Joint Special Interest Group meeting between euspen and ASPE
Advancing Precision in Additive Manufacturing
KU Leuven, Belgium, September 2023
www.euspen.eu

Atomistic simulations of laser powder bed fusion

Fabio Oelschläger[1], Azad Gorgis[1], Jonas Schmid[1], Kevin Vietz[1], Dominic Klein[1], Sarah Müller[2], Johannes Roth[1]

[1]Institute for Functional Matter and Quantum Technologies, FMQ, University of Stuttgart, Germany
[2]Graduate School of Excellence advanced Manufacturing Engineering, GSaME, University of Stuttgart, Germany

Johannes.roth@fmq.uni-stuttgart.de

Abstract
New applications for additive technologies continue to demand an improvement in quality and reproducibility. Using simulations and physical models we are able to better understand the root causes for defects and may be able to derivate actions for defect avoidance. This paper presents a novel approach to the simulation of additive manufacturing using molecular dynamics simulations. By solving Newtons equations of motion iteratively we are able to yield the time evolution of the system and can simulate the melting of single particles or particle clusters. A big challenge to the simulations are the scales: although we use multi-million atom systems and run "long" simulations we have to scale parameters like particle size, laser power, power density, scanning speed, laser focus diameter and gravity.
Using parameter studies for scanning speed and laser power while also including the influence of protective argon gas, different inclusion defects in pure aluminum particles are shown. The simulation of powder beds formed by spheres of different size show holes which vanish if filled with vacuum but persist if the simulation box is filled with protective gas allowing insight into the defect formation. Additionally, different configurations of binary materials made of aluminum and titanium are simulated: the study compares spheres from by a core of aluminum and an outer shell of titanium or vice versa, and homogenous sphere of a TiAl alloy.

Aluminium, Modelling, Laser power bed fusion (LBPF) Simulation

1. Introduction

Additive manufacturing (AM) of products plays an increasing role today. Although AM is widely promoted as a method with a big future, it is still far away from working perfectly and being competitive with other methods. Deviation of size and defects are frequent. To understand the defects and failures on an atomistic level, large scale molecular dynamics (MD) simulations on supercomputers are carried out with the simulation code IMD [1] which is well suited for this purpose and has been demonstrated to run effectively with billions of atoms. For the simulation of AM presented here only a few modifications have to be made, for example the setup of the moving laser beam, the absorption of the laser power, including protective gas in the simulations, and the addition of gravitational force.

A main challenge is the gap between manageable simulation sizes and industrial scales which typically differ by one to two orders of magnitude in the current case. In principle the supercomputers are large enough to reach industrial scales but such simulations would require the complete state-of-the-art machine for weeks together with sufficient resources for storage, analysis, and visualization.

For the time being we have to resort to running smaller simulations and to scale the results suitably. Having optimized the simulation code and collected experience from the simulations it will be possible to go to the limits of the available computing power. In the present study we have demonstrated already that all components of the model work quite well.

The report is organized as follows: First we discuss the simulation model, followed by the first proof of principle studies. Then we show results of binary alloy and resolidification studies, followed by a summary and conclusion.

1.1 Simulating Laser Powder Bed Fusion (LPBF)

The principle setup for the LPBF simulations is as follows: the objects which are to be irradiated are placed on a fixed plate which is modeled by immobile atoms. Currently only single spheres or one-dimensional arrangements of spheres are studied. Later stacked layers of powder particles will follow and the fixed plate will be included in the simulation. A laser beam is moving across the objects with a fixed, but adjustable velocity. Its shape, size, and absorption length can be varied.

2. Modeling of LPBF by Molecular Dynamics (MD) Simulations

The dynamics of the powder as well as the interaction between powder and laser is modeled by molecular dynamics simulation using the IMD [1]. The classical Newtonian equations are integrated at discrete time steps, typically fractions of femto-seconds for atomistic systems. Interactions in metals are modeled by embedded-atom potentials (EAM) [2].

The total interacting energy of the system

$$E_{tot} = \sum_i \left[F(\rho_i) + \frac{1}{2} \sum_{i \neq j} \phi(r_{ij}) \right]$$

contains of the electrostatic core-core repulsion $\varphi(r_{ij})$, as well as an embedding function F depending on the host electron density ρ_i which incorporate the properties of the free electron gas. To represent a specific material these effective interactions are fitted to the quantum mechanical properties.

