

Supplementary information

Efficient texture prediction for additive manufacturing

Xiaohui Liang¹, Jianing Zhu^{1*}, Vera Popovich¹, Marcel Hermans¹, Ian Richardson^{1,2}
Cornelis Bos^{1,3}

¹Material Science and Engineering, TU Delft, Mekelweg 2, 2628 CD, Delft, The Netherlands

²IR Welding Consultancy, Berkel en Rodenrijs, The Netherlands

³Tata Steel, Research & Development, P.O. box 10000, 1970 CA IJmuiden, The Netherlands

1 Calibration of the analytical thermal model

In this work, an analytical thermal model is employed to calculate the temperature profile, in which two ellipsoidal heat sources with Gaussian distributions are adopted to approximate the heat input in conduction-mode or transition-mode melt pools generated by a laser. This model is calibrated for each additive manufacturing case by tuning parameters including absorptivity (η_1 and η_2) and shape parameters ($\sigma_{x,1}$, $\sigma_{z,1}$, $\sigma_{x,2}$ and $\sigma_{z,2}$) to fit the cross section shape of the melt pools obtained from the experiment.

$$T = T_0 + f(x, y, z, t, \eta_1, \sigma_{x,1}, \sigma_{y,1}, \sigma_{z,1}) + f(x, y, z, t, \eta_2, \sigma_{x,2}, \sigma_{y,2}, \sigma_{z,2}). \quad (1)$$

The details of the calibration procedure are given below. First, melt pool shapes in the cross section perpendicular to the scanning direction are extracted from secondary electron microscope (SEM). For each NiTi sample, seven melt pool boundary curves are averaged to obtain a curve between w^{exp} and h^{exp} in a coordinate system defined with its axes parallel to the width and height directions, and its origin at the center of the melt pool. A set of points is sampled from the averaged melt pool curve with evenly spaced values w_i in the width direction and the local depth in the experiment is denoted by h_i^{exp} . The sampled points from the averaged melt pool curve are then employed as the experimental dataset to calibrate the analytical thermal model.

With the thermal model, the 3D melt pool shape can be determined by solving the conditions defined by,

$$\frac{\partial T}{\partial t}(x, y, z) = v \frac{\partial T}{\partial x}(x, y, z) = 0, \quad (2)$$

and

$$T(x, y, z) = T_l, \quad (3)$$

where $\partial T/\partial t$ is the derivative of the temperature with respect to time t , $\partial T/\partial x$ the derivative of the temperature with respect to distance x , v the scanning velocity, and T_l the liquidus temperature. The x , y and z axis are parallel with the scanning direction, the transversal direction and the vertical direction, respectively. In the modelled thermal profile, the local depth value h_i^{model} at w_i can be determined by solving

$$\frac{\partial T}{\partial x}(x, w_i, h_i^{model}) = 0, \quad (4)$$

and

$$T(x, w_i, h_i^{model}) = T_l. \quad (5)$$

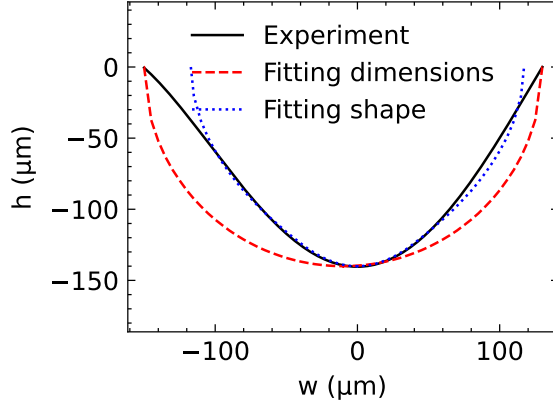
A weighted root mean square error is then employed to quantify the difference between the experimental melt pool shape and the modelled melt pool shape,

$$error = \sqrt{\frac{1}{n} \sum_i^n \left(\left(2 - \frac{w_i^2}{w_{max}^2} \right) (h_i^{exp} - h_i^{model}) \right)^2}. \quad (6)$$

*Correspondence email address: J.Zhu-2@tudelft.nl

where w_{max} is the maximum absolute value of the sampled points in width direction and n is the number of points. $(2 - w_i^2/w_{max}^2)$ is a weighting factor, which emphasizes the differences in the bottom of the melt pools. This is because the shape in the bottom of the melt pool governs the final microstructure, while the upper part will be remelted by subsequent scanning passes. A dual-annealing optimizer is employed to minimize the error by optimizing η_1 , η_2 , $\sigma_{x,1}$, $\sigma_{z,1}$, $\sigma_{x,2}$ and $\sigma_{z,2}$.

In traditional CA model for texture prediction, analytical or numerical thermal models are calibrated by matching the dimensions (width and height) of the experimental melt pool. In this work, the analytical thermal model is calibrated for each NiTi sample by fitting the cross-section shape of the melt pool. The two different methods are then compared by fitting the melt pool in NiTi sample-B. The experimental and fitted melt pool cross-section shapes are given in Supplementary Figure 1. When the thermal model is calibrated by fitting melt pool dimensions, a large difference exists between the experimental melt pool shape and the modelled melt pool shape, especially in the bottom of the melt pool. This means the directions of the temperature gradients near the bottom of the melt pool are not correctly modelled, which may lead to an inaccurate prediction of the microstructure and texture in CA simulations. When the thermal model is calibrated by fitting melt pool shape, the lower part ($h < -50 \mu\text{m}$) of the experimental melt pool is well fitted with the thermal model. In the upper part ($h > -50 \mu\text{m}$), the modelled melt pool shape deviates from the experimental shape as the thermal model does not include fluid dynamics. However, during additive manufacturing, the upper parts will be remelted by subsequent laser passes. Consequently, deviations in the upper part of the melt pool have little influence on the final microstructure.



Supplementary Figure 1: Comparison of different fitting methods for thermal model calibration. The analytical thermal model is calibrated for NiTi sample-B with two different fitting methods: fitting melt pool dimensions and fitting melt pool shape. Fitting melt pool dimensions results in a larger error than fitting melt pool shape.

2 Parameters

In this work, additive manufacturing simulations are performed for two different materials, namely a 316L steel and a Ni-Ti alloy. The material properties of the 316L steel are taken from the work of Teferra and Rowenhorst [1], while the material properties of the Ni-Ti alloy are obtained from Thermo-Calc. To match the dilute solution approximation, the Ni-Ti alloy (49.4 at%) is considered as a binary system (NiTi-Ni) with Ni (1.2 at%) dissolved in NiTi. The parameters for the 316L steel and the transformed parameters for the NiTi-Ni system are given in Supplementary Table 1. Processing parameters and other simulation parameters are given in Supplementary Table 2. In the simulation for the 316L steel sample, to benchmark the simulation performed by Zinovieva et al. [2], the fitting function [2] between the growth velocity v_g and the undercooling ΔT is employed,

$$v_g = 2.49 \times 10^{-7} \Delta T^2 + 6.2 \times 10^{-8} \Delta T^3. \quad (7)$$

The relationships between the growth velocity v_g and the undercooling ΔT for the 316L steel and the NiTi alloy are plotted in Supplementary Figure 2. In addition, for the 316L steel sample, calibration

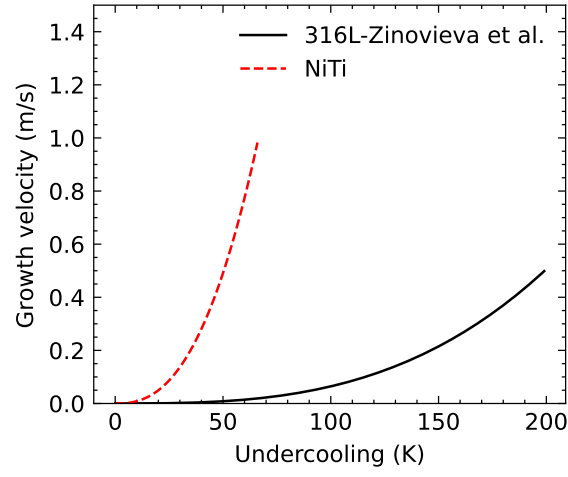
of the thermal profile is performed by fitting the width and the height of the melt pool, as melt pool curves are not available. In this case, only one ellipsoid heat source is employed in the analytical thermal model during fitting. The laser beam diameters used to manufacture NiTi samples are also given in Supplementary Table 2, which nevertheless are not used in the simulations.

Symbol	Description	Value for 316L	Value for NiTi
c_0	The nominal concentration	4.85 wt%	1.2 at% (NiTi-Ni)
k	The partitioning coefficient	0.48	0.50 (NiTi-Ni)
m_l	The slope of the liquidus line	$-10.9 \text{ K/wt}\%$	$-7.70 \text{ K/at}\%$ (NiTi-Ni)
D_l	The diffusion coefficient in the liquid	$3 \times 10^{-9} \text{ m}^2/\text{s}$	$3 \times 10^{-9} \text{ m}^2/\text{s}$
Γ	The Gibbs Thomson coefficient	$1 \times 10^{-7} \text{ K} \cdot \text{m}$	$2 \times 10^{-7} \text{ K} \cdot \text{m}$
ρ	The density	8000 kg/m^3	6450 kg/m^3
κ	The thermal conductivity	$18 \text{ W}/(\text{m} \cdot \text{K})$	$30 \text{ W}/(\text{m} \cdot \text{K})$
c_p	The specific heat	$500 \text{ J}/(\text{kg} \cdot \text{K})$	$489 \text{ J}/(\text{kg} \cdot \text{K})$
T_l	The liquidus temperature	1609 K	1583 K

Supplementary Table 1: Material properties of a 316L steel [1] and a NiTi alloy.

