

黏结剂喷射增材制造陶瓷全过程数值模拟：现状、挑战与展望

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摘 要: 高性能陶瓷在高温结构、耐蚀绝缘与精密型芯等场景中的需求持续增长。黏结剂喷射(BJ)具备室温成形与高几何自由度优势, 但铺粉-喷射-脱脂-烧结的跨尺度耦合使陶瓷零件易发生难以预测的缺陷。本文面向陶瓷材料 BJ 成形过程, 凝练全过程数值模拟进展: 离散元法(DEM)量化层厚、粒径级配与刮刀/辊筒运动对孔隙率与表面粗糙度的影响; 计算流体力学/流体体积法(CFD/VOF)、格子玻尔兹曼方法(LBM)及 DEM-CFD 耦合描述液滴冲击、毛细渗透与干燥固化过程黏结剂与粉床的作用机制; 脱脂阶段汇总热重分析(TGA)驱动的多步动力学、扩散-对流-达西输运、相场网络运输与热-质-力有限元模型, 建立残余黏结剂、空隙变化与裂纹风险的预测框架; 烧结部分对比连续体本构、Monte Carlo 与相场方法在颈部长大、致密化、晶粒演化及各向异性收缩中的适用性。文末归纳参数定义与实验验证方法, 提出跨尺度耦合与数据闭环驱动的陶瓷 BJ 过程建模方向。

关键词: 增材制造; 黏结剂喷射; 多尺度模拟; 性能预测

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高性能陶瓷因其优异的高温力学性能、化学稳定性、电绝缘性能以及生物相容性, 在航空航天、能源电力、化工冶金以及电子封装等领域发挥着日益重要的作用。随着行业的高速发展, 对陶瓷成形的轻量化、复杂化和可靠性提出了新的挑战。但传统模压、注浆、等静压等成型工艺与机械加工手段在复杂三维结构、内部流道和多尺度孔隙可设计性方面存在天然局限, 并且模具开发周期长、成本高、形状自由度有限。增材制造为复杂净成形提供了新的技术路径。粉末床熔融(SLM)、黏结剂喷射(BJ)、立体光固化(DLP)和熔丝沉积成形(FDM)等多种工艺已被用于 Al_2O_3 、 ZrO_2 、 SiC 、 Si_3N_4 等体系陶瓷的制备, 部分工艺在制备小批量复杂构件上已具备工程应用可行性。研究表明, 相比熔融型工艺, 基于粉床的 BJ 具有室温成形、无内应力、可适配高熔点脆性材料等优势, 尤其适合尺寸较大、结构复杂且形状精度要求较高的陶瓷构件, 无须激光热源和支撑结构, 显著降低了设备与运行成本, 并能自由构建 SLM 等技术难以完成的复杂中空或晶格结构。但

是打印后坯体需要经过烧结才能使用, 最终零件难以达到完全致密状态^[1-3]。

黏结剂喷射打印是一类典型的粉床型增材制造工艺, 其基本原理是: 在铺展好的粉末床上, 通过喷头按截面轮廓选择性喷射液态黏结剂, 使粉末颗粒在目标区域被局部黏结, 层层堆叠构建三维坯体。主要有粉末铺展、黏结剂喷射打印、固化与除粉、脱脂与烧结等步骤。表 1 归纳了现阶段已有的 20 种陶瓷材料通过 BJ 打印成功应用于众多领域的相关情况。然而, BJ 成形过程中工艺链条长, 影响因素繁多, 任何一步(铺粉、喷射、干燥、脱脂、烧结)中的微观偏差都可能放大为最终宏观缺陷^[4-6]。因此, 工业端迫切需要一套能够包括粉末 坯体 烧结体全流程的数值模拟框架, 以指导工艺窗口设计、缺陷预判和优化结构-性能协同。

近年来, 围绕 BJ 工艺链, 金属领域已经形成了相对完整的建模体系, Ramalingam 等^[46]、Zhu 等^[47]的综述系统梳理了金属 BJ 在粉床致密度、黏结剂与粉床相互作用、坯体力学与烧结致密化方面的建模

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表 1 黏结剂喷射打印陶瓷种类及应用

Table 1 Types and applications of binder jet printing ceramics

Material category	Applications	References
Al ₂ O ₃	Ceramic crucibles	[8]
	Sensor shells	[9]
	Catalytic fixed bed reactors	[10]
	Hubs	[11]
	Glass-based grin lenses	[12]
ZrO ₂	Bone repair	[13]
	Porous structures	[14]
SiC	Space telescope mirrors	[15]
	Turbine discs	[16]
	Gears	[17]
	Nuclear-grade fuel	[18,19]
	Gradient lattice trusses	[20]
AlN	Pipes, boxes	[21]
Si ₃ N ₄	Filter elements	[22]
	Wave-shaped transparent ceramics	[23]
TiC/TiO ₂	Porous prefabricates	[24]
BN	Red blood cell plates	[25]
BaTiO ₃	Piezoelectric elements	[26,27]
	Pressure sensors	[28,29]
HA	Bone substitutes	[30]
	Bone scaffolds	[31]
Ca ₃ (PO ₄) ₂	Bone substitutes	[32]
	Tissue-engineered bone scaffolds	[33]
Dental porcelain	Porcelain teeth	[34–36]
SiO ₂	Investment casting shells	[37]
MgAl ₂ O ₄	Refractory ceramic crucibles	[38]
B ₄ C	Scattering beam collimators	[39]
Y ₂ O ₃	Investment casting cores	[7,40]
CaO/CaCO ₃	Soluble ceramic cores	[41]
SMM	Toroidal cores	[42]
Cordierite	Honeycomb filtration substrates	[43]
KNN	Piezoelectric ceramics	[44]
CaSiO ₃	Medical fields	[45]

进展。相比之下，陶瓷 BJ 领域的数值研究虽然在粉床铺展与单液滴渗透等子过程中已取得一系列成果，但整体上仍呈现出“局部建模、经验优化为主”的特点。并且与金属 BJ 相比，陶瓷 BJ 在“粉末流动性—孔结构—后处理致密化”链条上呈现更强的脆弱性与不确定性：1) 陶瓷粉末常呈非球形或团聚形貌，堆积结构更疏松且孔隙率更高，导致渗透率(K)与有效扩散系数(D_{eff})对铺粉参数与粒度级配高度敏感；2) 陶瓷坯体在脱脂与升温阶段骨架强度低、

断裂韧性差，在产气压强梯度与热应力共同作用下更易开裂，因此脱脂模型需把“产气/排气能力匹配”与“应力峰值”作为核心评价指标；3) 相比金属常见的致密化到近全致密，陶瓷体系往往需要液相助烧、反应烧结、渗透等工艺以降低收缩或提高致密化效率，使烧结阶段的本构、边界摩擦与微结构演化参数完全按具体致密化路径分别标定与传递。基于上述应用需求与方法差异，本文聚焦陶瓷型芯、耐火构件与高温绝缘件等典型工件，系统梳理并有选择地借鉴金属 BJ 领域以及其他陶瓷脱脂与烧结已有的建模思想和数值方法，分别从粉床铺展、黏结剂—粉床相互作用与渗透行为、脱脂、烧结 4 个层面系统总结现有研究，并在此基础上讨论 BJ 陶瓷全过程数值模拟的关键问题以及挑战。

1 基于离散元法的粉床铺展行为与工艺参数影响

1.1 铺粉原理与 DEM 建模框架

在 BJ 工艺中，粉床铺展是构件成形的首个关键步骤，其结果直接决定粉床的堆积密度、孔隙率与表面粗糙度，进而影响黏结剂渗透情况、初坯强度和烧结致密化行为。Miao 等^[48]在系统综述中指出，粉床质量通常通过平均堆积密度和表面粗糙度 2 个指标综合表现。

在粉床铺展过程中，颗粒运动呈高度离散特征，频繁接触与局部压实并存，因此，可将其归类为典型颗粒流问题。离散元法(DEM)将单个颗粒视为刚体，通过显式求解颗粒与颗粒及颗粒与壁面之间的碰撞接触、摩擦滑移、滚动阻力与黏附作用，被广泛用于粉床铺展行为的数值研究^[49,50]。在常见 DEM 粉床模型中，颗粒接触通常采用 Hertz–Mindlin 模型，并叠加库仑摩擦与滚动阻力项；当粉末粒径进一步减小(通常低于 20 μm)时，为捕捉细粉间的黏结趋势，需引入基于 JKR/DMT 接触模型的范德华黏附力项^[49]。围绕非球形陶瓷颗粒的形貌效应，Haeri^[51]采用球簇/杆状颗粒表示方法，系统分析了形貌参数对铺层质量的影响，结果表明细长度与扁平度增大往往对应更大的休止角与更低的铺层致密度，从而证明粉末形貌通过改变颗粒堆积与重排动力学影响粉床成形质量。

为便于跨材料的对比，若干 DEM 研究^[48]将粉床质量归纳为无量纲指标体系(表 2)：相对密度用于表征压实程度；无量纲表面粗糙度用于量化表面平整度；归一化层厚用以刻画层厚相对于颗粒尺度

