Simulation models for 3D inkjet printing – Material and Process Design

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Abstract

Due to the ability to produce complex parts with no need for pre-tooling, Additive Layer Manufacturing (ALM) is a future technology with 3D inkjet printing being one of them. The latter is based on the polymerization of a liquid dispensed into a powder bed. However, the special challenges which have to be met here are to increase product quality such as tensile strength und density on a repeatable base. Consequently multi-scale simulation models were developed to support material researchers as well as users of the technology in their daily work and therefore to contribute to process stability and material reliability of 3D printers and their products.

Introduction

Manufacturing technology is facing even bigger challenges, due to increasing product-requirements caused by the globalization of production. Rising trends for individualization as well as a receding product life cycle play a growing role [1]. Trends to one-piece-production with ever shorter time-to-market and small quantities will strengthen in the coming years [2]. Hence, it is necessary for manufacturing technology to react to these challenges. Rapid Manufacturing can be a part of the solution as it is possible to produce devices of nearly any geometry without the need for pre-tooling. On the one hand a batch size of one is not a challenge anymore; on the other hand the achievable material qualities do not meet the expectations. Therefore, it is necessary to develop the Rapid Prototyping to Rapid Manufacturing. To improve the product quality and to simplify the discovery of new materials, it is necessary to develop simulations. These models will help to a further understanding of process and material.

State of the art

The technique of Rapid Manufacturing (RM), also called Additive Layer Manufacturing (ALM), is based on fabricating three-dimensional models and devices layer by layer [3]. Therefore, adequate CAD-data of the component is converted to STL (Standard Triangulation Language) and then to layer-data, often based on CLI (Common Layer Interface). This information is transferred to the system, where it is consequently produced layer-wise with no need for tooling or writing of individual CNC-codes. The global market offers several systems to fit this purpose, which have to be categorized as follows. On the one hand there are systems, which build up metal parts; on the other hand there are polymer- and ceramic-based techniques. The material can be powder, wire or liquid, which is essentially solidified by laser, electron beam or a liquid second phase (binder).

The three-dimensional inkjet printing process is one of the technologies of Rapid Manufacturing. It is based on printing a liquid binder in a powder bed, where solidification takes place. By repeated recoating a thin powder layer, selectively printing the liquid and lowering the fabrication platform, a physical model is generated as can be seen in Figure 1. Depending on the printing process and the material it can take up to 24 hours until the device can be removed which is completely wrapped with powder.

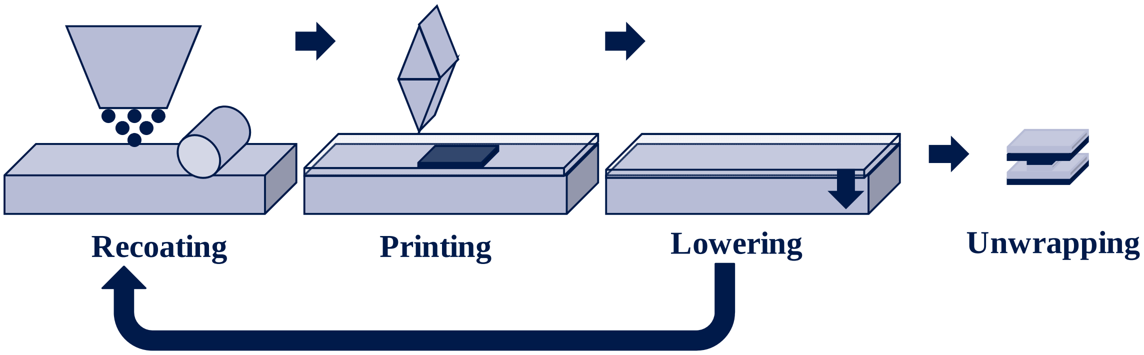


Figure 1: Principles of 3D inkjet printing

The material is always defined by its mechanical, thermal and physical characteristics. For design of devices the mechanical properties are particularly important. A brief overview on tensile testing and its general results shall be given. Figure 2 shows a stress-strain diagram of PolyPorA as a result of tensile testing according to DIN 527 [4].

