SAMPLE: A Software Suite to Predict Consolidation and Microstructure for Powder Bed Fusion Additive Manufacturing

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Powder bed fusion comprises all layer-by-layer additive manufacturing technologies of parts built from a powder bed. To exploit the advantages of near-net shape manufacturing of complex geometries, in contrast to conventional manufacturing techniques, it is essential to understand the underlying physical phenomena occurring during processing for a broad range of different process scenarios. Experimental approaches are costly in time and material and provide only limited access inside the process. However, to understand the process behavior and predict final properties of parts, numerical approaches are powerful tools. This work presents the software suite SAMPLE (Simulation of Additive Manufacturing on the Powder scale using a Laser or Electron beam) which simulates the consolidation and microstructure evolution during beam-based powder bed fusion processes. It is based on a mesoscopic approach, in which statistical powder beds, melt pool dynamics, evaporation effects, and microstructure evolution are considered and can simulate the build-up of more than 100 layers. The underlying models and algorithms of the software including a newly applied thermal model are described. Finally, the unique potential of the software is demonstrated by reviewing the influence of various powder bed properties, the effects of evaporation, and the grain structure evolution in the process.

1. Introduction

Powder bed fusion (PBF) describes additive manufacturing (AM) techniques that form solid parts from a loose powder bed, usually in a layer-by-layer manner.[1] This is usually done by melting thin powder layers in predefined areas. The heat source used to selectively melt the powder is usually a deflected laser or electron beam.[2] Depending on the source, selective laser melting (SLM)[3,4] and selective electron beam melting (SEBM)[5] are the most common technologies. According to Wohlers report 2018, there is an increasing demand for these technologies: approximately 80% more AM machines were sold in 2017 than in 2016.[6]

Despite this demand, PBF processes are still challenging and require detailed knowledge about how various process parameters and strategies influence the final properties of parts: for example, residual stresses, porosity, surface roughness, and microstructure formation. One strategy for process optimization is to use in situ real-time measurement systems to adjust parameters during the process, to circumvent defects.[7–9] Nevertheless, for a controllable, predictable, and reliable process, it is necessary to understand the underlying physical mechanisms during powder deposition, melting, and solidification in each layer, to derive optimal process strategies. Experiments allow only limited access to quantities such as spatial temperature evolution, melt pool dynamics, and solidification pathways.

To support experimental observations, simulation is often the only way to obtain a deeper insight into the process. Furthermore, it provides the opportunity to study different effects independently from each other, which is rarely possible in experiments. PBF processes are modeled by several approaches, ranging from the powder and microstructure scale (mesoscale) to continuum descriptions (macroscale).[10] Continuum methods, such as finite elements (FE), are suitable for calculating stresses and resulting deformations on the scale of whole components, up to the range of meters. However, continuum methods cannot describe statistical effects caused by a random powder bed or melt pool dynamics. These effects are crucial for obtaining information about how, when, and where defects evolve. A variety of different mesoscale approaches exist,[11,12] which are capable of describing such effects.

The aim of this work is to give a comprehensive overview of our mesoscopic software suite SAMPLE (Simulation of Additive Manufacturing on the Powder scale using a Laser or Electron beam) for PBF processes. The software is based on a previous version,[13] which has been significantly improved in recent years. This article summarizes all individually published methods and models and their coupling within the software. In the first part, we outline the structure, workflow, and modules of...
the software, including the physical and numerical models. The core module of the software is used for modeling the melt pool evolution; this module uses a new thermal model, which is more stable to the previous one. Furthermore, the software incorporates a powder module for the powder bed, an absorption module for the beam source, an evaporation module for concentration changes, and a microstructure module for solidification and microstructure evolution. The second part reviews example applications for the influence of the powder bed and evaporation on process windows, and for the study of the grain structure evolution process.

2. SAMPLE

The software suite SAMPLE is designed to simulate beam-based PBF processes for all types of materials. Currently, metals and polymers are already considered. There exist three different implementations in the software suite: one in two dimensions and two in three dimensions. In this work, we focus on the most comprehensive version in two dimensions called SAMPLE2D. The 3D versions are briefly mentioned and referenced for further reading in Section 3 and 4.2.

The single steps of a PBF process are preheating, powder delivery, and melting. First, the powder particles of the complete upper layer are heated up to the preheating temperature. This step is only necessary for some PBF processes, such as the SEBM process. In the second step, the cross sections, according to the model design of the part, are melted. The hatching strategy is often used to deposit the beam energy during melting: the beam scans single lines of the desired area in alternating directions with a small line offset perpendicular to the scan direction. Once the beam has finished and the melt is solidified, the process platform is lowered by the layer thickness and the build cycle is repeated by starting with the distribution of a new powder layer.

