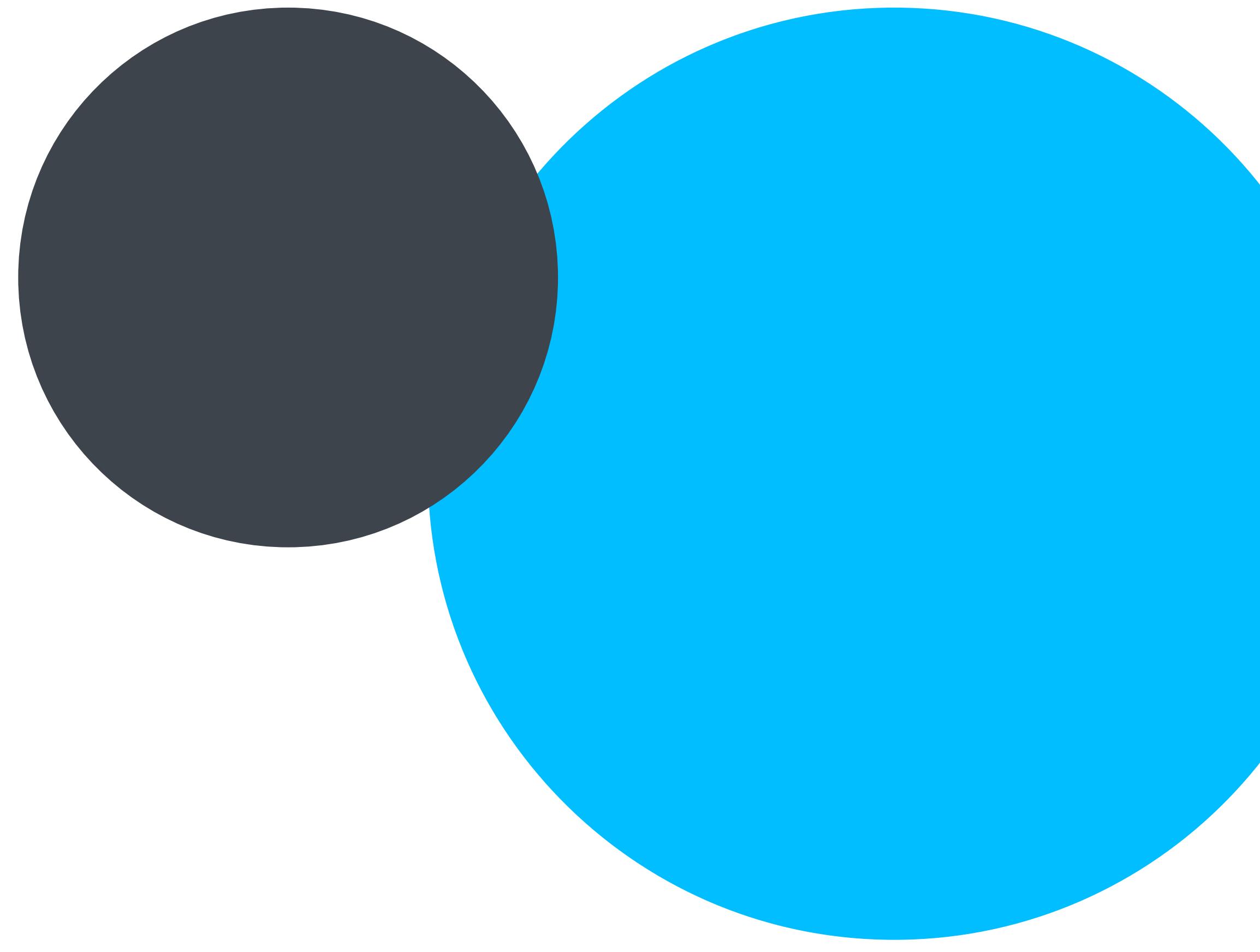


Molecular dynamics simulation of additive manufacturing

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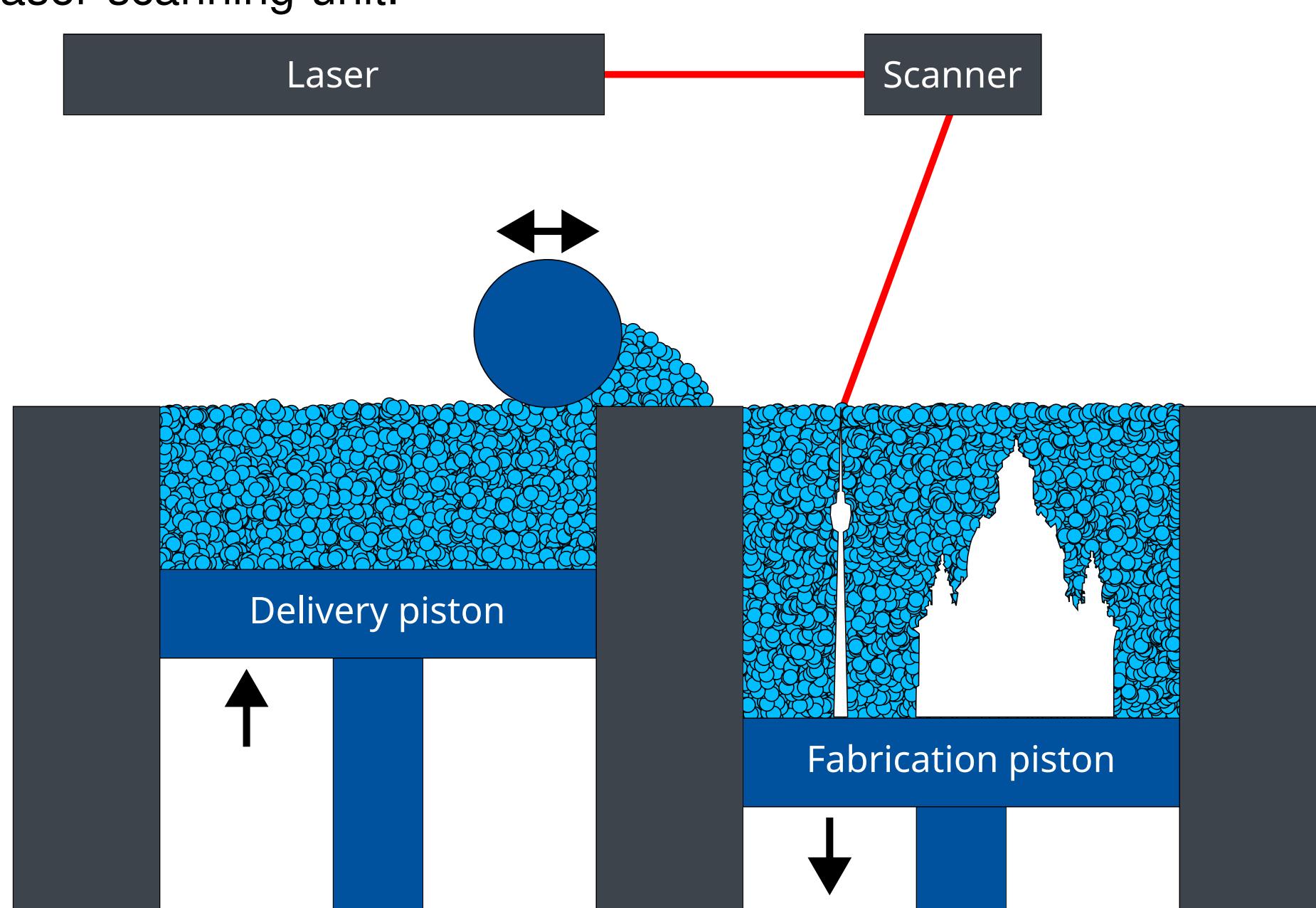


Motivation

Up to now, most simulation studies on additive manufacturing treat metals in vacuum. However, most common defects such as spherical pores arise from trapping a protective gas. To study the underlying mechanisms we extend the treatment by the inclusion of argon as protective gas. Also we investigate the impact of coated metals for the manufacturing of binary alloys.

Powder-bed additive manufacturing

Powder-bed additive manufacturing is a process that melts the powder with a laser beam, layer upon layer. The schematic construction consists of two separated powder containers, as well as a laser-scanning-unit.



