

Article

Model of the Selective Laser Melting Process-Powder Deposition Models in Multistage Multi-Material Simulations

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Featured Application: This holistic model for full-scale modeling of the selective laser melting process can be applied for the study, development, and design of multi-material processes. It can be adapted to other powder-bed fusion processes.

Abstract: This paper presents one of the final stages in the development of a holistic model of the selective laser melting (SLM) process. The holistic model developed previously allows for modeling of only one stage of SLM, which limits simulations to one cycle with one material. The lattice Boltzmann method is applied for simulation of laser treatment, melting, fluid flow, and solidification. Several models of powder bed generation were developed within the framework of the holistic model and are described in this paper. They were developed on the basis of static and dynamic physical principles with the use of cellular automata, their own code, and the Unity[®] platform. They employed continuous and discrete particle representation and incorporated a model of powder deposition with particles of atomized or arbitrary shape. The closing of the external simulation circuit, which contains the powder bed generation model, cycle initialization, its realization by the model based on the Lattice Boltzmann Method (LBM), and the powder removal model, allows us to finish one simulation cycle of laser treatment and initialize the next, thereby enabling multistage multi-material simulations. The simulation results of the multistage SLM process with the Ti-6Al-V alloy and bioactive glass are presented in this paper. These simulation results confirm the possibility of modeling several SLM stages with two different materials. The holistic model can be used for simulation, design, and optimization of multistage, multi-material SLM processes.



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1. Introduction

This paper is a continuation of a project connected with biotechnologies, e.g., for the manufacture of bioresorbable scaffolds in tissue engineering for the repair of skeletal defects. Additive manufacturing (AM) or 3D printing methods enable effective control over the structure of the scaffold, which in turn dictates the geometry of the newly formed tissue. The ability of AM to manufacture anatomically shaped scaffolds with designed structures made of biocompatible, bioactive, and bioresorbable composite materials at high filler loadings allows the fabrication of scaffolds with a high degree of geometric complexity and enables the direct conversion of the digital representation of any object into its physical realization. These methods also enable the development of tissue and patient-specific reconstruction strategies.

Products consisting of materials of different mechanical and thermal properties can be manufactured in several stages. For example, first, a material melted at a higher temperature forms a matrix, and then materials with a lower melting temperature fill the matrix. However, often the final products with a complicated shape and requirements for properties (for example, porosity) cannot be produced in several stages with one

material, but must be produced in one stage or multiple stages with different materials. The development of such a multi-material process was defined as the main goal of this project.

Among the different branded powder bed fusion (PBF) techniques of AM, selective laser sintering (SLS) and selective laser melting (SLM) appeared to be the most useful and suitable methods to develop such a multi-material process. The SLS and SLM processes are very similar. During the SLM process, the powder is completely melted by a high-energy laser, with consequent solidification into the final product in a layer-by-layer method. The mechanical properties of the final product are close to those of the products manufactured by the conventional method. In contrast, during the SLS process, the powder is not melted but softens to a state at which the particles sinter together. A choice between SLS and SLM depends mainly on the material properties. The SLS process is more difficult for modeling; therefore, attention was focused on the development of the platform for modeling the SLM process from the perspective of joining SLS.

Reviews on modeling and simulations of AM including laser PBF and SLM can be found in [1–4].

Probably the first analysis and simulation of single layer formation by SLM was performed by Matsumoto et al. [5]. They calculated the distribution of temperature and stress within a single metallic layer using two-dimensional finite element methods (FEMs) with very low resolution. Next, Contuzzi et al. [6] simulated the powder–liquid–solid change by measuring the temperature of the nodes and evaluating the distribution and evolution of the temperatures in the SLM process. Another simulation was performed by Hussein et al. [7]. Their study used 3D FEM simulation to investigate the temperature and stress fields in single 316L stainless steel layers built on the powder bed without support in the SLM and using code developed in ANSYS. A simulation of temperature fields during the SLM of AlSi10Mg powder was carried out by Li and Gu [8] using FEM. The effects of laser power and scan speed on the SLM thermal behavior were investigated. Then, Yuan and Gu [9] applied the 3D finite volume method (FVM) model to investigate the temperature evolution during SLM of a TiC/AlSi10Mg nanocomposite. SLM experiments were also conducted. Some important physical phenomena, such as the transition from powder to solid, nonlinearities produced by temperature-dependent material properties, and fluid flow, were taken into account in the calculation. Masoomi et al. [10] developed a continuum-scale 3D FEM model to simulate the temperature response of a Ti-6Al-4V in a two-layer parallelepiped during laser powder bed fusion. The model was also validated. Kollmannsberger et al. [11] developed a hierarchical computational model for moving thermal loads and phase changes. The model was based on hp-finite elements, which varied the size of the element and the high polynomial degree because of strong gradients. The mesh was refined towards the entire laser path and kept fixed at all time steps. Luo and Zhao [12] surveyed the temperature and thermal stress fields of SLM/SLS and electron beam melting (EBM).

Khairallah and Anderson [13] developed a 3D mesoscopic model to simulate selective laser melting processes using the ALE3D multiphysics code. They studied the laser-induced melting of a random bed of 316 atomized stainless steel particles on a solid substrate and its solidification. The simulations were used for further powder homogenization. Gürtler et al. [14] developed a transient three-dimensional (3D) beam-matter-interaction model to simulate the process dynamics of laser beam melting of metals in the powder bed. The simulations were realized by the software OpenFOAM (Open Field Operation and Manipulation), and studies were performed on the regularly deposited powder with atomized (spherical) particles of the same sizes. The effects of powder layer thickness, heat source intensity, scan spacing, and scanning velocity on the process dynamics were simulated. Körner et al. [15] investigated the melting and resolidification of a randomly packed powder bed with round particles using a 2D model based on the lattice Boltzmann method (LBM). Numerical simulation considered individual powder particles and took into account any physical phenomena, e.g., the influence of the relative powder density, the

stochastic effect of a randomly packed powder bed, and capillary and wetting phenomena. Similar principles are applied in the project presented in this paper.

Foroozmehr et al. [16] simulated the size of a single-layered 316L stainless steel melt pool during the SLM process using a 3D FEM model. They modeled the optical penetration depth of the laser beam into the powder bed and its dependence on the powder size and the heat source. The results were validated with the experimental results. The model was used to predict the effect of different scanning speeds on melt pool depth, width, and length. Russell et al. [17] simulated laser fusion additive manufacturing processes using the smooth particle hydrodynamics (SPH) method. It is a Lagrangian mesh-free numerical scheme adapted to resolve thermal–mechanical–material fields. They noted that the SPH method is a viable and promising numerical tool for simulating laser fusion-driven additive manufacturing processes. They applied the model to powders with regularly deposited spherical particles of the same sizes.

Many publications are devoted to microstructure evolution during the SLM process, e.g., [18–24]. Helmer et al. [18] studied local solidification conditions to develop a scanning strategy to achieve grain orientation by changing the thermal gradient during solidification. They used a model based on a 2D LBM. An interesting complex approach is presented by Panwisawas et al. [19]. They studied the thermal fluid flow and microstructural evolution of a set of single tracks scanned with a laser with different thicknesses of the powder layer and scanning speeds during SLM and analyzed single-track morphology, porosity formation, and melt flow behavior. They used both computational and experimental approaches. A computational fluid dynamics (CFD) calculation was developed using the C++ open-source CFD toolbox (OpenFOAM) to model the interaction between the laser heat source and the randomly distributed Ti-6Al-4V powder materials. AlMangour et al. [20] used Layerwise Additive Manufacturing Predictions and Simulations (LAMPS) software to analyze the full-scale temperature field response and quantitatively explain the experimental results of the 6061 Al alloy and the TiC-reinforced 316L stainless steel SLM process. Liu et al. [21] also analyzed the microstructure evolution of AlSi10Mg on a single track using FEM. Kundin et al. [22] analyzed the microstructure evolution of the Fe-18.9Mn and Fe-18.5Mn-Al-C alloys solidified during the SLM process and presented 2D results. Ao et al. [23] applied a 3D FEM model for a thermal task and a 2D cellular automata (CA) for simulation of microstructure evolution with dendritic grain growth. Jiang et al. [24] investigated the complex solidification process during laser welding of the 5083 aluminum alloy. The model combines a macroscale model for heat and mass transfer, a microscale model for polycrystalline alloy solidification, and the continuous Gaussian nucleation distribution model for heterogeneous nucleation.

