MADE-3D



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# MADE 3D

## HORIZON EUROPE EUROPEAN HEALTH AND DIGITAL; EXECUTIVE AGENCY (HADEA)

# MADE-3D

## **Multi-Material Design using 3D Printing**

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# = Deliverable D2.2 =

Building and application of microscale simulation

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#### **Executive Summary**

This report explains in details finite element thermomechanical model built to simulate monomaterial and bimaterial L-PBF (Laser Powder Bed Fusion) process at microscale and mesoscale. All equations for thermal and mechanical behavior are explained, as all boundary conditions and loading induced by the process. This model has been built using in-house finite element software.

The model has been used to simulate different generic cases, waiting more detailed process parameters. These cases are:

- Microscopic scale with one track simulation (for AlSi10Mg)
- Mesoscopic scale with up to ten coincident tracks and layers for monomaterial configuration (for AlS10iMg)
- Same with bimaterial configuration

Thermal and mechanical field obtained permits to define the geometry scale to be considered to achieve representativeness of thermal history and residual stresses. First simulation with bimaterial configuration show a very complex stress generation at interface wich leads us to conclude on the importance of near interface lasing strategy as material consolidation order (A then B, B then A).

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#### MADE-3D

#### **1. Introduction**

This deliverable is dedicated to microscale and mesoscale simulations of dissimilar L-PBF manufacturing (Laser Powder Bed Fusion). This work is realised in the frame of the WP2 of the project (Design & Modelling). This work package is subdivided in four tasks:

- Computational path planning for joining dissimilar materials by DED (T2.1)
- Baseline alloy modification for improved joining by PBF-LB (T2.2)
- FEM modelling of residual stresses, thermal history, melt pool temperatures at micro level scale (T2.3)
- Use Case component design and simulation (T2.4)

The first main topic of this workpackage is to define materials or materials assembly (in case of DED process) to optimise manufacturing reliability as part properties. The first difficulty induced by these two high temperature processes involving bimaterial manufacturing is to manage inter diffusion between both materials. Inter diffusion leads often to intermetallic precipitation. Generally, intermetallic phases are brittle. In the case of DED process, diffusion aspects can be controlled using intermediate layers. It is also the case for others bimaterial processes like brazing, HIP (High Isostatic Pressing, welding,...). For L-PBF process, the only solution is to choose a compatible chemical composition for both materials and limiting diffusion mechanism. This work is dedicated to first two tasks (T21 and T2.2).

If we want to optimise chemical compositions in L-PBF process in that way, we need to have an idea of the thermal history at interface between materials. Knowing this thermal history, we can be able to predict numerically inter diffusion zones at interface.

Another difficulty of these bimaterial processes are residual stresses. Residual stresses induced by material contraction during cooling, moreover with multimaterial processes inducing local thermal expansion mismatches (see **Figure 1**), is the main cause for small or large cracking in dissimilar material assemblies, and so by extrapolation to high temperature multimaterial 3D printing processes, whatever the process used (cold spray, L-PBF, DED, etc...). This cracking is of course also dependent on materials ductilities.



Figure 1: thermal gradient effect for monomaterial L-PBF process [1]

As a result, we need to consider three different main aspects in our materials/process optimisation:

- Limitation of residual stresses induced by the process
- The best mechanical compatibility between both materials, i.e thermal expansion and ductility in first order
- The best chemical compatibility between materials, i.e. intermetallic precipitation.

The numerical tool which will be developed in this T2.3 work will permit the project to develop best materials couples and process parameters to achieve bimaterial parts with good mechanical properties. Results form with workpackage will be usefull for other tasks from this workpackage, as we need inputs form other workpackages. The interaction chart of this T2.3 is presented **Figure 2**.



Figure 2: T2.3 interaction chart

The last topic of this workpackage WP2 is dedicated to the design and optimisation of use cases using DED or L-PBF process (T2.4).



Figure 3: global simulation strategy

During this project, we will focus our work on Copper/Aluminium L-PBF configuration, as it is the most challenging couple in terms of inter-diffusion and mechanical residuals stresses. More precisely, we will deal with AlSi10Mg/CuCrZr bimaterial configuration.

All the work realised during this first year as explanations on simulation strategy are given in APPENDIX A.