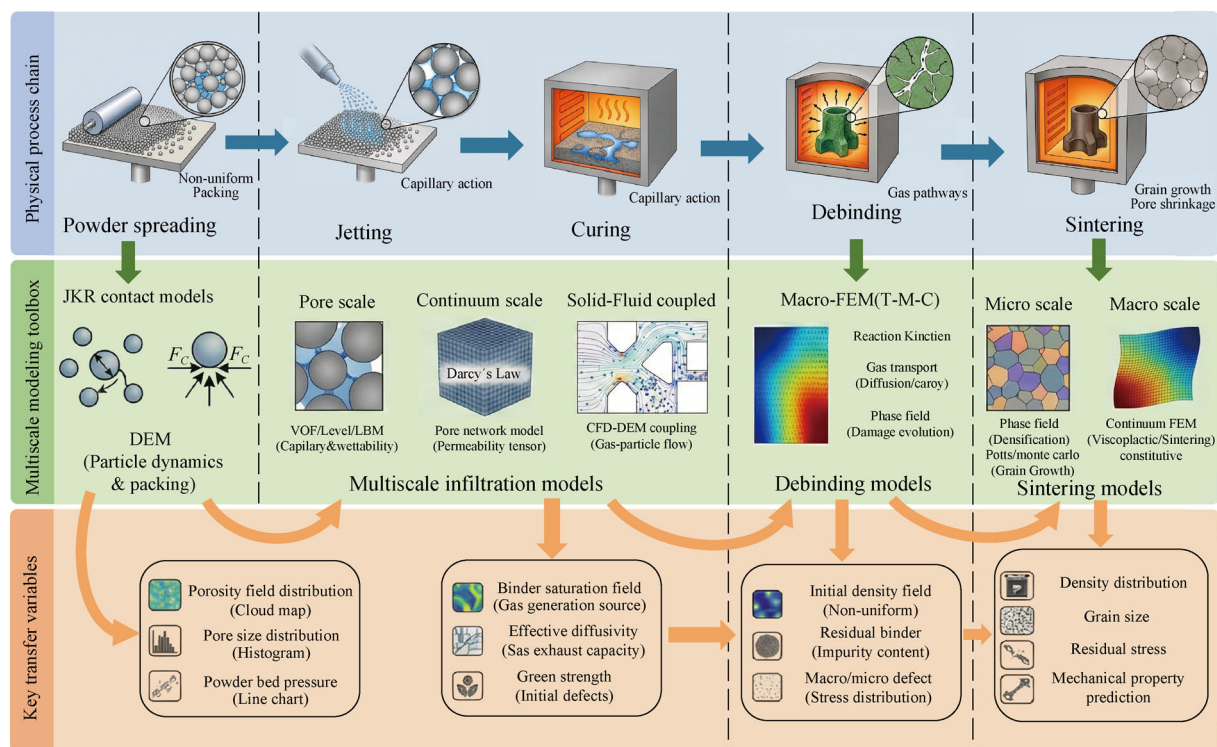
图 1 BJ 陶瓷制备流程图、数值计算方法和材料参数^[7]Fig. 1 BJ ceramic preparation flow chart, numerical calculation method and material parameters^[7]

表 2 黏结剂喷射打印模拟涉及参数及含义

Table 2 Binder jet printing simulation involved parameters and meanings

Symbol	Name	Definition/Expression	Unit
t	Time	Process time	s
$\mathbf{x}$	Position vector	Position vector	m
D_{50}	Granulometric distribution	Powder particle size at 50% mass cumulative	m
S_v	Solid surface area	$S_v = A_s / V_s$; For spherical particles $S_v \approx 6/d_p$	m^{-1}
φ	Solid phase volume fraction	$\varphi = V_s / V_{\text{total}} = 1 - \varepsilon$	1
ε	Porosity	$\varepsilon = V_{\text{void}} / V_{\text{total}} = 1 - \varphi$	1
ρ_{th}	Theoretical density	Density of a fully dense material	$\text{kg} \cdot \text{m}^{-3}$
ρ_{pb}	Powder bed density	$\rho_{\text{pb}} = m_{\text{bed}} / V_{\text{bed}}$	$\text{kg} \cdot \text{m}^{-3}$
ρ^*	Relative density	$\rho^* = \rho / \rho_{\text{th}}$; Powder bed: $\rho^*_{\text{pb}} = \rho_{\text{pb}} / \rho_{\text{th}}$	1
R_a	Surface roughness	Arithmetic average roughness	m
R'_s	Dimensionless surface roughness	$R'_s = R_a / D_{50}$	1
h	Powder layer thickness	BJ print layer thickness	m
h^*	Dimensionless layer thickness ratio	$h^* = h / D_{50}$	1
ρ_l	Binder liquid density	Binder density	$\text{kg} \cdot \text{m}^{-3}$
μ_l	Viscosity	Binder viscosity	$\text{Pa} \cdot \text{s}$
σ_{lv}	Surface tension, liquid-gas interface	Binder liquid-gas surface tension	$\text{N} \cdot \text{m}^{-1}$
θ	Contact angle	Static contact angle of binder on powder	$^\circ$
d_d	Droplet diameter	Equivalent diameter of jet droplet	m
u_d	Droplet impact speed	Impact speed of droplet on powder bed	$\text{m} \cdot \text{s}^{-1}$
P_l, P_g	Liquid/Gas phase pressure	P_l : Liquid pressure; P_g : Gas pressure	Pa
P_c	Capillary pressure	$P_c = P_g - P_l$	Pa
K	Permeability	Permeability of porous media	m^2
$K_{\text{r}}(S)$	Relative permeability function	Relative permeability	1

(Continued Table 2)

Symbol	Name	Definition/Expression	Unit
S	Binder saturation	$S=V_i/V_{\text{void}}$	%
S_B	Process set saturation	$S_B=V_{\text{jet}}/V_{\text{void}}\times 100\%$	%
Re_d	Reynolds number	$Re_d=\rho_l\cdot u_d\cdot d_d/\mu_l$	1
We_d	Weber number	$We_d=\rho_l\cdot u_d^2\cdot d_d/\sigma_{lv}$	1
Ca_d	Capillary number	$Ca_d=\mu_l\cdot u_d/\sigma_{lv}$	1
Bo_d	Bond number	$Bo_d=\rho_l\cdot g\cdot d_d^2/\sigma_{lv}$	1
Oh_d	Ohnesorge number	$Oh_d=\mu_l/(\rho_l\cdot\sigma_{lv}\cdot d_d)^{1/2}$	1
T	Temperature	Process temperature	K
β	Heating rate	$\beta=dT/dt$	K·s ⁻¹
c_B	Binder mass fraction/concentration	$c_B=m_B/m_{\text{total}}$	1
k_{rxn}	Reaction/Decomposition rate constant	$k_{\text{rxn}}(\text{Arrhenius: } k=A\cdot e^{-E/RT})$	s ⁻¹
D_{eff}	Effective diffusion coefficient	$D_{\text{eff}}=D_0\cdot\epsilon^m/\tau$	m ² ·s ⁻¹
τ	Tortuosity	$D_{\text{eff}}=D_0/\tau$	1
k_{th}	Thermal conductivity	Material thermal conductivity	W·m ⁻¹ ·K ⁻¹
h_c	Convective heat transfer coefficient	Convective heat transfer	W·m ⁻² ·K ⁻¹
ϵ_{sh}	Linear shrinkage	$\epsilon_{\text{sh}}=(l_0-l)/l_0$	1
σ_{ij}	Stress tensor	Cauchy stress	Pa
γ_s	Surface energy	Solid surface energy	J·m ⁻²
η_i	Phase field orientation order parameter	Orientation order parameter for the i -th grain	1
G	Grain size	Average grain size	m
g	Gravitational acceleration	Acceleration due to gravity	m·s ⁻²
R	Gas constant	Molar gas constant	J·mol ⁻¹ ·K ⁻¹
A	Pre-exponential factor	Arrhenius pre-exponential factor	s ⁻¹
E	Activation energy	Activation energy	J·mol ⁻¹
c_p	Specific heat	Constant pressure specific heat	J·kg ⁻¹ ·K ⁻¹
α	Thermal diffusivity	$\alpha=k_{\text{th}}/(\rho\cdot c_p)$	m ² ·s ⁻¹
C_K	Kozeny-Carman structural constant	Kozeny-carman constant	1

的匹配关系。基于该框架，Miao 等^[52]在陶瓷 BJ 研究中采用上述无量纲量统一 DEM 与实验的对比，说明其能够有效表征铺粉质量随粉末与工艺条件的变化。进一步地，Li 等^[53]建立了 DEM 预测的粉床相对密度与实际打印绿件密度之间的对应关系，指出对于自由流动粉末，粉床致密度在较大程度上约束初坯致密化水平。Mariani 等^[11]针对 Al₂O₃ 细粉 BJ 通过几何堆积算法与 DEM 预测给定粒度分布下的堆积极限与初坯相对密度，并在实际打印中观察到初坯相对密度达到与模拟一致，随后通过高温烧结获得明确的最终密度与力学性能数据。

1.2 铺粉方式以及运动参数

在 BJ 中，最常见的铺粉方式包括刮刀式铺粉与反转辊筒式铺粉。Miao 等^[48]指出其主要差异体现在：刮刀式铺粉会对粉堆施加显著法向压实载荷，反转辊筒式铺粉会导致颗粒流动轨迹存在循环对流。

刮刀式铺粉的主导因素包括刮刀几何结构、移动速度与刮刀间隙，这些参数共同决定粉堆前缘的剪切重排方式，进而影响致密度与表面质量。Miao 等^[48]的对比结果表明，椭圆形刮刀更易获得较高密度粉床并保持铺展稳定性；矩形刮刀因接触面积较大，有利于颗粒再排列，从而降低表面粗糙度。对于倾斜刮刀，角度存在最优区间(约 15°)，可在压实提升与表面扰动之间取得更合理的平衡(图 2a)。Haeri^[51]的参数扫描进一步指出，减小刮刀与床之间的间隙通常有助于提高粉床密度，但当间隙小于铺粉层厚时易诱发“刮空”、破坏局部床面，导致铺粉连续性下降。刮刀尺寸亦会改变压实区尺度：较宽且较短的刮刀更利于提高密度，但过宽可能破坏床面平整。基于 Taguchi-DEM 的敏感性分析，Avrampos 等^[54]认为，刮刀速度与间隙高度是影响铺层厚度与表面质量的关键变量，而振动辅助可在一定程度上削弱细粉黏结带来的铺展缺陷。