Parameter	316L sample	NiTi sample-A	NiTi sample-B	NiTi sample-C
Laser power P (W)	175	250	400	950
Scanning velocity v_s (m/s)	0.5	1.25	1.2	0.65
Absorption efficiency η_1	0.413	0.304	0.330	0.165
Absorption efficiency η_2	-	0.355	0.448	0.216
Shape parameter $\sigma_{x,1}$ (μm)	30.0	30.3	129.5	281.8
Shape parameter $\sigma_{z,1}$ (μm)	26.2	54.8	54.3	41.6
Shape parameter $\sigma_{x,2}$ (μm)	-	34.8	51.4	174.7
Shape parameter $\sigma_{z,2}$ (μm)	-	0.1	133.9	2.1
Initial temperature T_0 (K)	523	523	523	523
Hatch distance h_d (μm)	140.0	120.0	120.0	180.0
Layer thickness l_t (μm)	30.0	30.0	30.0	40.0
Nucleation density n_n (10^{14} m^{-3})	0.1	2.0	2.0	2.0
Rotation angle (degree)	0	67	67	67
Laser beam size (μm)	-	80.0	80.0	500.0

Supplementary Table 2: Parameters for the CA simulations and experiments.



Supplementary Figure 2: The relationship between the growth velocity v_g and the undercooling ΔT for the 316L steel and the NiTi alloy. To benchmark the simulation performed by Zinovieva et al. [2], the fitting function [2] between the growth velocity v_g and the undercooling ΔT is employed for the 316L steel.

3 Multi-level capture algorithm

The pseudocode of the multi-level capture algorithm is given in Supplementary Algorithm A1.

Supplementary Algorithm A1: The multi-level capture algorithm.

```

1  $N_0$  ; // set of interface cells at the beginning of the time step
2  $N_c \leftarrow N_0$  ; // set of valid capture nodes in the current level
3  $N_v \leftarrow \{\}$  ; // set of valid capture nodes in the current and previous levels
4 /* Iterate until there are no nodes in the current level */
5 while  $N_c \neq \emptyset$  do
6    $N_n \leftarrow \{\}$  ; // set of valid capture nodes in next level
7    $N_i \leftarrow \{\}$  ; // set of invalid capture nodes in  $N_v$ 
8   /* Add nodes in current level into  $N_v$  */
9    $N_v \leftarrow N_v \cup N_c$ ;
10  /* Pre-pruning */
11   $N_c \leftarrow \{\text{the capture node with the shortest capture time for each captured cell in } N_c\}$ ;
12  /* Loop over all valid nodes in the current level to get nodes in the next level */
13  foreach  $n_c \in N_c$  do
14    /* The corresponding interface cell  $c_c$  */
15     $c_c \leftarrow$  the interface cell related to  $n_c$ 
16    /* Update growth length  $l$  of cell  $c_c$  */
17    Update growth length  $l$  of cell  $c_c$ ;
18    /* Check all neighboring cells in the neighborhood of cell  $c_c$  */
19     $C_{nb} \leftarrow \{c_{nb} | c_{nb} \text{ is a cell in the Moore neighborhood of the cell } c_c\}$ ;
20    foreach  $c_{nb} \in C_{nb}$  do
21      /* Check if  $c_{nb}$  is captured by  $c_c$  */
22       $l_{crit} \leftarrow$  the critical growth length to capture  $c_{nb}$ ;
23      if  $c_{nb}$  is not Liquid or  $l \leq l_{crit}$  then
24        continue;
25      /* Calculate the capture time  $t_{cap}$  for  $c_{nb}$  */
26       $t_{cap} \leftarrow$  the capture time for  $c_{nb}$ ;
27      /* Check if  $c_{nb}$  is captured in the current or previous level */
28       $N_{nb,v} \leftarrow \{n_v | n_v \text{ is related to } c_{nb} \text{ and } n_v \in N_v\}$ ;
29      if  $N_{nb,v} \neq \emptyset$  then
30         $n_{nb,v} \leftarrow$  the node with the shortest capture time in  $N_{nb,v}$ ;
31        if  $t_{cap} > \text{capture time of } n_{nb,v}$  then
32          /* Collect invalid node in  $N_v$  and save it into  $N_i$  */
33           $N_i \cup \{n_{nb,v}\}$  ;
34        else
35          /* Pre-pruning by ignore this capture event safely */
36          continue;
37      /* Collect the new capture node for the next level */
38       $N_n \cup \{\text{the new capture node related to } c_{nb}\}$  ;
39  /* Post-pruning by remove invalid nodes in  $N_v$  and  $N_c$  */
40   $N_c \leftarrow N_c - N_c \cap N_i$ ;
41   $N_v \leftarrow N_v - N_v \cap N_i$ ;
42  /* Update nodes in current level */
43   $N_c \leftarrow N_n$ ;
44  Update interface cells based on  $N_v$  for next time step;

```

The critical growth length to capture a neighboring cell is given below. Consider a growth envelop

centered at (x_e, y_e, z_e) in a coordinate system defined based on the sample geometry. The coordinates of the considered neighboring cell is (x_n, y_n, z_n) . At the center of the growth envelop, a local coordinate system can be defined with its axes aligned with the $\langle 001 \rangle$ crystallographic directions. The relative coordinates of the considered neighboring cell in the local coordinate system is (x_r, y_r, z_r) , which can be calculated with

$$\begin{pmatrix} x_r \\ y_r \\ z_r \end{pmatrix} = \mathbf{R}^{-1} \begin{pmatrix} x_n - x_e \\ y_n - y_e \\ z_n - z_e \end{pmatrix}, \quad (8)$$

where $\mathbf{R}$ is the rotation matrix for the crystal orientation. The critical growth length l_{crit} to capture the considered cell is given by

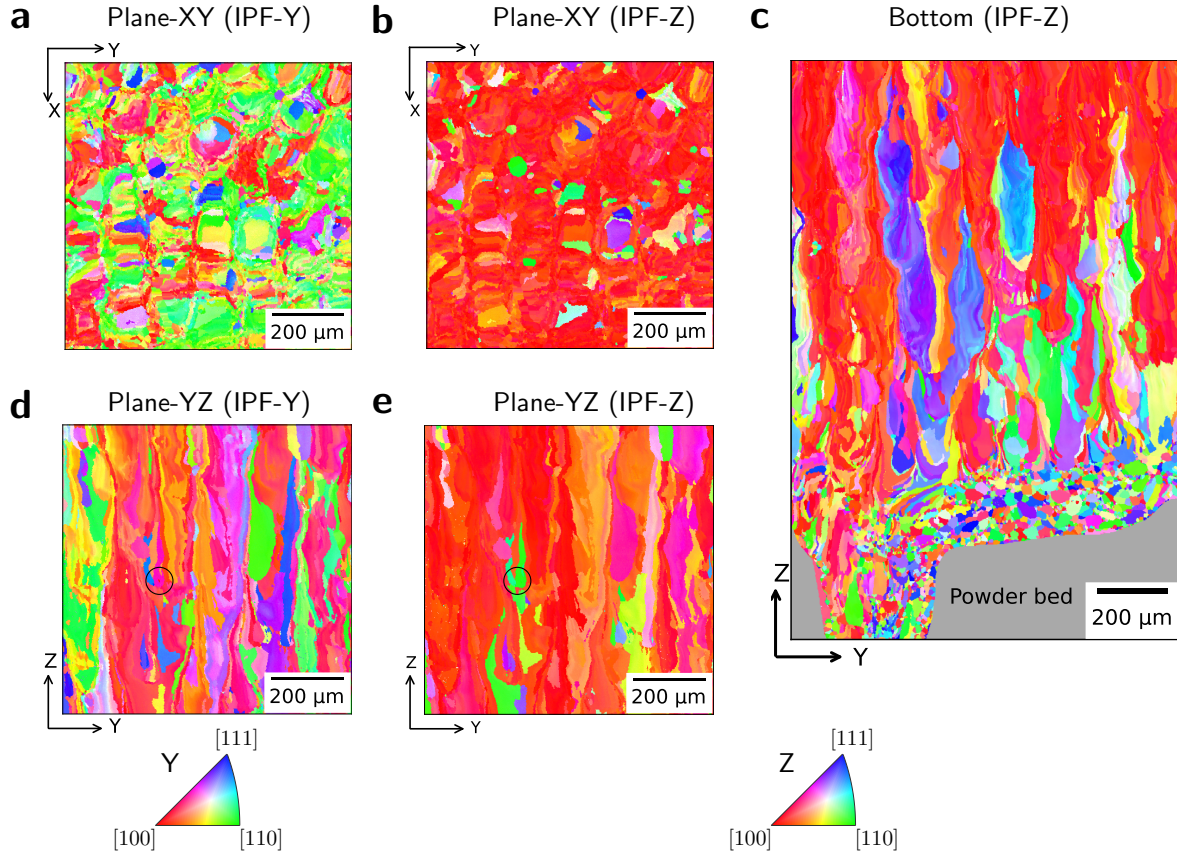
$$l_{crit} = |x_r| + |y_r| + |z_r|. \quad (9)$$

4 Determination of cell size for CA simulations

In CA simulations for texture prediction, cell size has a large impact on the orientation selection effects. With decreasing cell size, the selection effect becomes larger and gradually approaches a geometrical limit proposed by Pineau et al. [3]. According to Pineau et al. [3], a suitable cell size should be employed to achieve a physically reasonable CA simulation. In the current work, in order to benchmark the simulations of Zinovieva et al. [2] and Teferra and Rowenhorst [1], the same cell sizes were employed for 316L steel sample. For microstructure simulations of NiTi samples, an appropriate cell size is determined as a balance of the selection rate requirement and the computational cost.