Liu and Wen [25] studied vaporization and its influence during powder bed fusion processes. Chen et al. [26] simulated the SLM powder-layering process, powder movement, and packing on the particle scale. On the basis of the discrete element method (DEM), their study investigated the flowing behavior of powder layered by a blade, and the model was validated by the results of the experiment. Chen et al. [27] performed experimental studies of the thermal and fluid behavior of the powder layer during SLM and then applied computational research to the SLM process, where DEM and CFD were used to simulate the spread of the powder layer and the fusion of the powder layer, respectively. Wu et al. [28] used DEM to simulate the random distribution of particles of spherical shapes of different sizes and the 3D finite difference method (FDM) for thermal simulations. He et al. [29] presented a multiphase and multiphysics model developed for the selective laser melting process, where fluid flow, solidification, and heat transfer were included. The DEM and volume-of-fluid (VOF) methods were applied to generate the powder bed and capture the free surface of the melts, respectively. Physical behaviors such as surface tension, the Marangoni effect, vapor recoil, and radiation were considered. The remolten region between two neighboring tracks in the horizontal and vertical directions was predicted, and the effects of the scanning spacing and laser power on the width and depth of the remolten region were investigated.

Liu et al. [30] proposed a ray-tracing heat source model for a mesoscale computational fluid dynamic (CFD) simulation of the SLM process. Multiple reflections of the laser beam at the surface of the metal powders were taken into account in the modeling. It was integrated into the commercial software, FLOW3D. A single laser path was simulated. Tian et al. [31] used DEM and the finite volume method (FVM) to build a 3D numerical model to simulate the SLM process of SS316L stainless steel. The single track was verified. A CFD model was set up and implemented in the FLOW-3D CFD software. Rehman et al. [32] simulated a similar laser melting deposition process with a single track using a mesoscopic CFD model for AISI 304 stainless steel with experimental verification. Spherical particles were deposited in one layer.

Recently, multi-material AM processes have also been modeled. Shinjo and Panwisawas [33], using the coupled level-set and volume-of-fluid method for multiphase thermal fluid flow simulation of very complicated AM processes, simulated and analyzed the fluid flow dynamics and mass loss characteristics due to metal vaporization. They obtained, among others, results connected with the formation of the melt pool, keyhole, and flow for different elements, as well as the mass loss rate resulting from vaporization. A multi-material model for the lattice Boltzmann-based simulation of the mixing of two elements to a binary alloy via PBF is presented by Küng et al. [34]. The thermodynamic model comprised mass, momentum, and enthalpy conservation equations, including element-specific mass conservation and the effect of enthalpy diffusion. The material model considered concentration-dependent material parameters such as heat capacities and latent heat. In particular, melting and solidification were modeled in accordance with the phase diagram, for which an isomorphous example was provided. They simulated a single melt track in a multi-material powder mixture and predicted the partitioning of the melt pool into an inner well-mixed region. A multitrack and multilayer simulation shows that unmolten particles and high surface roughness are unwanted side effects in multi-material PBF processes. Tang et al. [35] simulated the multi-material laser PBF process using a volume-of-fluid CFD model. They modeled two-, three- and four-component powders with mixed titanium Ti, niobium Nb, and vanadium V particles. The resulting materials of the product obtained in the AM presented in [34,35] are different alloys with uncontrolled inhomogeneity. Such processes probably cannot be applied to manufacturing products that contain, for example, titanium alloys and bioactive glasses (ceramics). In real SLM processes, materials can be mixed uniformly before the process, especially when they are metals and can form alloys. When materials such as metal and glass (ceramics) are used, where materials have very different properties and should not form alloys, and the structure of the product should be accurately controlled because materials play different roles in the product, the mixture before the process cannot be performed. For example, titanium alloy is inert, long-term biocompatible, and able to perform its intended function without eliciting any undesirable local or systemic effects. Metallic glasses based on magnesium are biodegradable materials. A scaffold or matrix for tissue engineering products should support appropriate cellular activity, including facilitation of molecular and mechanical signaling systems, to optimize tissue regeneration, without causing undesirable effects in those cells. One technology uses SLM for the creation of a regular metallic matrix or foams which is followed by a coating with bioactive glass. The matrix is dipped into the molten glass or the molten glass is sprayed onto the surface. However, both methods have disadvantages that can be avoided in the proposed approach.

The author of this paper, together with a team, presented the first concept of AM modeling processes in a previous paper [36]. Then, Svyetlichnyy et al. [37] developed a holistic numerical model based on CA and LBM. Their model was devoted to laser-assisted PBF, focusing mainly on SLS/SLM processes. The 2D LBM-based fluid flow model was presented in detail in [38] in an investigation of the effects of surface tension and liquid flow on the free surface, as well as the results of melting and solidification. The first qualitative results of the simulation of one track of SLM technology were presented in [39]. The results of the 3D PBG model with atomized particles were transferred to the 2D domain. Then, the

laser beam passed through the domain and the melted particles, and the molten material flowed and solidified. The authors of [40] presented a further development of the numerical platform for modeling SLM. Another study [41] focused on the thermal interaction between a laser beam and a powder bed using a ray tracing algorithm for opaque, translucent and transparent materials; another study considering this in more detail is being considered for publication. The publication [42] presents quantitative simulations of titanium alloy (Ti-6Al-4V) in the SLM process in one cycle with three tracks. It describes in detail the calculation of modeling parameters on the basis of real ones. It presents the results and some elements of verification.

In summarizing the current state of this field, some important achievements can be stressed. Several research groups have demonstrated the possibility for accurate simulation of one cycle of SLM and similar processes on a particle scale, sometimes with more than one track and with mixed metals. They use different methods and combinations. Multilayer simulations are often performed with homogenization of the material properties of the powder, liquid, and solid domains. This approach is used mainly for simulation of the microstructure evolution. Most publications are devoted to simulations of metallic powders with atomized particles represented by spheres of different diameters. Studies with particles of another shape (arbitrary shape) are difficult to find. Most studies on the particle scale are limited to one cycle of the process and one material, although simulations with several layers and several metals have recently been published [33–35]. The holistic model of the entire SLM process developed and presented in [36–43] had the same limitation related to the imperfection of the powder deposition models. The improved model presented here allows for the simulation of multistage multi-material SLM processes.

The objective of this paper is to present a new calculation scheme, a deposition model, an interface between modules, and the results of simulations of multistage multi-material SLM processes.

2. Holistic Model of the SLM Process and Main Algorithm

2.1. Holistic Model and Algorithm

The holistic model was developed after an analysis of SLM at three levels: technological, associated physical processes and phenomena, and associated mathematical models (Figure 1) [39]. The latter, with appropriate connections or interfaces, is the content of the holistic model. On the first technological level, SLM can be schematically represented as a cyclic process consisting of the sequence: powder deposition, pause, laser beam treatment, pause, and powder removal. This sequence can be repeated many times until the product is finished. The following six basic processes are considered at the second level of analysis and can be consequently modeled: powder deposition, laser beam heat treatment, melting, liquid flow (free flow of melted material), solidification, and powder removal. The defined processes and phenomena associated with SLM are modeled using the following five sub-models: a powder deposition model, a heat transfer model with laser treatment, a phase transition model, a fluid flow model with a free surface, and a powder removal model. The work to develop the model required some adjustments to the structure of the holistic model and its components. The main algorithm, the structure, and the functioning of the model can be represented as a block diagram (Figure 2) [39]. The algorithm has two circuits. The first external circuit contains the powder bed generation (PBG) model, cycle initialization, and its realization (represented by the internal circuit—LBM calculation module), and the powder removal (PR) model.

