方法有助于增材制造材料微观结构的可视化,指导加工工艺参数的优化。

纹理合成的优势在于通过搜索图像局部像素分布来捕获微观结构中细微的形态学特征,适用于金属晶体、多相复合材料等复杂形貌结构,但因该过程通常是隐式的,不具备描述微观结构物理意义的显示表达式,导致难以控制重建微观图像中组分含量、颗粒数量等与样本图像保持一致。针对该问题,解曦宇等^[131]提出一种面积分数可控的MCR纹理合成算法,以AlSi-PHB封严涂层三相结构为例,以样本图像的颗粒数量与各相面积分数为参数

对纹理合成算法优化,计算重建结果的两点相关函数误差评价算法有效性,如图8所示,可以看出优化后算法的方差 V_{ar} 约降低两个数量级。因此,纹理合成与统计方法结合,在重建过程中加入预先提取的微观结构表征参数进行优化,便于深入理解并建立材料结构-性能关系,这一研究方向值得进一步探索。

3 讨论与展望

3.1 微观结构表征与重建技术的应用

MCR技术在材料科学领域的应用主要体现在以下几个方面:

(1)加工-结构-性能关系的建立。通过MCR技术能够获得大量材料微观结构模型,以这些微观结构作为PSP关系的中心环节,结合有限元模拟等方法,既可以分析材料结构对性能(structure-property, S-P)的影响,又可以探究加工对结构(processing-structure, P-S)的影响。Seibert等^[93]将 β -Ti/TiFe合金的MCR重建结果和有限元模拟结合,计算重建结果与样本图像的弹性模量与屈服强度,既从性能角度验证重建结果有效性,又有助于探究微观结

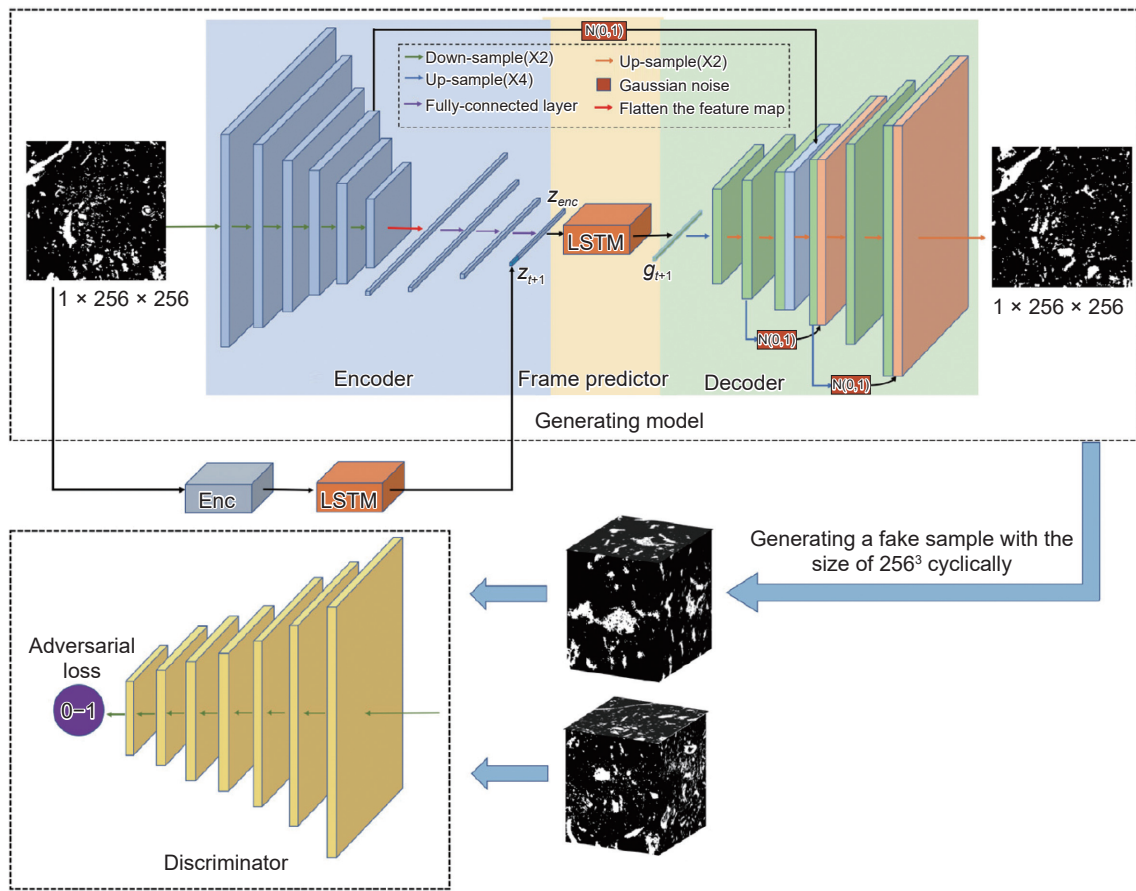


图 6 基于对抗递归神经网络的多孔介质微观结构表征与重建^[114]