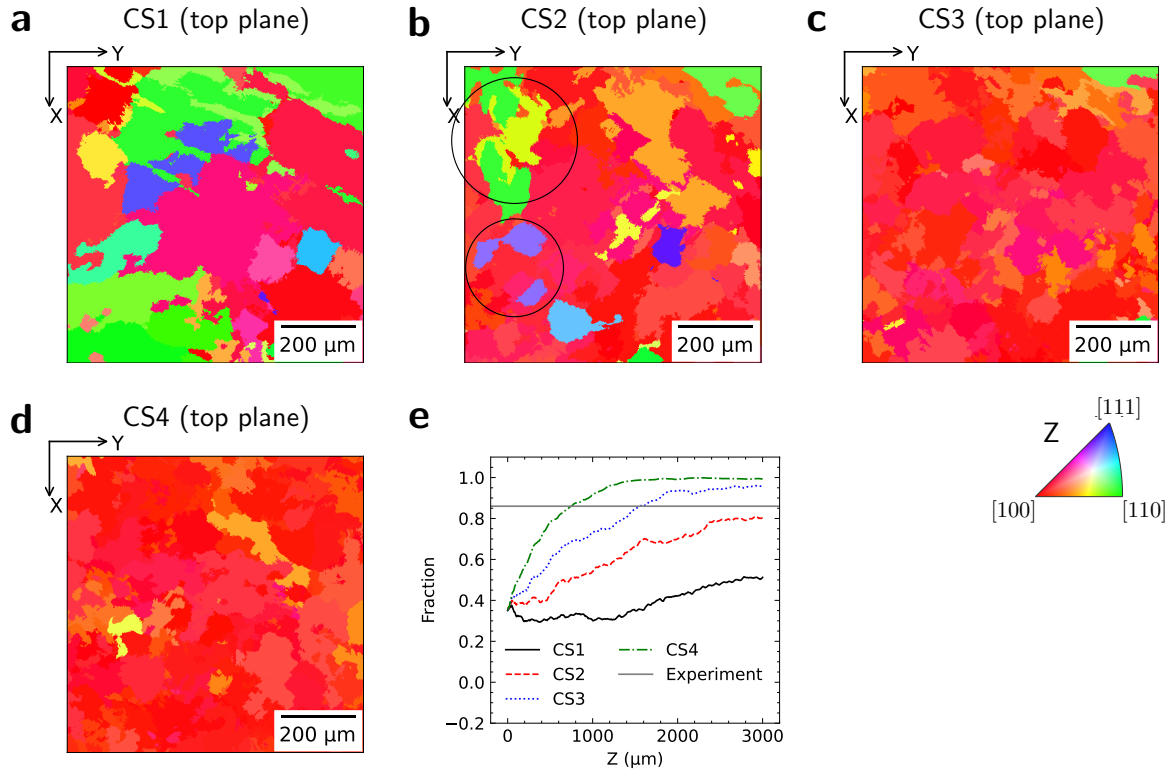
In this work, an appropriate cell size is determined based on the simulations of NiTi sample-B. To do that, important features are extracted from the experimental microstructure of NiTi sample-B, which are given in Supplementary Figure 3, where the bulk microstructure in plane-XY and plane-YZ are colored with IPF (inverse pole figure) color with respect to different axes. In NiTi sample-B, as shown in Supplementary Figure 3b, red grains with globally favorable orientations ($\langle 100 \rangle \parallel Z$ orientations) dominates the bulk microstructure. Some small grains with global unfavorable orientations (non-red) locates in the red matrix randomly, as shown in Supplementary Figure 3b and Supplementary Figure 3e. There are two possible explanations for the existence of small grains with globally unfavorable orientations. The first one is that those stripe-like grains originate from the sample bottom and propagate in a direction inclined to the Z axis, which explains why those grains have limited lengths in plane-YZ. The other explanation is that those grains come from nucleation in melt pools. The first explanation for the existence of small grains with globally unfavorable orientations is not valid. If those grains originate from the sample bottom, then they will develop branch-like features after growing through multiple layers. However, branch-like features are barely observed in the experimental microstructure. From Supplementary Figure 3b, it can be inferred that those small green ($\langle 110 \rangle \parallel Z$) grains which are close to each other may come from branches of the same grain. However, by checking the IPF map with respect to Y axis, the orientations of those grains are different. In this case, branch-like features are rare in NiTi sample-B. In Supplementary Figure 3e, a pseudo branch-like feature is observed in a green ($\langle 110 \rangle \parallel Z$) grain (highlighted with a circle). However, by checking Supplementary Figure 3d, those branches are in fact from two different grains. Given the fact that branch-like features are not commonly observed in smaller grains with globally unfavorable orientations, those small grains with globally unfavorable orientations are more likely to originate from nucleation. If nucleation does not exist, then the microstructure should be completely $\langle 100 \rangle \parallel Z$ (red) grains. The bottom microstructure is given in Supplementary Figure 3c, where grains with different orientations grows epitaxially from the substrate. Initially, some large columnar grains with globally unfavorable orientations are observed. After depositing around $1000 \mu\text{m}$, $\langle 110 \rangle \parallel Z$ (red) grains dominate the microstructure, which is close to the bulk microstructure. In this case, the length of the transition zone from a random microstructure to a region dominated $\langle 110 \rangle \parallel Z$ (red) grains is roughly $1000 \mu\text{m}$.

The microstructure of NiTi sample-B is simulated with different cell sizes, which are $2.0 \mu\text{m}$ (CS1), $1.5 \mu\text{m}$ (CS2), $1.25 \mu\text{m}$ (CS3) and $1.0 \mu\text{m}$ (CS4). The domain size is $800 \times 800 \times 3000 \mu\text{m}^3$. To simplify the problem, no nucleation is considered in the simulations. The simulated microstructures in the top plane (taken at $z = 3000 \mu\text{m}$) are given in Supplementary Figure 4. With decreasing cell size from CS1 to CS4, more $\langle 100 \rangle \parallel Z$ (red) grains appear in the top plane. In the simulation CS3 and CS4, $\langle 100 \rangle \parallel Z$ (red) grains dominate the microstructure in the top plane. This indicates that the selection rate on $\langle 100 \rangle \parallel Z$ orientations increases with decreasing cell size. The fraction of red grains at different heights in the simulations CS1-CS4 are given in Supplementary Figure 4e, where the influence of the cell size



Supplementary Figure 3: Experimental bulk microstructure and bottom microstructure in NiTi sample-B. Different IPF (inverse pole figure) colors are employed: IPF-Z (IPF color with respect to Z axis) and IPF-Y (IPF color with respect to Y axis). **a, b** Plane-XY in experiments colored with IPF-Y color and IPF-Z color. **c** Near bottom microstructure in NiTi sample-B (colored with IPF-Z color). In practical laser powder bed fusion processes, thin-wall grid supports have been manufactured firstly to enhance printability and facilitate the removal of samples from the substrate. Thus, grain growth originates from either the grids or the powder bed (marked as grey background). **d, e** Plane-YZ in experiments colored with IPF-Y color and IPF-Z color.

on the selection rate can be confirmed. As mentioned before, if nucleation is not considered, the bulk microstructure should be completely $\langle 100 \rangle \parallel Z$ (red) grains, which is satisfied by CS3 ($1.25 \mu\text{m}$) and CS4 ($1.0 \mu\text{m}$). Moreover, the length of the transition zone from a random microstructure to a region dominated by $\langle 110 \rangle \parallel Z$ (red) grains should be roughly $1000 \mu\text{m}$, as indicated by the experimental microstructure. Note the simulations are performed with the melt pool measured from top layers, which is larger than the melt pool in the bottom layers and has a more pronounced selection effect. In this case, the desired transition zone length could be smaller than $1000 \mu\text{m}$. Considering the requirement of the transition zone length, the cell size is determined as $1.0 \mu\text{m}$, which is employed for all the NiTi simulations. Note the top-plane microstructure in simulation CS2 seems to be close to the experimental microstructure. However, due to the low selection rate, branch-like features are observed in simulation CS2. As shown in 4b, neighboring small grains (highlighted with circles) with globally unfavorable orientations are branches from the same grain. As those features are not observed in the experimental microstructure, it supports the argument that small grains with globally unfavorable orientations originates from nucleation in the melt pool instead of growth from substrate.