While printing a new layer, the piston on the left lifts the delivery powder which will be transported to the fabrication container by the coating unit. Thereby the piston on the right is lowered so far that there is space for the new powder layer. The laser beam is then directed across the printing plane scanning the desired structure which fuses the powder above the already printed object.

Simulation basis

Embedded Atom Method (EAM) potentials are used to describe the interatomic interactions of metals and metallic alloys. The pair potential term ϕ_{ij} has the electrostatic core-core interaction and F_i accounts for the energy increment when embedding an atom into the local electron density ρ_i . With this, the total energy of the system can be written as [1]

$$E_{\text{tot}} = \sum_i F_i(\rho_i) + \frac{1}{2} \sum_{i \neq j} \phi_{ij}(R_{ij}).$$

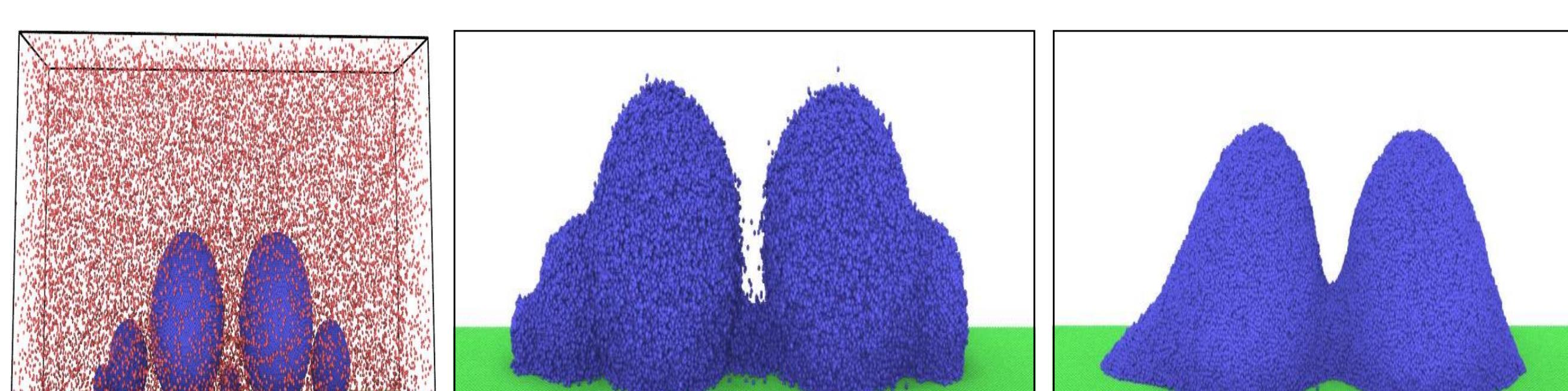
The Laser interaction is depicted by a gaussian intensity profile. Therefore a kinetic energy change of the form

$$\frac{dE}{dVdt} = (1 - R) \cdot \frac{\mu P_{\text{tot}}}{2\pi\sigma^2} \cdot \exp\left(-\frac{(x-vt)^2 + y^2}{2\sigma^2}\right) - \mu z$$

is applied to the atoms per volume unit dV and time step dt . Here R is the reflection coefficient, μ the absorption coefficient, σ^2 is the variance and P_{tot} the total power of the laser.

Influence of protective argon gas

The influence of argon as protective gas during additive manufacturing simulations was investigated by using various initial proportions of argon atoms in a system with multiple aluminum powder grains. Among other things we examined the percentage of molten material by performing common neighbor analysis and determine remaining lattice structures.