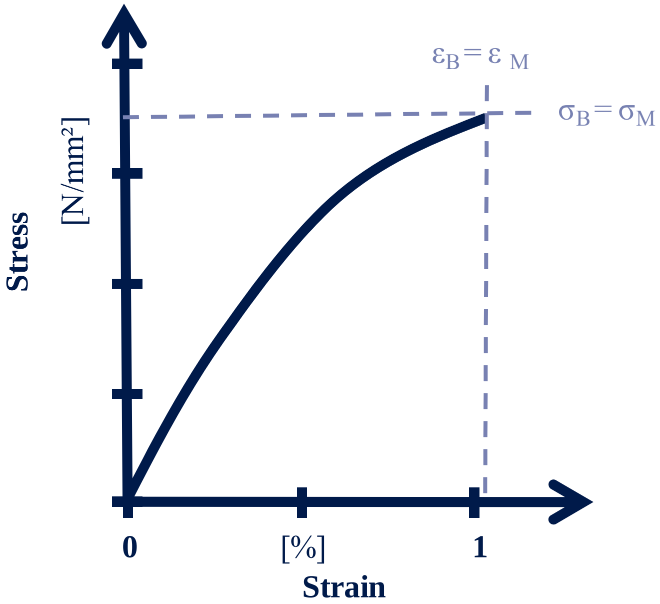


Figure 2: Stress-strain diagram of PolyPorA

The relevant parameters are tensile stress at break σ_B, tensile strength σ_M and the related strains ε_B and ε_M. Strain is defined as the change of length regarding the effective distance. The modules of elasticity in tension (Young's modulus, according to equation (1)) E_t, to measure the stiffness of the material can be obtained as well:

$$E_t = \frac{\sigma}{\varepsilon} \qquad (1)$$

Tensile stress at break defines the stress which the specimen stands at break. Analogue the tensile strain at break is measured. The tensile strength is the maximum stress, which the specimen bears during tensile testing; the tensile strain at tensile strength is the related strain at maximum stress. The material used for this work is PolyPorA, which is a PMMA-blend; their characteristics are:

Table 1: Mechanical characteristics of PMMA and PolyPorA

Parameter	Abbr.	Unit	PMMA [5]	PolyPorA
Tensile strength	σ_M	MPa	80	3,6
Tensile strain at tensile strength	ε_M	%	10	1,1
Young's modulus	E_t	MPa	2000	400
Poisson's ratio	ν	-	0,3	0,31

These values are important input quantities for the simulation models. As a matter of course, various approaches for simulation of 3D inkjet printing are close at hands. On the one hand it is possible to set up a model of the fluid dispensed by the printing head and its flow in the powder bed by the Finite Elements Method (FEM). Similar was done by [6], who evaluated the flow of a Newtonian liquid in a trapezoidal cavity. On the other hand it seems to be more useful for the problem of diminutive material properties to simulate the strength of the material. This can be done by a micro-macro-structural model. A promising approach appears to be the building of an inner material model for the micro-structure based on [7] to optimise material properties and to estimate the shrinkage of the resulting macro-structure by a layer model, as presented by [8] to improve accuracy.

Aims

During this work, which is supported by the Bavarian Research Foundation, mechanical properties shall be improved and material behavior will be simulated. The parts, to be analyzed, are fabricated of polymer material (PolyPorA) on a machine of voxeljet technology. Other systems for 3D printing are not focused in this work.

To be able to produce devices and not only physical models and prototypes it is particularly important to increase mechanical properties such as

- Young's modulus
- Tensile strength
- Tensile strain at tensile strength

and to decrease

- Porosity.

Hence, it is necessary to modify the materials used as well as to alter the processing equipment. As a first step it is reasonable to simulate the material used in production run and to change its composition as well as the processing equipment later in addition. In this paper several simulation models will be presented:

- Multiscale material design to foretell mechanical properties of binder
- Modeling of material micro structure to estimate its properties
- Simulation of stress and its resulting deformation and derivation of principles
- Configuration of a simulation model for prediction of shrinkage

The first three steps are linked with one another, the last one stand can be implemented parallel. An overview is given in Figure 3.