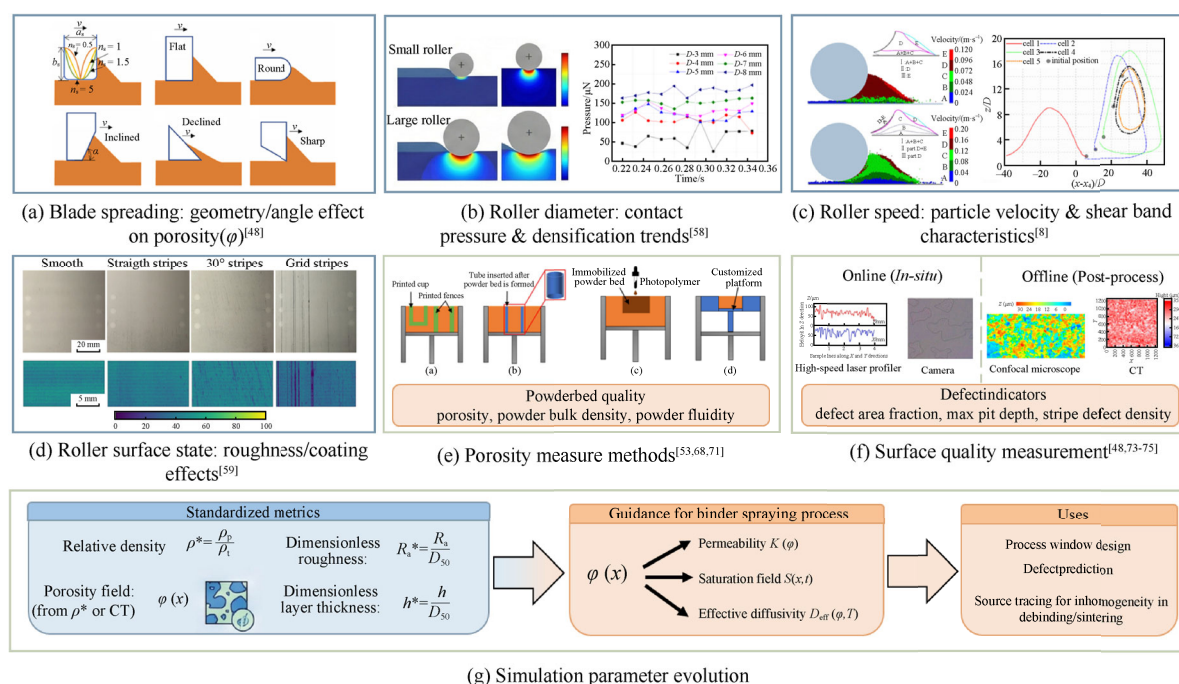


图 2 粉末铺展阶段: 工艺参数影响、床层质量及验证方法

Fig. 2 Powder spreading stage: process parameter effects, bed structure and validation methods

反转辊筒式铺粉主要受辊轮移动速度、自转速度及辊轮直径控制。Ramalingam 等和 Miao 等^[46,48]的 DEM 与实验对照显示, 移动速度对应较窄的工艺窗口: 速度过高会增强剪切并引发床面滑移与欠料, 速度过低则可能因过度压实与颗粒滑移导致床面起伏增大。与此相关的是, 辊轮反向旋转会在接触区产生促使颗粒翻转的剪切作用, Nan 等^[55]指出当转速过大时粉末易飞溅, 从而破坏均匀性。Zhang 等^[56]认为辊子自转会施加一个对粉堆有压实作用的法向力。Meyer 等^[57]将自转速度与铺粉速度之比作为关键参量, 发现二者相近时可兼顾压实与低扰动; 自转速度远小于铺粉速度时辊轮“拖拽不足”导致欠料, 自转速度远大于铺粉速度时床面被过度搅动、粗糙度上升。Zhang 等^[58]报道辊轮直径由 3 mm 增至 8 mm 时堆积密度提高且法向接触力增大(图 2b)。辊轮直径增大通常会强化压实区法向载荷并扩大有效压实体积(图 2c)。除运动学参数外, 辊筒表面状态同样构成重要边界条件: Oropeza 等^[59]实验证明, 光滑表面辊筒可获得更高堆积密度与更平整的床面, 而网格纹理辊筒铺粉质量较差, 表明辊筒表面光洁度对稳定铺展具有直接约束作用(图 2d)。

1.3 铺粉层厚

铺粉层厚 h 是 BJ 工艺中基础却也是关键的工艺参数之一。直观观察, 层厚越大, 单位面积储粉量越多, 但在给定铺粉方式和粉末流动性的前提下,

过大的 h 往往会降低粉床压实程度、增加层内孔隙; 过小的 h 则易受床面缺陷与设备几何误差影响, 引发推粉等问题^[46,60]。

Miao 等^[60]近期工作专门研究了层厚对粉床密度的影响, 并指出自由流动陶瓷粉末的铺粉状态主要与 h^* 有关: 当 h^* 过小(<2)时, 粉床受基板粗糙度与铺粉设备间隙波动影响显著, 粉床均匀性严重受影响, ρ^* 和 R_s 波动较大; 当 h^* 过大($>4\sim5$)时, 粉床中上部的颗粒无法充分压实, 平均 ρ^* 下降且层内易形成孔隙梯度。Li 等^[61]通过实验结合 DEM 研究发现: 对于球形造粒的 Al_2O_3 与 ZrO_2 粉末, $h^*\approx 3$ 左右可获得兼顾较高粉床密度与较低表面粗糙度; 当采用更细、更易团聚的颗粒时, 则需要适当减小层厚以抑制局部空隙缺陷。多层 DEM 研究表明, 层厚不仅影响平均孔隙率, 还直接决定孔隙在厚度方向上的分布均匀性。Weissbach 等^[62]基于 BJ 多层 DEM 模型, 分析了不同 h^* 条件下的粉床各向异性力学性能, 指出过大的 h^* 会放大层间堆积差异, 使得粉床在 Z 方向上的弹性模量与渗透率表现出明显各向异性。从工程应用角度, 可以将层厚设计视为在“ h^* 过小会导致粉床不均匀, 床面缺陷会增加”与“ h^* 过大导致平均孔隙率升高与各向异性增强”之间寻找平衡。对于大多数 BJ 陶瓷体系, 目前文献与工业实践都倾向于将 h^* 控制在 2~4 内, 并通过 DEM 结合实验来确定具体值^[52,60]。

1.4 粉末特性

粉末特性主要包括粒径分布和粉末形状两方面, 粒径分布常常通过级配(粗粉与细粉进行一定比例混合)进行优化。粉末特性是决定粉床孔隙率与表面粗糙度的最重要因素之一。研究表明: 对于细小的粉末, 粉末床的密度通常较低。由于细颗粒之间的相互作用力(如范德华力、静电相互作用、氢键作用以及毛细管桥接作用)可能与重力相当, 甚至更大^[63–65]。因此, 在这种强大的相互作用力的影响下, 细粉的流动性较差, 所以在铺展过程中很难重新排列^[66]。对于粗粉而言, 进一步增大颗粒尺寸并不会显著增加粉末层的密度, 甚至可能会降低粉末层的密度^[46,65,67]。原因在于颗粒尺寸变大, 颗粒之间的间隙也会变大。所以常常采用级配方式对粉末粒径进行优化, 粗粉与细粉按照最优配比进行混合, 细粉可填充粗粉之间的间隙, 以此增加粉床的密度, 并保持较好的流动性。

Ali 等^[68]在制备 Al_2O_3 陶瓷时, 通过引入少量纳米粉与粉床压实相结合, 提高了粉床致密度, 烧结后密度可达 72%, 表明“纳米粉+机械压实”可以在不显著恶化流动性的前提下, 提高粉床填充程度。针对真正意义上的双峰陶瓷粉末, Shahed 等^[69]近期系统研究了 1–20 μm 范围内多种双峰 Al_2O_3 粉末的铺展行为与力学性能。DEM 结果表明, 随着细粉体积分数增加, 粉床平均密度先升高后降低, 而表面粗糙度则在细粉中等含量时达到最小; 实验进一步证实, 对于其研究体系, 细粉体积分数约 30%~40%时可在流动性、粉床致密度与烧结力学性能之间取得较优平衡。

1.5 铺粉实验验证

为了保证 DEM 粉床模型的可靠性, 必须通过实验对关键接触参数(摩擦系数、滚动阻力系数、表面能/黏附力等)进行系统标定。主要通过霍尔流速计对粉末休止角、堆积密度、振实密度以及流动性进行测量计算, 然后在 DEM 中扫描接触参数组合, 使模拟堆积与流动行为与实验结果最接近。通过进一步实验对 DEM 模拟粉末床堆积密度和表面质量的结果进行验证。主要测试粉床密度与表面质量。粉末床堆积密度主要通过测量粉床的质量和体积求得。一般采用栅栏法^[69]、插管法^[70]、光固化法^[67]以及定制收集法^[53](图 2e)。粉末床表面质量主要从表面平整度与表面缺陷(如凹坑、空隙)两方面进行评估。其中, 表面平整度指粉末床表面沿法线方向与理想表面之间存在的偏差。目前, 测量方法主要

分为在线测量(激光轮廓仪^[71]、工业相机^[72])和原位测量[激光共聚焦^[48]和工业计算机断层成像 CT^[73]] 2 种方式(图 2f)。

2 黏结剂–粉床相互作用与渗透行为的多尺度建模

2.1 黏结剂在陶瓷粉床中的渗透与扩散机理

在 BJ 打印过程中, 单个液滴自喷嘴射出后经历飞行、撞击粉床、表面铺展、毛细渗透等一系列耦合过程, 其中, 黏结剂在多孔粉床中的浸润渗透行为对成形质量至关重要。黏结剂渗透主要受粉床孔隙结构和液滴本身特性驱动, 包括毛细作用(表面张力驱动)、润湿性(液–固接触角)、重力以及扩散迁移机制等物理因素共同影响^[46,74]。按时间尺度划分, 通常可将其分为 3 个阶段: 液滴与粉床接触后几十微秒内的因惯性驱动的铺展阶段、随后由表面张力主导的回缩—再平衡阶段(几十至数百微秒)、以及以由毛细压差驱动的渗透阶段(微秒至秒级)。