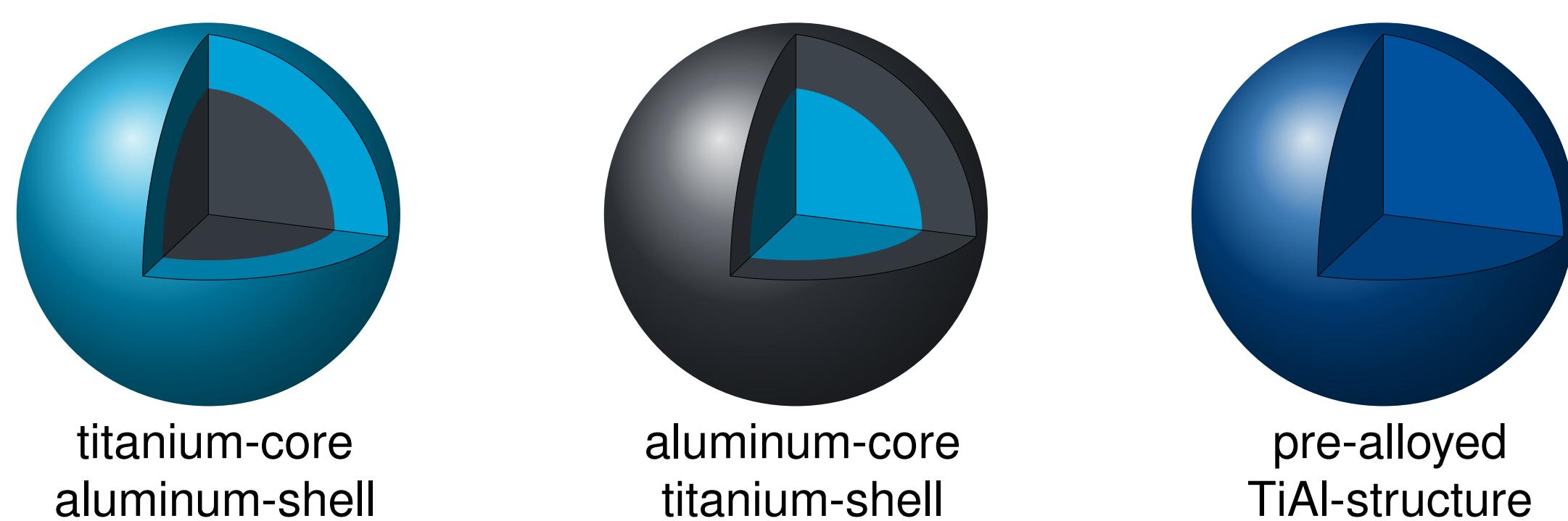


Left: The setup with protective argon gas equilibrated to room temperature during NVT simulation. The argon atoms are depicted in red. **Center:** After running a selective laser simulation including argon. For clearer illustration, the argon atoms have been hidden. **Right:** After running a selective laser simulation without argon atoms.

We use sub-burst laser parameters to evaluate the behavior of the protective argon gas. Despite the fact that the aluminum grains did not burst, fusing is clearly visible and we observe that the argon cools the aluminum causing an increased surface roughness.