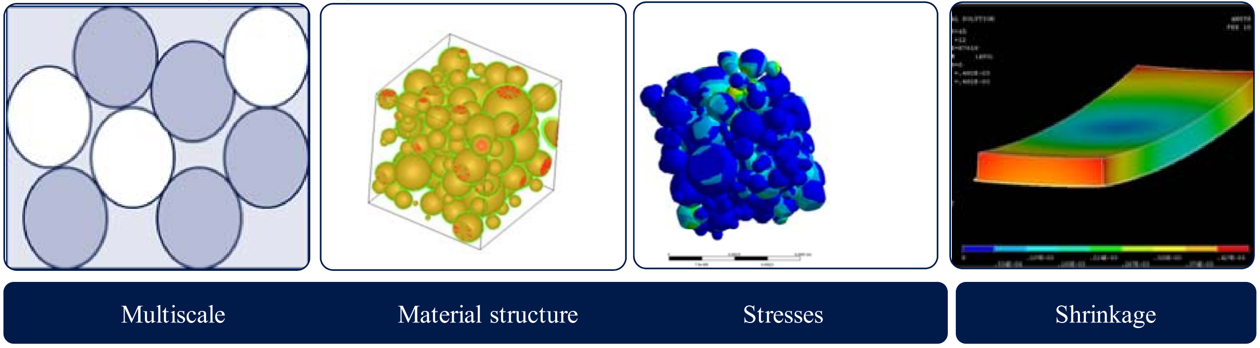


Figure 3: Approaches of simulation models for 3D printing

Approach

Multiscale material design

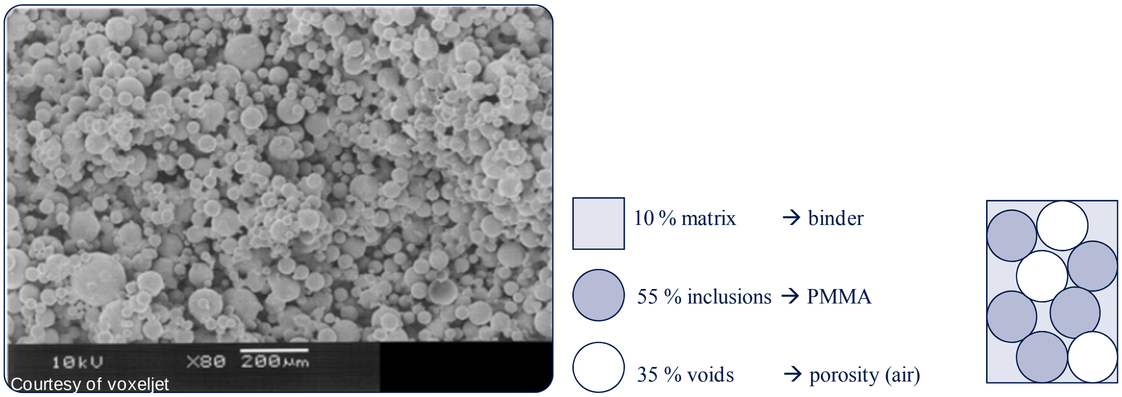
The multiscale material design is based on the distribution of the phases after the 3D printing process and the scanning electron micrograph (SEM), which can both be seen in Figure 4. The material consists of

- 10 % binder
- 55 % PolyPorA pellets
- 35 % air-filled voids.

On that base it was possible to set up a scheme of the material. Preliminarily a model is set up to gain the properties of the binder (glue) by reverse engineering in digimat MF. Therefore, it is necessary to make the following presuppositions for the mechanical properties of the PMMA (base of PolyPorA) pellets:

- Linear elastic approach
- Values presented in table 1 are well known from literature (PMMA) [5] and experimentations in this project (PolyPorA)

Furthermore the geometry microstructure of the pellets can be estimated from electron microscopy samples



Courtesy of voxeljet

Figure 4: Distribution of the phases

The voids can be estimated by the characteristics of air such as:

- Cannot bear stress
- Infinite strain possible

The mechanical properties of the glue as well as the strength of the bonding between the pellets are unknown and have to be evaluated in the simulation using the suppositions of nonlinear material properties and an elastoplastic approach.

Modeling of material micro structure

Knowing the grain size distribution of the material and under the presumption of a particle overlap of 10 %, several models of the microstructure can be modeled. The overlap is realistically based on the assumption the binder etches the PolyPorA balls. This part of the simulation takes part in digimat FE. Giving these boundary conditions several material structures are set up.

Using this new approach, it will be able to predict the mechanical strength of the system depending on its material, microstructure and amount of powder and binder, which is used. As a consequence it will be possible to design the optimal material in terms of grain distribution, powder and binder input.