粉床的孔隙率和渗透率决定了黏结剂渗透的难易程度: 高孔隙率/高渗透率的陶瓷粉床对液体阻力小, 液体更易穿透; 而致密粉床将产生更高的毛细管阻力和入口压力, 使黏结剂难以渗入^[75,76]。除孔隙结构外, 重力也会影响垂直渗透行为: 当液体渗透高度增加时, 液柱的重力与毛细吸力相抗衡, 最终在一定深度达到平衡。衡量重力相对毛细作用的重要无量纲参数是邦德数(Bo_d)。 Bo_d 表示重力与毛细力之比; 对于细孔陶瓷粉末, Bo_d 往往很小, 说明毛细管力主导渗透过程, 而重力影响可以忽略。在打印过程中, 浸渗深度至少超过单层粉末厚度, 以实现层间结合; 如果黏结剂仅停留在层表面而未充分下渗至下层粉末, 层间将无法有效胶结而导致强度缺陷。

此外, 初始液滴速度对渗透行为也有重要影响。高速液滴撞击粉床时, 动能可能引起局部粉末颗粒移动、液滴铺展甚至飞溅分裂, 造成更深的局部渗透和孔隙填充不均; 而低速液滴则主要受毛细力牵引, 趋向于原地渗入并横向润湿扩散。这一效应常用雷诺数(Re_d)和韦伯数(We_d)等无量纲数刻画(表 2): Re_d 反映惯性与黏性之比, We_d 反映惯性与表面张力之比。

在典型陶瓷 BJ 中, Re_d 通常为几十到数百量级, We_d 接近临界值以形成稳定液滴。中等速度(适中 Re_d 、 We_d)的液滴会较充分地铺展并渗透; 过高速(高 Re_d 、 We_d)可能导致液滴破裂、反弹或粉末冲击

溅出, 反而降低有效渗透深度。黏结剂在陶瓷粉床中的浸润渗透是多种因素共同作用因素的结果: 毛细吸力提供主要驱动力, 重力和惯性影响次之, 而孔隙结构、润湿接触角以及液滴参数决定了渗透前沿形态和深度。这些物理机制为后续多尺度建模提供了依据和参数参考。

2.2 黏结剂渗透模型

2.2.1 连续介质模型 连续介质模型将粉床等效为多孔介质, 或在孔隙尺度直接求解 Navier-Stokes (N-S) 方程, 用于描述黏结剂渗透的宏观规律。孔隙尺度求解 N-S 方程需解析液/气界面、黏性阻力与表面张力, 能够捕捉液滴在孔道内的细节, 但真实粉床孔隙数量巨大, 网格解析成本极高。工程上更常采用体积平均并引入 Darcy 定律, 将黏结剂视为多孔介质内渗流^[77]。Wang 等^[78]采用 COMSOL 软件建立 2D 多孔介质模型, 研究了接触角、孔隙率和黏结剂滴落高对黏结剂渗透面积的影响。他们通过调整 Darcy 模型中的润湿边界条件, 发现提升润湿性和提高孔隙率都会增大黏结剂在粉床中的铺展渗透面积(图 3e)。Gao 等^[79]则提出将每层粉末渗透简化为圆柱渗透体的多层叠加模型, 用 Darcy 定律近似计算各层液柱上升高度, 以模拟多层打印过程中的黏结剂渗透(图 3f)。Darcy 模型计算成本低, 适合预测一定时间下渗透深度和饱和度场, 并且可以用于接触角、孔隙率等参数的分析。基于比表面积与孔隙率的 Darcy 毛细平衡模型已被用于推导平衡饱和

度并与实验较好吻合, 显示其在黏结剂用量优化中的实用价值。但是 Darcy 模型由于未显式包含界面形变动力学, 无法直接预测液滴形状的演化 and 局部毛细桥形成等微观现象。

2.2.2 LBM 模型 格子 Boltzmann 方法(LBM)属于介观统计流体方法, 通过离散格点上的分布函数迁移与碰撞求解多相流动, 相较传统 N-S 方程求解器, LBM 对复杂几何(如随机堆积的陶瓷颗粒孔隙)具有天然优势, 且易于并行计算。LBM 在模拟黏结剂与粉床相互作用方面的一个关键进展是实现了高密度比两相流的计算。Zhou 等^[80]采用彩色梯度多相 LBM 模型模拟了黏结剂液滴撞击并渗入三维颗粒床的动态过程, 系统研究了粉床孔结构和黏结剂参数对渗透行为的影响。得出以下结论: 对于细颗粒陶瓷粉末, 应选择较低的液滴速度以充分发挥毛细润湿作用, 从而均匀渗透; 而对于较粗颗粒或多孔预制体, 可以适当提高喷射速度以确保足够的渗透深度。除了单液滴行为, Hu 等^[81]进一步将 LBM 用于多液滴连续沉积过程的研究, 考察多滴相继喷射对渗透饱和度和液桥连通性的影响。这对于模拟实际打印中喷头多次喷射同一区域(如轮廓加固或高填充区域)的情形非常重要。LBM 方法的优点在于精细解析: 它可以在颗粒尺度捕获黏结剂在陶瓷粉床中的细观渗流和界面动力学等特征, 得到黏结剂浸润过程中瞬态速度场、压力场以及多相界面状态等详细信息^[80]。当关注单滴或少量液滴局部行为以

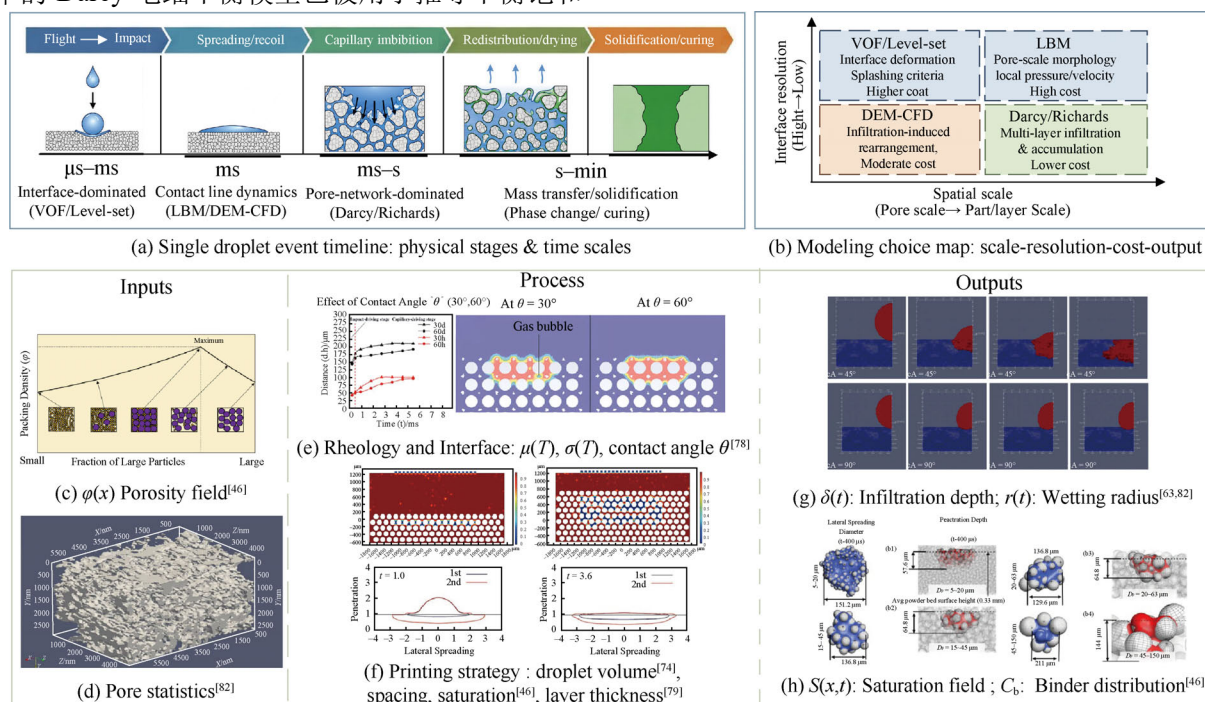


图 3 液滴撞击和粉床渗透: 物理阶段、模型选择

Fig. 3 Droplet impact and powder bed infiltration: physical stages, modeling choices

及毛细现象时, LBM 提供的高保真度模拟结果能弥补宏观 Darcy 模型的不足。随着计算能力提升和算法优化, LBM 有望在陶瓷 BJ 多孔介质流动研究中发挥更大作用。

2.2.3 界面捕捉模型 VOF 法和 Level Set 法是传统 CFD 中用于处理多相界面的数值技术, 已广泛应用于黏结剂液滴在粉床上的动力学模拟^[46,82]。两者思路略有不同: VOF 方法通过在网格中引入组分体积分数函数, 利用流体对流方程追踪液相/气相的体积分数分布, 从而定位界面; Level Set 方法则引入一个连续的水平集函数, 其零值面代表界面位置, 通过求解 Level Set 方程来更新界面状态。VOF 以体积分数追踪界面, 具有较好的质量守恒。Tan 等^[83]采用 VOF 技术, 对直径几十微米的液滴撞击堆积粉末的过程进行了三维数值模拟。研究了液滴以 1、5、10 m/s 3 种速度入射时的行为, 发现液滴入射速度对渗透有明显影响: 高速时液滴穿透力最强, 渗透深度最大但伴随较多粉末被击飞; 中速时渗透深度和润湿范围均衡; 低速时液滴主要滞留表层, 横向润湿面积较大但下渗不足。这些结论与 LBM 模拟和实验观察一致。Level Set 方法则以更光滑的方式捕捉界面且易于计算界面曲率, 在处理表面张力精度上有优势。Choi 等^[84]利用 Level Set 法模拟液滴渗入多孔介质, 探讨了孔隙率和接触角对渗透形态的影响。成功模拟出不同润湿性条件下液滴在孔隙中推进的界面形状。结果表明, 润湿角从 90°降低到 30°会显著改变渗透模式: 前者液滴更倾向于停留表面, 后者则迅速吸入孔隙形成“指状”突进。VOF/Level Set 等界面捕捉 CFD 模型的一大优势在于细节丰富: 能够直观呈现黏结剂液滴变形、铺展、渗透的连续过程, 例如液滴形状从球冠状逐渐塌陷润湿粉层、液体沿颗粒表面形成液桥、部分液体在颗粒间下渗深度随时间变化等^[85,86]。当然, 界面捕捉 CFD 模型的计算成本较高: 要求细密网格刻画颗粒表面和孔隙流场, 三维模拟单个液滴渗透常需耗费数小时乃至更长时间。因此, 其适用范围多局限在单液滴-局部多孔结构的场景^[87]。在陶瓷 BJ 领域, 当关注例如液滴撞击动力、瞬态润湿铺展、局部毛细桥形成等现象时, VOF/Level Set 模型能够发挥无可替代的作用。