2.1 Laser Absorption

The laser power P_0 is described by a Gaussian power profile. The laser velocity is set to a constant, and the total laser power is also approximately constant due to the short time scale of the simulation. The laser absorption is modelled by an energy re-scaling on an atomistic base. The radiant power inside the metal

at a depth z is calculated according to the Lambert-Beer law given by

$$P(z) = P_0\ e^{-\alpha z}$$

depending on the material specific absorption coefficient α.

The laser excites the electrons and the energy will eventually be transformed into thermal energy of the atoms. Thus the rescaling method has been applied since the time scales of the thermalization processes are shorter than the interaction time scales of the laser. The velocities of the atoms are rescaled such that the added laser energy increases the temperature due to the equipartition principle. For details see [3].

2.2. Sample Sizes

The size of MD simulation samples have increased tremendously in recent years up to about 10^{13} atoms. But simulations of such a size would require full-time simulations on entire top-level supercomputers. The sizes of powder particle in the LPBF process in the range of a few µm is beyond the limit of current production simulations. The size of the system has been scaled down to a few hundred Å.

Scale factors have to be introduced to connect simulation and experiment. The approach can be motivated by the work of Glosli et al [4] who could demonstrate that the Kelvin-Helmholtz instability in fluids for example occurs at relatively small particle numbers already. Laser power bed fusion depends on the behavior of fluids in a similar way. If the simulations are carried out at different length scales, laser power and velocities, then the fit of the results can be extrapolated to relatistic LPBF parameters.

The scaling will have to include an increase of the gravitational force also. Here the specific size of the force does not change the behavior of the system, it is only necessary to add a preferential up-down-direction to the system.

3. First simulations

The initial sample is a sphere cut out of a crystal and equilibrated at 300 K taking gravity into account which causes the sphere to settle down slightly. The sphere is placed on a fixed plane. For details see [3]. A typical laser velocity which can be realized in MD simulations is 1 Å/fs.

The laser power melts the system rapidly on a scale of 5 ps and stays constant for about 50 ps. A laser power of P = 16 eV/fs is required for complete melting in this phase. It is observed, however, that on the longer time scale of 200 ps a lower power P = 10 eV/fs is already sufficient for complete melting since the molten fraction increases slowly.

A further phenomenon was observed for partial molten spheres: they tip over and generate inclusions which is often a problem in LPBF. Since the current simulation was carried out in vacuum, the inclusion vanished after some time. If the process is simulated with a protective gas, then vapor may fill the inclusion and protect it from removal.

A relation between the laser velocity and the laser power was determined: if the velocity is reduced, for example from v = 1 to 0.5 Å/fs, then the laser power has to be reduced since the interaction time increases. This is really the case. The laser power has to be reduced from P = 8 to 5 eV/fs to get the same melting behavior.

The general behavior of the melting sphere is remarkable: it strongly depends on the specific absorption coefficient α. If this value is small, only the upper part of the sphere is molten, the lower stay crystalline. If the applied laser power is too large many droplets are formed which lead to splashing and balling. Thus it is recommended to apply a laser power as small as possible. Then the surface deforms but stays smooth or a pillar develops which spawns a single drop and finally falls back into the bulk.

3.1 Gas coverage

Usually LBPF is carried out in ambient atmosphere or under protective gas and not in vacuum as in the first simulations. This possibility has also been modelled. First simulations show that the gas suppresses melting and reduces evaporation. Few gas-filed inclusions are generated.

4. Laser-based powder bed fusion of TiAl

We investigate the applicability of binary alloys for additive manufacturing by performing simulations of laser-bed powder bed fusion with titanium aluminide and studying the material dynamics. Therefore we compare coated powder grains with pre-alloyed grains and investigate the influence of the laser scanning speed.