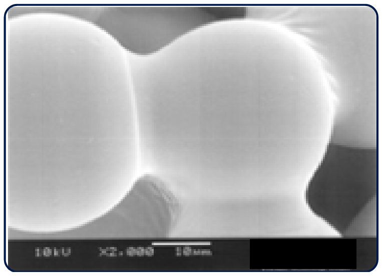


Figure 5: Overlap of 10 %

Simulation of stress

By using established material data of microstructures, the tensile load was simulated by the tool ANSYS. The resulted stresses and distortions were evaluated. The maximums were accounted for every structure and a classification of the topologies took place.

Modeling of shrinkage

To consider the influence of shrinkage it is also necessary, to establish a model, by implementing the thermo-mechanical shrinkage based on reduction of volume as a function of time and binder input. This will be set up in layers and therefore be able to give an idea of the influence of shrinkage on several aspects like accuracy, different kinds of distortion and impact of layer-wise fabricating of polymers.

Results

Multiscale material design

Based on this information, a model is set up, which is content of Figure 6, giving an overview of the properties of PMMA, printed PolyPorA, strength of the binder and air. The binder properties are modeled in a way to fit the simulated and the experimental stress-strain-diagram. It is clearly visible, that the PMMA pellets have a much higher strength than printed PolyPorA. Anyway, the binder is the weak point.

Therefore, it is necessary to have a closer look at that part of the diagram, which can be seen in Figure 6. The Young's modulus will be $E_t = 18$ MPa and Poisson's ratio $\nu = 0.3$. This is one order of magnitude less than the PMMA tensile properties and requires a closer look on the connection of the pellets.

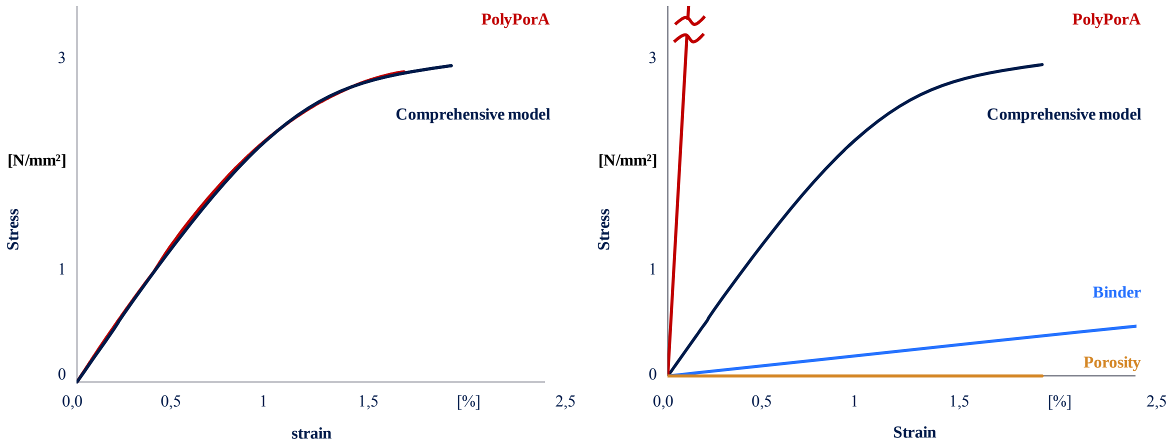
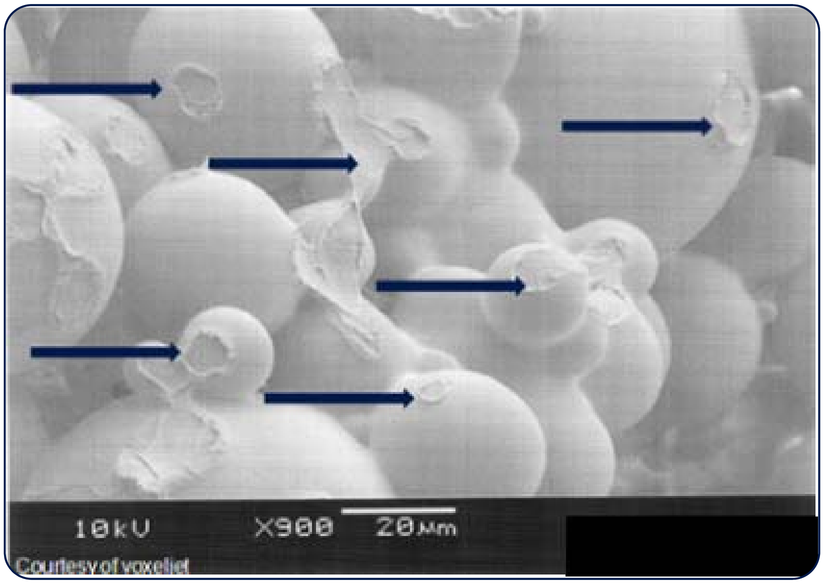