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### 2. Results and Discussion

Before to go in details on simulation building and results, we present Figure 3 the global simulation strategy wich will be conducted during this project. Three simulation scales will be studied:

• **Microscale simulation**. We focus here on the study of a single track lasing. Main outputs at that scale are melt pool dimension. Melt pool dimension is very important for thermal history and residual stresses generation. At that scale, we can fit numerous thermal loading and boundary conditions involved in this process (see **Figure 4**) before going to upper scales, generally involving lot of more computation times.



Figure 4: thermal model at micro scale [2]

- **Mesoscale simulation**. At that scale, we deal with several contiguous lasing tracks and several layers. This scale permits to have a good access to thermo-mechanical phenomenoms acting during the process. At that scale we will introduce bimaterial L-PBF configuration. This scale will permit to extract proper thermal history for diffusion calculations and residuals stresses. Moreover, these simulation at that scale will permit to extract inherent strains ([3]) for macroscale simulations.
- **Macroscale simulation.** At that scale we will be able to compute simulation on whole parts. These simulations are needed to predict part deformation during process and in a certain way, induced stresses. Macroscale simulation building will be done during next year.

From this first year T2.2 work, we present in this deliverable:

- Building of base thermomechanical model with associated process thermal loading and boundary conditions.
- Microscale simulations with AlSI10Mg
- Monomaterial mesoscale simulation with AlSi10Mg
- Bimaterial mesoscale simulation with AlSi10Mg/CuCrZr

We focused on simulations on AlSi10Mg for model building, but similar simulations can be run using CuCrZr. As process parameters are not known at that time, there is no needs to conduce simulation for both materials.

#### MADE-3D

#### 2.1. Model building

For these simulations, we built a thermomechanical model (sequential iterative coupling) using in-house open source software (Cast3M **[4]**). Main things to consider for our L-PBF application are:

- Properly model all boundary conditions, in particular thermal ones (convection, radiation, laser source model)
- Manage powder behavior. Indeed, powder layer (see Figure 5) have a very low thermal conductivity and close to none mechanical rigidity.
- Include latent heat effects during solid/liquid phase change. It is a little bit tricky to integrate this phenomenon for high-speed liquefaction/solidification processes.

As bimaterial process parameters are not yet consolidated in terms of process parameters, we used process parameters from litterature.



Figure 5: powder and bulk material configuration during L-PBF process [5]

#### 2.1. Single track simulation (AlSi10Mg)

We present **Figure 6** the temperature field obtained for AlSi10Mg. From this thermal information, we can compute melt pool size. Computed melt pool size is quite coherent with the one computed from classic analytical model using Rosenthal equation ([6]).



**Figure 6**: temperature during lasing of a single line (AlSi10Mg) **D2.2 Building and Application of Microscale Simulation** Page 7 of 44

For mechanical behavior materials, we choose in first step a simple perfectly plastic behavior depending on temperature. Residual stresses induced are mainly traction ones due to material contraction during cooling. We observe laser ignition and stop effect due to different thermal cooling speed at that points.



Figure 7: V.M. stress field during lasing of a single line (AlSi10Mg)

Integrating more thermal non-linearities as properties depending on temperature and liquid conductivity change melt pool dimensions, but we pay the price in terms of computation times as seen **Table 1**. If computation time is not problematic for monotrack simulation, computations times are important (>1 day) for mesoscopic one when we compute several tracks/layers.

If we want to accelerate computation times, we can neglect non-linearities in a first approach. It makes sense for lasing strategy optimisation and various sensibility analysis.

							melt po	ool dimei	nsion
Ν	NL thermal	liquid	powder/bul	latent	time	factor	length	widt	depth
	properties	conductivit	k phase	heat	(min)		[μm]	h	[µm]
		У	change					[µm]	
1					10	1.00	530	195	120
2	Х				30	2.94	485	195	120
3	Х	Х			89	8.79	394	260	120
4	Х	Х	Х		93	9.19	432	195	120
5	Х		Х		39	3.90	545	195	120
6				X	41	4.05	909	195	90
7	Х	х		X	269	26.66	667	195	90

Table 1: Evolution of melt pool dimensions and computation times depending on thermal non-linearities assumptions

#### 2.2. Mesoscopic monomaterial simulation (AlSi10Mg)

We conducted a mesoscopic simulation with five contiguous laser lines during five layers (total of 25 laser lines). We made here the assumption of a lasing strategy without rotation between layers Deep analysis of thermal evolution might lead us to conclude that scans with ten layers (10x10 laser lines) is necessary to achieve a kind of stable thermal periodicity (see **Figure 9**).