2.1. Physical Effects

SAMPLE2D focuses on the simulation of the melting step, as shown in Figure 1a. The figure shows the temperature distribution in the melt pool and the solid material after melting of a hatching scan line perpendicular to the simulation domain.

A variety of different physical effects are covered. The most important are heat conduction, phase transitions between liquid and solid, evaporation, convection, capillarity, and wetting. During heating of the solid material, heat conduction is the main physical effect, which distributes the temperature from the source into the solid material. Because of the continuous absorption of the beam, the temperature increases and the material is melted. The applied absorption and reflection models depend on the beam source and the material. Evaporation, capillarity, and wetting forces convect the melt, which further spreads thermal energy. After melting, the material cools down and solidifies, and the final shape is determined.

Further effects, such as radiation, gravity, Marangoni convection, or solidification shrinkage, are not covered. High radiation rates, applying the Stefan–Boltzmann law at high processing temperatures, only occur locally and for very short durations where the material is molten. Marangoni forces arise from temperature or concentration dependencies of the surface tension. Marangoni forces are neglected because the software is designed to predict stable melt pools within the conduction or near keyhole melting mode. Once unstable keyhole melting is reached, Marangoni forces become important.[16] Gravitational forces are neglected because they are much smaller than the main driving forces (evaporation and capillarity).[16] Solidification shrinkage and thermal expansion are important effects because they are the reason for residual stresses and distortion. However, the applied numerical method is not able to model these effects, corresponding to constant and equal mass density in all phases.

2.2. Numerical Basics

The simulation domain is defined by a Cartesian grid with a spacing of $\delta x$. Typical spacings are between 1 and 10 $\mu m$ to resolve the smallest powder particles by at least five cells. This assumption is necessary to compute reliable surface normals and curvatures.[21]

Each cell of the grid has a certain state named cell type, as shown in Figure 1b.[22] In solid cells only heat conduction is solved, whereas both heat conduction and convection of the melt pool are computed in liquid cells. Gas cells are neglected during simulation and are therefore thermally isolating.
SAMPLE$^{2D}$ applies explicit solvers for the different physical effects. The most important effects of thermodynamics and hydrodynamics are solved by coupling volume of fluids and lattice Boltzmann methods.$^{[22]}$ Additional effects, such as evaporation and grain structure evolution, are modeled by finite difference or cellular automaton approaches.$^{[23,24]}$ The specific methods used are described in more detail in the following sections, which present the various modules.

2.3. Software Flow

Figure 2 schematically shows the SAMPLE$^{2D}$ software flow. At the beginning, the whole setup and simulation domain is initialized by reading the material data, process parameters and the geometry of the domain, the built part, and the beam scan path. After initialization, the powder is deposited; this is illustrated by one particle, showing the orientation of the grain structure regarding the build direction. During beam absorption, the beam position is adjusted at each time step, and the beam energy is deposited into the material. If the evaporation module is activated, thermal energy is lost during evaporation. Subsequently, the core functions of the software, the thermodynamics and hydrodynamics, are evaluated. Optionally, grain structure evolution during solidification is computed. The update procedure, starting with the beam absorption, is repeated until the beam path is finished. For each new powder layer, this update procedure is repeated. If the predefined number of layers is built, the simulation is finished. The small images on the right show schematically the melting and solidification of the particle on the base plate, within three time steps.

3. Core Modules

The core modules are mandatory modules for simulating the consolidation during PBF. They comprise the functions for adding a powder bed, absorbing a beam source, and for thermodynamics and hydrodynamics, including phase transitions. The core modules are also implemented with few modifications in a 3D software called SAMPLE$^{3D}$. Due to the high computational demand, no additional modules are implemented and a special high performance platform designed for supercomputers$^{[23]}$ is used. Further model details$^{[19]}$ and applications$^{[26]}$ on PBF are published.
3.1. Powder Module

The powder module ensures the deposition of a random powder bed, with a nominal powder layer thickness, onto the current surface. Therefore, each individual powder particle is placed by maintaining a specified powder size distribution and powder bulk density at the end of deposition. The simulation only considers circular powder particles with a defined diameter normally between 10 and 150 μm. After deposition, the particles are completely rigid in the solid state.