Figure 6: Stress-strain diagram of PolyPorA, PMMA, Air and the expected strength of binder

Consequently some SEM micrographs of a broken PolyPorA tensile testing specimen are taken and the results can be seen in Figure 10. Obviously, the fracture face is situated at the bonding of the pellets.



[redacted]

Figure 7: SEM micrograph of 3D printed and broken PolyPorA

Modeling of material micro structure

In line with the modeling several structures with a filling degree of 40 - 62 % have to be created. The binder is presumed to be the coating on the particles. Therefore, the 10 % input of binder is not sufficient to glue all grains. About 5 - 10 % of the grains have no connection at all. Therefore, the binder seems to increase the density and the filling degree of the material structure. But as parts of the grain do not have any connection to the base material, the material cannot bear stresses. The tensile stress area is reduced. Figure 8 shows the modeled microstructure and its resulting non-bonding effect. The grains are pulled out of the rest of the structure, showing no connection.

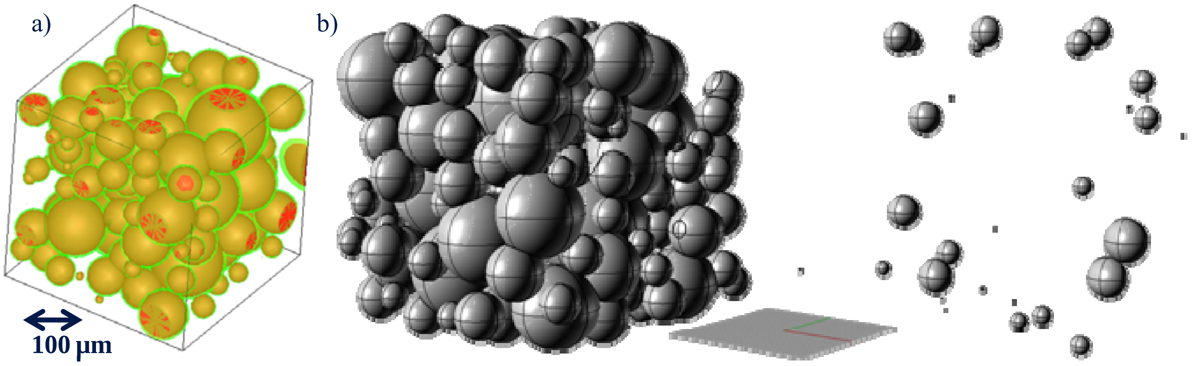


Figure 8: Modeled microstructure (a) and demonstration of non-bonding (b)

Simulation of stress

Exemplary for all structures, two are shown in Figure 9. A quite equal stress limit all over the grains with a maximum of 12.1 MPa can be seen in a). The particle arrangement is reminiscent of a spherical structure. On the contrary structure b) has less inner connection and therefore a maximum stress level of 37.3 MPa. Some of the balls take an elliptical form, which in reality, would result in breakage.