2.2.4 离散元-流体动力学模型 纯流体模型通常将粉床视为静止骨架, 难以反映液滴冲击引发的颗粒重排以及液桥产生的毛细凝聚力对骨架稳定性的影响。DEM-CFD 耦合通过 DEM 求解颗粒碰撞、摩擦与运动学响应, 并与 CFD 流场双向耦合, 可更

真实地反映黏结剂与粉末之间的相互作用^[74,81,88]。

Rehman 等^[89]将单个液滴渗透砂床的过程用 DEM-CFD 耦合模拟, 发现液滴撞击区域的粉末在液体冲击下发生轻微松动和重排, 随时间推移, 黏结剂进一步渗入这些松动区域, 渗透深度相对未耦合模型有所增加。进一步串联铺粉与喷射过程的耦合研究表明, 初始床密度不均匀会导致黏结剂迁移路径差异, 多液滴间距也会改变局部饱和度进而影响黏结剂深层渗透迁移。DEM-CFD 耦合在陶瓷 BJ 数值模拟中扮演着连接微观与宏观的角色。一方面, 它从微观上描述黏结剂与粉床相互作用导致的介观结构演变; 另一方面, 其结果可提升宏观模型对粉床非均匀性和动力学效应的准确度

不同模型各有侧重: Darcy 模型适用于宏观快速评估, 但细节欠缺; N-S 直接模拟(VOF/Level Set)和 LBM 注重微观精确, 能提供丰富细节但计算成本昂贵; DEM-CFD 耦合则在考虑粉体响应方面独具优势, 但当前只能在有限规模上应用。在陶瓷 BJ 研究中, 往往需要多种模型结合: 可先用 Darcy 模型确定一个合理的黏结剂饱和度范围, 再用 VOF/LBM 深入研究该条件下液滴渗透微观形态, 最后, 若关注颗粒重排, 再辅以 DEM-CFD 验证。在实际工程应用中, 则可依据需求选择模型: 要求快速优化工艺参数时用 Darcy 等简化模型, 研究细节机理时用高保真度模型。

2.3 黏结剂渗透实验验证

为验证数值模型并研究黏结剂在陶瓷粉床中的真实渗流行为, 通常需结合多尺度实验表征。实验不仅用于提供关键参数与边界条件, 还可通过与模拟结果的同尺度对照检验预测精度, 从而反向推动模型修正与工艺优化(表 3)。渗透深度可通过在单层或少层粉床上喷射定量黏结剂, 待固化/干燥后进行纵截面观察并测定渗透前沿位置; 借助染色或树脂本征颜色可清晰识别渗透区, 部分研究显示模拟预测的平均渗透深度与实验测量具有良好一致性^[74]。为获取瞬态信息, 可采用高速成像记录液滴撞击、粉体扰动与渗透前沿演化^[74]; 可见光侧视适用于观测透明容器截面, 而同步辐射高速 X 射线可实现对不透明粉床内部渗流的原位透视。润湿性测试则通过粉床或致密陶瓷基底上的动态接触角表征界面润湿参数, 并可在不同温度下评估黏度与表面张力变化对黏结剂与粉末润湿性的影响。微观层面, 可通过冷冻劈裂或抛光制备粉床截面, 利用 SEM/EDS 识别黏结剂桥连、孔隙填充及其分布范围; 进一步采

用 XCT 实现三维可视化, 尤其适用于反应固化体系以分割固化相并与模拟三维渗透形貌对照。宏观上, 初坯弯曲/拉伸强度等力学测试可作为黏结剂分布

与均匀度的间接响应, 用于验证饱和度-强度-精度的耦合趋势, 并反向校准毛细压力饱和度关系或固化收缩等参数。

表 3 黏结剂渗透实验验证
Table 3 Binder penetration experiment verification

Measurement	Data-Out	Calibration Model
High-speed imaging	Splash/rebound threshold, spreading factor	VOF/Level-set contact line model
Dyed sectioning/Confocal	Front morphology, layer-to-layer infiltration	Darcy/Richards
XCT saturation mapping	3D pore connectivity, filling topology	LBM/VOF pore-scale
Rheology and wetting tests	$\mu(T)$, $\sigma(T)$, θ	All model input parameters
Green strength mapping	Strength mapping/ Layer interface weak zones	Condition for debinding crack risk
Mass change/ Evaporation rate	Evaporation/ Curing kinetics	Evaporation/ Curing models
IR thermal imaging	Temperature field	$\mu(T)$ dependence, curing exothermic reaction

经过黏结剂喷射打印后的粉床经过高温或者常温干燥固化, 除去多余的粉末后得到陶瓷初坯。BJ 陶瓷初坯通常具有高孔隙率、低强度、层间各向异性的典型特征。初坯相对密度往往由粉末堆积能力所主导, 可通过铺粉模拟与实验对照获得; 层层铺粉与喷射路径引入的结构差异可在烧结阶段放大为收缩与性能的各向异性。初坯的孔隙率场、渗透率、有效扩散系数与相对密度变化由铺粉及黏结剂渗透共同作用产生。

3 脱脂过程的数值模拟

3.1 脱脂方法与机制

BJ 成形后初坯中残留的有机黏结剂在致密化烧结前必须通过脱脂去除。若去除不充分, 残余组分在烧结阶段的 2 次分解将引入孔隙并造成应力集中; 若升温速率过高, 温差与分解放气诱发的内压叠加, 坯体更易产生裂纹。根据工艺路径通常包括: 1) 热脱脂^[90]: 分阶段升温/保温, 利用热能有机黏结剂裂解挥发; 2) 溶剂脱脂: 将坯体浸入能溶解黏结剂某一组分的溶剂中, 溶解除去大部分黏结剂, 然后干燥并再经热脱脂清除残余; 3) 气相辅助脱脂: 利用特定气氛加速黏结剂降解的脱脂方法。在 BJ 中, 通常采用简单高效的热脱脂。

陶瓷坯体的热脱脂实质上包括 2 个同时进行的过程: 有机黏结剂的热分解, 以及分解产物在孔隙中的传输扩散。从黏结剂的逸出机理来看, 主要包括 3 种模式: 1) 蒸发: 低分子量有机物受热直接从坯体表面挥发逸出; 2) 热降解: 高分子量黏结剂在加热下大分子链断裂生成小分子产物, 后者扩散到表面后挥发; 3) 氧化降解: 在有氧气氛中, 高分子链发生氧化裂解产生小分子, 随后扩散逸出。并且脱脂气氛对热解动力学和缺陷形成影响显著。在低温阶段

(200~300 ℃), 氧气参与使黏结剂分解速率降低, 质量损失较小; 而在更高温时, 氧化气氛会加速聚合物随机断链, 促进快速裂解。Zhou 等^[93]对比了 Al_2O_3 坯体在氩气和空气中的脱脂行为, 结果显示氩气中主要发生热降解和蒸发, 生成的气体以低分子碳氢化合物为主; 而空气中由于发生氧化反应, 生成了更多 CO_2 等气体, 导致坯体内部应力更强, 出现了严重的裂纹缺陷。

3.2 初坯脱脂模型

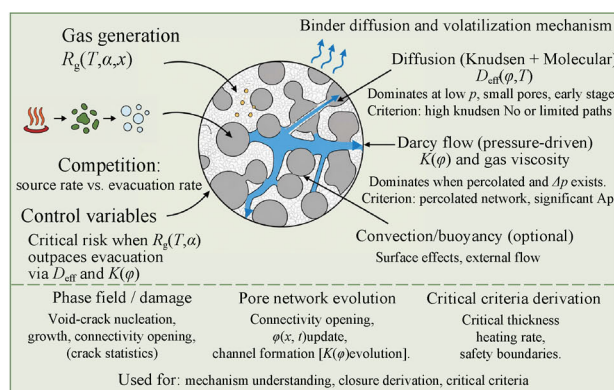
3.2.1 有限元模型 有限元模型(FEM)可以建立热传导、化学反应动力学、流体质量传输和固体力学本构关系的温度-形变-应力耦合模型。FEM 模型擅长在给定脱脂曲线与零件形状下求解残余黏结剂富集区、解决是否存在临界厚度或需要设定保温平台等问题^[91, 92]。研究人员可以定量预测脱脂过程中的内部应力演化, 从而设计出既能保证完整性又能缩短周期的最优热处理工艺。Belgacem 等^[94]在 316L 金属粉末体系中建立了温度-黏结剂残余量耦合模型, 利用 COMSOL 对热分解、热传导和体积变化进行耦合求解, 准确预测了黏结剂残余分布和温度场分布。余一帆等^[95]利用自研求解器, 对 BJ 成形氧化铝陶瓷芯脱脂过程中的温度场、应力场以及位移场的变化进行了预测。探究升温速率以及保温时间对其的影响(图 4c)。Li 等^[96]利用 COMSOL 实现输出任意时刻金属初坯的残余黏结剂分布、温度分布与变形场, 该方法对 BJ 陶瓷热脱脂具有直接可迁移性, 差异主要体现在初始孔隙率与黏结剂含量更低、孔隙连通性更强。