Figure 8: temperature field during first and last laser line for 5x5 mesoscopic simulation (AlSi10Mg)



Figure 9: upper thermal history at third scan (AlSi10Mg)

Concerning mechanical residual field, a quick stabilisation of stress field is observe with contiguous tracks is observed (**Figure 10**). Last two tracks present side effects. We observe a lower residual stresses zone below approximatively five manufactured layers, wich probably correspond to a kind of stress relieve phenomenon induced by medium temperatures without melting. Therefore, five layers is not sufficient if we want to quantify internal residuals stresses of our material. To quantify upper residual stresses wich are quantitatively more important, five layers seems sufficient.



Figure 10: V.M. residual stress field at the end of last track of the fifth deposited layer (AlSi10Mg)

Taking into account these preliminaries consideration, we successfully launched a 10x10 thermomechanical configuration. We can now really observe that we have a relative homogenous stress concentration in last fifth layers due to layer remelting. Below this zone, we observe a stress relieving do hight temperatures attempt (see **Figure 11**). This result is very important because that mean that for XR residual stresses measurements, as-built surface analysis (gauge depth of about 30-50µm) will give different results as inside material.



Figure 11: V.M. residual stress field at the end of last track for ten deposited layer (AlSi10Mg)

#### 2.3. Mesoscopic bimaterial simulation (AlSi10Mg/CuCrZr)

We simulated 5x5 bimaterial thermomechanical simulation for AlSi10Mg/CuCrZr couple. As expected, we obtain a complex residual stresses field with again two distinct zones which are near surface one ( $\approx$ 5 layers) and sub-surface one (<5 layers).

An example of thermal fields are given **Figure 12**. As material properties and lasing parameters are different between two materials, this induce complex thermal history at interface. These results can now be used to complete diffusion simulation at the interface. Near interface, bimaterial configuration induce more remelting as melt pool from one material can penetrate the other. That means that positions of the laser near interface has an important effect on residual stresses, as the order of consolidation between first and second material.



Figure 12: temperature field during first line for each material for 5x5 mesoscopic bimaterial simulation

The presence of two materials with different thermal/mechanical properties generate highly complex residual stress field at interface, like we can see



Figure 13: stress field along lasing direction for 5x5 mesoscopic bimaterial simulation

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#### 3. Conclusion

During this first-year project period, we built a complete Finite Element thermomechanical model for mono and bimaterial L-PBF process at micro and meso-scale, including liquid/solid latent heat, powder to bulk evolutions as layer deposition.

Concerning thermal results, this model permit to access complete thermal history, in particular at interface for bimaterial configuration. These informations are usefull for diffusion calculations at interface. 10x10 tracks/layers seems to be sufficient to be representative.

For mechanical stresses generated by the process, we need less coincident tracks to be simulated (around four or five tracks). Computation of five deposited layers are sufficient to characterise near surface residual stresses. If we want to have an idea of inside material residual stresses, at least 10 layers will be needed.

In bimaterial configuration, complex residual stresses are observed near interface. As a result, order of material consolidation as lasing strategy are preponderant.

Thermal non-linearities consume a lot computation times. As thermal solver of our in-house code is not parallelized, computation times are quite long. A first work of next year will be to transfer models inside commercial F.E. software ANSYS©

#### 4. Degree of Progress

All main tasks of this T2.3 WP are listed **Table 2**. According to first results presented in this report for this first year, we had a task consisting in building same model inside commercial F.E. ANSYS©.

Deadline	sub-tasks	status	commentes
M12	thermal model	100%	
M12	mechanical model	90%	
M12	monotrack simulation on generic case	100%	done on AlSi10Mg and CuCrZr
M12	multilayer scan pattern on generic case	100%	done on AlSi10Mg
M12	Model building inside ANSYS©	20%	
M24	monotrack line simulation on real case	0%	wait process parameters from ICGV. Need to be done on both materials
M24	bimaterial multilayer scan pattern on real case	0%	wait process parameters from ICGV. Need to be done on both materials
M24	multilayer scan pattern on generic case	100%	done on a simplified case
M24	bimaterial multilayer scan pattern on real case	0%	wait process parameters from ICGV. Need to be done on both materials
M24	inherent strain tensor identification using mesoscopic simulations	0%	
M24	building of macroscopic simulation	0%	
M38	experimental validation on monomaterial process	0%	
M38	experimental validation on bimaterial process	0%	
M38	experimental/simulation comparaison		samples need to be defined (in progress with WP4)