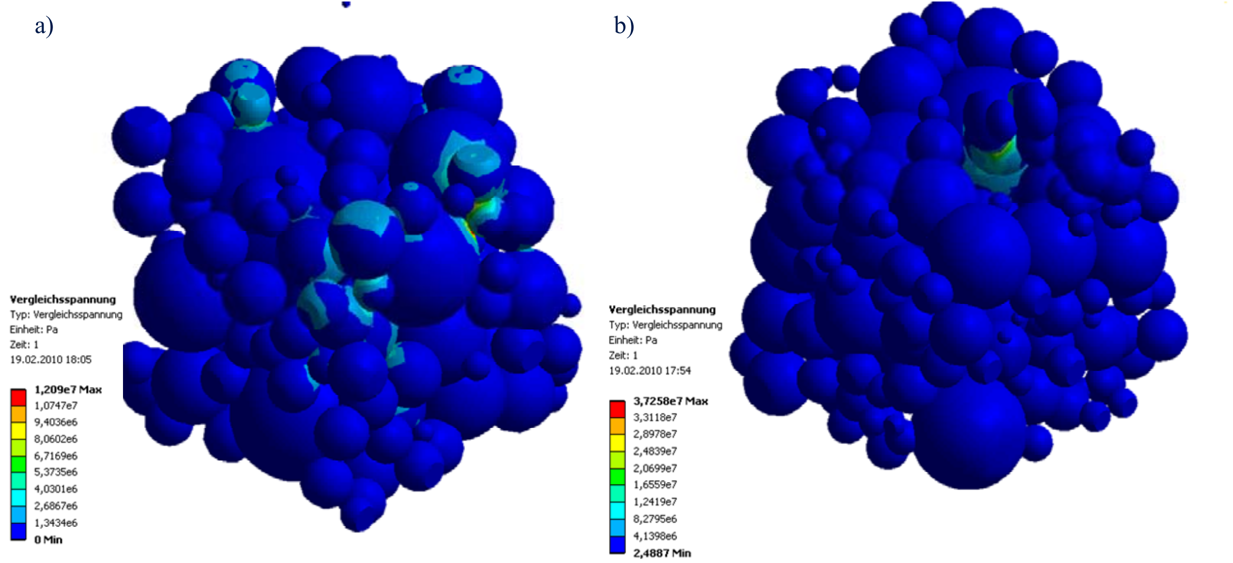


Figure 9: Stress and resulting distortion in two structures

Three different grain distributions could be determined (Figure 10), which are classified into the general types:

- z shaped structure
- c shaped structure
- o shaped structure

As a matter of course hybrids can appear as well. All structures can be rotated arbitrarily, which results in diverse stress and distortion limits. The stress peaks differ strongly as well, which leads to very different tensile strengths. As they cannot be determined before 3D printing, but are generated by coincidence, repeatable material properties cannot be predicted.

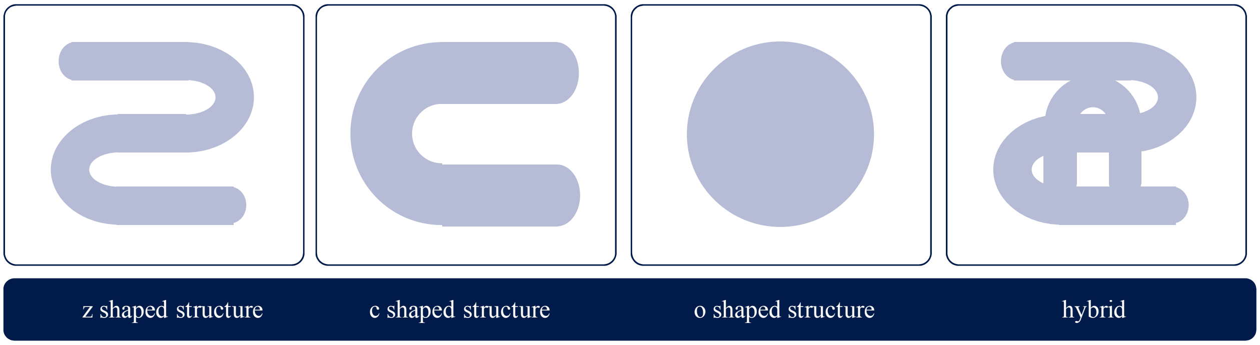
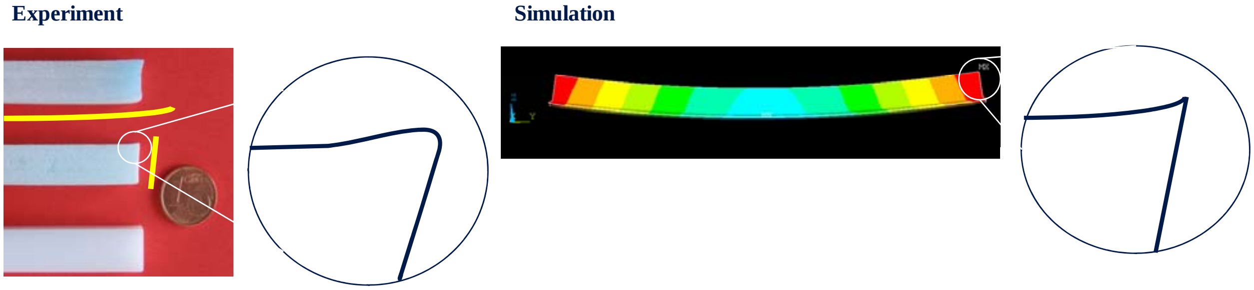