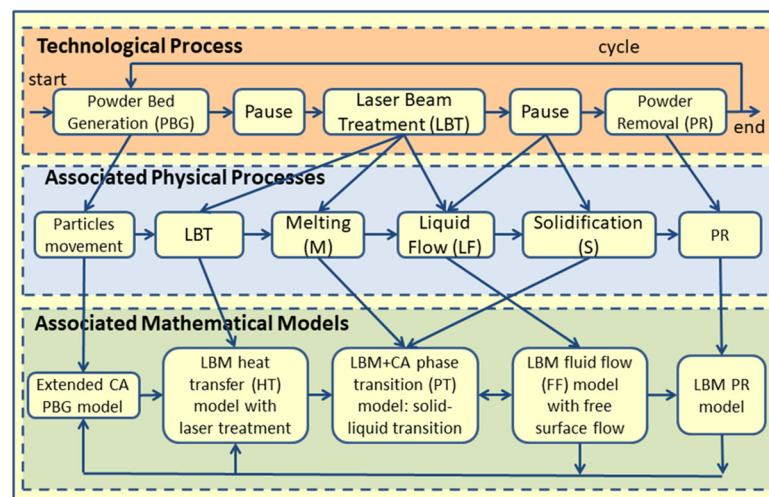


Figure 1. SLM process with associated physical phenomena and submodels [39].

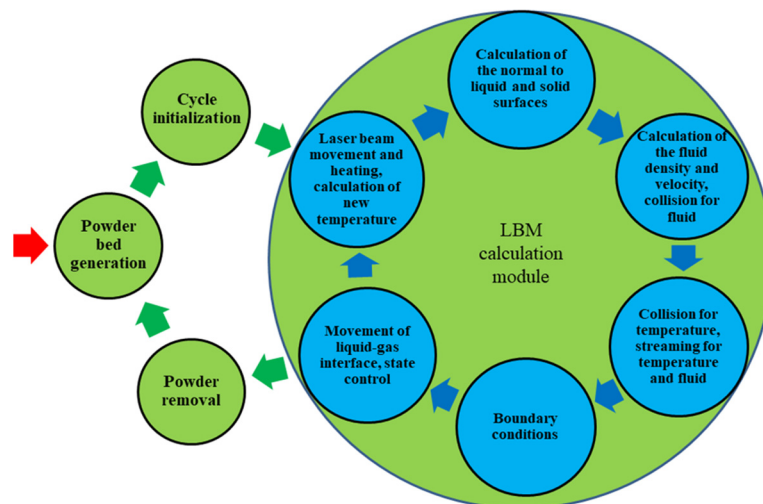


Figure 2. Graphical representation of the main algorithm [39].

Details of the development, testing, verification and validation of the 2D and 3D submodels and the entire holistic model of the SLM process, as well as several examples of simulations of separated phenomena by submodels and the entire process, can be found in previous papers [33–40]. The paper [39] presented the main algorithm, but it was only partially implemented. The external circuit was not closed, and the results of the simulations performed by the LBM calculation module were not transferred to the PBG model for further deposition of the next powder layer. The LBM calculation module allows modeling of only one stage of the SLM with several laser tracks on a distributed level of the powder. A file with a structure after the stage was prepared but could not be used by the PBG model. This can be explained by the logic of developing a holistic model. Until the internal circuit has been developed and verified, the external circuit was not worked on and the PBG model was simplified and could perform only the necessary functions. Closing the external circuit required the development of a new version of the PBG model that provides feedback communication from the LBM calculation module.

2.2. Powder Bed Generation Models

Four variants of the powder deposition model have been developed. The first three variants use a quasi-kinematic approach with a simplified static stability test and are based on a similar algorithm. The simplified representation of the algorithm is shown in Figure 3a.

Briefly, each particle falls onto the basement (flat, curved, or arbitrary shape after treatment) or onto the previously deposited particles. First, the first contact of the falling particle with the basement is searched, which restricts the first degree of freedom. Then, the particle begins to roll, slide, or rotate over the surface or other particles until it finds the second contact. After the tests, the algorithm can go further or return to the previous stages. Next, the particle continues to move with a restriction of two degrees of freedom. When the third contact point is found and the last degree of freedom is restricted, the stability of the particle is tested. If the stability conditions are satisfied, the location of the particle is treated as final, and the algorithm passes to the next particle. The algorithms of the variants differ in detail depending on the shape of the particles and the accepted assumptions.

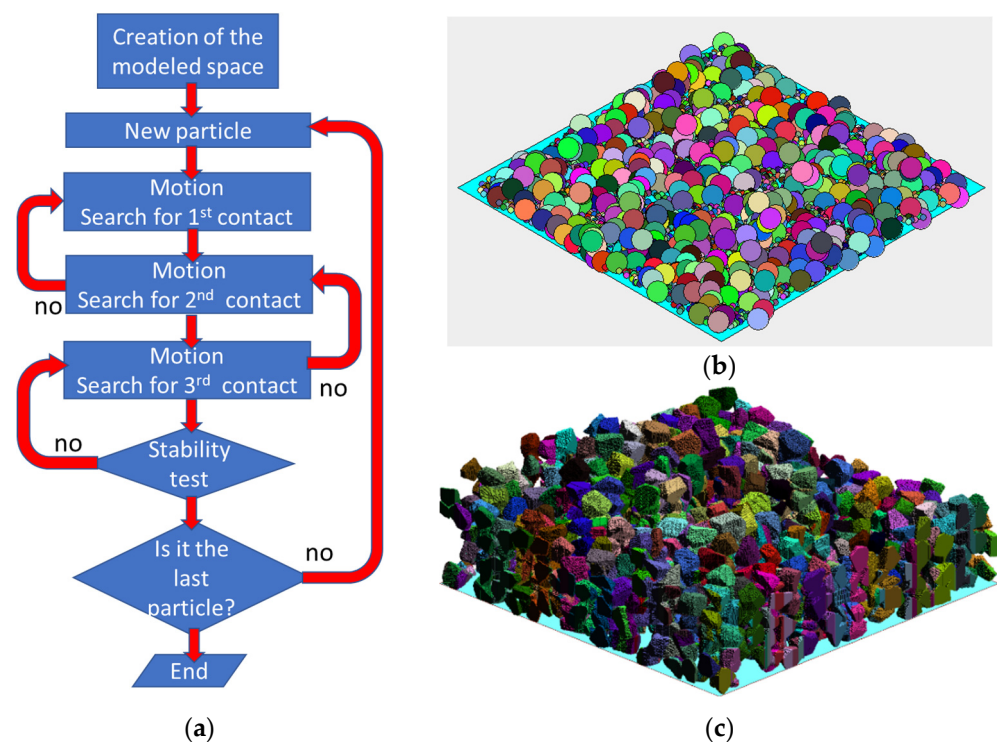


Figure 3. A simplified algorithm of the powder deposition model (a), and examples of particle deposition obtained by the first (b), and second (c) variants of the model.

The first variant based on 2.5D CA considers a powder with atomized particles (spherical shape) (Figure 3b). The algorithm considers only rolling movements. A detailed description of this variant, simulation results, and model verification and validation can be found elsewhere [33]. The validation confirms high accuracy in terms of packing density.

The second variant based on 2.5D CA has been developed for arbitrary-shaped particles. A database containing 50 particles was created. The particles are modified before deposition by their rotation on three random Euler angles with consequent random scaling along three independent axes, giving an unlimited number of unique particles. The particles are represented by a cloud of points on the surface of the particles. The particle can be translated (fall or slide) or rotated around an axis fixed by one or two points. The simulation results can be found in [34,36,38] and are presented in Figure 3c.

The third variant was created after the development and implementation of the laser beam heating (LBH) model based on the ray-tracing algorithm in the holistic model. The LBH model requires a parametric (continuous, vectorizing) representation of the material surface that could not be achieved with the previous variants. Surfaces are represented by vertices, edges, and faces (triangles). During the particle movement (translation and rotation), two types of contacts are analyzed: vertex-to-face and edge-to-edge. After deposition, the results can be represented in two forms: vector (continuous) and discrete.

Discrete representation is necessary for LBM models. An example of deposition presented in the parametric and discrete forms are presented in Figure 4. The other simulation results with this variant can be found elsewhere [39].