3.1.1. Powder Size Distribution

The powder size distribution used in the software depends on the material and powder used in experiments. Generally, all types of size distribution can be used, for example, bimodal distributions. Normally, the powder size distribution used has a logarithmic Gaussian shape (monomodal).\(^{\text{[27]}}\) It is based on discrete experimental measurements of the distribution, where the distribution is interpolated stepwise in a linear fashion.\(^{\text{[28]}}\)

3.1.2. Powder Bed Generation

The powder deposition algorithm\(^{\text{[22]}}\) is based on the rain drop model for random packing with multiple restructuring.\(^{\text{[29]}}\) To create the powder bed, a particle is generated at a random horizontal position above the current maximum powder height. The size of the particle is chosen based on the predefined powder size distribution. The particle falls downward until it hits solid material. Subsequently, it additionally minimizes its potential energy by rotating around its circumference until the lowest possible vertical position for this particle is reached. Particles with their center above the maximum powder height are removed. The particle deposition is repeated until the powder layer between a specified minimum and maximum height

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**Figure 2.** Flowchart of SAMPLE\(^{\text{[24]}}\) including thumbnail images showing the temperature distribution in liquid material and either the temperature distribution or the grain structure with misorientation to the build direction in solid material. Each simulation starts (after the initialization step) with the application of a powder layer. During beam absorption the material is heated. The evaporation step computes the energy and mass loss as well as the exerted recoil pressure on the surface. During thermodynamics and hydrodynamics, heat is conducted and the melt pool moves because of exerted forces. In the final step the melt pool solidifies and the grain structure evolves. Depending on the beam movement, melt pool state and number of layers, it is decided, whether the simulation exits or continues in the loop.
(layer thickness) is filled and no new particles can be added. The density needs to be adjusted, by removing particles from the powder bed, because the rain drop algorithm produces much denser packings in two dimensions than experimental values. To achieve this, particles are removed randomly from the current powder layer until a predefined powder bulk density is reached.

3.2. Absorption Module

The lateral energy distribution of the beam is assumed to be a 2D Gaussian with a defined width of 4 times the standard deviation of the Gaussian. As the beam moves through the simulation plane, the 1D section through the Gaussian is calculated for each time step. In general, the direction of the beam movement to the simulation plane is arbitrary. The two normal use cases are in-plane and out-of-plane movement.\(^{[10]}\) The in-plane movement applying an averaged 1D Gaussian distribution is suitable to study single-line effects during processing.\(^{[10,31]}\) However, the in-plane movement neglcts the main heat distribution perpendicular to the beam movement (that is the heat conduction out of the simulation plane). This would overestimate the heat preserved along the melt line. Therefore, the temperature predictions are more accurate the higher the angle between beam direction and simulation plane is. The recommended beam direction is consequently perpendicular to the simulation plane. This beam direction is also necessary to study the effects of hatching strategies like different line offsets.

3.2.1. Electron Beam

The electron beam can only be applied to metals because the material needs to be electrically conductive to discharge the absorbed electrons. When electrons impinge on metal, they are either backscattered, transmitted, or absorbed until a certain depth, the mean penetration range, is reached. The absorbed energy at a certain depth is calculated from an empirical model.\(^{[10]}\) This depends on the electron energy, acceleration voltage, and material properties such as atomic number, atomic weight, and bulk density.

3.2.2. Laser Beam

A laser source can be applied for metals and polymers. Here, the reflectance of the surface is important because only a small amount of the laser is directly absorbed, whereas the rest is reflected, transmitted, or refracted. The current ray-tracer model is applied on a subgrid that simulates the laser pathway caused by reflection and reflectance (between solid and fluid) in the material.\(^{[32]}\) For metals, the transmitted part of the laser is absorbed in the first material cell because the penetration depth of a laser is much smaller than the standard grid resolution of a few microns. In contrast, the transmitted laser part inside a polymeric powder particle has the potential to escape the particle, to be reflected and refracted again.

3.3. Thermodynamics and Hydrodynamics Module

The core module of the simulation software comprises basic methods for melting and solidification, hydrodynamic movement and heat convection, and conduction. The governing equations are solved on a Cartesian grid, applying a free surface lattice Boltzmann method.\(^{[15]}\)

3.3.1. Physical Model

Three conservation equations have to be satisfied within the model: the conservation of mass, momentum, and energy. For an incompressible fluid, the conservation of mass can be written as

\[
\nabla \cdot \mathbf{u} = 0 \quad (1)
\]

where \( \mathbf{u} \) is the fluid. Conservation of momentum is described by the Navier–Stokes equation

\[
\frac{\partial \rho \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \rho \mathbf{u} = -\nabla p + \mu \nabla^2 \mathbf{u} \quad (2)
\]

where \( \rho \) is the density, \( t \) is the time, \( p \) is the pressure, and \( \mu \) is the dynamic viscosity. Both equations are only solved in the liquid melt pool. Conservation of energy in the solid and liquid material is described by the convection–conduction equation for the specific enthalpy \( h \)

\[
\frac{\partial h}{\partial t} + \mathbf{u} \cdot \nabla h = \nabla \cdot \left( \frac{\lambda}{\rho c_p} \nabla h \right) + S_h \quad (3)
\]

where \( \lambda \) is the thermal conductivity, \( c_p \) is the heat capacity, and \( S_h \) is a thermal source or sink term (e.g., beam absorption or evaporation losses).