**Table 2:** Progress table for tasks involved in T2.3 WP.

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## Appendix: Model building and first results (global presentation)







Micro and Meso thermal model for L-PBF bimaterial configuration

27-11-2023

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## **Global modelisation approach**





## **Models description: Thermal**

Physics

 $\rho C_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( k \frac{\partial T}{\partial y} + \right) \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right) + Q$ Heat conduction equation

Q is volumetric heat: volumetric laser source and/or latent heat effects





6

## **Models description: Thermal**



[Makoana et al., 2018] 
$$Q(x,y) = \frac{2\lambda P_L \beta}{\pi r_L^2} exp\left(\frac{-2[(x-x_0)^2 + (y-y_0)^2]}{r_L^2}\right) exp(-\beta|z-z_0|) \quad \text{For } z \in \Omega$$
$$\beta = \frac{1}{L_{ep}} \text{ as few laser penetration through bulk material}$$

8



Models description: Thermal



 $h_{eq} = 24.1 E^{-4} \xi (T-273)^{1.61}$ [Goldak et al., 1984]



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with  $\xi = 0.9$ 

## Models description: Thermal

- Boudaries conditions
  - Fixed temperature at bottom of studied part

$$T = T_B$$
 for  $\lceil_2$ 

 $\rightarrow$  bottom temperature depends on process parameters, plate configuration and wich layer considered

→ temperature fixed at T<sub>B</sub>=80°C (first layers)

→ bottom temperature can be simulated using aggregated macroscopic approach



GA number: 101091911





10

9

#### Powder zone properties

→ Packed bed powder conductivity can be approximated by:



→ As powder zone is considered geometrically as consolidated

 $\rho_p = \rho_b$  $C_p = C_b$ 

<u>08</u>2



## **Models description: Thermal**

Liquid/Solid transformation

→ Phase change is take into account by parameters dépendance in temperature (no metallurgical change in our case)

→ conductivity:

$$k_L = k_S$$
 for  $T < T_m$  [Ren et al., 2019]  
 $k_L = 2.5k_S$   $T < T_m$ 

→ heat capacity:

$$C_L = C_S \qquad \text{for} \qquad T < T_m - 0.5\Delta T_m \qquad \text{or} \qquad T > T_m - 0.5\Delta T_m$$
$$C_L = C_{S+} \frac{L}{\Delta T_m} \qquad \text{for} \qquad T_m - 0.5\Delta T_m < T < T_m + 0.5\Delta T_m$$
$$[Promoppatum \ et \ al., \ 2017]$$

 Bad.....too much step size dependant. I programed phase change and so heat generation with phase change within convergence iterations











## **Materials thermal properties**

→ precipitation won't occurs on top layers, so evolutions in this zone are excluded



→ First cycle properties are considered (as built state)

## Materials thermal properties







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**Models description: Mechanical** 



### Physics

- $\nabla \cdot \{\sigma\} + \rho \vec{b}$  Quasi-static stress equilibrium
- {σ} stress tensor
- B Internal body force per unit volume



## **Models description: Mechanical**

Material behavior



Models description: Mechanical

We suppose isotropic purely 
$$J_2$$
 plasticity:  $f({\sigma}) =$ 

 $\sqrt{\frac{\{S\}:\{S\}}{2}} - \sigma_y \qquad \qquad \{S\} = \{\sigma\} - \frac{1}{3}Tr\{\sigma\}$  $\sigma_y \qquad \qquad \forall ield stress$ 

For powder material domain  $\Omega_2$ :  $\{\sigma\} = [C][\{\varepsilon^t\} - \{\varepsilon^{th}\}]$  Purely elastic material Same as bulk material

Powder has no rigidity → Epowder=Ebuk. 10-7



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NO 180



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**Mechanical properties of AISI10Mg** 



w W

n wy

## Mechanical properties of CucrZr

Thermo-elastic properties

#### [Ferraiuolo, 2023]

Temperature [K]	Mass Density [kg/m <sup>3</sup> ]	Thermal Conductivity [W/mK]	Specific Heat [J/kgK]	Thermal Expansion Coefficient [1/K]
300	8933	320	390	$15.7 \times 10^{-6}$
600	8933	290	390	$17.9 \times 10^{-6}$
900	8933	295	400	$18.7 \times 10^{-6}$