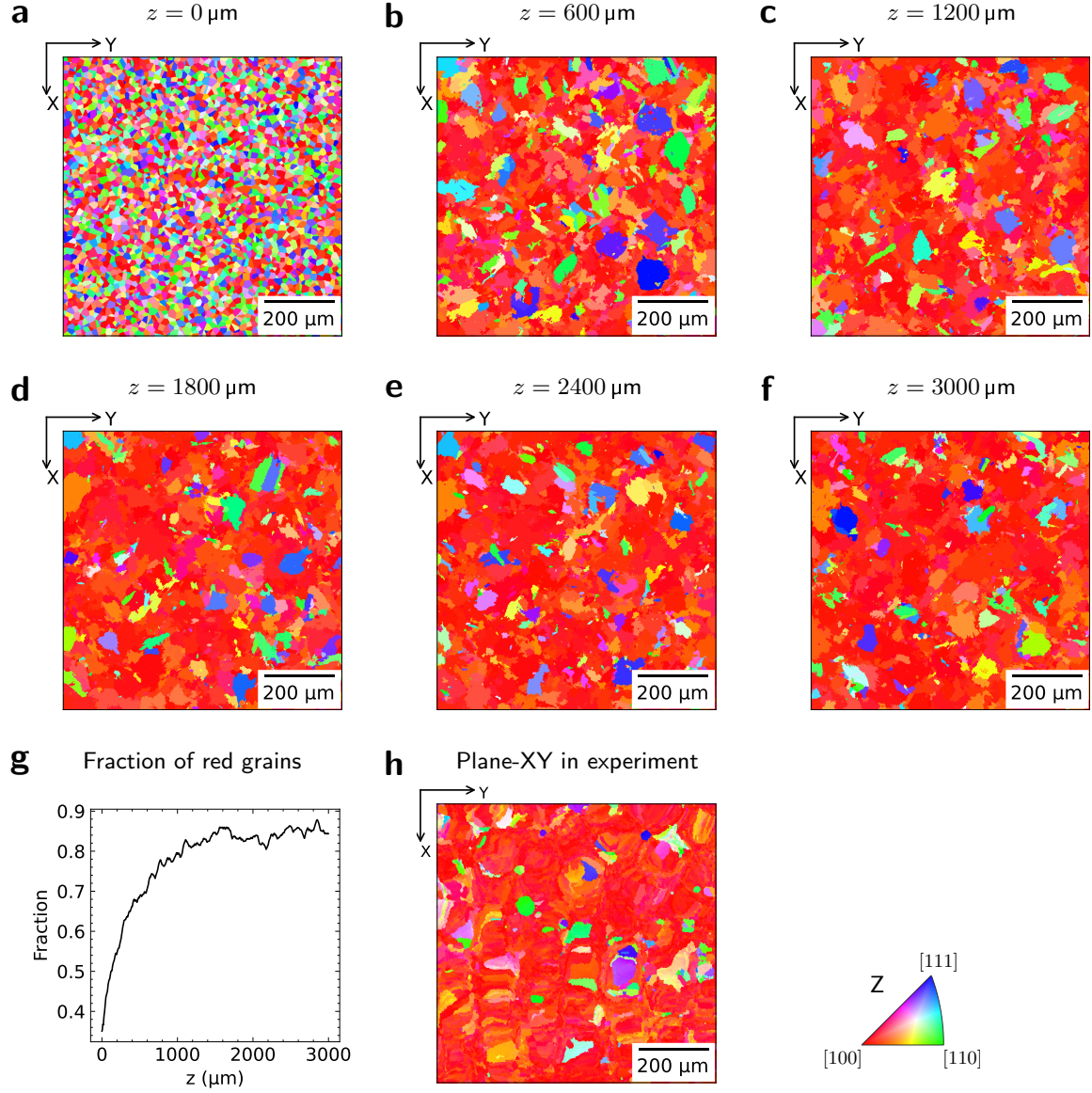
Supplementary Figure 4: Simulated microstructures in the simulations for NiTi sample-B with different cell sizes. The employed cell sizes are 2.0 μm (CS1), 1.5 μm (CS2), 1.25 μm (CS3) and 1.0 μm (CS4). **a, b, c, d** Microstructure in the top plane (taken at $z = 3000 \mu\text{m}$) in simulation CS1-CS4. Grains with globally unfavorable orientations show branch-like feature in figure b, which are highlighted with circles. **e** The fraction of red grains at different heights in the simulations CS1-CS4. Red grains are defined as grains with $\theta < 20^\circ$, where θ is the minimum angle between the $\langle 100 \rangle$ crystallographic directions and Z+ direction. IPF (inverse pole figure) colors with respect to the Z axis are employed in a-d.

5 Simulation of bulk microstructure

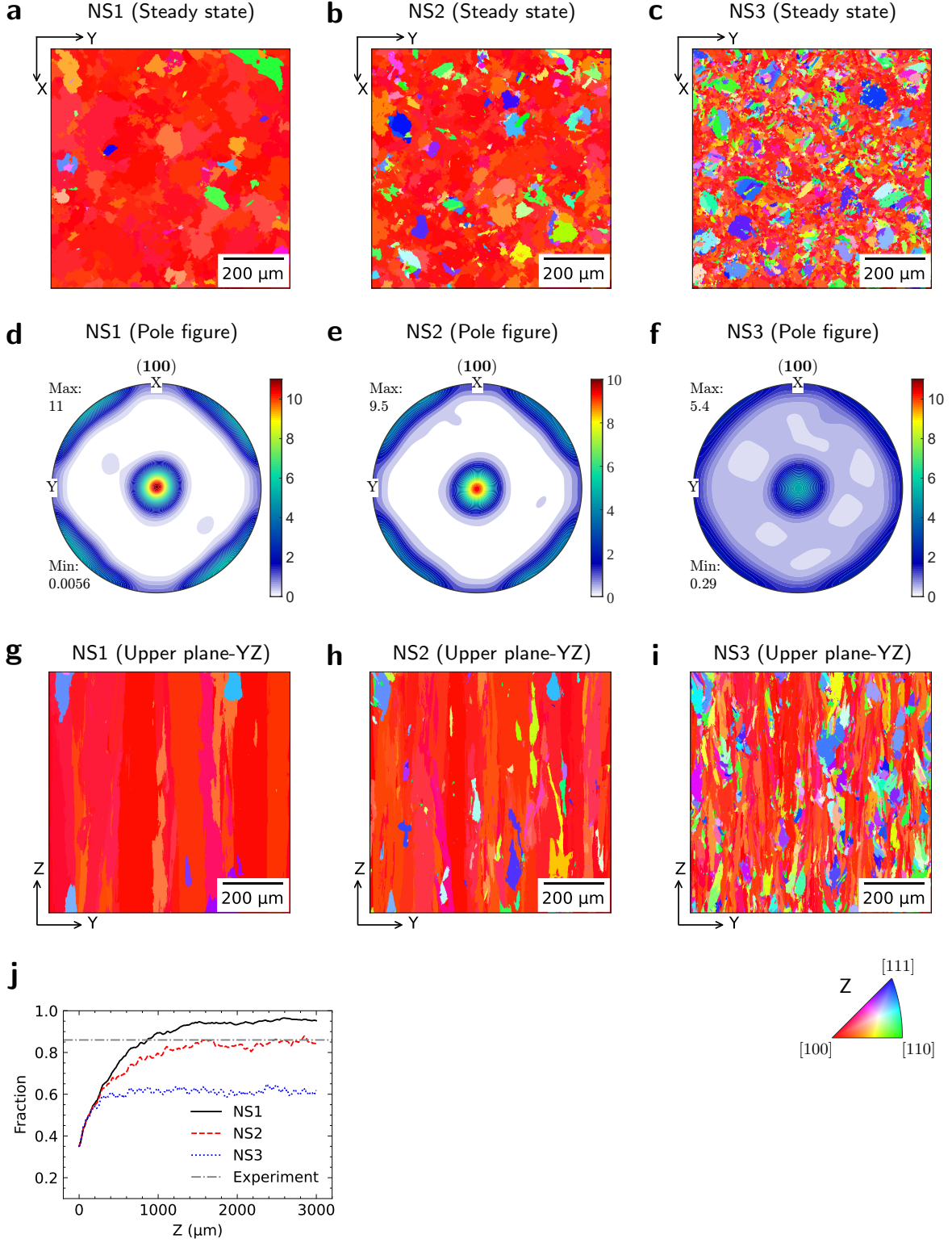
The intention of the current work is to validate the developed CA model by comparing simulated bulk microstructures with experimental ones under different processing conditions. In additive manufacturing, when enough layers have been deposited, the deposited microstructure reaches a steady state condition. The steady-state microstructure is obtained as a balance between an orientation selection effect and nucleation. With increasing height, grains with unfavorable orientations gradually disappear due to orientation selection of temperature gradients, while nucleation introduces new grains with different orientations. The balance between orientation selection and nucleation will be illustrated with NiTi sample-B.

The simulation of NiTi sample-B was performed with a domain of $800 \times 800 \times 3000 \mu\text{m}^3$ and a cell size of $1.0 \mu\text{m}$. The microstructure in plane-XY at different heights are given in Supplementary Figure 5. The simulation starts from a random microstructure, as shown in Supplementary Figure 5a. With increasing height, temperature gradients from different laser passes select grains with favorable orientations ($\langle 100 \rangle \parallel Z$ grains, namely, red grains), and the fraction of non-red grains decreases, until a steady-state microstructure is reached at a height around $1800 \mu\text{m}$. As shown in Supplementary Figure 5d, 5e and 5f, the microstructures at $1800 \mu\text{m}$, $2400 \mu\text{m}$ and $3000 \mu\text{m}$ are similar, where small non-red grains are located randomly in the matrix of $\langle 100 \rangle \parallel Z$ (red) grains. The fraction of red grains as a function of height (Z) is given in Supplementary Figure 5g. Here, red grains are defined as grains with $\theta < 20^\circ$, where θ is the minimum angle between the $\langle 100 \rangle$ crystallographic directions and Z+ direction. With increasing height, the fraction of red grains increases until a plateau is observed at a height of around $1800 \mu\text{m}$. The fluctuation observed in Supplementary Figure 5g is caused by nucleation. The existence of a plateau confirms the steady-state condition.

The steady-state microstructure in NiTi sample-B is a balance between orientation selection and nucleation. The fraction of red grains in the steady-state microstructure is influenced by nucleation density n_n . To demonstrate this effect, the steady-state microstructure from simulations (NS1, NS2 and NS3) with different nucleation densities n_n ($2 \times 10^{13} \text{m}^{-3}$, $2 \times 10^{14} \text{m}^{-3}$ and $2 \times 10^{15} \text{m}^{-3}$) are compared in Supplementary Figure 6. In simulations of NiTi sample-B, $\langle 100 \rangle \parallel Z$ (red) orientations are globally favorable, while other orientations (non-red) are not globally but locally favorable. In the simulation domain, there are some regions where the locally favorable orientations are not $\langle 100 \rangle \parallel Z$ orientations but orientations which are globally unfavorable. For simplicity, those regions are referred as LF (locally favorable) region. Whether LF regions are occupied by $\langle 100 \rangle \parallel Z$ (red) grains or grains with LF orientations depends on nucleation density. With a small nucleation density n_n , the chance of LF oriented grains appearing in the corresponding LF regions is small and those regions are filled by $\langle 100 \rangle \parallel Z$ (red) grains, as shown in Supplementary Figure 6a and 6g. With a larger nucleation density n_n , most LF regions are occupied by corresponding LF oriented grains, as shown in Supplementary Figure 6c and 6i. Subsequently, the fraction of $\langle 100 \rangle \parallel Z$ (red) grains decreases with increasing nucleation density n_n . The fraction of $\langle 100 \rangle \parallel Z$ (red) grains with respect to height (Z) in the simulations NS1, NS2 and NS3 are given in Supplementary Figure 6j. The existence of plateaus confirms that steady states are obtained within the simulations. As the nucleation density n_n increases from $2.0 \times 10^{13} \text{m}^{-3}$ to $2.0 \times 10^{15} \text{m}^{-3}$, the fraction of $\langle 100 \rangle \parallel Z$ (red) grains decrease from 0.9 to 0.6. The fraction of $\langle 100 \rangle \parallel Z$ (red) grains in the experimental microstructure is around 0.86, which is close to the that in the steady-state microstructure in the simulation with $n_n = 2.0 \times 10^{14} \text{m}^{-3}$. In this case, $2 \times 10^{14} \text{m}^{-3}$ is employed as the nucleation density n_n for all the NiTi simulations presented in the main article. Note this value is close to the nucleation density ($3 \times 10^{14} \text{m}^{-3}$) employed in the work of Teferra and Rowenhorst [1].