3.3.2. Numerical Model

To compute the hydrodynamic movement of the liquid and interface cells, the lattice Boltzmann method is applied. This method does not solve Equation (2) directly, but solves the Boltzmann equation on a 2D lattice for particle distribution function \( f_i(x, t) \). The distribution function defines the probability of finding a particle at a specific position \( x \) and time \( t \) with a certain velocity inside a specific volume. The index \( i \) refers to one of the nine discrete velocities \( \mathbf{c}_i \) of the stencil D2Q9. The time is discretized by the time step \( \delta t \). The time evolution of the distribution function reads\(^{[13]}\)

\[
f_i(x + \mathbf{c}_i \delta t, t + \delta t) = f_i(x, t) - \frac{1}{\tau_f} \left( f_i(x, t) - f_i^\text{eq}(x, t) \right) \quad (4)
\]

where the first term of the right-hand side represents streaming of material from one cell to another. The second term of the right-hand side is the collision term, which produces the relaxation of the distribution function towards its equilibrium \( f_i^\text{eq} \).\(^{[14]}\) with the relaxation time constant \( \tau_f \). Equation (4) fulfills the Navier–Stokes equation with the relation between relaxation time, viscosity, and resolution given by
The relation
\[ t_f = \frac{1}{c_{e}^{2} \rho} + 0.5 \delta t, \quad c_s = \frac{\delta x}{\sqrt{3} \delta t} \]  
(5)

The macroscopic quantities \( \rho \) and \( u \) are calculated as moments from the distribution functions
\[ \rho = \sum_i f_i, \quad \rho u = \sum_i c_i f_i \]  
(6)

To ensure mass conservation, a volume of fluid approach is applied, whereby mass is interchanged between neighboring cells within the liquid phase.[22]

To solve the energy conservation equation, the passive scalar approach of Zhang et al.[14] is applied for the enthalpy density \( h \), instead of the temperature. The time evolution of the enthalpy distribution functions \( h_i \) is given by
\[ h_i(x + c_i, t + \delta t) = h(x, t) + \left( 1 - \frac{1}{c_{e}^{2} \rho} \right) \phi_i(x, t) + \Psi(x, t) \]  
(7)

\[ \phi_i(x, t) = \frac{c_i - u(x, t)}{c_{e}^{2} \rho} \sum_j c_j f_j(x, t) \left( h_j(x, t) - h(x, t) \right) \]  
(8)

The equation for the macroscopic enthalpy
\[ h = \frac{1}{\rho} \sum_i f_i h_i \]  
(9)

serves additionally as the equilibrium distribution. The energy of the beam source or evaporation losses are applied by \( \Psi \). The term \( \phi_i \) can thus be described as the relaxation of the non-equilibrium proportion of the distribution functions. Applying the Chapman–Enskog expansion, Equation (7) is related to the heat convection–conduction (3) by the thermal relaxation time
\[ \tau_h = \frac{\lambda}{c_{e}^{2} \rho c_p} + 0.5 \delta t \]  
(10)

This model replaces the passive scalar approach,[15] which was previously applied. This modification significantly improved the stability of the software, especially in the interface region. The stability improvement results from the incorporation of the hydrodynamic distribution function \( f_i \) in the thermal model. Consequently, no thermal fluctuations are induced by surface stresses; this was the case in the previous approach and was a possible reason for simulation instabilities.

3.3.3. Boundary Conditions

The lattice Boltzmann method and the passive scalar approach require a full set of distribution function values after streaming to neighboring cells. However, gas cells are neglected and hydrodynamics are only computed in liquid cells. Therefore, neighboring cells lack these distribution function values, and they need to be reconstructed before the collision is computed.