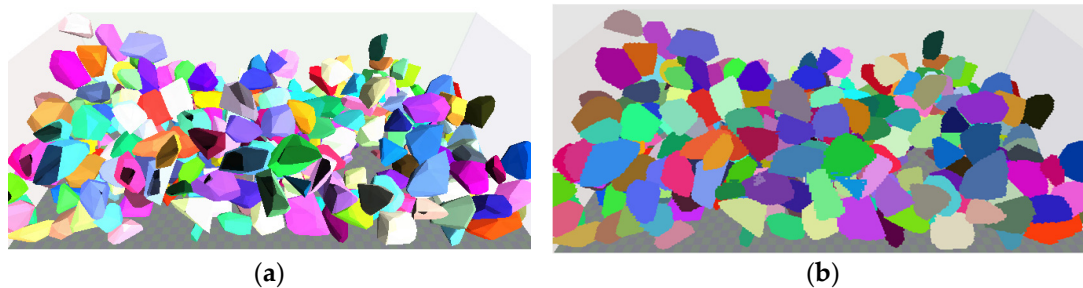


Figure 4. An example of particle deposition obtained by the third variant of the model with parametric (a) and discrete (b) representations.

The last variant presented here uses the Unity[®] platform with the same database of particles of arbitrary shape extended by the spherical (atomized) particle. Unity is a cross-platform game engine developed by Unity Software Inc. (doing business as Unity Technologies) is a video game software development company based in San Francisco (USA). The particles in the database were adapted to Unity by creating so-called prefabs. The particles are considered to be rigid bodies with bounce. They move and rotate under gravity and forces of interaction with the terrain and other particles. The movement is described by the Newton and Euler equations. Collisions are identified by colliders. Atomized particles use a spherical collider, and particles of arbitrary shape use a convex mesh collider, a basement (or previously deposited and processed particles) mesh, or a terrain collider. The physical principles used by Unity ensure appropriate results for the deposition of free-falling particles or re-coating (smoothing and flattening of the top layer of powder after the fall). However, the packing density obtained by Unity is less than in real deposition and smoothing and flattening because the contact test results in some gaps between the surfaces (particles, basement, terrain). The gap is an almost constant value. Therefore, the largest sizes of representative space and smallest particles result in errors. Increasing the sizes of the particles, which removes the gap after deposition, allows us to obtain the real packing density. The resulting particle deposition in two forms is transferred to the holistic model to prepare one layer for the SLM cycle modeling in the LBM calculation module.

Examples of powder deposition and re-coating with atomized and arbitrary particles are presented in Figure 5.

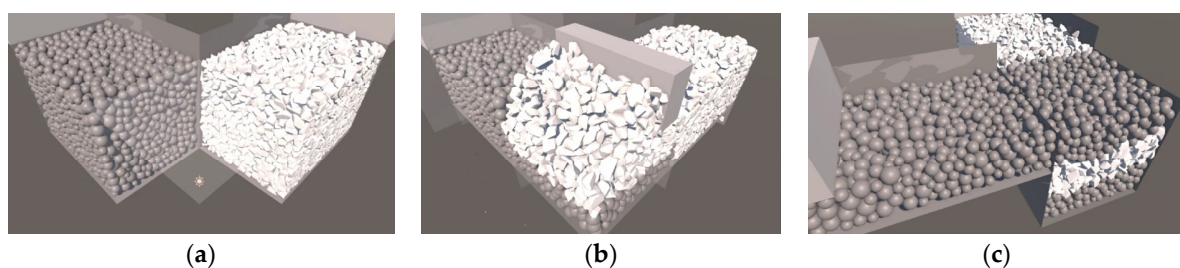


Figure 5. Results of deposition of free-falling atomized and arbitrary-shaped particles (a), re-coating of the second layer (b), and after the re-coating of the third layer (c).

2.3. Powder Removal Models

Powder removal models remove loose powder particles from the powder bed. One such model aims to support multiple material SLM systems with a point-by-point micro vacuum material removal system [41]. It has been designed to remove a single layer of

powder selectively and precisely at the specific locations, in combination with several dry powder dispensers that deposit powders according to the designed pattern.

After the generation of the powder bed and the completion of the single processing stage of the SLM, some of the untreated powder material should be removed. To simulate this operation and process, two variants of new powder removal models have been developed.

The first variant was developed to analyze the effectiveness of the loose particle removal operation. It was developed in a 2D version. The model uses the same principles and algorithms as the other LBM models of the holistic SLM model (e.g., the LBM calculation module presented in Figure 2). The objective of this variant is to simulate the gas flow, allowing for local removal of loose particles. The model contains equations that describe the motion of particles entrained in the gas stream. Particles of different masses and sizes are considered in the simulation, although they are assumed to be small enough to influence the gas flow. Then, Newton's laws are applied to the linear motion of a particle of constant mass without consideration of particle rotations. Because this variant is not used in the holistic model, the details are omitted and only some simulation results are presented here. The intensity of the color shows the vertical component of the velocity of the gas flow (red—upward, blue—downward). In this case, the trajectories of particles of three different sizes are simulated: the violet trajectories correspond to very small particles, green ones represent medium particles, and blue trajectories are related to the largest particles.

Only in the case of a 'vacuum' (Figure 6a) does the gap between a vacuum tube and the surface become a crucial parameter. If the gap is too small, the inflowing gas flow is too weak to entrain the particles in the flow. An increase in the gap is accompanied by an increase in the gas flow, and the removal device becomes more effective. When the gap becomes too large, the turbulences that can appear in the tube can lead to asymmetrical flow and instabilities; the effectiveness of the device drops significantly, even for a highly symmetric case. The observed instabilities are typical for wider tubes and diminish as the diameter of the tube narrows. Considering the simulation results from the technological point of view, it can be concluded that efficient control of particle removal using a device with only a vacuum function is fraught with difficulties. This is due to the high dependence of the device effectiveness on the gap, which is difficult to maintain at an optimal level.

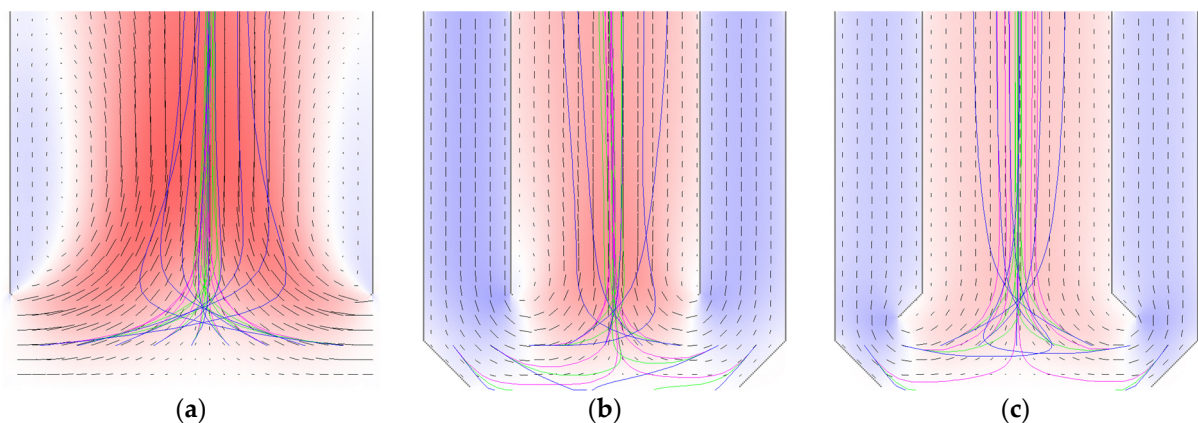


Figure 6. Gas streams and trajectories of moving particles predicted by the LBM model. The case of vacuum only with a big gap (a). The cases of inflows and outflows for different tube profiles and higher pressure (b,c).

