University of Stuttgart
Germany

Institute for Functional Matter and Quantum Technologies

MD Simulation of 3D Laser Printing

Jonas Schmid, Kevin Vietz, Dominic Klein, Johannes Roth

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3D Laser Printing Setup

- Components are printed layer by layer
- New powder is distributed for each layer
- The metal powder is fused onto the previous layer using laser beam

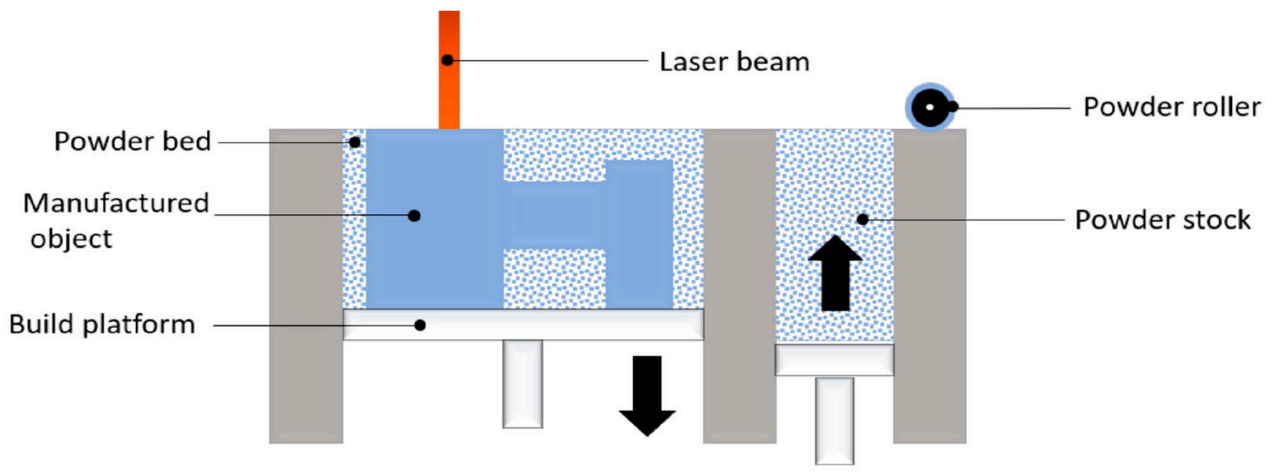

Figure: Schematic representation of 3D laser printing setup (PBF)[1]

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Powder Composition

- Size distribution of powder particles is adopted form experimental data [2] [3]
- Powder particles consist of fine and coarse particles, while the particle sizes are Gaussian distributed

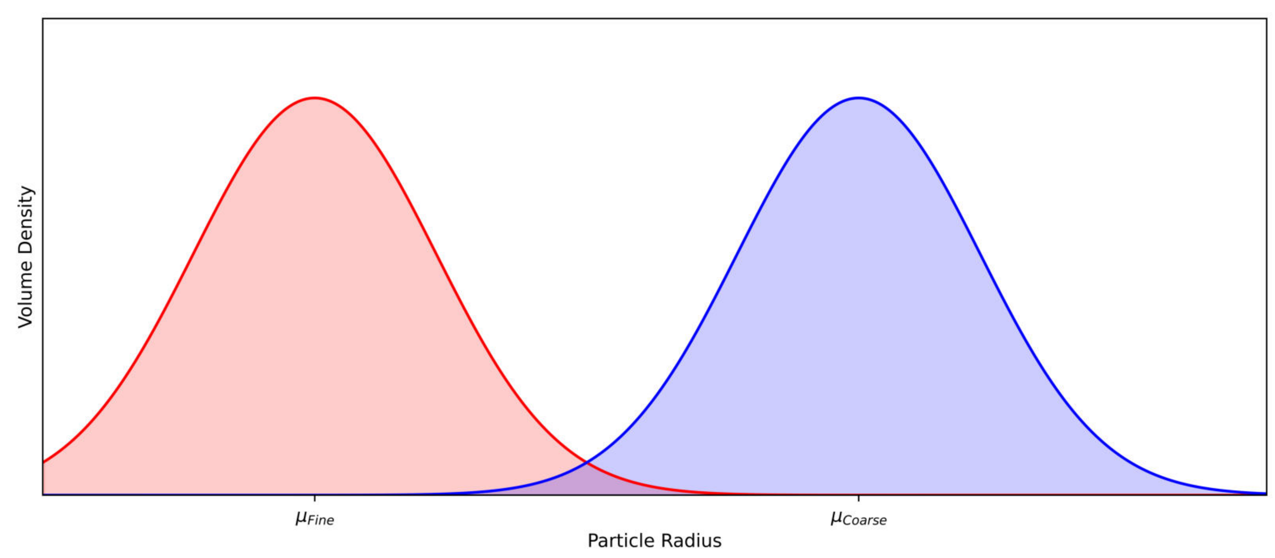

Figure: Powder Particle Distribution

- Powder are particles random distributed in the sample
- Total volume fractions are 35% for coarse particles and 20 % for fine particles