Regarding hydrodynamics, the no-slip boundary condition between solid and liquid cells is achieved by a bounce-back method; the missing incoming distribution function value is initialized by the outgoing distribution function value.[23] In interface cells, the unknown incoming distribution functions from the gas phase must be reconstructed from the distribution functions of the surrounding fluid that are known.[15] The force that the fluid exerts on the surface is calculated from distribution functions and the surface velocity. The missing distribution functions are computed by the equality of this force to all other surface forces from the gas phase (such as gas or evaporation pressure and surface tension). At the triple point between gas, solid, and interface, the wetting force is considered as a local variation of the capillary force that depends on the deviation between the local contact angle and the equilibrium contact angle.[21]

There are two kinds of boundaries applied for thermodynamics. At the bottom of the simulation domain, the temperature is held constant, that is, the missing value \( h_i \) can be directly computed from the temperature.[34] Between interface or solid cells and gas cells, we assume an isolating boundary, which is calculated via the bounce-back method because of the complex interfaces that can occur between powder particles.

3.3.4. Phase Transformations

For phase transformations, melting and solidification are considered, whereas the gas phase is treated as a noninteracting phase. A phase transformation occurs when a cell passes the temperature threshold value which corresponds to a specific solid fraction of 55%. The solid fraction is assumed as a linear interpolation between solidus and liquidus temperature.[15] The relation between temperature and specific enthalpy is given by[22]
\[ h = \int_0^T \tilde{c}_p(T) dT \]  
(11)

where \( \tilde{c}_p \) is an effective specific heat capacity that includes the latent heat of melting \( l \).[22]
\[ \tilde{c}_p = \begin{cases} c_{p,s} + \frac{l}{T_{l} - T_{s}} & \text{for } T \leq T_{l} \\ c_{p,s} + \frac{l}{T_{l} - T_{s}}(T_{s} - T_{l}) + L(T_{l} - T_{s})^{-1} & \text{for } T_{s} < T \leq T_{l} \\ c_{p,s} & \text{for } T_{l} < T \end{cases} \]  
(12)

The heat capacities in the solid phase \( c_{p,s} \) and the liquid phase \( c_{p,l} \) are approximated as constants. To keep the relationship between temperature and enthalpy reversible, a liquidus and solidus temperature has to be assumed for pure materials as well.

4. Additional Modules

The additional modules are optional. On the one hand, they provide additional information about element distributions and grain structure, but on the other hand they increase the computational effort. These modules are only applicable for metals and alloys.

4.1. Evaporation Module

Evaporation mostly occurs during melting with high beam powers. The resulting effects (Figure 1c) include a repulsive evaporation recoil pressure on the melt pool surface, as well
as mass and temperature losses.\cite{23} In case of in-plane movement, high evaporation pressures lead to an unphysical material accumulation in front of the melt pool. Therefore, the evaporation module requires a beam movement perpendicular to the simulation plane. If an alloy contains volatile elements, the evaporation also has an effect on the local alloy concentration.\cite{16} A low influence of the concentration changes regarding the overall thermo- and hydrodynamic calculations is assumed, i.e., the material parameters are applied for the base alloy.

### 4.1.1. Evaporation

Because the gaseous phase is not explicitly simulated, the evaporation module does not perform a full modeling of the liquid gas transition; instead, only the effects of evaporation on the fluid are considered. This encompasses the energy loss, mass loss, the concentration change, and evaporation recoil pressure on the fluid surface, which are all dependent on the particle flux that leaves the fluid (Figure 1c). In the multicomponent model, the particle flux off the fluid surface of each element $\alpha$ is\cite{36}

$$ f^\alpha = \chi^\alpha \gamma^\alpha \rho_e^\alpha(T_s) \frac{m_\alpha^\alpha}{2\pi k_B T_s} $$ \hspace{1cm} (13)

The product of the mole fraction $\chi^\alpha$ and the activity coefficient $\gamma^\alpha$ is the component’s activity. If evaporation is not regarded selectively, the value is one and the model reduces to the single-component evaporation model.\cite{23} The latter part of the formula is the Hertz–Knudsen formula for evaporation. It contains the saturated vapor pressure $p_v^\alpha$, the fluid’s surface temperature $T_s$, the atomic mass of the component $m_\alpha^\alpha$, and the Boltzmann constant $k_B$. The saturated vapor pressure is calculated from the Clausius–Clapeyron equation.\cite{36}

However, not all of the particles that leave the fluid surface also leave the Knudsen layer above it. Some are back-scattered into the fluid. Therefore, the evaporation flux is multiplied by a recondensation coefficient $\phi^\alpha$. This coefficient is, in general, dependent on temperature and the surrounding pressure. For vacuum conditions (e.g., in SEBM), the assumption $\phi \approx 0.82$ is valid.\cite{30}

From the net flux leaving the Knudsen layer, the mass, energy, and concentration loss can easily be calculated. Because particles that do not leave the Knudsen layer are reflected back on the surface, the recoil pressure depends not only on the vapor pressure but also on the pressure in the Knudsen layer. For each interface cell, the mass loss is applied as a change of the cell’s filling rate. Energy loss is added as a sink in the energy calculation (Equation (3) and (7)), and the recoil pressure is added to the ambient pressure for the hydrodynamic boundary condition.