3.2.2 反应动力学模型 反应动力学模型基于黏结剂的热分解机理, 通过多步化学反应(通常采用广义的 Arrhenius 方程)描述黏结剂分解的路径和速

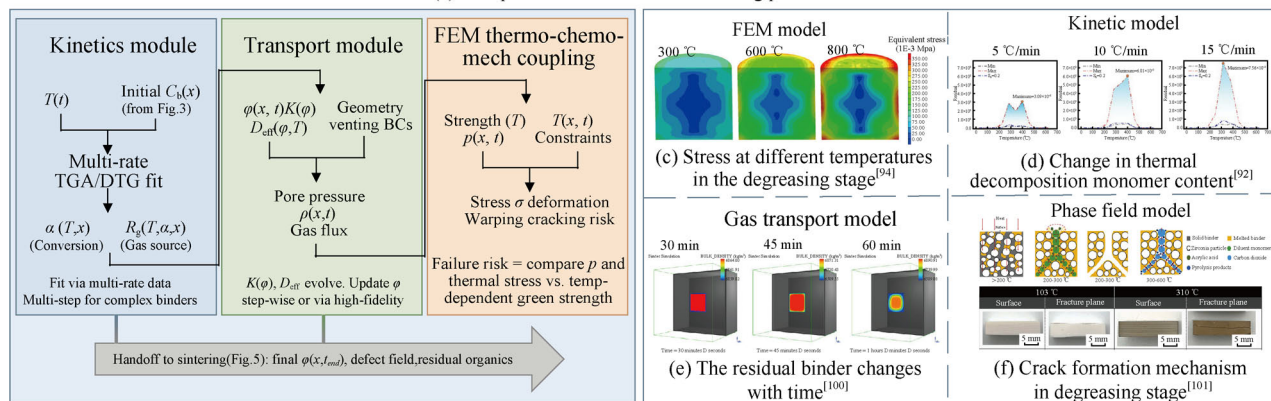
率。并基于热重分析(TGA)拟合出多峰热解模型或采用分布活化能模型(DAEM/M-DAEM)来表征复杂的交联树脂体系^[92,97]。Wang 等^[98]利用多分布活化能模型拟合光敏树脂的热重数据,获得多个组分的活化能分布,实现高精度拟合(拟合优度 $R^2 > 0.9999$)。反应动力学模型的核心在于准确反映黏结剂分解过程的热力学和动力学特性,并关联分解产物和残余物分布。Zhao 等^[92]基于 Arrhenius 方程研究了三乙二醇二甲基丙烯酸酯黏结剂的热分解动力学,并分析了黏结剂从热解生成物到气相的物理扩散过程(图 4d)。Zhao^[99]进一步针对金属 BJ 研究报告了基于 TEG-DMA 黏结剂热解动力学的扩散控制模型,揭示黏结剂热解后的气体扩散行为。

3.2.3 气体输运模型 气体输运模型用于描述脱脂过程中热解产生的挥发物在多孔初坯中的运动。其控制方程一般结合质量守恒、动量守恒和物质输运方程。气相传输主要包括扩散和对流 2 种模式:在气体分压较低或孔隙细小情况下,传质受分子扩散控制;当气压升高、孔隙连通性较好时,可通过达西流动或扩散-对流并存传输^[92]。早期研究中,German^[100]提出 3 种热脱脂控制机制:扩散控制、

渗透控制和毛细管吸引控制。对于高孔隙率的 BJ 陶瓷初坯,由于喷射黏结剂体积分数低于粉末床孔隙率,一般认为,气体流动以扩散为主。在模型中,常采用达西定律描述气体在孔隙中的黏性渗流,并结合欧拉-拉格朗日方法或有限体积法求解速度场;菲克定律用于气体组分的分子扩散。通常假设热解气体为理想气体,质量传输可由气体浓度梯度和压力梯度驱动。Yan 等^[101]应用 CFD 方法模拟 MBJ 脱脂过程,联立能量、动量和物质守恒方程,计算多种生成气体在孔隙结构中的流动。他们模型考虑了流场随时间、温度和粘度的变化,用 PVA 黏结剂反应产生 CO_2 、 H_2O 、 $\text{C}_2\text{H}_6\text{O}$ 等气体,并求解对应的速度场和压力场,结果表明脱脂从外层向内部推进,对气体组分浓度、速度和压力分布进行了详细分析(图 4e)。类似地,Zhao 等^[92]在 BJ 初坯中建立了基于扩散方程的脱脂模型,研究了热解气体扩散系数对 TGA 结果的影响,模型与实验结果吻合良好。数值模拟时,边界条件通常为固体-气相界面浓度或压强条件,初始参数(如孔隙率、渗透率)可根据初始黏结剂含量和实验测定确定,并随着脱脂进程迭代。



(a) Transport mechanisms and controlling parameters



(b) Modeling chain: kinetics → transport → FEM coupling

图 4 脱脂过程: 路线、耦合物理

Fig. 4 Debinding process: routes, coupled physics, modeling chain

3.2.4 相场模型 相场模型用于模拟脱脂过程中微观结构和成分的演化, 尤其适用于多组分黏结剂体系或伴随裂纹形成和孔洞聚并的情形。其基本思想是通过一个或多个描述相分离和界面演化的连续场变量, 在能量泛函下采用 Cahn–Hilliard 方程或 Allen–Cahn 方程描述界面演变和相互转变。相场模型能够自然捕捉黏结剂与陶瓷粒子、空气之间的相分布, 以及由于黏结剂溶解或热解产生的空洞和微裂纹的形成与演化^[93,102](图 4f)。Liu 等^[103]开发了基于 Cahn–Hilliard 方程的相场模型, 用于模拟金属 ME 打印件的溶剂脱脂过程, 跟踪聚合物-溶剂体系的分相分离动态及孔隙结构演变, 该模型考虑了黏结剂溶解、扩散以及由此导致的孔洞逐渐形成和网络结构的变化, 为孔隙对随后的热脱脂和烧结行为提供了微观解释。相场方法可扩展到热脱脂场景: 通过定义不同相场来表示黏结剂、陶瓷颗粒和气相, 可模拟脱脂过程中黏结剂浓度梯度驱动下的相分离、孔洞生长甚至微裂纹萌生。相场模拟适用于研究多组分黏结剂体系或在脱脂过程中出现宏观缺陷(如裂纹)时的机理分析; 但其高精度也意味着计算效率较低, 不适合大尺度工程直接应用。

3.3 脱脂模型实验验证

可通过 TGA 质量曲线求得反应动力学模型中的转化率(表 4)。通过脱脂中断实验, 由工业 CT 测得脱脂过程中孔隙率变化, SEM 观测陶瓷组分变化以及定位裂纹萌生位置。通过热电偶与红外热像实现外表面温度场验证以及换热边界条件的反演。可用三维扫描仪检测脱脂后零件尺寸变化情况。

4 烧结过程的数值模拟

4.1 烧结机制

脱脂后获得的陶瓷棕坯孔隙率较高且脆, 需经高温烧结促使颗粒键合并削减孔隙, 方可得到致密制件。由于 BJ 棕坯初始相对密度多为 50%~60%, 线收缩通常达到 10%~20%, 且收缩往往呈各向异性; BJ 研究显示, 构建方向收缩率可比平行粉层方向高约 15%, 这一现象表明堆积微结构会放大不均匀致密化与热应力。基于此, 尺寸设计通常预留足够的收缩补偿, 并通过提高烧结温度、延长保温或辅以热等静压降低残余孔隙, 以提高强度。相较传统成形, BJ 坯体致密度更低, 使常压直接烧结达到高密度更具挑战^[104–105]。

表 4 脱脂模型实验验证
Table 4 Experimental verification of degreasing model

Measurement	Data-Out	Calibration Model
Multi-rate TGA/DTG	$\alpha(T)$, $R_g(T, \alpha)$	Kinetics model (E , A , reaction order/steps)
Off-gas analysis (MS/FTIR)	Evolution of species	Reaction pathway, charring; BCs and safety window
Interrupted debinding +XCT	$\phi(x,t)$, connectivity, crack initiation sites	$D_{eff}(\phi, T)$, $K(\phi)$ evolution, damage criteria
Thermocouple/IR	$T(x,t)$	Thermal BCs and thermo-chemical coupling strength
3D Scan / CMM	Strength mapping	FEM prediction; constraints and residual stress effects
Crack statistics (SEM)	Evaporation, curing kinetics	Critical heating rate, defect sensitivity parameters

在烧结过程中按液相是否出现及化学反应是否参与, 可将烧结机制概括为 3 类: 1) 固相烧结完全在固态下进行, 颈部生长主要受表面/晶界扩散控制, 常需接近熔点的高温长时保温, 并易伴随晶粒异常长大与致密化停滞^[106]; 2) 液相辅助烧结通过少量低熔点助剂生成液相, 借润湿–毛细重排及溶解–再沉积加速传质, 从而降低烧结温度与时间; 3) 反应烧结则利用原位反应形成骨架或结合相以减小收缩并降低开裂风险。在实际工程应用中, 针对不同烧结机制需选用适配的烧结模型进行模拟。

4.2 棕坯烧结模型

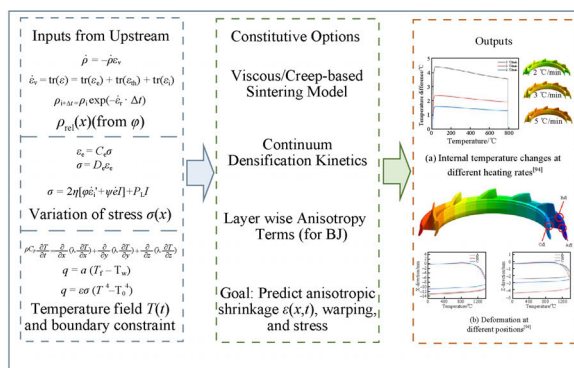
4.2.1 有限元模型

在宏观尺度上, 将多孔坯体

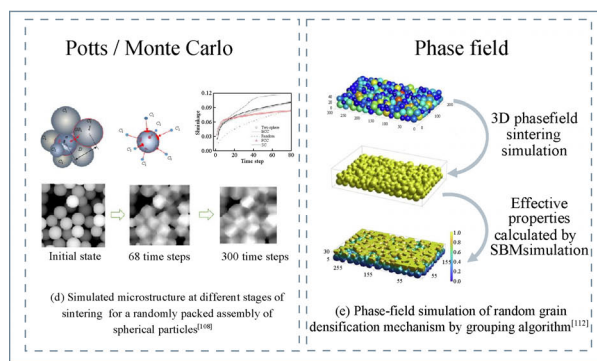
视为黏弹塑性连续介质, 通过本构方程描述烧结收缩和蠕变变形。典型模型引入烧结应力和有效黏度等参数, 将烧结致密化类比为黏性体在自身收缩应力驱动下产生体积应变的过程。Olevsky^[107]提出的烧结理论以相对密度为状态变量, 建立了烧结体应变速率与应力和烧结驱动力的关系, 可用于有限元计算不均匀加热或复杂外形坯体的变形。有限元烧结模拟适用于预测器件尺度的收缩不均和翘曲开裂等问题, 可将各向异性收缩、重力、自重支撑等因素纳入考虑。其核心方程通常包括: 质量守恒方程(描述致密化速率与扩散流密度的关系)、动量守恒方程(高温下颗粒骨架的流变行为)以及状态方程(例如孔隙率演化方程)。关键参数如烧结激活能、黏度