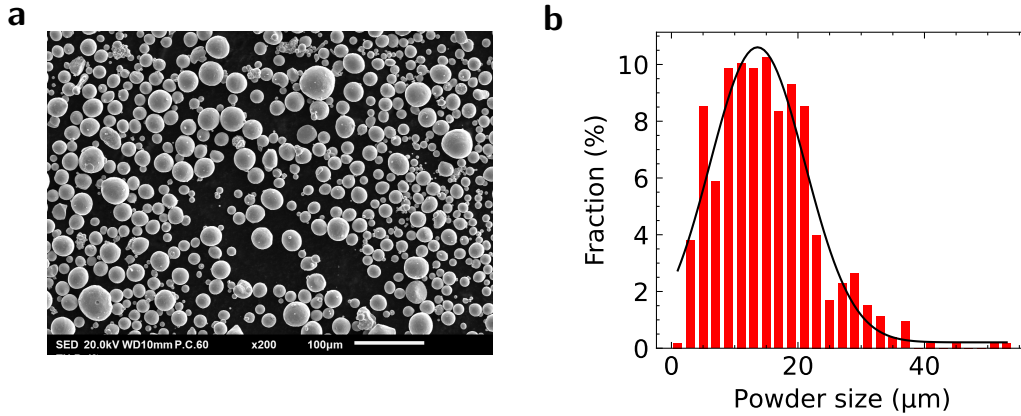
Supplementary Figure 5: A steady-state microstructure is obtained after depositing enough layers in NiTi sample-B. a, b, c, d, e, f Microstructure in plane-XY at different heights ($0 \mu\text{m}$, $600 \mu\text{m}$, $1200 \mu\text{m}$, $1800 \mu\text{m}$, $2400 \mu\text{m}$ and $3000 \mu\text{m}$). **g** The fraction of red grains increases with increasing height. Red grains are defined as grains with $\theta < 20^\circ$, where θ is the minimum angle between the $\langle 100 \rangle$ crystallographic directions and Z+ direction. **h** Experimental microstructure in plane-XY. IPF (inverse pole figure) colors with respect to the Z axis are employed in a-f and h.



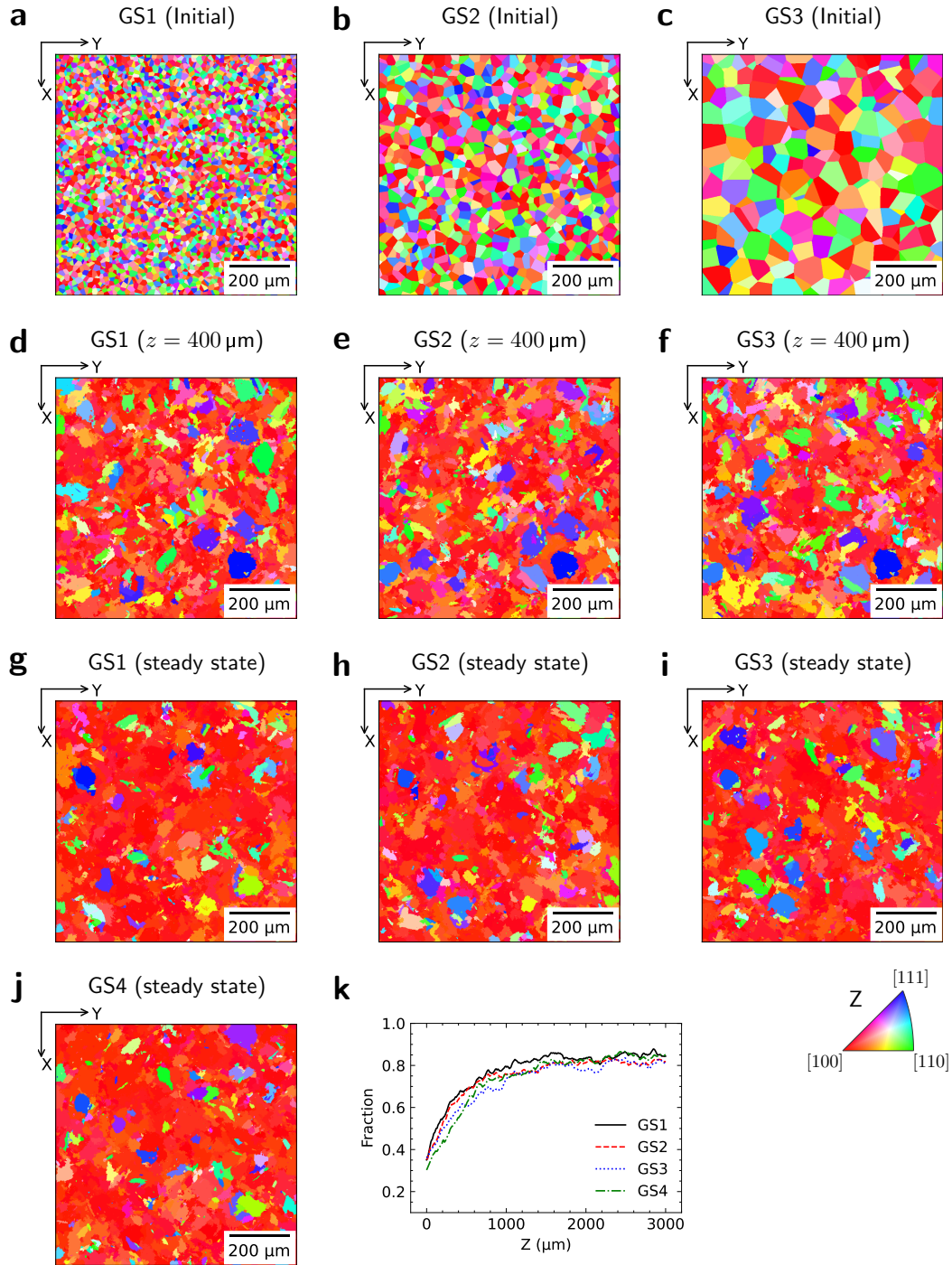
Supplementary Figure 6: Influence of the nucleation density on steady-state microstructure. Simulations (NS1, NS2 and NS3) are performed for NiTi sample-B with different nucleation density n_n ($2 \times 10^{13} \text{ m}^{-3}$, $2 \times 10^{14} \text{ m}^{-3}$ and $2 \times 10^{15} \text{ m}^{-3}$). The domain size is $800 \times 800 \times 3000 \mu\text{m}^3$. **a, b, c** Steady-state microstructure (taken from plane-XY at $z = 3000 \mu\text{m}$) in simulations NS1, NS2 and NS3. **d, e, f** Pole figures for simulations NS1, NS2 and NS3, generated based on the microstructure in a, b and c. **g, h, i** Microstructure in the upper part of plane-YZ ($2200 \mu\text{m} \leq z \leq 3000 \mu\text{m}$ at $x = 400 \mu\text{m}$) in simulations NS1, NS2 and NS3. **j** The fraction of $\langle 100 \rangle \parallel Z$ (red) grains with respect to height (Z) in the simulations NS1, NS2 and NS3. With increasing nucleation density, the fraction of $\langle 100 \rangle \parallel Z$ (red) grains in the steady-state microstructure decreases. IPF (inverse pole figure) colors with respect to the Z axis are employed in figures a-c and g-i.