### 4.1.2. Concentration Distribution

The concentration distribution inside the melt pool is important for selective evaporation and indispensable for monitoring element loss during manufacturing. Because powder is prealloyed, an initial constant mass concentration $c_0$ of the main evaporating element is assumed. Because we calculate the mass losses of the matrix and the most volatile element of the alloy, the concentration change in one interface cell can be calculated from the different mass losses. These changes in concentration are distributed inside the melt pool according to the convection–diffusion equation. Here, convection dominates because of low diffusion coefficients inside the fluid ($D = 10^{-9} - 10^{-7} \text{m}^2 \text{s}^{-1}$).\cite{18} Therefore, we apply a passive scalar transport algorithm that takes advantage of the fluid distribution functions known from the hydrodynamic calculation.\cite{36} The mass change of one cell into its neighboring cell in direction $\theta$ is $\delta m = f_{\theta}(x) - f_{\theta}(x + \delta t)$, where $i$ denotes the direction opposite to $\theta$. If the mass change is negative, concentration streams out of cell $x$ and into the adjacent cell. Otherwise, if $\delta m > 0$, concentration is distributed from the neighbor into the cell itself. The full concentration change is given as the sum over all directions

$$ c(x, t + \delta t) = c(x, t) + \sum_{\theta} \begin{cases} \delta m_{\theta} & \text{if } \delta m_{\theta} \leq 0 \\ m_{\theta}(x, t + \delta t) & \text{if } \delta m_{\theta} > 0 \end{cases} \frac{c(x + \delta t, t) - c(x, t)}{\delta t} $$ \hspace{1cm} (14)

The method does not prevent numerical broadening of distributions, but keeps it to areas where material is mixed anyway because of high fluid velocities.\cite{37} Because the diffusion coefficient is even lower in solid cells ($D = 10^{-15} - 10^{-19} \text{m}^2 \text{s}^{-1}$), the concentration in all solid cells is kept constant.

### 4.2. Microstructure Module

The microstructure module provides the opportunity to gain information about the grain structure evolving in PBF processes for cubic crystal lattice structures without solid–solid phase transition. Figure 1d shows a growing grain structure inside the melt pool, with some schematically drawn dendrites and their square approximations. The algorithm modeling crystal growth is based on a cellular automaton model.\cite{38} When using the microstructure module, solidification of cells is controlled by the growth algorithm and not by the solid fraction. Melting of cells is not affected by the module.

The algorithm is implemented in the 2D software SAMPLE\cite{22,24} as well as in a standalone 3D software called SAMPLE\textsuperscript{GS}.\cite{19} In three dimensions, an analytical heat solver is applied on a continuum description of each layer neglecting the powder bed. These simplifications are necessary to allow large-scale simulations based on a high performance implementation for supercomputers.

### 4.2.1. Numerical Model

The so-called 2D decentered squares algorithm allows the description of dendritic growth of materials with a cubic crystal structure. The crystal growth is only considered for the main growth directions, which are the (100) directions in the cubic lattice and the (10) directions in 2D. Therefore, a dendrite in a 2D lattice has the main growth directions: [10] and [01]. The dendritic shape is approximated by a square, where the four corners represent the dendrite tips of the corresponding main growth directions. The square is characterized by its size (expressed by its half diagonal length ℓ), the grain orientation angle, and an identification number (ID) that specifies the grain
to which the square belongs. All cells with the same grain ID compose one grain. The temporal evolution of \( L \) is described by

\[
L(x, t + \delta t) = L(x, t) + v(\delta T(x, t))\delta t
\]

where \( v \) is the dendrite tip velocity. Based on the columnar growth model, the dendrite tip velocity \( v \) is a function of local undercooling \( \delta T \). This relationship is normally simplified as a polynomial expression

\[
v = \sum_{j=0}^{N-1} a_j (\delta T)^j
\]

with a polynomial of order \( N \) and coefficients \( a_j \). In addition, other expressions (e.g., power laws) are possible. The velocity model can have a substantial influence on the solidification pathway and final grain structure. A so-called active cell is solid, has at least one liquid neighbor and contains a growing square. If the growing square of an active cell overlaps with the center of an adjacent liquid cell, the latter cell is captured and inherits the grain ID and orientation from the active cell. The new square is set in such a way that two sides of the growing square and the captured square are aligned and the corner of the growing square nearest to the center of the captured cell overlaps. A liquid cell can be captured in one time step by different adjacent active cells. In this case, the cell is captured by the faster growing cell. If an active cell no longer has a liquid neighbor, it becomes inactive.