—温度曲线、烧结应变能等可由实验测定(热膨胀仪、多步烧结实验)并通过拟合获得。余一帆^[95]已经成功利用有限元模拟对 BJ 成形氧化铝复杂陶瓷芯的烧结情况进行了模拟,准确预测了在不同升温速度及

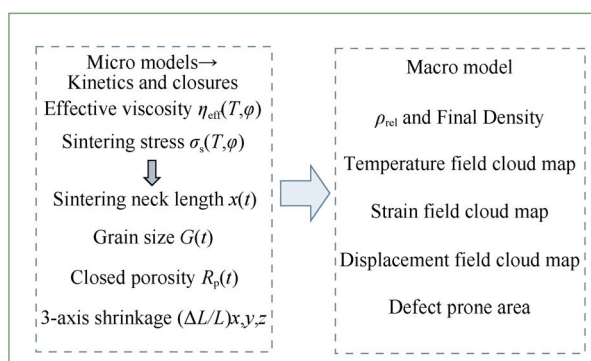
烧结温度下,复杂陶瓷芯尺寸收缩以及应力集中情况(图 5a~图 5b)。有限元模型擅长宏观形变和应力分析,为烧结工艺制定(如烧结支撑设计、炉温均匀性要求等)提供了指导。



(c) Macro model (FEM model)



(f) Micro models (Potts / Monte Carlo and Phase field)



(g) Micro-macro parameter correspondence

图 5 烧结阶段多尺度建模框架、参数传递

Fig. 5 Multi-scale modeling framework, parameter transfer & validation chain for sintering stage

4.2.2 Potts 模型 蒙特卡洛方法通过统计规律模拟烧结微结构演化,是研究烧结颈部形核长大和空隙迁移的有力工具之一。常用的是晶格 Potts 模型:将多晶材料离散为格点,每格赋予一个晶粒编号,通过 Monte Carlo 迭代更新格点状态,趋向于使系统总界面能最小。该方法可直观展现烧结过程中晶粒长大和孔隙位移合并的现象(图 5d)。其核心在于定义晶界能和表面能,以及考虑体积(密度)变化的规则,然后通过大量随机试移和能量判断,模拟出随时间推进的微观结构变化^[108–109]。蒙特卡洛模型参数主要是晶界能/表面能比值、晶粒取向数(Potts 状态数)等,时间步与实际烧结时间没有直接对应关系,但可定性比较不同条件下的致密化速率。该方法适用于中观尺度(数百颗粒以内)的烧结过程研究,能揭示如异常晶粒出现、气孔被截留等微观机制。Wang 等^[110]的研究表明,粒度级配改变了初始堆积密度与空隙排列,从而改变孔隙闭合规律;

当孔隙在晶粒快速粗化过程中被包裹,其消除难度显著上升,易在末期残留大孔或形成气孔截留。Potts 模型^[111]模拟显示若初始粒径分布很宽,大颗粒可能通过吞并机制抑制小颗粒周围的致密化,导致烧结末期残留大孔洞;这一结果在实验中也屡有观察。蒙特卡洛方法的局限是无法直接引入连续时间尺度,但结合实验标定后,可用于半定量预测微观演变趋势,被广泛用于陶瓷烧结颈/孔结构研究。

4.2.3 相场模型 相场法是在细观尺度模拟多相界面和形貌演变的强大工具,已被成功应用于烧结的数值研究。相场模型以连续“相场变量”描述材料的相/晶粒分布,引入自由能泛函来表征系统的热力学状态,通过偏微分方程演化相场以模拟界面迁移和物质扩散^[112–113]。针对烧结,可设定一个密度场 ρ (或孔隙相浓度)和若干晶粒取向场 η ,构造包含体积自由能、表面能和晶界能的总自由能 $F[\rho, \eta]$,以及 $\nabla \rho$ 、 $\nabla \eta$ 的梯度能系数项。演化方程通常采用变分

形式的 Cahn-Hilliard 方程(保持总物质守恒, 模拟致密化驱动下孔隙体积分数变化)和 Allen-Cahn 方程(控制晶界迁移和晶粒长大)耦合而成。相场模型的核心参数包括: 表面能和晶界能(决定不同相场的相互作用势垒)、界面宽度参数、各扩散通量的动力学系数(界面迁移的动力学参数)等。这些可部分由实验或原子模拟获得。相场模拟能够自然地呈现烧结过程中的颈长大、孔洞迁移合并以及晶粒粗化过程, 且无须预先跟踪界面, 使其非常适合复杂形状、多颗粒体系的烧结研究。Kumar 等^[114]最早用多相场模拟了不同大小双粒子的烧结过程, 清晰展现了颈部形核、颈径稳定、小粒溶解、晶界快速包络小粒直至消失的全过程, 其颈长大速率与经典烧结理论结果相符。Termuhlen 等^[112]在相场法中创新采用分组算法来计算大量粒子系统的致密化行为和由此产生的刚体运动, 发现 2 个相邻规则排列的颗粒层能够协同合并, 导致孔隙相的曲折度大幅增加(图 5e)。Nakazawa 等^[115]在多相场模型与图形处理单元(GPU)/并行计算框架上取得进展, 使得更大颗粒集合与更长时间尺度下的致密化与晶粒演化预测成为可能, 为连续体模型参数反演与跨尺度耦合提供了更可靠的微观依据。相场方法目前主要用于学术研究和微结构演化预测, 计算量较大, 但随着算法优化和算力提高, 有望在烧结工艺优化(如添加剂设计、烧结路径对微观结构的影响等)中发挥越来越重要的作用。

4.3 不同陶瓷体系的烧结特征

黏结剂喷射工艺涉及氧化物、氮化物、碳化物等多种陶瓷材料, 各自的烧结温度、气氛要求及收缩行为有所差异, 本文对于每一类别选取一种材料加以说明。 Al_2O_3 为稳定氧化物, 可在空气中 $\geq 1550^\circ\text{C}$ 固相烧结获得高致密度, 但 BJ 件常有 15%~20% 线收缩且对排胶/升温制度敏感, 宜采用阶梯升温与真空辅助排胶, 并配合浸渗/助烧剂与控晶粒手段以降低残孔和翘曲风险^[10]。 Si_3N_4 无助剂难以

常压致密化(约 $1800\sim 1900^\circ\text{C}$), 通常引入 Y_2O_3 — Al_2O_3 等氧化物助剂(量级 5%~10%, 质量分数)并在约 $1700\sim 1750^\circ\text{C}$ 、流动 N_2 气氛下液相助烧^[116]; 同时需管理 $\alpha\rightarrow\beta$ 转变与长柱晶诱发的各向异性。若追求低收缩, 可先打印 Si 并在 $\sim 1400^\circ\text{C}$ 氮化制得 RBSN, 再 2 次烧结/等静压提高密度^[117-118]。 SiC 纯无压烧结需 $>2000^\circ\text{C}$ 且仍难全致密, BJ 更宜采用反应/熔渗或 PIP 路线。通过在 1450°C 左右真空或氩气中熔融硅充填 SiC 坯体孔隙, 实现高密度 SiC 制品^[16]。该法产品含有少量残余硅, 但因无烧结收缩, 能精确保持打印形状, 已成功应用于大型耐热 SiC 部件制造。若必须采用无压烧结, 也应考虑在烧结后增加等静压工序将闭孔压合, 提高最终密度。

4.4 烧结模型实验验证

为验证烧结数值模型并阐明 BJ 陶瓷在致密化阶段的真实演化规律, 通常需要以“动力学曲线—形貌场—孔隙与组织”多层级实验表征构建同尺度对照体系(表 5)。宏观层面, 可通过推杆式膨胀仪获取的线收缩曲线; 配合阿基米德法得到的相对密度可得到尺寸收缩以及空隙变化规律, 从而求得黏度或烧结应力等参数。并以不同升温速率下的独立曲线检验模型的可迁移性^[119]。为求得各向异性收缩与受限边界效应, 应采用定向取样的三向收缩测量, 并在自由烧结与局部支撑 2 种条件下对照; 烧结前后通过三维扫描或工业 CT 外形重建翘曲与尺寸偏差, 与有限元预测的位移场和密度梯度驱动的差异收缩区域进行匹配, 从而判断摩擦边界、重力与初始密度不均匀对形变的影响^[120]。介观层面, 中断烧结结合 CT 扫描可得出孔隙率、孔径分布与连通性随时间和温度的变化规律, 并与相场等微观模型输出的孔形迁移与闭孔转变行为对照^[121]; 必要时辅以汞压法或气体渗透率测量, 将孔结构统计量进一步计算为渗透率或扩散通道演化, 为跨工序耦合提供实证支撑^[122]。微观组织方面, 可通过分段淬冷后的 SEM 图像分析统计烧结颈尺寸与空隙, 并用电子背散射

表 5 烧结模型实验验证
Table 5 Experimental verification of sintering model

Measurement	Data-Out	Calibration Model
Dilatometry	Shrinkage of T/t	Densification kinetics and constitutive parameters
Archimedes density	Final prel or porosity	Endpoint consistency and closure validity
3-axis shrinkage	$(\Delta L/L)_{x,y,z}$	Anisotropy and size shrinkage law
3D scan/CT	Warping, internal defects	FEM warping prediction and defect inheritance assumption
SEM/EBSD	$G(t)$, Pore morphology, distribution	Micro-models and micro-macro closures
Mechanical tes	Strength scatter, fracture origins	Defect sensitivity and quality consistency