As can be seen in Figure 6a, there is some movement in the opposite direction, and turbulences can appear within the tube. It is possible to enforce such movement by applying an additional inflow channel with a much higher gas pressure. Some simulation results are presented in Figure 6b,c. A simple liner shape is less effective due to a strong gas stream in a downward direction (Figure 6b). The device becomes more effective in the presence of a

stream in the horizontal direction. It is possible to obtain more effective design options by using different profiles of the internal and external tubes. This would have the additional advantage that the two-tube solution results in easier control of the minimal gap between the external tube and the surface.

The second variant of the particle removal model simply removes untreated particles from the modeled space after simulation of the SLM process cycle. This variant of the model is combined with an interface to transfer results from the LBM calculation module to the PBG model and requires a small modification of the LBM calculations.

The particles that are exposed to the laser and begin to melt, at least partially, are noted as particles that lose their freedom of movement after solidification. They are attached to the built product and cannot be removed by the removal system.

Then, after the cycle that includes the treatment of one powder layer, the results can be transferred with or without particle removal. The removal does not need to be performed if the next level is filled with the same material or another material with the same shape of particles or if removal is not expected according to technology. In this case, the solidified product and untreated particles remain in the modeling domain and are transformed into the terrain collider for Unity. Some examples of such a transformation are presented in the simulation section of this paper.

If, according to the technology, untreated particles are removed and another material is deposited in their place, information about the untreated particles is not used during the transformation into the terrain collider for Unity. Examples of this case are also presented below in the simulation section of this paper.

3. Modeling

3.1. Modeling Domains and an Interface between Them

Two modeling tools are used to model the SLM process. The first one based on Unity implements the PBG model. The domain of size $100 \times 100 \times 100 \text{ m}^3$ is applied. Such a large domain is caused by the relatively large gaps between the particles and between the particles and other elements of the modeled domain (walls, floor, or terrain). The gap is almost independent of the domain size and in the range of about 0.1–0.5 m or 0.1–0.5% of the modeling domain but it reaches about 2–10% of the particle size. The scale of the disposed particles depends on the sizes of the modeling domain of the second modeling tools and the real sizes of the particles. To reduce the gap and reach the real packing density, the sizes of the deposited particles are slightly increased during the transfer from Unity.

The input data for powder deposition include the type of particle shape (atomized or arbitrary), distribution of particle size, and deposition basement, which can be presented by the terrain collider described using heights in the nodes of the horizontal mesh.

The output information consists of a list of the particles in parametric form. There are several types of grains, coordinates of the center of mass, scales of three local axes of the particle, and three Euler rotation angles. There are 50 types of particles of arbitrary-shaped and spherical particles. When the atomized particles are deposited, the scales of three local axes are the same. They determine the radius of the sphere, and the rotation angles are irrelevant.

The second tool for modeling is the code developed the author of this study for parallel calculations on a GPU (graphics processing unit) and CPU (central processing unit) and visualization with OpenGL. It performs the internal circuit of the algorithm (Figure 3) and is based on the LBM. The interfaces between the Unity and LBM modules in both directions are part of this code and include the cycle initialization and powder removal model.

Transfer of the disposed particles from the Unity domain to the LBM domain takes place in parametric and discretized forms with scaling. The sizes of the discretized Unity and LBM domains can be set independently, but the sizes of the cells in both domains should be the same. The name 'cell' originates from the CA method and defines the volume of the LBM nodes. The neighboring cells are in contact with each other without a gap; that is, the sizes are equal to the length between the nodes. Then, the sizes of the discretized Unity

and LBM domains are defined by the number of cells in three dimensions. Therefore, the number of cells of the LBM domain in each direction should be equal to or less than those in the Unity domain. The size of the cell is mainly defined by the conditions of the simulated process. This means that the sizes of the particles in Unity should be in agreement with the sizes of the cells before the simulation of powder deposition in Unity. For example, if the two domains in the horizontal plane are of the same number of cells (equal to 256×256), the cell sizes in the LBM domain are $1.25 \mu\text{m}$, and the particle radius is $10 \mu\text{m}$, then the radius of this particle in the Unity simulation is 3.125 m ($= 25/1.25 \times 100/256$). The more general equation for such calculations is as follows:

$$R_U = \frac{RL_U}{N_U l_c} \quad (1)$$

where R_U is the particle radius in the Unity domain (m), R is the real particle radius in the LBM domain (μm), L_U is the size of the Unity domain (m), N_U is the number of cells in one direction in the Unity domain, and l_c is the cell size in the LBM domain (μm).

The initialization of the cycle also contains a schedule of the laser movement and pauses between the subsequent tracks. The schedule is loaded from the previously prepared file.

After preparing the simulated geometry and schedule, a cycle simulation begins in the LBM calculation module. After the cycle simulation, the geometry should be transferred to Unity if it is not the last cycle. First, the information about the material is separated into two parts: the untreated particles and the material processed. The untreated particles are those that were not heated by a laser beam or other means to the melting temperature and retained their shape. The processed material comprises particles which were melted completely or partially, changed shape, flowed, and solidified. Untreated particles remain in the list of particles; the other particles are removed from the list. Information about the material is used differently depending on the next cycle of laser treatment, which consists of either the same material without powder removal or with another material and powder removal. Both cases are shown in the next section.

If the next cycle proceeds with the same material without powder removal, the untreated particles and the processed material are used together to create the terrain collider for Unity. After the deposition of a new layer, new particles are added to the list of particles. The list of the particles after deposition in Unity contains all particles disposed in Unity even if they lie outside the modeled space of the LBM model.

If the next cycle proceeds with another material or with powder particles of another shape, only the processed material is used to create a terrain collider for Unity. The list of particles is emptied and filled with new particles after powder deposition in Unity.

3.2. Modeling Parameters

The first quantitative results obtained by the 3D model for one layer of Ti-6Al-V powder were presented in the previous paper [39] but were unrealistic due to the arbitrary shape of the particles. The previous paper also details the properties of Ti-6Al-V, bioactive glass, and air (nitrogen) needed for adequate modeling and describes the methodology for the calculation of the simulation parameters. Some parameters of the materials are collected in Table 1, which is based on [39] with corrections and extension.

Four stages of the simulation of the SLM process are presented here. The first three layers are filled with Ti-6Al-V alloy powder with atomized particles with diameters of $12.5\text{--}25 \mu\text{m}$, and the last layer is filled with bioactive glass powder with particles of arbitrary shape and sizes of about $20\text{--}40 \mu\text{m}$. The laser power is 300 W . The diameter of the laser spot is $80 \mu\text{m}$. The velocity of the laser movement is 1 m/s . The initial temperature of the powder and atmosphere is $T_i = 373 \text{ K}$ (100°C). The representative volume element (RVE) for the LBM simulation is represented by the space with $256 \times 256 \times 80$ ($= 5,242,880$) cells with cell size $\Delta x_r = 1.25 \mu\text{m}$; that is, the RVE sizes are $320 \times 320 \times 100 \mu\text{m}^3$. The time step is about $\text{tr} = 26 \text{ ns}$.

Table 1. Properties of the materials.

Properties	Ti-6Al-V	Glass	Air (Nitrogen)
Melting temperature, T_m (K)	1922	1336	-
Boiling temperature T_b , (K)	3560	2503	-
Heat capacity, C_p (J kg ⁻¹ K ⁻¹)	560	500	1 ÷ 1.25
Specific latent heat, L (J g ⁻¹)	360 ÷ 370	-	-
Thermal diffusivity, α (m ² s ⁻¹)	2.9×10^{-6}	$37 \div 67 \times 10^{-6}$	$200 \div 300 \times 10^{-6}$
Convective heat transfer coefficient, h (Wm ⁻² K ⁻¹)	50	50	-
Density, ρ (kg m ⁻³)	4420	2700	0.6 ÷ 0.35
Dynamic viscosity, μ (Pa s)	4.42×10^{-3}	0.1 ÷ 500	$30 \div 55 \times 10^{-6}$
Kinematic viscosity, ν (m ² s ⁻¹)	10^{-6}	$3.75 \times 10^{-5} \div 0.2$	$20 \div 250 \times 10^{-6}$
The surface tension of the liquid–gas interface, γ (N m ⁻¹)	1.55	0.25	-
Thermal expansion coefficient, α_l (K ⁻¹)	6.5×10^{-5}	8.5×10^{-6}	1.22×10^{-3}
Rayleigh number, Ra	676	$0.2 \div 2.5 \times 10^{-6}$	0.005 ÷ 0.1
Bond (Eötvös) number, Bo(Eo)	11.4×10^{-6}	43.2×10^{-6}	-

According to the assumptions, all the variables in the LBM calculations are dimensionless. The cell size and time step are equal to unity: $\Delta x = \Delta t = 1$. The temperature scale is chosen based on the initial $T_i = 0$ and the melting temperature of the titanium alloy ($T_{mTi} = 1$). The density of the titanium alloy is $\rho_{Ti} = 1$.