### 4.2.2. Initialization

To initialize the grain structure in a solid base plate at the beginning of a simulation, a nucleus base plate density is defined. Based on this density, randomly oriented squares with zero size are placed in the middle of random cells in the base plate. Subsequently, these cells grow with a constant velocity until the whole base plate has been captured. Thus, using the nucleus base plate density, it is possible to control the grain size in the base plate. Equivalently, a nucleus powder density is defined and the grain structure of particles in a newly added powder layer is generated.

### 5. Applications

**SAMPLE** was successfully applied to investigating several aspects of beam-based PBF processes, of which we outline some SEBM examples here. Numerical predictions are only useful, when the applied software was previously validated with experimental results. Four different SEBM machines (Arcam AB: Arcam A2, A2X, Q10, ATHENE (modified S12)\(^{[7]}\)) are applied to manufacture test samples and parts of various alloys (titanium, nickel, or aluminum alloys). A bunch of measurement devices allow to detect porosity, layer binding defects, alloy concentration, and microstructure. These measurements are compared with numerical results to determine the accuracy of the numerical predictions for single-line melting up to process windows.

One goal for a specific material is to determine process windows: defined parameter ranges in which reproducible and desirable results can be obtained. The points of interest can differ between applications. First, parameter sets for producing dense parts for maximum load-bearing capacity are investigated (Figure 3a left). Increasing energy input generally increases the part density, although excessively high energy inputs cause evaporation and build failures. Volatile elements strongly evaporate for high surface temperatures, and decrease the homogeneity of the alloy (Figure 3a right). Furthermore, because of high evaporation pressures, the surface roughness and final porosity increase. Thus, there is always a minimum and maximum energy applicable, which spans the process window. A third property is the final microstructure (Figure 3b). This can vary from single crystalline over columnar to equiaxed structures. Scan strategies can alter the growth direction of columnar grains because of varying heat transport. Therefore, tilted columnar grains with varying anisotropic properties in certain directions are possible.

### 5.1. Powder Bed Effects

One essential aim during PBF is to minimize porosity, to ensure optimal mechanical properties. Generally, three different types of porosity features occur: single- and multilayer binding faults and gas pores. Multilayer binding faults can include up to hundreds

![Figure 3. Sketch of different process window properties. a) By increasing the deposited energy, the porosity decreases until the porosity limit is reached and the process window is entered. By applying too much energy, the top surface becomes uneven and no new powder layer can be applied. This build failure marks the upper boundary of the process window. Different concentrations of the most volatile element are caused by different evaporation rates. b) For a constant build rate and area energy density (circles in process windows in a), different grain structures can be adjusted by changing the process parameter combinations (denoted by P-A, P-B, and P-C) or the scan pattern rotation in each layer (CS1) or in every tenth layer (CS10).](image)
of layers and produce channel-like cavities. The reasons for the formation of such channels were identified and demonstrated with the software. After a successful validation, in comparison with experiments, the software was applied to predicting further process windows with modified process conditions. Thus, the influence of the powder bulk density and powder size distribution were altered to increase the process window. One key factor in the simulations is that it is possible to isolate different properties, such as powder bulk density and powder size distribution, which are naturally related, and study how, and to what extent, they influence the process.

As an example, Figure 4 shows a comparison between experimental microsections and corresponding simulations for Ti–6Al–4V. An overall sample size of 5 × 5 mm² with 100 layers is required to gain an impression of the statistical occurrence of defects. The beam power is varied by keeping the scan velocity and line offset constant. The experimental porosity and porosity features, such as multilayer (a, d) and single-layer binding faults (b, e, f), were reproduced with the software.

An increase in the powder bulk density results in a decreased porosity for a constant powder size distribution. This results in lower energy inputs needed for eliminating porosity and finally extends the process window. Similarly, the powder size distribution was varied for a constant powder bulk density. With a decreasing mean particle diameter, the probability of binding faults decreases. The effect on process windows is comparable with the increase in powder bulk density.