4.1. Suitability of coated powder grains

We perform laser melting simulations of coated powder grains as well as pre-alloyed titanium-aluminide powder grains. The schematic illustrations of the initial grain structures are shown in figure 1. We construct the initial powder grains with a diameter of 400 Å and place them on a fixed ground of atoms. The initial titanium:aluminum ratio is set to 50:50 which leads to about 2 000 000 atoms per powder grain.

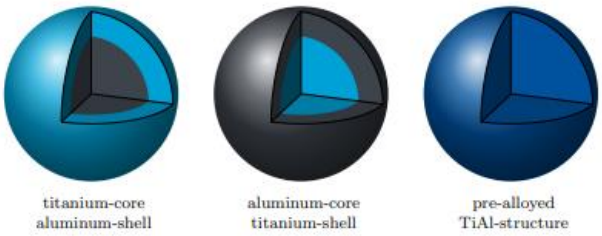

Figure 1. Schematic illustration of the investigated powder grain structures.

The time evolution during laser melting simulations for the different structures is shown in figure 2. Due to the chosen laser parameters we observe that all grains burst and melt completely. But despite infusing enough energy to melt the grains completely we observe an inhomogeneous mixing for the coated structures in the long time limit. For the investigation of the distribution ratios we perform a cluster analysis and consider only atoms within the biggest leftover cluster. We then find titanium:aluminum ratios of 58:42 for the aluminum coated titanium core, 52:48 for the titanium coated aluminum core and 55:45 for the pre-alloyed grain simulation. So we are left with less aluminium in all simulations, but the more aluminium atoms are protected by surrounding titanium atoms the less aluminium is vaporized.