6 Influence of initial grain size on microstructure and texture

In the CA simulations, the initial microstructure is generated randomly with a Voronoi tessellation, accounting for the microstructure in the base plate and powder layers. The random microstructures in the substrate plate and powder layers provide a sufficient number of grains for orientation selection during epitaxial growth. The initial grain size employed in the simulations of NiTi samples is $15\text{ }\mu\text{m}$ (GS1), which has been determined from the average powder size, as shown in Supplementary Figure 7. To study the influence of initial grain size on the microstructure evolution, three more simulations have been performed for NiTi sample-B with different initial grain sizes, namely $30\text{ }\mu\text{m}$ (GS2), $60\text{ }\mu\text{m}$ (GS3) and $90\text{ }\mu\text{m}$ (GS4). The domain size is $800 \times 800 \times 3000\text{ }\mu\text{m}^3$ and the cell size is $1.0\text{ }\mu\text{m}$. Nucleation is considered with a nucleation density of $2 \times 10^{14}\text{ m}^{-3}$. The initial microstructure (taken from plane-XY at $z = 0\text{ }\mu\text{m}$) and the steady-state microstructure (taken from plane-XY at $z = 3000\text{ }\mu\text{m}$) in the simulations GS1-GS3 are given in Supplementary Figure 8. As shown in Supplementary Figure 8a, 8b and 8c, with increasing initial grain size from GS1 to GS3, the number of initial grains decreases. As a result, the number of initial grains for orientation selection decreases, which limits the selection rate on $\langle 100 \rangle \parallel Z$ (red) grains. Consequently, at the same height ($z = 400\text{ }\mu\text{m}$) near the bottom, the fraction of $\langle 100 \rangle \parallel Z$ (red) grains decreases with from GS1 to GS3, as shown in Supplementary Figure 8d, 8e and 8f. However, the influence of the initial grain size has little influence on the steady-state microstructure. The steady-state microstructures in simulations GS1, GS2, GS3 and GS4 are similar, as shown in Supplementary Figure 8g, 8h, 8i and 8j. This is because nucleation introduces new grains with different orientations, which compensates for the effect of insufficient number of initial grains. Due to randomness in the initial microstructure, the fraction of grains $\langle 100 \rangle \parallel Z$ (red) grains in the steady state may be smaller compared to other simulations (GS1, GS2 and GS4). The fraction of $\langle 100 \rangle \parallel Z$ (red) grains with respect to height (Z) in the simulations GS1, GS2, GS3 and GS4 are given in Supplementary Figure 8k. Initially, the fractions of $\langle 100 \rangle \parallel Z$ (red) grains in the simulations GS1-GS3 are around 0.35, while the the fraction of $\langle 100 \rangle \parallel Z$ (red) grains is smaller due to the large initial grain size and insufficient number of initial grains. With increasing height, the fraction of $\langle 100 \rangle \parallel Z$ (red) grains increases. In the simulation with a smaller initial grain size, the selection rate is higher, and the steady state is reached earlier. However, as a result of the balance between the orientation selection and nucleation, as shown in Supplementary Figure 8k, the fraction of $\langle 100 \rangle \parallel Z$ (red) grains tends to converge to a value around 0.85 in all the simulations, which agrees with the steady-state microstructures.



Supplementary Figure 7: The powder size in additive manufacturing experiments. a Observation of powder under SEM (secondary electron microscopy). **b** The powder size distribution.



Supplementary Figure 8: Influence of the initial grain size on the steady-state microstructure and texture. Simulations (GS1, GS2, GS3 and GS4) are performed for NiTi sample-B with different initial grain size (15 μm , 30 μm , 60 μm and 90 μm). The domain size is $800 \times 800 \times 3000 \mu\text{m}^3$. **a, b, c** The initial microstructure (taken from plane-XY at $z = 0 \mu\text{m}$) in the simulations GS1, GS2 and GS3. **d, e, f** The bottom microstructure in plane-XY (taken from plane-XY at $z = 400 \mu\text{m}$) in the simulations GS1, GS2 and GS3. **g, h, i, j** The steady-state microstructure (taken from plane-XY at $z = 3000 \mu\text{m}$) in the simulations GS1, GS2, GS3 and GS4. Figures a-j are colored with IPF (inverse pole figure) colors. **k** The fraction of red grains with respect to height (Z) in the simulations GS1, GS2, GS3 and GS4. With decreasing initial grain size, the selection rate is higher, and the steady state is reached earlier. However, the initial grain size has little influence on the steady-state microstructure. Due to the limitation of figure size, the microstructure in GS4 is not shown here.

7 Influence of heat accumulation on microstructure and texture

During multi-layer additive manufacturing, heat may accumulate from the bottom to the top, leading to an increase in the initial temperature of newly deposited layers and thus an expansion in the melt pool shape. In this work, experimental melt pool shapes are extracted from top layers in the manufactured samples, where the melt pool has expanded due to accumulated heat from previous layers. To account for the accumulated heat in the simulation, an initial temperature of 523 K higher than room temperature (298 K) is employed when calibrating the analytical thermal model. In the simulations presented in the main article, constant initial temperature and melt pool shapes are employed throughout the simulations. In this case, the simulated microstructures in the bottom layers are shaped with a melt pool which is larger than the real melt pool. In this section, the influence of the melt pool change on microstructure evolution is studied by considering a layer-dependent initial temperature.

To calculate the initial temperature for each layer, the analytical model proposed by Hagenlocher et al. [4] has been employed, in which the change ΔT_0 in the initial temperature after depositing n layers is given by

$$\Delta T_0 = \frac{Q}{\rho c_p 4\pi\alpha} \sum_{i=1}^n \frac{1}{i/f} \exp\left(-\frac{f(r-i \cdot l_t)^2}{4i \cdot \alpha}\right), \quad (10)$$

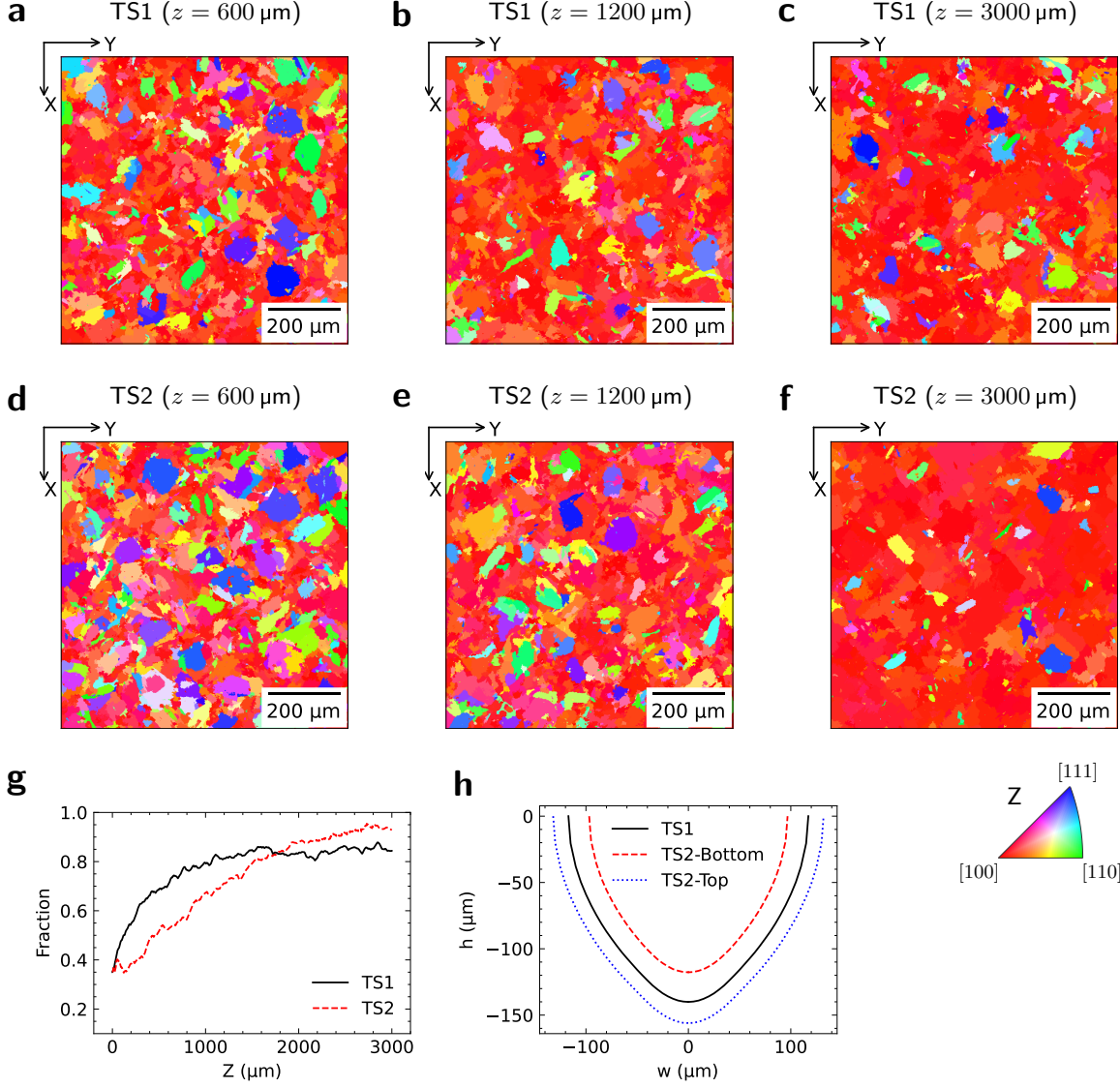
with

$$Q = \frac{\eta P}{l_t v}, \quad (11)$$

where Q is the generalized 1D energy input, α the thermal diffusivity, n the number of deposited layers, f the frequency and $r = 0$ for the considered case. The initial temperature for the first layer is set to room temperature 298 K and it increases gradually during multi-layer additive manufacturing.

The microstructure of the NiTi sample-B is simulated with a constant initial temperature of 523 K (TS1) and with a layer-dependent initial temperature (TS2) based on Equation 10. The domain size is $800 \times 800 \times 3000 \mu\text{m}^3$ and the cell size is $1.0 \mu\text{m}$. The microstructure in the simulations TS1 and TS2 are compared in plane-XY at different heights ($600 \mu\text{m}$, $1200 \mu\text{m}$ and $3000 \mu\text{m}$), as shown in Supplementary Figure 9. In both simulations TS1 and TS2, the microstructure is dominated by $\langle 100 \rangle \parallel Z$ (red) grains; the fraction of $\langle 100 \rangle \parallel Z$ (red) grains increase with increasing height. In the lower part of the sample, at the same height ($600 \mu\text{m}$ or $1200 \mu\text{m}$), the fraction of $\langle 100 \rangle \parallel Z$ (red) grains in simulation TS2 is smaller than that in simulation TS1, indicating that the selection rate in simulation TS2 is lower than that in simulation TS1. The reason is that the melt pool dimensions in the lower part of simulation TS2 are smaller compared to the melt pool dimensions in simulation TS1, as shown in Supplementary Figure 9h. Thus, the selection rate in the lower part of simulation TS2 is lower than that in simulation TS1. After depositing more layers, the initial temperature for new layers increases and eventually goes beyond 523 K. This is because the model of Hagenlocher et al. [4] does not include heat loss through convection and radiation and could overestimate the increase in the initial temperature. Consequently, the melt pool in the top layers in simulation TS2 is larger than the melt pool in simulation TS1, as shown in Supplementary Figure 9h. As a result, a higher selection rate is expected in the top layers of simulation TS2. This agrees with the fact that the fraction of $\langle 100 \rangle \parallel Z$ (red) grains in the top plane of simulation TS2 is larger than that in the top plane of simulation TS1, as shown in Supplementary Figure 9c and Supplementary Figure 9f. The fraction of $\langle 100 \rangle \parallel Z$ (red) grains at different heights in the simulations TS1 and TS2 are given in Supplementary Figure 9g, where steady states can be confirmed. In simulation TS1, the steady state is reached earlier while in simulations TS2, the steady state is achieved near the end of the simulation. Near the end of simulation TS2, the fraction of $\langle 100 \rangle \parallel Z$ (red) grains tends to stabilize at a value around 0.95, which is higher than the plateau value (0.85) in TS1 due to the overestimated melt pool dimensions in the upper part of simulation TS2.