5.2. Evaporation Effects

Some alloys are prone to evaporation of volatile elements. The consequences are concentration inhomogeneities, which result in anisotropic material properties and, in the worst case, promote local part failure. In particular, in the high line energy regime of process windows, the additional energy is mainly lost in evaporation, and only a small proportion increases the amount of remelting consolidated material. To avoid these disadvantageous effects, modified process strategies need to be developed. Our single-component numerical model was validated with experimental data and applied on different acceleration voltages. Here, higher acceleration voltages were beneficial because they reduce evaporation.

The multicomponent model was applied on Ti–48Al–2Cr–2Nb sample cubes with different beam velocities and line offsets, and constant beam power and area energy. Here, the new heat solver resulted in more stable numerical simulations and allowed coarser grid and time resolutions. The excellent agreement

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**Figure 4.** Comparison between experimental microsections a–c) and simulation d–f) for Ti–6Al–4V (cubes with 15 × 15 mm², different area energies, scan speed 20 m s⁻¹, line offset 50 μm). The depicted areas have 5 × 5 mm² base area. Several defects are highlighted and magnified in the insets: multilayer binding faults a,d), single-layer binding faults b,e,f), and gas pores c). Reproduced under the terms of the CC BY 4.0 license. Copyright 2017, MDPI AG.
between experiment and simulation is shown in Figure 5. The main influence on the evaporation rate was found to be the peak melt pool temperature, which is a quantity only available through simulations. High beam velocities and low line offsets reduce the peak temperatures, and consequently the aluminum loss, significantly.\[42\]

5.3. Solidification Microstructures

The solidification microstructures of PBF samples range from equiaxed over columnar to single crystalline. Different process parameters and strategies influence the microstructure, and accordingly the mechanical properties. For example, columnar grains arranged along certain directions in different regions establish anisotropic local properties for different loading conditions. The goal of the microstructure module is to reveal process strategies to tailor the microstructures locally.\[43\]

Figure 6 shows the comparison of simulation and experimental results for a cylinder sample made of CMSX-4. The 3D results are computed with SAMPLE\[44\]. All types of orientations are present in the powder particles and the polycrystalline base plate. During solidification, aligned grains (with respect to the build direction) overgrow grains with high misorientations in the center part of the sample. In this area, the mean temperature gradient points along the build direction and a columnar grain structure evolves. At the side walls, new orientations from partially molten particles can penetrate into the sample because the direction of the temperature gradient is different here. The evolution of the columnar structure with grain selection and new grain formation from partially molten powder are in good agreement with experiments.\[44\]

6. Conclusions

In this work, the software suite SAMPLE for simulating beam-based PBF processes was described. The mesoscopic models implemented in SAMPLE\[2D\]—the core module with powder deposition, beam absorption, and hydrodynamics and the add-on modules for evaporation and microstructure—were presented. Various materials (metals, alloys, and polymers) and different beam sources (electron and laser) are available. The 3D
implementations SAMPLE\textsuperscript{3D} and SAMPLE\textsubscript{2D} are briefly introduced and referenced.

In addition, several successful applications of the software have been revisited to demonstrate the simulation capability. SAMPLE\textsuperscript{3D} reproduces the porosity of parts quantitatively as well as qualitatively (porosity features) from experiments. Therefore, it is possible to validate and predict process windows for dense parts without build failures. Here, the software enables the different effects resulting from different powders, machines, beam sources, process parameters, or materials to be studied. Furthermore, the evaporation of volatile elements, such as aluminum in titanium alloys, was shown. This module enables the prediction of process windows for more homogenous parts with reliable and reproducible properties. Finally, we described the grain selection process during solidification, which captures the epitaxial columnar growth in PBF processes. Predicting the final grain structure enables the local part properties to be tailored by modified process strategies. Thus, the software has proven its extensive support for understanding various effects during manufacturing and for improving the process for achieving better part properties.

Some aspects of the software have been omitted from this article and will be published separately in future work. A grid-coarsening algorithm has been developed and implemented in the software, to decrease simulation times. The elaborated laser beam model for polymers has already been extended for metals and alloys. In addition, the microstructure module has been extended by a nucleation model to improve predictability and to produce equiaxed grain structures in simulations. The concentration module is currently under development for further multimaterial functionality. Changes in the alloy concentration have to be coupled to the thermo- and hydrodynamics computations by concentration and temperature-dependent material parameters, such as solidus and liquidus temperatures. In addition, Marangoni forces may become important for high concentration changes. Furthermore, the conservation equations are currently under review to account for mixing during melting and advanced solidification effects. The final goal is to establish a multimaterial model for mixed powder beds of different materials.

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Conflict of Interest

The authors declare no conflict of interest.

Keywords

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