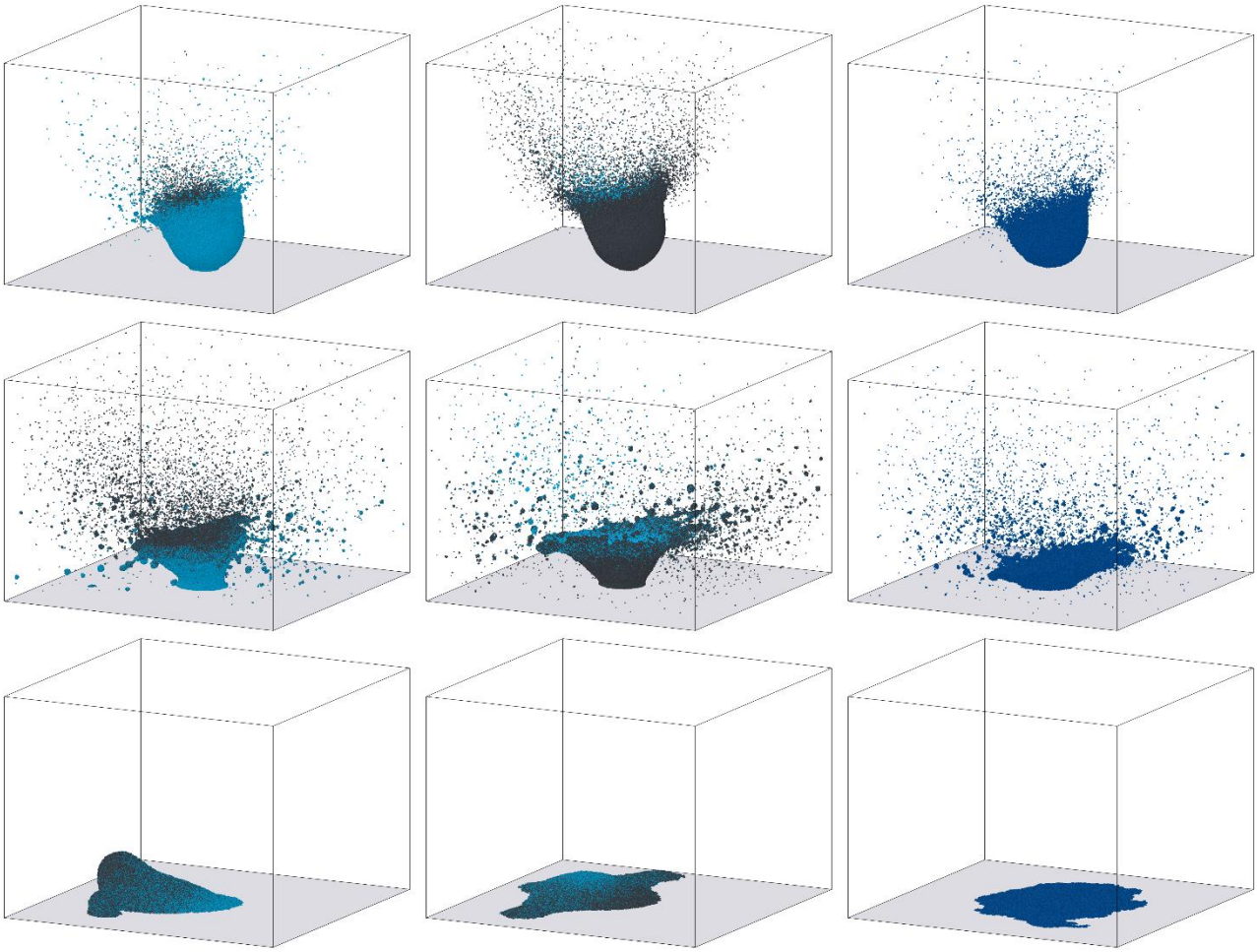

Figure 2. Time evolution of laser melting simulations for coated grains in comparison to pre-alloyed titanium-aluminide grains. From left to right: Ti-core Al-shell, Al-core Ti-shell, TiAl-alloy. From bottom to top: 300 ps, 80 ps, 40 ps.

4.2. Laser scanning speed comparison

Because of the different scaling between simulated and real powder grains and especially the scaling in time it is by far not trivial to choose a valuable set of laser parameters to depict the material dynamics in a good manner. Therefore we perform laser melting simulations and vary the laser scanning speed while keeping other parameters constant. The simulations are performed with the pre-alloyed TiAl-grains. Figure 3 shows a snapshot during the laser melting simulations for different laser scanning speeds. While the infusing energy varies greatly, we obtain very different behaviors during the simulation. The grain on the left shows a strong explosion, while the grain on the right side is not fully melted. Also a kind of splashing fountain effect can be obtained for increasing the scanning speed, results in the generation of bigger detached droplets.

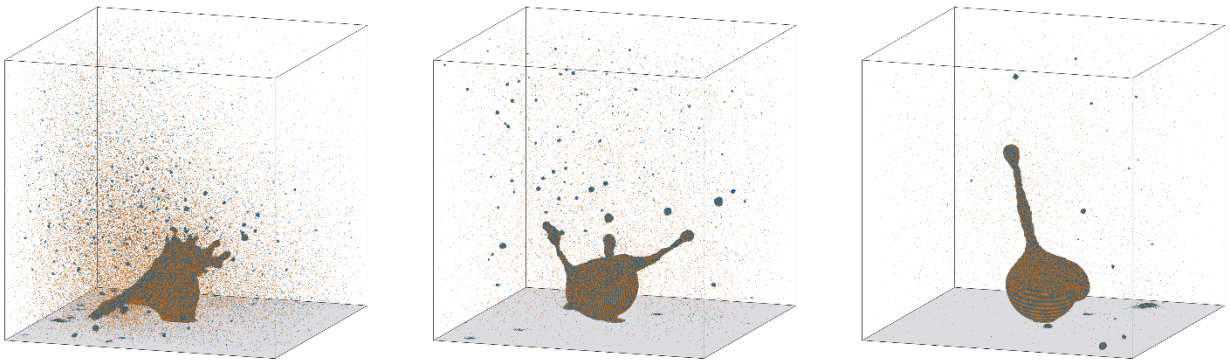

Figure 3. Snapshot after 80 ps of different laser scanning speeds. From left to right the used velocities are v = 0.01, v = 0.03 and v = 0.05 Å/fs.

5. Resolidification

Resolidification has been studied in a simulation of a bimodal distribution of spheres as shown in figure 4. The initial sample is composed of aligned spheres covered with argon gas (Figure 5).