Initial structures and simulation setup

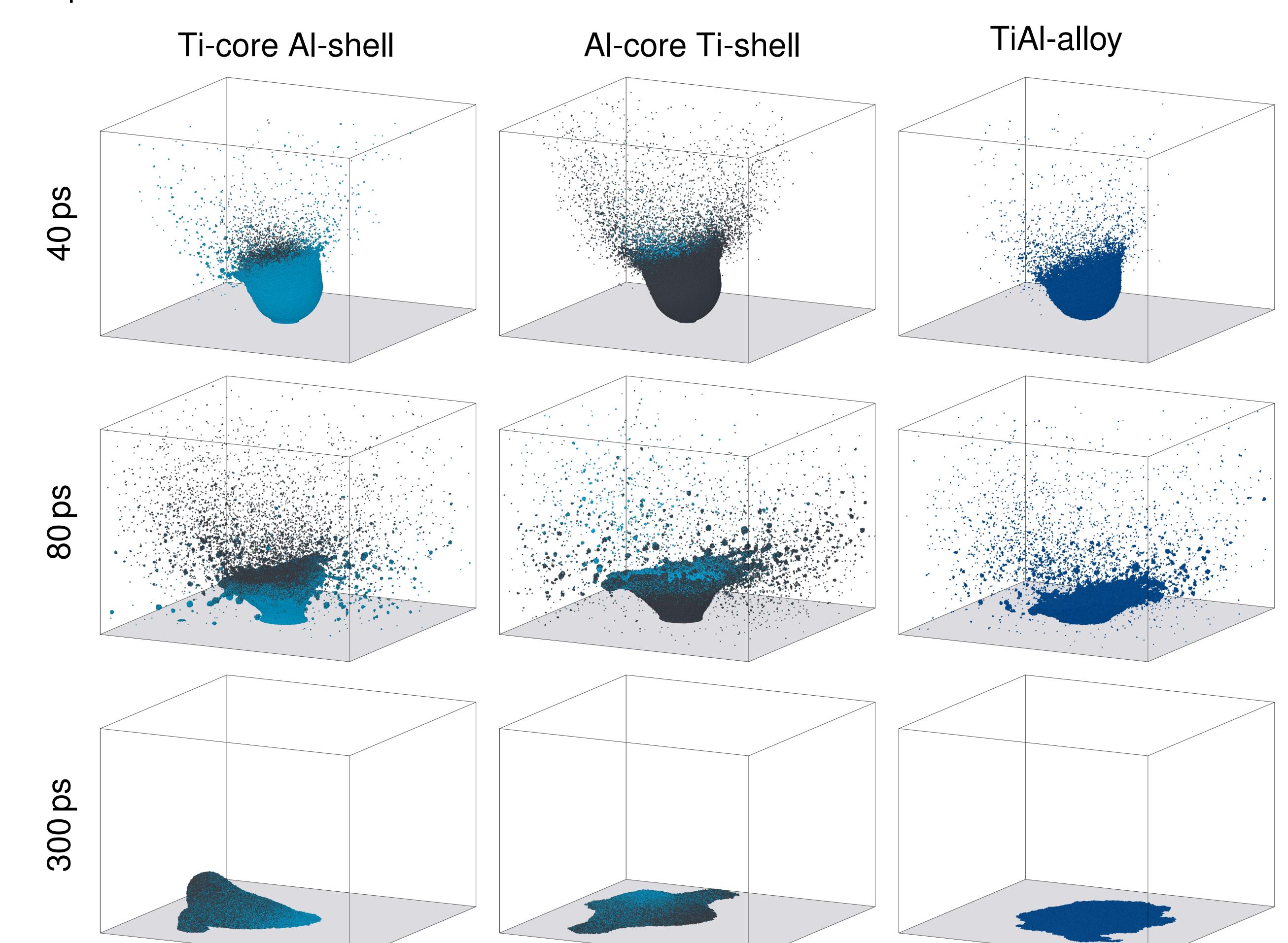
We investigate the applicability of binary alloys and perform additive manufacturing simulations of different powder grain structures. In principle we want to prove the suitability by comparing the core-shell-structures with pre-alloyed grains.



The initial powder grains are constructed with a diameter of 400 Å and placed on a fixed ground. All grains are distributed with a 50:50 titan-aluminum ratio. For the interatomic interaction we use an EAM-potential which has been fitted to a database of experimental data and ab initio calculations [2].

Really hot results

Here we show the time evolution of the simulations for the different structure types. While the simulation time increases from top to bottom, the different grain structures varies from left to right. Also we performed a cluster analysis to hide single atoms and tiny clusters from the picture.



The short time limit shows approximately the same behavior. All grains burst and the power of the laser was high enough to melt the whole powder grain. Despite infusing enough energy to melt the complete grains we observe an inhomogeneous mixing for the coated structures in the long time limit. However, the simplified assumption of the Lambert-Beer-law dominates the spatial energy infusion profile. More sophisticated implementations of laser light absorption could yield different material dynamics.

Conclusion

Results show that the protective argon gas cools the system and leads to a rougher surface. For the coated titanium-aluminum-system we found an inhomogeneous mixing in the long time limit. However, both studies have to be investigated in more detail and the current implementation of the laser interaction needs more improvements to better depict the material dynamics.

[1] Murray S. Daw and M. I. Baskes. Embedded-atom method: Derivation and application to impurities, surfaces, and other defects in metals. *Physical Review B*, 29, 1984.

[2] Rajendra R. Zope and Y. Mishin. Interatomic potentials for atomistic simulations of the ti-al system. *Physical Review B*, 68, 2003.