Then, the laser spot diameter is 64. The simulation laser velocity is 0.0208 or about 47 iterations (time steps) per cell for laser movement. The area of the laser spot is 3215.36. The laser heat per cell and iteration is about 2.43×10^{-9} J, and is used to calculate the temperature decrement ΔT . The calculated gravity acceleration is about 5.3×10^{-9} but due to very low Rayleigh and Bond numbers, the gravity acceleration is increased to a value of 8×10^{-4} . The simulated buoyancy coefficient is 0.01. Other simulation parameters dependent on the materials are collected in Table 2.

Table 2. Simulation parameters.

Properties	Ti-6Al-V	Glass
Melting temperature T_m , (-)	1.0	0.614
Boiling temperature T_b , (-)	2.031	1.358
Temperature decrement ΔT , (K)	452.3	645.1
Temperature decrement ΔT , (-)	0.288	0.411
Specific latent heat (enthalpy) L (-)	0.415	-
Convective heat transfer coefficient, h (-)	5.05×10^{-6}	7.72×10^{-5}
Relaxation time for fluid flow τ_F , (-)	0.55	25.5
Relaxation time for heat flow τ_T , (-)	0.75	0.53

The calculations are mainly performed on the CUDA (Compute Unified Device Architecture) developed by NVIDIA with the use of the GeForce RTX-3800 graphic card.

4. Results

4.1. The First Cycle

After deposition of the titanium alloy powder (the layer thickness is about 32 μ m), the laser beam moves along three parallel tracks and creates the first level of the product. Figure 7 presents the simulation stages of the first cycle of laser treatment. Untreated particles of titanium alloy are shown in olive color, a laser beam is shown in green, a liquid phase with blue, and solidified material is shown in brown. The laser beam moves forward in Figure 7. After the beam reaches the end of the track, the model simulates cooling till all the material transits into the solid state. Then, the next track begins. The pause between the tracks can be varied.

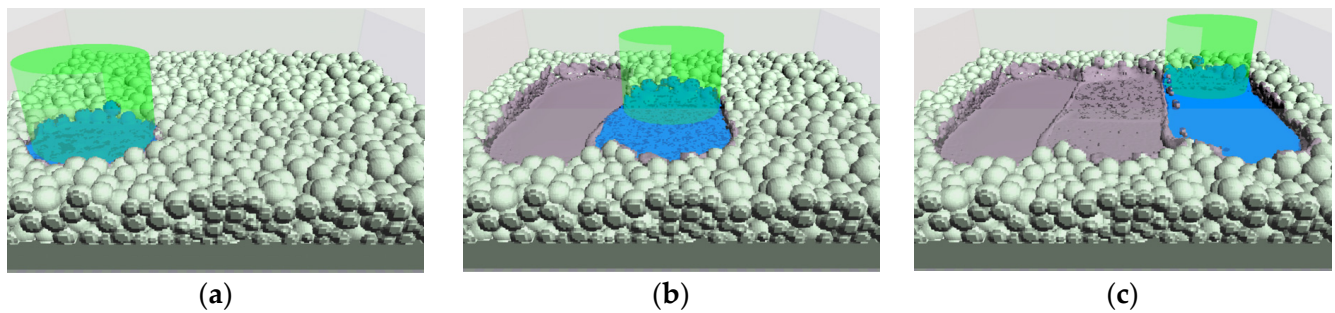


Figure 7. 3D snapshots of the simulation of the first cycle of the laser treatment: the beginning of the first laser track (a), the middle of the second track (b), and the end of the third track (c).

Figure 8a presents the temperature distribution in the cross-section across the movement immediately following the laser beam. The temperature scale is presented in Figure 8d, and it is the same in all the following figures. Blue represents low temperature and red represents high. Black, pink, and light blue correspond to the melting temperature of the titanium alloy and are somewhat higher and lower (about 10%) than the melting temperature. Figure 8b,c show the state of the material at the beginning and end of the track in the cross-section along the laser movement. Melting is seen to continue for a short time after the laser passes. The melting pool expands and deepens as a result of the heat accumulated in the liquid phase.

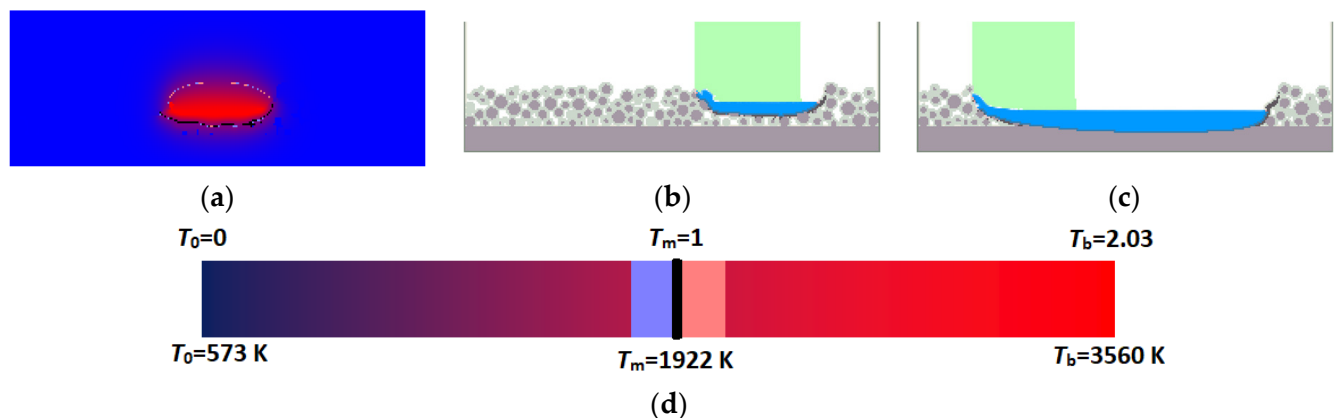


Figure 8. The first cycle. Temperature distribution (a) with the temperature scale (d) and the state of the material at the beginning (b) and end (c) of the track.

4.2. The Second Cycle

The first cycle ends with the preparation of information transferred from the LBM model to Unity. The second cycle begins in Unity with the introduction of the terrain into the modeling space. Because the second cycle is performed with the same material, the terrain completely reflects the result of laser treatment in the first cycle, i.e., without the removal of untreated powder. The terrain before powder deposition is presented in Figure 9a (it can be compared with Figure 7c). The modeling space is then filled with falling particles (Figure 9b). The final state after deposition is shown in Figure 9c. The level of the powder obtained with falling particles in Unity is somewhat higher than that used in the consequent LBM simulation. The re-coating operation is not shown here. The total thickness of the two powder layers is approximately 42 μm , and the thickness of the powder layer above the product is approximately 30 μm .