Figure 10: Different structures resulting from grain distribution

Modeling of shrinkage

The shrinkage simulation gives an overview of the distortion in z direction as could be seen in experiments as well. Only the sphericity of the angles (Figure 11) cannot be seen in the model, as their mechanism is not part of the simulation model. The developed model will be varied in future to minimize shrinkage by suitable processing parameters.



Experiment

Simulation

Figure 11: Model of shrinkage

Conclusion and future works

The developed simulation models were validated on a prototype machine, which is able to produce parts of the polymer material PolyPorA and can be seen in Figure 12. The material properties of the produced devices were examined and the challenges of porosity in addition to tensile strength were demonstrated. Hence, there is need to improve the achievable mechanical strengths as well as the materials in use for testing.

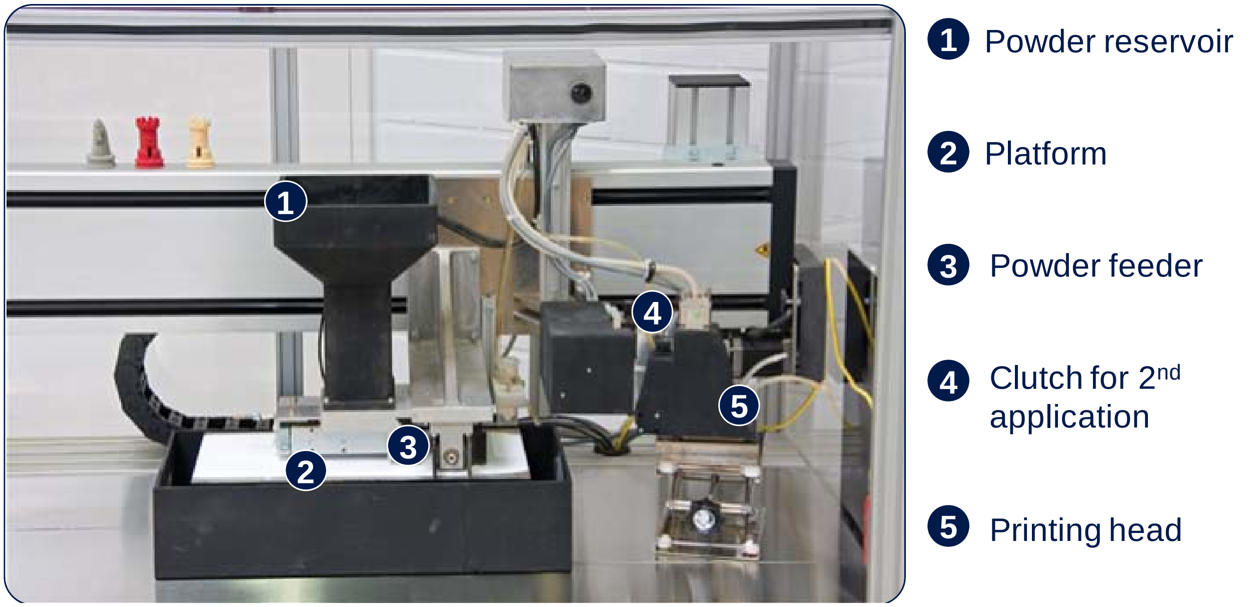


Figure 12: Developed 3D printing demonstrator

The simulation models could be determined and provide a first glance on possibilities to optimize the process as well as the characterization of materials for 3D printing. Yet, they have to be expanded in future works to integrate more characteristics as well as to model the macrostructure more precisely to be able to give a better insight into the problem of shrinking.

Acknowledgement

The presented studies are part of the research project “Activated polymerisation for 3D printing of polymers”, which is funded by the Bavarian Research Foundation (BFS).

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