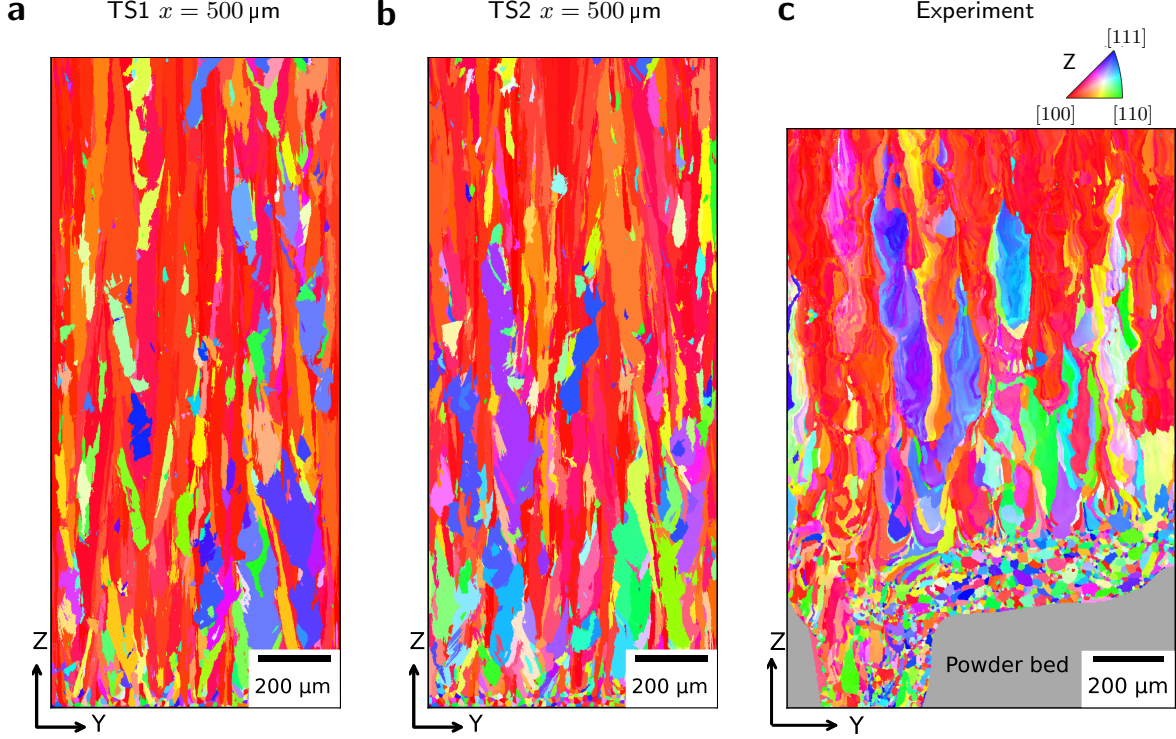
The microstructures in the two simulations are further compared in plane-YZ against an EBSD measurement at the bottom of NiTi sample-B, as shown in Supplementary Figure 10. In the simulation TS1, the fraction of $\langle 100 \rangle \parallel Z$ (red) grains increases from bottom to top and short stripes of grains with globally unfavorable orientations (non-red) propagate along the building (Z) direction, as shown in Supplementary Figure 10a. Similar to simulation TS1, stripe-like grains with globally unfavorable orientations are observed, as shown in Supplementary Figure 10b. However, the size of the stripe-like grains in simulation TS2 is larger, indicating the selection rate in simulation TS2 is lower than the selection rate in simulation TS1. The experimental bottom microstructure is given in 10c. In the first few layers of experiments, fine grains with different orientations are formed due to unstable melt pool and high nucleation rate. After depositing more layers, stripe like grains with globally unfavorable orientations (non-red) are observed, which propagate along the building (Z) direction. The length of



Supplementary Figure 9: Microstructure evolution in plane-XY in the simulations for NiTi sample-B. Two simulations are performed for NiTi sample-B: one (TS1) with a constant initial temperature, and the other (TS2) with a layer-dependent initial temperature. **a, b, c** The microstructure in plane-XY at different heights ($z = 600 \mu\text{m}$, $1200 \mu\text{m}$ and $3000 \mu\text{m}$) in simulation TS1. **d, e, f** The microstructure in plane-XY at different heights ($z = 600 \mu\text{m}$, $1200 \mu\text{m}$ and $3000 \mu\text{m}$) in simulation TS2. **g** The fraction of $\langle 100 \rangle \parallel Z$ (red) grains with respect to heights (Z) in the simulations TS1 and TS2. **h** Comparison between the melt pool shapes in simulation TS1 and TS2. IPF (inverse pole figure) colors with respect to the Z axis are employed in figures a-f.

the transition region from bottom to the region dominated by $\langle 100 \rangle \parallel Z$ grains in the experiment is approximately $1000 \mu\text{m}$, which is comparable to that in simulation TS2. A good match is obtained between simulation TS2 and experiments, as shown in Supplementary Figure 10b and 10c.

For thermal models including analytical models, finite difference models and finite elements models, which do not consider fluid flow in the melt pool, calibration is necessary. The calibration is usually performed based on post-measurement of melt pool boundaries in the top layers, where nearly complete melt pool boundaries are available. However, derivation of melt pool shapes in the bottom layers based on melt pool shapes in the top layers is challenging, as the shape parameters of the top-layer melt pools may be invalid for bottom-layer melt pools. An accurate bottom-layer melt pool shape can be obtained with post-measurements of single-track experiments or in-situ thermal topography measurements during



Supplementary Figure 10: Microstructure evolution in plane-YZ in the bottom of NiTi sample-B. Two simulations are performed for NiTi sample-B: one (TS1) with a constant initial temperature, and the other (TS2) with a layer-dependent initial temperature. **a, b** Microstructure in plane-YZ (taken with $0 \mu\text{m} \leq z \leq 1800 \mu\text{m}$ at $x = 500 \mu\text{m}$) in simulation TS1 and TS2. **c** Bottom microstructure in plane-YZ from experiment. In practical laser powder bed fusion processes, thin-wall grid supports have been manufactured firstly to enhance printability and facilitate the removal of samples from the substrate. Thus, grain growth originates from either the grids or the powder bed (marked as grey background).

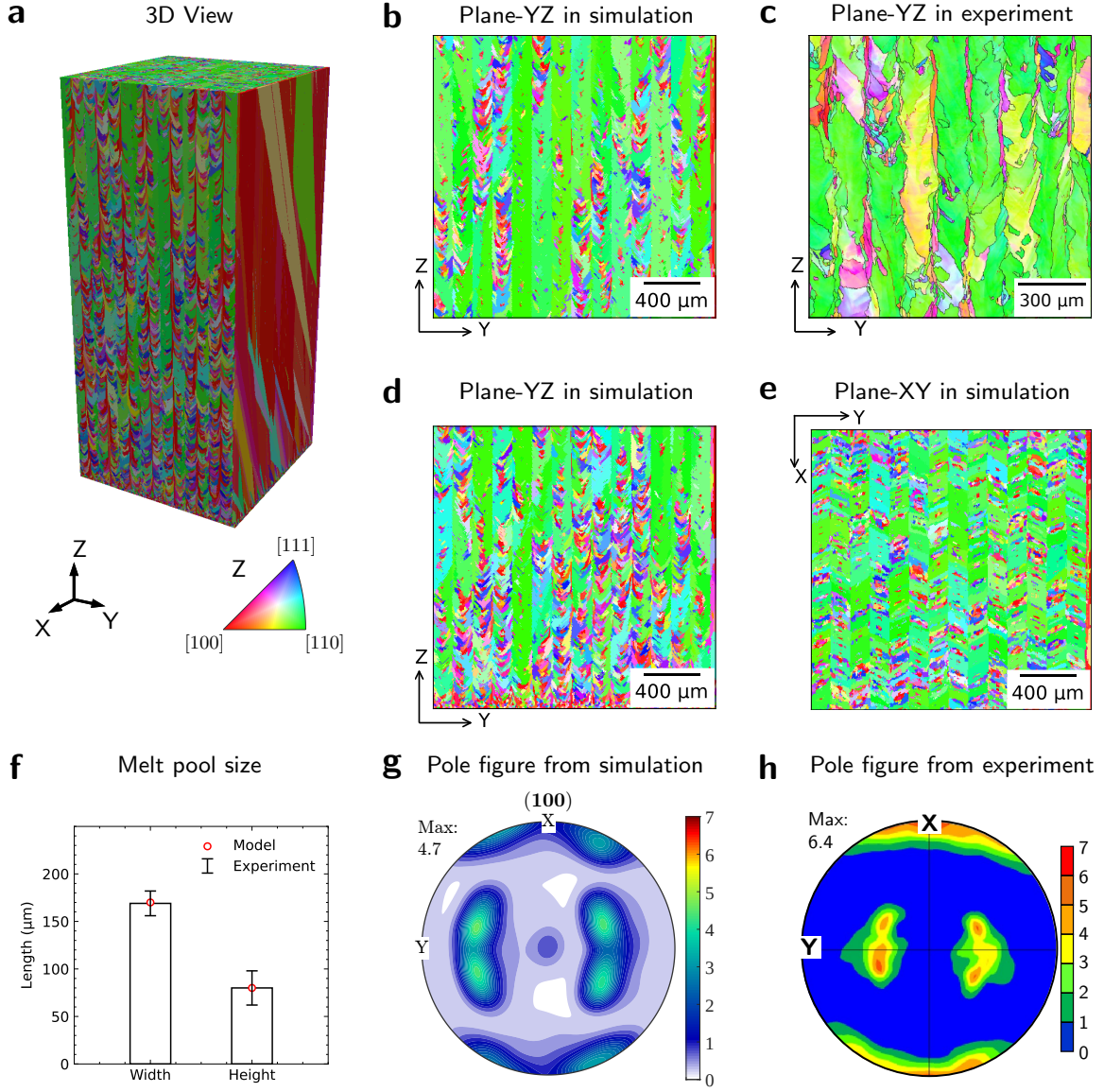
additive manufacturing. However, this is not worthwhile [5]. For real applications, bottom layers are always machined when samples are removed from the substrate. Thus, it is not meaningful to simulate microstructure evolution in the bottom layers. As the thermal model is calibrated against the melt pools in the top layers, it is thus more straightforward to simulate bulk microstructure with the top-layer melt pool.