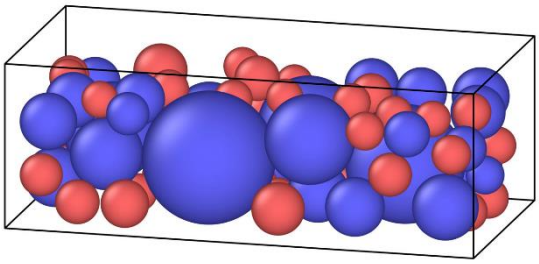

Figure 4. Bimodal distribution of spheres with Gaussian size distribution.

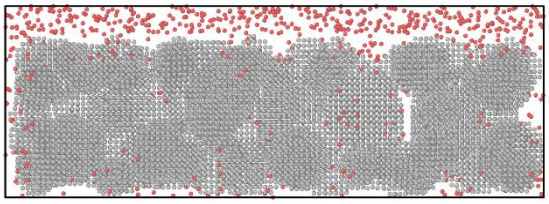

Figure 5. Crystal structure of the aluminum spheres (grey) covered by argon (red).

After the laser has passed the sample the material solidifies (Figure 6). Aluminum recovers its genuine crystalline fcc structure, some grains fuse coherently while others crystallize in random orientation and are separated by stacking faults, indicated by the hcp crystal structure. To study the distribution of stresses in the resolidified sample would be the next step but currently the samples are too small for reliable results.

The argon gas still plays a minor role: if gaps persist then they are closed and the gas escapes. Thus the geometry and the size of the sample have to be modified to increase the probability of gas pockets.

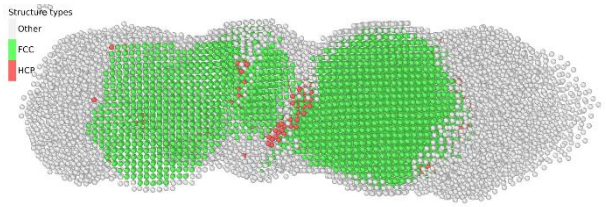

Figure 6. Cross section through the sample after resolidification. Colors should different crystal structure types and grain boundaries. Grey are liquid atoms or atoms with undefined crystal structure, red are grain boundaries or stacking faults (hcp) between grains with genuine aluminum crystal structure (fcc). At the left side two grains have fused coherently. In the center two grains in random orientation are separated by a stacking fault.

6. Summary and Conclusions

Our simulations have demonstrated that it is possible to achieve meaningful results for laser powder bed fusion (LPBF) with molecular dynamics simulations. A drawback are the long simulation times, short real time scale of the simulations and the small samples sizes. Some of this problems can be overcome by more experience and optimizations of the simulation code. Existing supercomputers are large enough for bigger simulations.

A huge advantage of molecular dynamics simulations based on ab-initio-interactions is the fact that much less assumptions have to be made compared to continuum descriptions used in finite element methods. All basic material properties can be derived directly from the simulations and compared to experiments. The MD permits a structural analysis of melting as well as the nucleation and the mixing of alloys on an atomistic level.

The simulations have resulted already in reproducing qualitatively basic problems of LPBF like inclusions, lack of fusion and boding defects, or balling. Cracks and pores are expected to follow. The observation of keyhole effects might be more difficult. It is expected that larger simulations can be used to produce quantitative results which can directly be compared to experiments.

References

[1] Roth J 2013: IMD: A Typical Massively Parallel Molecular Dynamics Code for Classical Simulations - Structure, Applications, Latest Developments, in Sustained Simulation Performance 2013, eds. Resch M M, Bez W, Focht E, Kobayashi H, and Kovalenko Y, Springer (2013) p 63-76

[2] Murray S D, and Baskes M I 1984 *Phys. Rev. B* **29** 6443

[3] Oelschläger F, Klein D, Müller S, and Roth, J: Molecular Dynamics Simulation of Selective Laser Melting, in High Performance in Science and Engineering ’21, eds. Nagel W E, Kröner D B, Resch M M, Springer (2023) p 65-80

[4] Glosli J N, Richards D F, Caspersen K J, Rudd, R E, Gunnels J A, Streitz, F H Extending stability beyond CPU millennium: a micron-scale atomistic simulation of Kelvin-Helmholtz instability, in: SC '07: Proceedings of the 2007 ACM/IEEE Conference on Supercomputing. 2007, pp. 1-11.