衍射(EBSD)获得晶粒尺寸分布与织构演变,用以约束界面能、晶界迁移率及扩散通道权重等关键参数;对非氧化物体系,还需引入X射线衍射(XRD)与截面EDS表征相组成与成分梯度,以校核气氛对致密化的影响^[123],上述“曲线–场–组织”的多证据链不仅用于验证预测精度,也可将误差反向归因到初始孔结构、边界条件与本构参数,实现模型修正与烧结工艺优化的闭环。

5 结论与展望

为避免分阶段模型并列导致过程链割裂,本文进一步将铺粉、渗透、脱脂、烧结4个阶段以统一变量集合贯通。铺粉阶段通过DEM/CT获取粉床固相体积分数 $\phi(x)$ 与孔隙率 $\varepsilon(x)=1-\phi(x)$,并以Kozeny–Carman型闭合把孔结构映射为渗透率 $K(x)$ 。在渗透阶段, $K(x)$ 与润湿参数(接触角 θ 、表面张力 σ)共同决定毛细压力–饱和度曲线 $P_c(S)$,从而通过闭合非饱和渗流方程得到黏结剂饱和度场 $S(x,t)$ 。随后,脱脂阶段将 $S(x,t)$ 作为初始黏结剂分布输入,用孔隙率–曲折度闭合得到有效扩散系数 $D_{\text{eff}}(\varepsilon)$,并与气体对流/压差驱动输运共同预测产气–排气能力匹配与裂纹风险。最终,脱脂后孔隙率场 $\varepsilon_{\text{brown}}(x)$ 映射为烧结初始相对密度 $\rho_{\text{rel}}(x)=1-\varepsilon_{\text{brown}}(x)$,作为连续体烧结本构或微结构模型的初始条件,形成孔结构–传输–致密化的可追溯过程链。

BJ陶瓷全过程数值模拟正在从单一子过程的机理阐释,向可传递的全流程预测体系演进。下一阶段的关键不在于继续堆叠模型类型,而在于建立跨尺度变量的一致表征与传递规则,使铺粉阶段得到的孔隙率场、孔径统计与各向异性指标能够自然进入渗透模型的渗透率与有效扩散系数闭合关系,并进一步作为脱脂阶段产气–排气能力匹配的初始条件,最终在烧结模型中以初始相对密度场和缺陷场的形式继承,从而把粉床结构非均、黏结剂饱和度分布、孔网络生成、烧结收缩串联为可计算的数据链。

模型可信度的提升将主要依赖多源一致性标定的实验–模拟闭环,而非单一曲线拟合。反应动力学应以多升温速率TGA/DTG反演的多步参数作为佐证,并通过不同气氛下分解挥发气体通量与残碳/残留有机物的空间分布实现2次校核。输运模型需要以孔结构演化(CT/MIP)、渗透率–孔隙率关系与有效扩散系数的独立测量来约束,避免以经验常数代替不同材料空隙结构。力学与失效预测则应把形貌

扫描、翘曲量与裂纹三维统计作为最终判据,使孔压峰值、温度梯度与骨架强度之间的联系具备可验证性。与此同时,不同陶瓷体系的差异会进一步推动模型模块化:氧化物更强调固相烧结的致密化与晶粒长大控制,氮化物与碳化物则更依赖气氛与反应路径,要求在脱脂与烧结阶段显式处理氧分压/氮分压、挥发相生成与界面反应对孔道和收缩行为的耦合影响。

面向未来,陶瓷BJ模拟体系的成熟标志将是基准确化、可比对与可移植。建立开放的标准算例与数据集,使粉床铺展、单滴/多滴渗透、标准脱脂试样与标准收缩试样在统一指标下被重复验证,将显著降低模型在不同研究间的对照难度,并推动参数与边界条件的透明化。在此基础上,融合过程监测与数据同化的数字孪生^[124]将成为最具牵引力的方向:通过在线温度、黏结剂分解挥发气体与形貌信息实时修正模型状态,动态更新孔隙率、渗透率与烧结本构参数,把缺陷风险从“事后解释”前移为“过程预警”,并最终服务于工艺路径设计、尺寸补偿与质量一致性控制。

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Full-Process Numerical Modeling for Binder Jetting of Ceramics: Current Status, Challenges and Outlook

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Extended Abstract

Binder Jetting (BJ) additive manufacturing emerges as a promising forming process for fabricating geometrically complex ceramic components, including thin walls, internal channels, and topology-optimized features. The process achieves forming through the selective deposition of a liquid binder onto a powder bed, typically without involving a melt pool. Consequently, it is inherently compatible with high-melting-point, brittle ceramic powders and is less constrained by melt-related instabilities. Despite these advantages, achieving robust manufacturing remains challenging. Defects and variability rarely originate from an isolated processing step. They emerge from the interaction of a series of strongly coupled steps like powder spreading, binder deposition and infiltration, drying/curing and depowdering, thermal removal of organics (debinding), and sintering. Heterogeneities introduced early in the process chain are often transmitted and amplified, ultimately manifesting as non-uniform shrinkage, warpage, cracking, residual porosity, and property scatter. In this context, full-process numerical modeling is increasingly required, serving for mechanistic interpretation and for predictive process-window design.

This review consolidates recent advances on numerical modeling of ceramic Binder Jetting (BJ) and proposes an organizing principle to enhance the coherence and utility of the literature, framing the process chain through transferable state variables that quantify process inheritance. Modeling approaches are evaluated not as isolated stage-specific problems, but according to three dimensions, *i.e.*, 1) the specific physical quantities predicted; 2) the transferability of these quantities as consistent inputs to subsequent stages; and 3) the practicality of calibrating and validating the relevant quantities through accessible experiments. Key transferable state variables highlighted include the spatial distribution of powder-bed porosity and pore-size statistics; permeability and its directional dependence; local binder saturation and organic distribution in the green body; evolving transport coefficients and gas-generation rates during debinding; and the initial relative-density and defect fields that control densification and shape evolution during sintering. Centering on these variables enables an explicit clarification of inter-stage coupling logic and charts a path toward engineering-grade predictability.

Powder spreading modeling defines the initial mesoscale structure controlling all downstream responses. The discrete element method (DEM) is widely adopted as it enables the direct representation of particle rearrangement, contact interactions, and localized compaction under blades or rollers. The existing studies demonstrate that particle size distribution, morphology, cohesion, layer thickness, and recoater kinematics jointly regulate bed density, surface roughness and structural anisotropy. For full-process simulation, key advantage of DEM converts these attributes into downstream-ready descriptors-including porosity maps, pore-network statistics and anisotropic permeability closures.

Binder deposition and infiltration determine the saturation field and organic distribution, which simultaneously control green body strength and subsequent gas evolution. At the component level, Darcy-type infiltration models remain an effective tool for

rapidly exploring printing conditions. When permeability and capillary effects are expressed through measurable parameters (*e.g.*, viscosity, surface tension, and wetting), these models can be enhanced to incorporate drying, evaporation, and curing/solidification kinetics. When pore-scale interfacial dynamics and droplet impact dominate, higher-resolution approaches are required. Interface-capturing computational fluid dynamics (CFD) and lattice Boltzmann method (LBM) simulations have been used to resolve transient interfaces and flow pathways in complex pore geometries, while coupled DEM-CFD frameworks have been introduced to capture infiltration-induced particle rearrangement in fine powders.

Debinding is typically the most failure-prone stage since gases generated by binder decomposition must vent through a pore network while the solid skeleton remains weak and thermally stressed. Consequently, predictive modeling necessitates a coupled treatment of reaction kinetics, transport and mechanical response. Decomposition kinetics is typically constrained through thermogravimetric analysis (TGA), commonly implemented with multi-step schemes that represent complex degradation pathways. Gas transport is treated through diffusion, convection, and pressure-driven Darcy flow, with permeability and effective diffusivity evolving with porosity and temperature. Coupled heat and mass transfer in actual geometries can be solved through the finite element method (FEM) implementations, with a failure risk evaluated by relating pore pressure, strength reduction, and constrained deformation.

Sintering consolidates the debound microstructure and determines densification, grain growth, and macroscopic shape change. Continuum constitutive laws embedded within FEM remain a dominant route for component-scale prediction, providing that temperature-dependent viscosities/creep parameters are calibrated and initial relative-density fields are supplied. These models are essential for predicting anisotropic shrinkage and warpage induced by inherent heterogeneity. In the microstructural scale, the Monte Carlo Potts models and phase-field approaches reveal the mechanisms of neck growth, pore evolution, grain-boundary migration, and coarsening. Despite high computational cost, they provide a basis for reduced-order kinetics and constitutive relations applicable to engineering-scale simulations, linking fundamental mechanisms to manufacturability.

A consistent thread across all stages is that predictive capability relies on effective parameter identification and validation. Accordingly, this review recommends establishing a validation matrix aligned with transferable variables. Powder spreading should be validated *via* bed density, surface roughness, and anisotropy metrics; infiltration *via* penetration depth, saturation mapping, and spatial green strength, debinding *via* multi-rate TGA/DTG constraints, independent characterization of pore-network evolution, and statistical measures of cracking/distortion as well as sintering *via* shrinkage anisotropy, warpage, final density, and defect populations. Designing validation around variables required for downstream transfer allows uncertainty to be localized and gradually reduced, thus avoiding implicit redistribution across the chain.

Summary and Prospects Future developments in the field are likely to follow three main trajectories. First, standardized definitions and transfer rules for transferable variables are required to reduce inconsistencies among models and to support reproducible coupled workflows. Second, the integration of uncertainty-aware calibration and sensitivity analysis into process-window design is warranted as fundamental constitutive relations and kinetic parameters are constrained by measurement limitations and condition dependence. Third, integrated workflows combining high-fidelity simulation, reduced-order modeling, and data-driven surrogates are essential for fast component-scale screening and optimization. Driven by these advances, full-process modeling can evolve from retrospective interpretation toward prospective control of process–structure–property linkages in ceramic BJ, thereby improving reliability, dimensional fidelity, and performance consistency across diverse material categories.

Keywords additive manufacturing; binder jetting; multiscale simulation; performance prediction