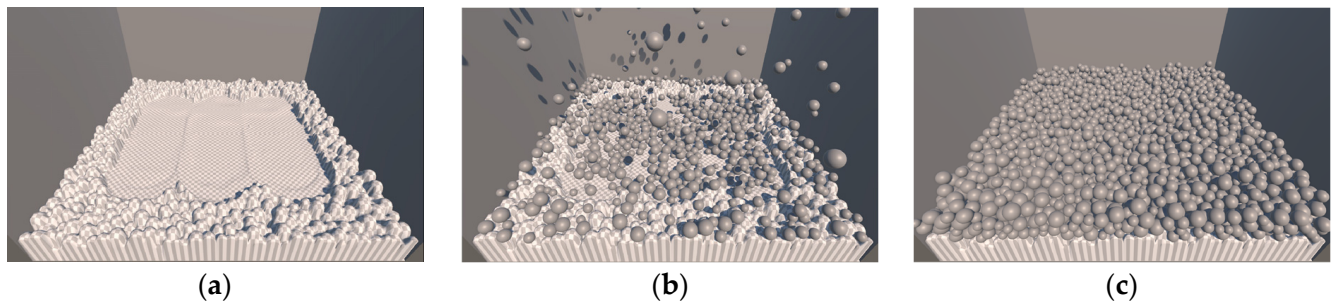


Figure 9. Powder deposition before the second cycle of laser treatment: state of the modeling space with the terrain collider after the first cycle and before deposition (a), the process of filling with powder (b), and the final state after deposition and before the second stage of laser treatment (c).

After the deposition of the second level of the powder and flattening with the roller, data were transferred to the LBM model. The second cycle of laser beam treatment along the closed track is then simulated. The beginning, end, and product view after the second cycle are shown in Figure 10.

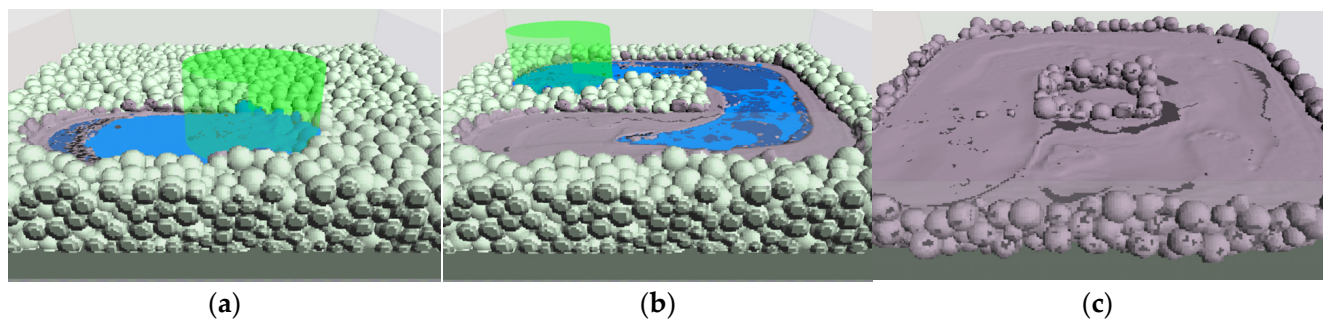


Figure 10. Simulation of the second cycle of the laser treatment along the closed track: the beginning (a) and the end (b) of the laser treatment, and a view of the product after the cycle (c).

Figure 11 presents a cross-section of the simulation of the second cycle. The laser begins to melt the highest particles of the new powder layer (Figure 11a). The elliptic shape of the bottom surface of the product obtained after deposition of the previous layer can be seen. The material melts, flows deep and wide, melts neighboring particles, and begins to solidify close to the end of the rightward movement of the laser beam (Figure 11b). When the laser beam is moved backward, the right part is incompletely solidified (Figure 11c).

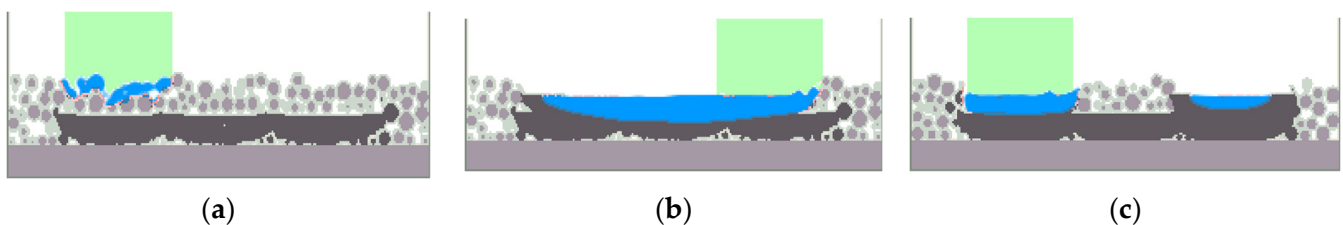


Figure 11. Cross-sections of the second cycle of laser treatment simulation: the beginning of the laser movement (a), the end of movement to the right (b), and the middle of the backward movement (c).

Figure 12 presents the temperature distribution during the second cycle at the same time as the last two images in Figure 11. The temperature scale is presented in Figure 8d. Light green shows the location of the laser beam. Pink represents a temperature slightly above the melting temperature and shows the liquid volume close to solidification.

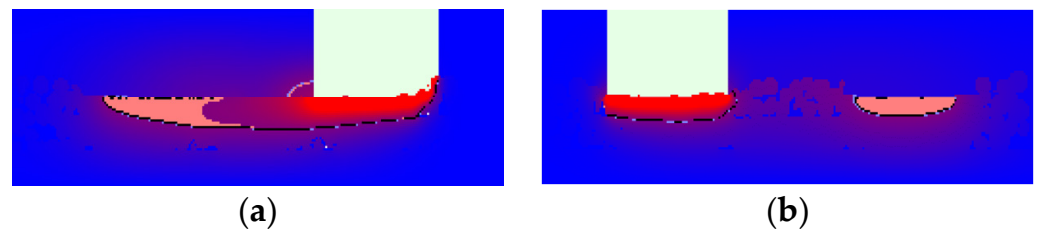


Figure 12. Cross-sections of the second cycle showing the temperature distribution: the end of the movement to the right (a) and at the middle of the backward movement (b).

4.3. The Third Cycle

The third cycle is very similar to the second one. The deposition process is shown in Figure 13. The overall thickness of the three powder layers is approximately 55 μm , and the thickness of the layer of powder above the product is approximately 30 μm .

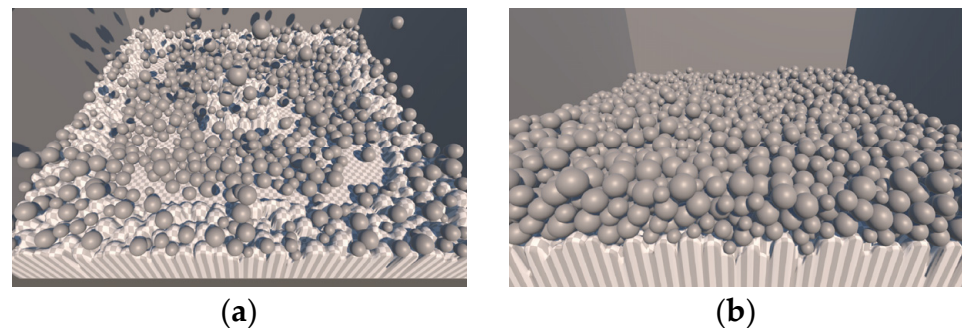


Figure 13. Simulation of the powder deposition process before the third cycle of laser treatment: filling with powder (a) and the final state after the deposition (b).

The third cycle of laser beam treatment also has a closed track. The beginning and end of the laser treatment are shown in Figure 14.

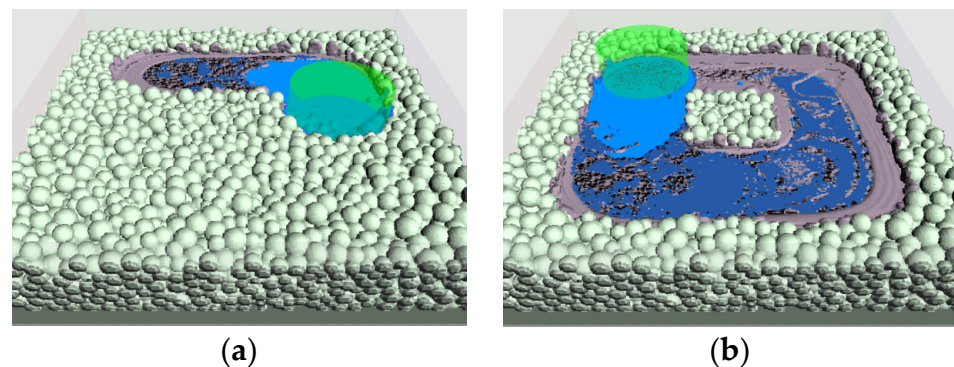


Figure 14. Simulation of the third cycle of the laser treatment: the beginning (a), and end (b).