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## **Mechanical properties of CuCrZr**





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## **Process parameters**

and the second	AISI10Mg [Rausch et al., 2017]	CuCrZr [Buchmayr et al., 2017]
Power [W]	350	370
speed [mm/s]	1650	300
hatch distance (mm)	0.13	0.11
layer thickness [um]	30	20

For both materials we will consider:

- 30µm layer thickness
- · 80µm laser diameter

All these parameters will be updated after material process consolidation



**Geometric configuration for monotrack** 







**Results for monotrack simulation** 

Comparaison with analytic model



simul 1Nt thermal propertieslequid conductivity powder/bulk phase changeintend (mis) (65171)factorlength (yn) (100)width (yn) (100)depth (y) (100)12x1001.005301951202x1730593302.444851951203XXX5317359898.793942601205xXX5561562939.194321951206X25327433.905451951207xX1613442226926.66667195907xXX1613442226926.66667195907xxX1613442226926.6666719590999999999999x1613442226926.6666719590999<
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4xxxsectors $33$ $9.19$ $432$ $106$ $120$ $5$ x $2362374$ $39.3729$ $3.90$ $545$ $135$ $120$ $6$ x $265344$ $4.1$ $4.05$ $909$ $136$ $909$ $7$ xx $16134422$ $269$ $26.66$ $667$ $195$ $90$ $n 5$ $5$ $5$ $5$ $5$ $5$ $106$ $567$ $195$ $90$ $n 5$ $5$ $5$ $7$ <t< td=""></t<>
s       x       282374       39.3728       3.90       545       195       120         6       x       2453484       41       4.05       909       195       90         7       x       x       16134422       269       26.66       667       195       120         15       x       x       16134422       269       26.66       667       195       90         15       Sim 7
x 263464 41 4.05 909 195 90 x x 16134422 269 26.6 667 195 90 15 Sim 7
r 5 x x x x x x x x x x x x x x x x x x
m 5 Sim 7 Sim 7 answerse section of the melt pool is the most important for residual stresses ineration $\rightarrow$ layent heat play a major role in transverse melt pool dimension
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**Results for monotrack simulation** 

Melted powder





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**Results for monotrack simulation** 

Residual stresses





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## **Results for monotrack simulation**

Residual stresses  $\sigma_{zz}$ 



Geometric configuration for mesoscopic simulation







## **Results for mesoscopic simulation**

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Temperatures evolution with contiguous tracks



**Results for mesoscopic simulation** 

Temperatures evolution with contiguous tracks



- If we want to reach representative thermal evolution, we need to have at least 2 more tracks
   → 5+2=7 tracks
- If we want at least 3 representative tracks → 7+2=9 tracks

## **Results for mesoscopic simulation**

Temperatures evolution with layers



A least 10 layers are necessary to acheive representative thermal evolution

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Approx. 6 previous layers are strongly mechanically affected

It is not necessarry to have a lot of tracks per layer





**Results for mesoscopic simulation** 



SZZ Stress field after last layer



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## **Results for mesoscopic simulation**









## **Results for mesoscopic simulation**



Geometric configuration for mesoscopic bi-material was simulation



Solver configuration: only linear thermal model

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Lasing strategy can be changed

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# Geometric configuration for mesoscopic bi-material





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# Geometric configuration for mesoscopic bi-material Simulation

Temperature evolution at interface with layers



Added remelting induced by other side material lasing

Geometric configuration for mesoscopic bi-material simulation



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Security from second material melt pool on previous consolidated material will change stress

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## conclusions

- We built a complete Finite Element thermomechanical model for mono/bimaterial L-PBF process at micro and meso-scale
- This model permit to access complete thermal history, in particular at interface for bimaterial configuration → input for diffusion calculations
- · Computation of five deposited layers are sufficient to characterise near surface residual stresses
- · A least 10 layers are necessary to characterise final residual stresses inside material
- · In bimaterial configuration, complex residual stresses are observed near interface
- A better thermal solver is necessarry for that kind of simulations → models will be integrated into commercial F.E. software ANSYS©

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