Fig. 6 Microstructure characterization and reconstruction of porous media based on adversarial recurrent neural network^[114]

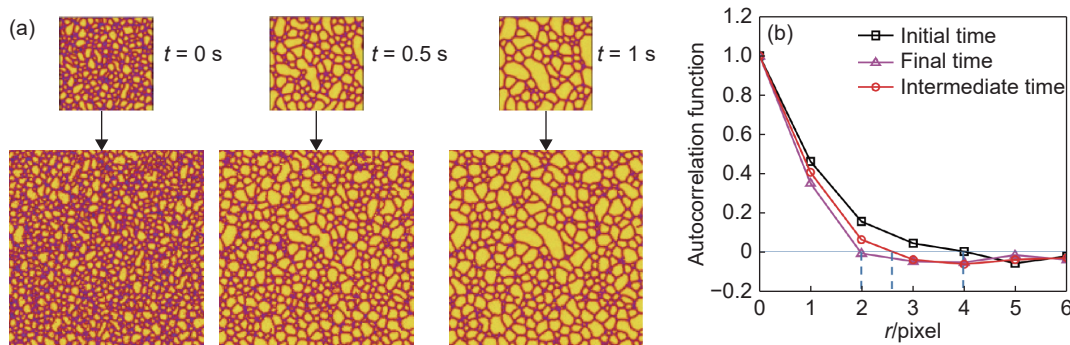


图 7 基于纹理合成方法的晶粒结构演化的表征与重建^[127] (a)基于纹理合成晶粒结构演化; (b)合成晶粒结构的相关函数

Fig. 7 Microstructure characterization and reconstruction of grain evolution based on texture synthesis technique^[127]

(a) grain structure evolution based on texture synthesis; (b) correlation function of the synthesized grain structure

构对力学性能的影响。Liu 等^[56] 提出将重建的微观结构与加工参数建立联系, 可以提高材料设计效率, 为材料设计研发提供理论基础。

(2)材料性能预测。在建立 PSP 关系基础上, 结合机器学习方法可对航空航天材料的力学性能^[93]、多孔材料的渗透性能^[136] 等材料特性进行预测。例如, Li 等^[137] 在单向 CFRP 复合材料微观结构重建的基础上, 进行细观力学有限元模拟并计算横向弹性模量、抗拉强度和抗压强度, 利用反向传

播神经网络建立微观结构与上述 3 种参数之间的关系, 实现材料力学性能的预测。

(3)材料结构设计和优化。基于 S-P 关系的建立, 在给定材料性能参数条件下可对微观结构进行反向设计, 如通过纳米光子材料的电磁响应预测所需性能的微观结构^[138]。基于 P-S 关系的建立, 也可在给定加工参数的条件下设计并优化微观结构, Cao 等^[121] 利用图像驱动的条件生成对抗网络重建增材制造 Ti-6Al-4V 微观结构, 依据激光功率、扫

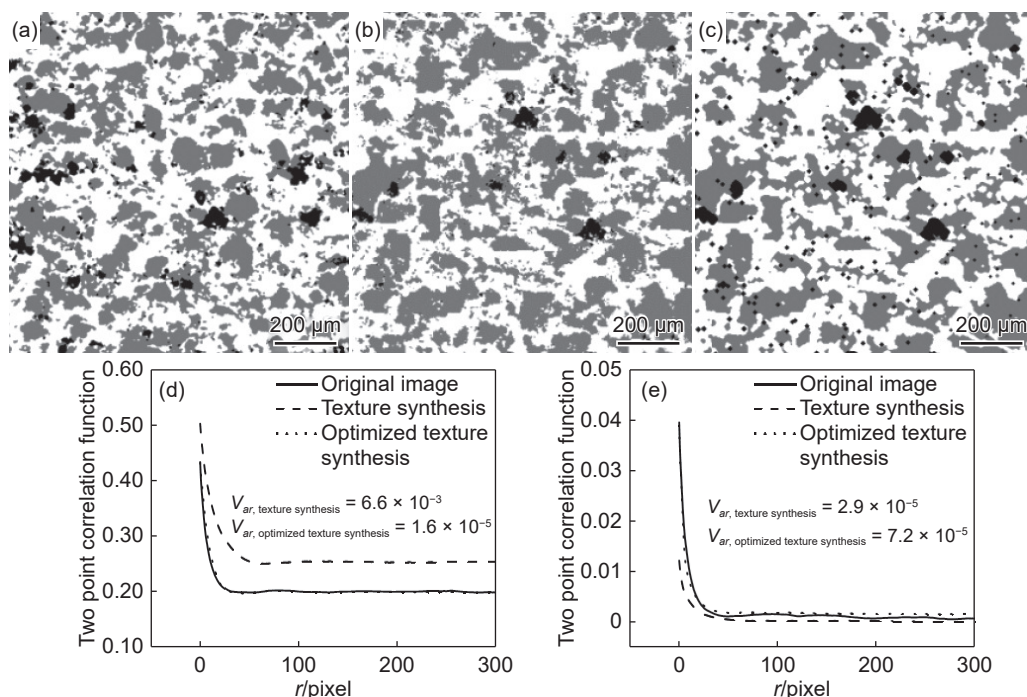


图8 基于纹理合成方法的三相 AlSi-PHB 封严涂层微观结构表征与重建^[131] (a)样本图像; (b)优化前纹理合成图像; (c)优化后纹理合成图像; (d)PHB 相两点相关函数; (e)孔隙两点相关函数