4.4. The Fourth Cycle

The fourth cycle differs from all previous cycles because another material is deposited and processed. After the third cycle, all unmolten titanium alloy particles should be removed from the working chamber, and the glass powder with arbitrary-shaped particles should be deposited instead. Then, the terrain prepared for Unity contains only the building product with fused or sintered particles which were incompletely melted. The created terrain is shown in Figure 15a. Then, falling particles with arbitrary shapes fill the modeling space (Figure 15b), and the space is filled to a certain level (Figure 15c). The thickness of the bioactive glass layer outside the product is approximately 65 μm . The thickness of the

powder above the higher metallic part of the product is approximately $19\ \mu\text{m}$, and above the hole in the middle of the product, it is approximately $47\ \mu\text{m}$.

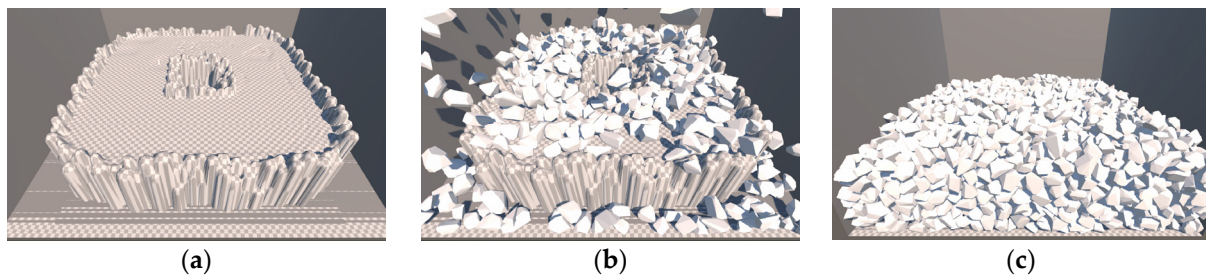


Figure 15. Simulation of the powder deposition process before the fourth cycle of laser treatment: before deposition and after the removal of the untreated powder (a), the process of filling with the powder (b), and the final state after deposition (c).

The fourth cycle is very simple and plays only the demonstrative role. The laser beam heats only the central part of the space. The properties of bioactive glass presented in Tables 1 and 2 are very simplified. Bioactive glasses (for example 45S5) have no exact melting temperature. The optical properties, thermal properties, viscosity and other properties vary in a wide range and strongly depend on temperature. However, in the presented simulations, they are mostly constant, independent of temperature or dependent on the state of matter only. An adequate model of the bioactive glass properties has not yet been developed, implemented, and verified. Simulations of the fourth cycle then have only a qualitative character, and hence, are very simple.

The laser beam does not move, remains in the same central position, and works in the pulse regime, giving two short pulses. Figure 16a,b present a 3D perspective view of this cycle and cross-section at the end of the second pulse. The molten glass closes the small hole with unmolten glass particles in the product of the titanium alloy.

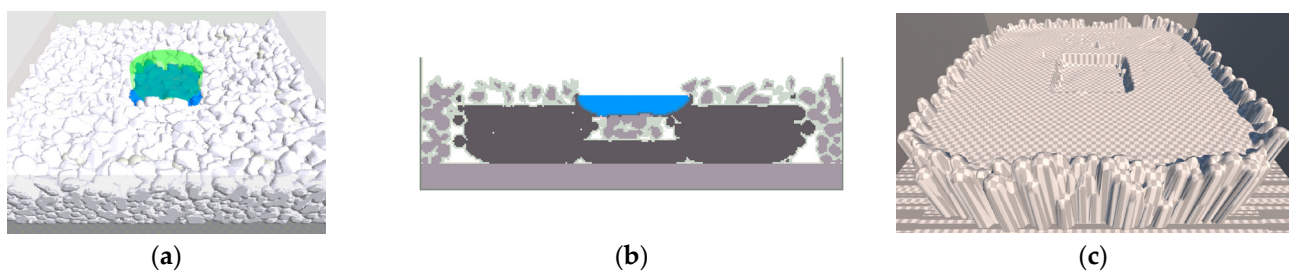


Figure 16. Simulation of the fourth cycle of the laser treatment: 3D view (a), cross-section immediately after the treatment (b), and another variant of the fourth cycle (c).

Figure 16c presents the result of another variant of the fourth cycle. The powder was removed from the working chamber (see Figure 15a) but another powder was not added. The laser beam was then directed at the central part of the product to smooth the edge of the hole by melting the bonded particles; molten material then flows down to the bottom of the hole and fills it evenly.

5. Discussion

Existing models presented by several research groups, including the author of this paper, demonstrate two approaches to the accurate simulation of SLM or similar processes. The first approach uses homogenization of the properties of the material in the powder, liquid, and solid states. This allows multilayer simulations on the mesoscale and is mainly used for simulations of the microstructure evolution. Another approach applied at a particle scale is limited to one cycle of the processes, sometimes with more than one track. This

approach, which is applied in this work, is more complex and allows the study of finer effects with high accuracy but requires more computational effort.

The next step in the development of the model presented in the previous sections is related to the extension of the simulation possibilities. The possibility of simulating several cycles of the process opens new perspectives for simulating, studying, and analyzing the process. To perform simulations of several cycles, it was necessary to add feedback from one module, which simulated a cycle, to the model responsible for powder deposition, that is, to close the algorithm circuit (see Figure 2). Such simulations are presented in previous sections.

Almost all publications present simulations of metallic powder with atomized particles of different sizes. Papers with deposition of particles of another shape (arbitrary shape) can be found but they are not dedicated to the simulation of PBF processes. The author implemented a powder with particles of arbitrary shape, which is characteristic of bioactive glass powder particles, in previous papers and this implementation is also shown here.

The ability to simulate several cycles also creates another possibility: the simulation of the process with different materials with very different properties and with different sizes and shapes of powder particles. This possibility is demonstrated in the previous section, where after the cycles with titanium alloy, the bioactive glass powder was deposited. However, this last cycle, should be treated as demonstrative and qualitative only because the properties of the glass are very simplified.

The optical, thermal, viscosity, and other properties of the bioactive glass vary in a wide range and strongly depend on the temperature. The development of a model of the properties of bioactive glass and its verification, validation, and implementation are the objectives of further research.

6. Conclusions

The development of a platform for modeling the multistage multi-material selective laser melting process is the main goal of this project, part of which is presented in this paper, and this objective was achieved. The powder bed generation model is connected to the LBM calculation module in a closed circuit, where the results of the one-cycle simulation can be used as feedback with or without the removal of untreated powder particles. This allows for multistage multi-material simulations.

Three cycles with titanium alloy (Ti-6Al-V) with different numbers and shapes of tracks were simulated. The model of the properties of titanium alloys was previously verified and validated; this part of the simulation was then treated as quantitative. The simulation of the fourth and last cycle demonstrates possibilities for the simulation of complex multistage multi-material SLM processes.

The novelty of the presented model is the possibility to model multistage multi-material SLM processes with materials that have extremely different thermal and mechanical properties and that should not be mixed before the process.

This paper presents several powder deposition models that enable the simulation of powder deposition with particles of different shapes. The arbitrary shape of the particles characterizing glasses and ceramics is a relatively new approach presented in this paper.

The powder removal system allows for the complete replacement of one powder with another, and the model of this removal system enabled the modeling of the multistage multi-material SLM process.

The main limitation of the presented platform is the simplified properties of the bioactive glasses. Moreover, the properties of the bioactive glasses impose an application of the selective laser sintering (SLS) process along with SLM.

Further development of the platform is connected with the modification of the SLM LBM-based model in the direction of the SLS/SLM model, with the implementation of a model of the properties of bioactive glass, as well as its verification, and validation.

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