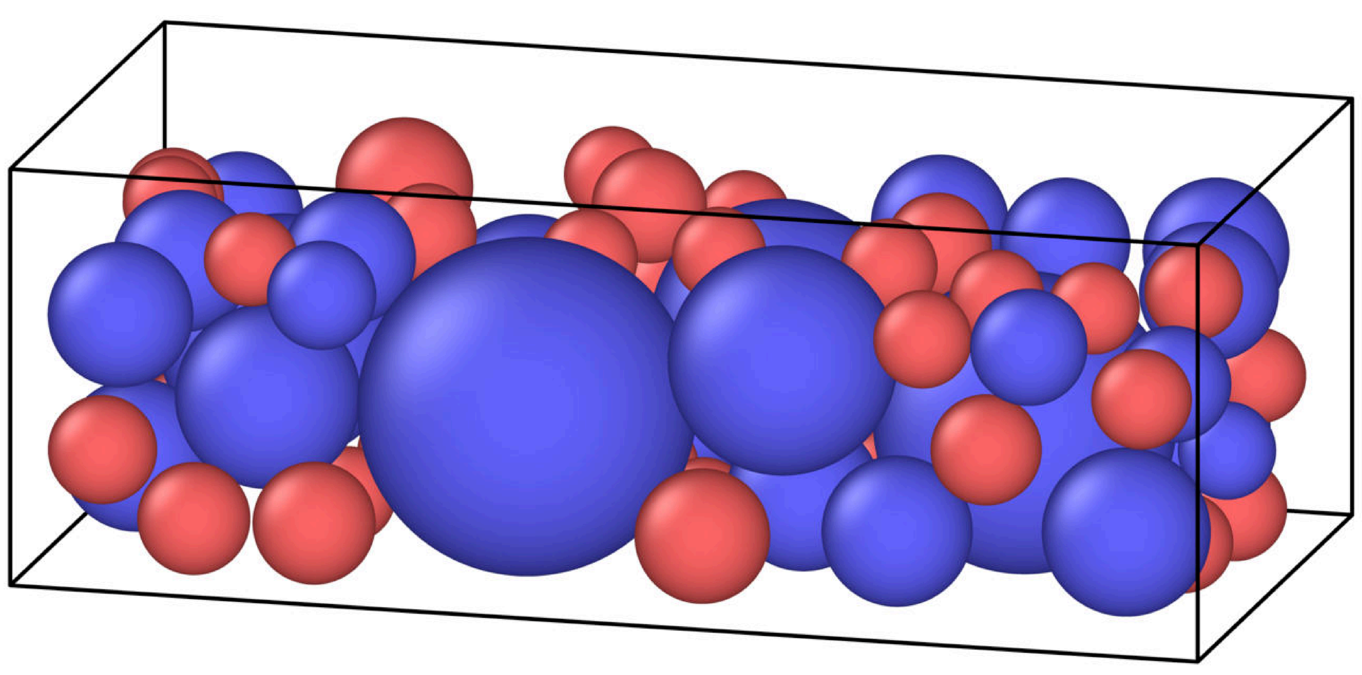

Figure: Powder bed including find (red) and coarse (spheres).

Discussion and Outlook

- Escape of the gas mainly due to the small size of the sample
- Larger escape trajectories and a higher number of gas atoms in bigger sample increase probability of gas pockets
- Recrystallization onto the previous layer is experimentally important
- Simulation until complete recrystallization to perform stress test of the final sample depending on aluminum powder composition
- Further investigation on laser parameters

Simulation Setup

- Forces between the atoms in the Molecular Dynamic simulation are calculated using the Embedded Atom Model.
- Laser absolution is calculated using the Lambert-Beer law:

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

- The specific abstention coefficient ε depends on the local metal density
- No interaction between laser and gas
- NVE ensemble is used while penetrating the sample with the laser.
- Cooling is performed uniformly using a Nosé-Hoover thermostat

Al Powder Laser Melting in Ar Gas Environment

- Powder spheres are filled with aluminum atoms in FCC-structure.
- The config consists of 32,000 atoms