8 Influence of melt pool dimensions on the 316L steel simulation

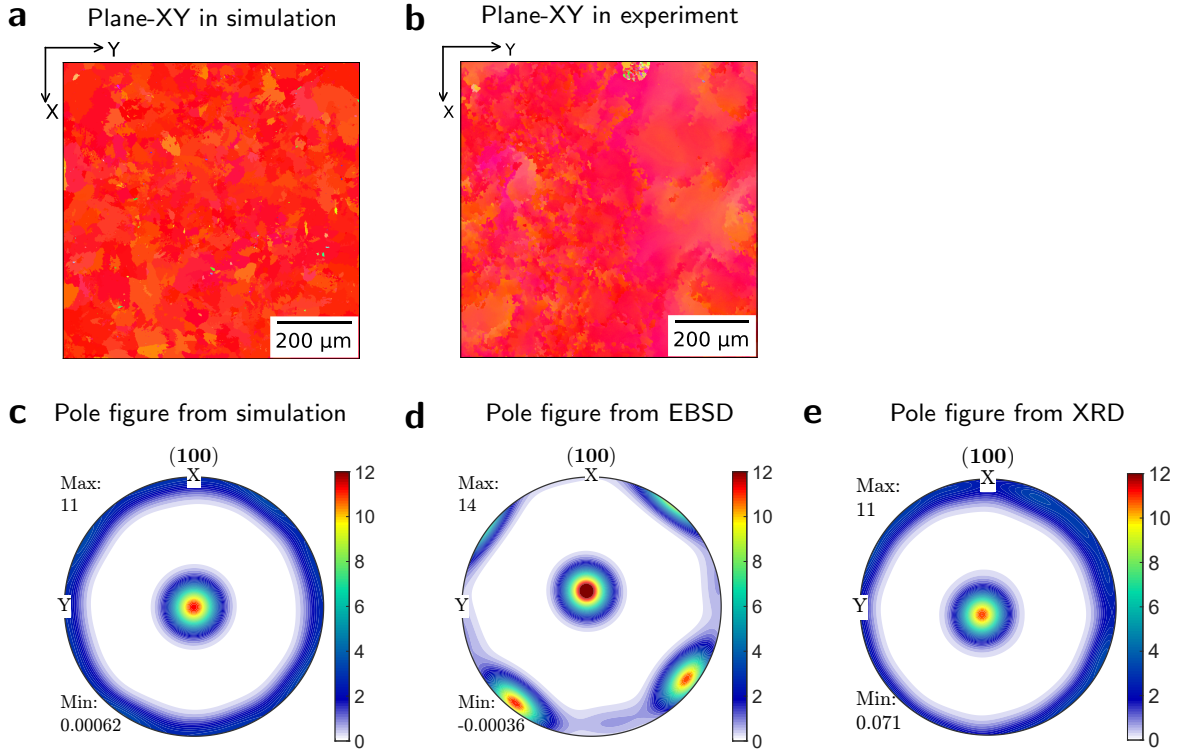
In the 316L steel simulation (LS1) presented in the article, the width and the height of the simulated melt pool deviates from the experimental melt pool by $5\text{ }\mu\text{m}$. With this deviation, a good match is obtained between the simulated bulk microstructure and the experimental microstructure. To check the influence of the deviation in the melt pool dimensions, an additional simulation (LS2) is performed with a melt pool that has the same dimensions as the experimental melt pool. The simulation results are given in Supplementary Figure 11. In simulation LS2, as shown in Supplementary Figure 11b, 11d and 11e, the microstructure is dominated by $\langle 110 \rangle \parallel Z$ (green) grains, which agrees with the experimental bulk microstructure shown in Supplementary Figure 11c. However, different from the experimental microstructure, more small grains with different orientation are observed in the junction region between neighboring melt pools. In the lower part of plane-YZ in simulation LS2, the transition region from a random microstructure to a microstructure dominated by $\langle 110 \rangle \parallel Z$ (green) grains is longer compared to simulation LS1, which is presented in the main article. This indicates that the selection rate in simulation LS2 is smaller compared to that in simulation LS1, due to the smaller melt pool dimensions in simulation LS2. In simulation LS2, a $\{110\}\langle 001 \rangle$ Goss texture is developed, as shown in Supplementary Figure 11g. However, due to the existence of small grains with different orientations, the maximum texture intensity (4.9) in simulation LS2 is lower than that in simulation LS1 (6.8) or the experiment (6.4). The differences in the microstructures and texture of simulation LS1 and LS2 shows that the simulated microstructure is sensitive to melt pool dimensions.

9 Pole figures of NiTi sample-C

The pole figure shown in the article is not generated based on the EBSD (electron backscatter diffraction) result. Instead, it is plotted based on an XRD (X-ray diffraction) measurement. The microstructure in plane-XY and the pole figures for the NiTi sample-C are given in Supplementary Figure 12. The pole figure in Supplementary Figure 12c is generated based on Supplementary Figure 12a, showing a $\langle 100 \rangle$ fiber texture. However, the experimental pole (Supplementary Figure 12d) generated from the EBSD result (Supplementary Figure 12b), indicates a $\{001\}\langle 110 \rangle$ texture. The reason is that the grain size in Supplementary Figure 12b is too large and there are not enough grains to give a quantitative evaluation of the texture. In this case, an XRD measurement was performed in a larger domain. The pole figure from the XRD measurement shows a $\langle 100 \rangle$ fiber texture, as shown in Supplementary Figure 12e, which agrees with the simulation results.



Supplementary Figure 11: Results from the simulation and the experiments for the 316L sample. The simulation domain size is $2000 \times 2000 \times 4500 \mu\text{m}^3$. The simulation is performed with a melt pool which matches the mean size of the experimental melt pool. **a** 3D view. **b, d** Simulated microstructure in the upper part ($2500 \mu\text{m} \leq z \leq 4500 \mu\text{m}$) and the lower part ($0 \mu\text{m} \leq z \leq 2000 \mu\text{m}$) of plane-YZ ($x = 1000 \mu\text{m}$). **c** Experimental microstructure in plane-YZ. In both the simulation and the experiment, $\langle 110 \rangle \parallel Z$ (green) grains dominate the microstructure. Many small grains exist in the simulation which are not common in the experiment. **e** Simulated microstructure in the plane-XY ($z = 4500 \mu\text{m}$). **a-e** are colored with IPF (inverse pole figure) color with respect to the Z axis. **f** Melt pool dimensions in the experiments and simulations. **g** Simulated pole figure (generated based on e). **h** Experimental pole figure. A $\{110\}\langle 001 \rangle$ Goss texture is identified in both the simulation and the experiment. Figures 2c, 2f and 2h are adapted from Andreau et al. [6].



Supplementary Figure 12: Microstructure and texture of NiTi sample-C from the simulation and experiments. **a** Microstructure in plane-XY in the simulation. **b** Microstructure in plane-XY from EBSD (electron backscatter diffraction) experiment. **c** Pole figure in the simulation (generated based on a), where a $\langle 100 \rangle$ fiber texture is observed. **d** Pole figure from experiment (generated based on b), indicating a $\{001\}\langle 110 \rangle$ texture. **e** Pole figure from an XRD (X-ray diffraction), which agrees with the simulated pole figure.

References

- [1] K. Teferra and D. J. Rowenhorst, *Acta Materialia* **213**, 116930 (2021).
- [2] O. Zinovieva, A. Zinoviev, V. Romanova, and R. Balokhonov, *Additive Manufacturing* **36**, 101521 (2020).
- [3] A. Pineau, G. Guillemot, D. Tournet, A. Karma, and C.-A. Gandin, *Acta Materialia* **155**, 286 (2018).
- [4] C. Hagenlocher, P. O'Toole, W. Xu, M. Brandt, M. Easton, and A. Molotnikov, *Additive Manufacturing* **60**, 103263 (2022).
- [5] W. F. Templeton, S. Hinnebusch, S. Strayer, A. To, and S. P. Narra, *Materials & Design* **231**, 112069 (2023).
- [6] O. Andreau, I. Koutiri, P. Peyre, J.-D. Penot, N. Saintier, E. Pessard, T. De Terris, C. Dupuy, and T. Baudin, *Journal of Materials Processing Technology* **264**, 21 (2019).