Fig. 8 Microstructure characterization and reconstruction of three-phase AlSi-PHB seal coatings based on texture synthesis technique^[131] (a) sample image; (b) reconstructed image by texture synthesis before optimizing; (c) reconstructed image by texture synthesis after optimizing; (d) two-point correlation function of PHB; (e) two-point correlation function of pores

描速度等加工参数预测微观结构中马氏体形态特征,为增材制造领域的材料微观结构调控提供巨大的应用潜力。

(4)材料微观机制的分析。MCR 技术可以作为实验的有力补充,分析力学实验中难以观测到的微观行为,例如, Huang 等^[85]基于二次电子成像和电子背散射衍射对珠光体钢进行微观结构重建及晶体塑性模拟,将模拟得到的应力-应变场与高分辨原位 SEM 及拉伸性能结果相结合,分析拉伸过程中材料微观变形诱导剪切传递等力学行为,这对于材料微观机制的深层理解具有重要意义。

(5)材料建模及无损检测。由于非均质材料微观结构复杂,传统无损检测方法难以有效检测其内部缺陷,通过结合 MCR 和无损检测仿真,可以模拟缺陷在材料微观结构中的存在状态及其对检测信号的影响,提高缺陷检测能力。例如, Lin 等^[139]基于随机场方法重建热障涂层的孔隙结构,借助超声检测仿真探究声速和孔隙特征参数之间关系,实现涂层孔隙的表征。该研究团队还针对 CFRP 层压板建立考虑层状结构的仿真模型,分析超声波的传播特性,提高超声检测的成像精度^[140]。

3.2 存在问题与发展方向

非均质材料的种类繁多,具有多相、多尺度、形

貌复杂的特征,在评估微观结构重建结果时需要考虑是否充分体现这些特征。因此,如何有效评价 MCR 结果的质量存在挑战,目前主要通过两类参数进行评价:

(1)采用相关函数评价重建图像质量。相关函数主要包括两点相关函数、两点聚类相关函数、线性路径函数等,微观图像的相关函数曲线中隐含材料各组成相的面积分数、尺寸、分布状态等特征的统计信息,通过比较重建图像与样本图像相关函数曲线的相似性,可评价重建图像的质量。相关函数评价方法应用广泛,目前很多研究人员^[37,41,56-58,66,75,88,106-109,115,131-132]采用该方法验证重建图像与样本图像的统计结果等效性。

(2)通过对比微观结构的量化参数评价重建图像质量。材料微观结构的量化参数主要包括各组成相含量、颗粒或晶粒数目、取向角、形状、尺寸分布函数等,这类参数比相关函数更具体直观,可以捕获目标图像最为典型的结构特征。例如,当对多孔材料或颗粒材料微观结构进行重建时,采用颗粒尺寸分布函数和两点相关函数结合比较,能够提供更全面的评价结果^[108-109]。

目前上述评价方法多用于验证 MCR 方法的有效性,对各类方法优劣的比较,尚未形成统一的评

价体系,后续可考虑综合多种评价指标,建立并完善更规范的评估准则。

随着越来越多 MCR 方法不断涌现,为适应材料类型逐渐多样化,亟待建立包含不同材料微观结构的 MCR 数据库,为发展高通量的微观结构表征与重建提供数据共享平台。此外,以 MCR 为关键环节的高通量计算模拟与高通量实验相结合^[14],可作为建立存储材料微观结构和性能特征的综合数据库,提升材料表征的智能化水平,加速推进以数据为中心的材料研发、设计、性能优化等研究进程,这也是未来值得探索的发展方向之一。

4 结束语

基于统计方法的微观结构表征与重建技术能够获得材料微观结构特征的物理参数或统计性描述,具备显式表达式,有助于微观结构的进一步量化分析和加工-结构-性能关系的构建,但仍存在效率较低、模型近似引起的形态学丢失问题。

基于机器学习及纹理合成的微观结构表征与重建技术能够再现非均质材料的复杂形貌,有助于高通量计算的材料建模替代昂贵的实验方法,预测具有特定属性的结构,但表征过程通常是隐式的,缺乏材料微观结构特征的物理意义描述,对加工-结构-性能关系的可解释性较差。

在高通量计算材料科学时代的发展进程中,微观结构表征与重建作为材料建模的关键环节,实际问题中需要根据不同的材料特性合理运用最佳方法,未来必将发挥更加重要的作用。

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收稿日期: 2024-12-23; 录用日期: 2025-03-24

基金项目: 国家自然科学基金项目(U22B2068, 52075078, 52175496)

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