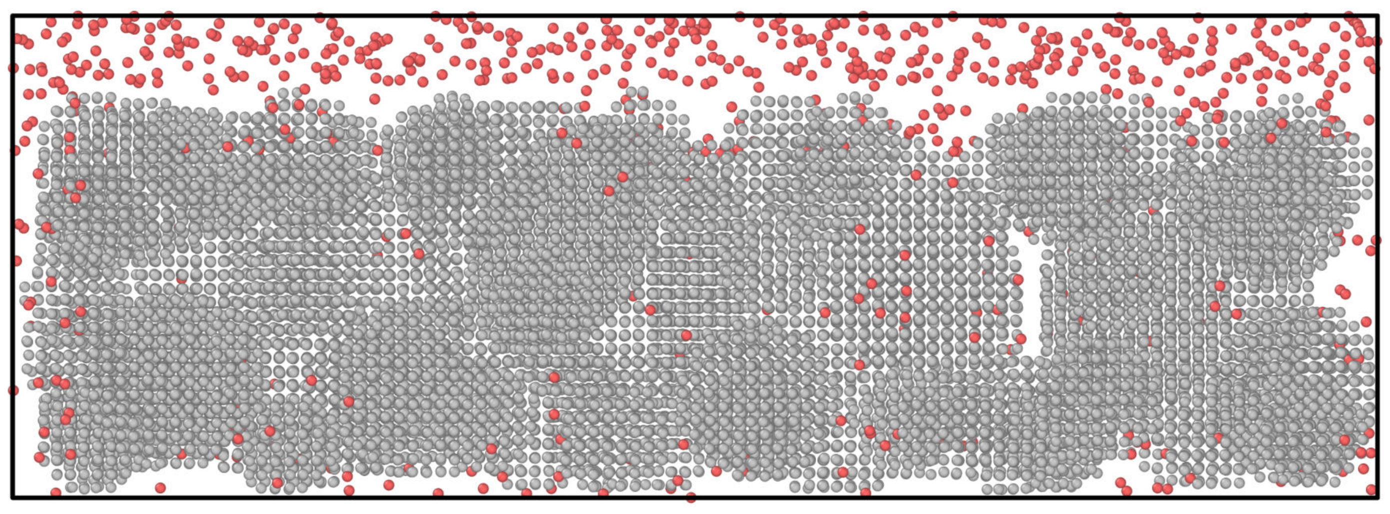

Figure: Aluminum powder (white) surrounded by Argon gas (red).

- While melting and resolidification the gas atoms are forced out of the sample.
- No major structure difference compared to melting without gas.

Structure Analysis of Al Powder Melting

- Recrystallizing of FCC structure starts from the unmelted powder centers
- Twisted orientations of the FCC crystals leads to defects (HCP structure) and cracks
- No vacuum pockets arise in the final sample

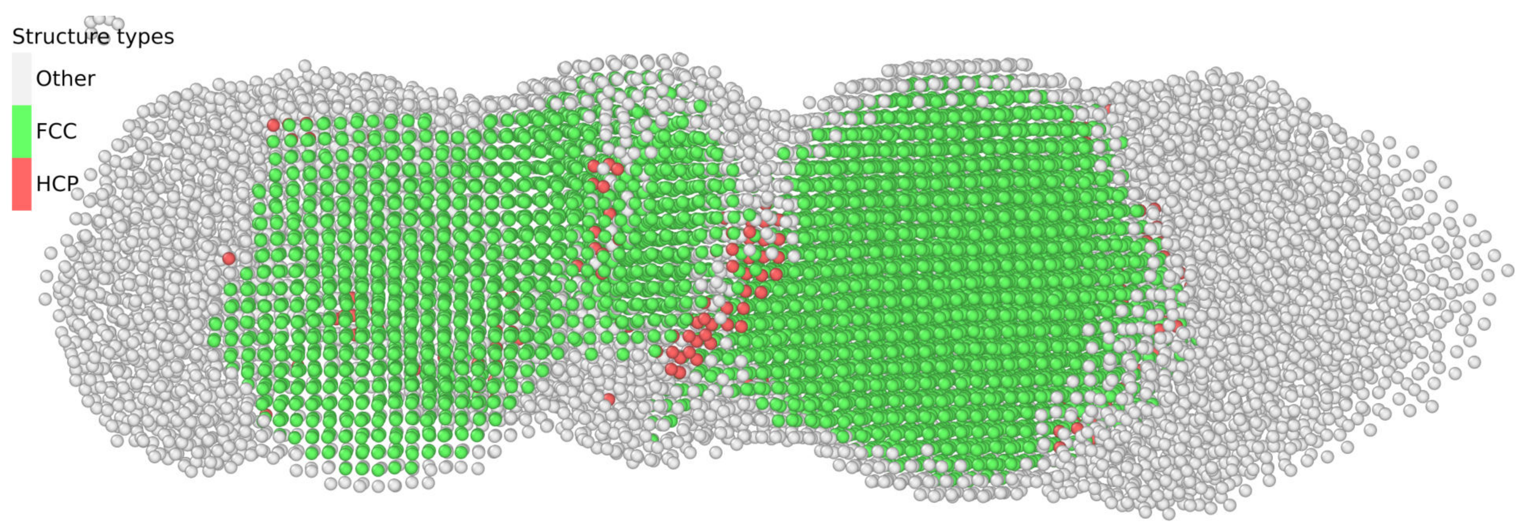

Figure: Cross section of aluminum powder while the resolidification

[1] Dejene Naol Dessalegn et al. Current status and challenges of powder bed fusion-based metal additive manufacturing: Literature review. *Metals*, 13(2), 2023.

[2] M.A. Balbaa et al. Role of powder particle size on laser powder bed fusion processability of alsi10mg alloy. *Additive Manufacturing*, 37:101630, 2021.

[3] Masaya Higashi et al. Effect of initial powder particle size on the hot workability of powder metallurgy ni-based superalloys. *Materials Design*, 194:108926, 2020.