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Thermomechanical modeling of additively manufactured structural parts - different approaches on the macroscale

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Abstract. Modeling the metal additive manufacturing process can be done on different length scales depending on the field of interest. However, due to the moving heat source and the narrow heat affected zone, a fine mesh and fine time resolution are required to analyze detailed information on various length scales. In this paper, the focus is on macro-scale temperature, deformation and residual stresses. The inherent strain method is applied layer by layer on the full part, to include the thermal contraction and inelastic strains generated by the moving heat source. The inherent strain components are mapped from the mesoscale simulations, where different boundary conditions can be used to resemble different regions from the macroscale. As an alternative to the inherent strain method and to include the thermal simulation on macroscale without simulating the moving heat source, a layer-by-layer approach is proposed and applied in the paper. The price to pay is the loss in detail of the thermal load. However, for the suggested layer-by-layer approach, the energy corresponds to the energy delivered from the laser. The proposed and implemented methods are applied to two examples and compared to measurements. Finally, large structural parts are simulated to evaluate the application on new trends in the automotive industry.

1. Introduction
Application of additive manufacturing has steadily been growing for many years and today the process is generally used to build complex parts in a wide range of alloys. The design freedom of the parts has been the main driver of the process. The possibility to build complex parts without expensive tooling has made the process interesting for prototyping and small series, especially for cases with a focus on service load analysis and an associated topology optimization. In laser powder bed fusion (LPBF), the building process of the parts comes with a price, in terms of steep thermal gradients around the moving heat source generated by the laser. Already solidified material is re-melted and affected by heating when new layers are added. High stress and inelastic strain can develop during the building process, which sometimes lead to large deformations when the part is cut off from the base plate and the support structure is removed. Heat treatment of the parts is often used to relax the stress level and to minimize these deformations. To analyze the influence of the process parameters on stability and the part quality, the process simulation is increasingly used today.

This paper presents the implementation of a general thermomechanical model, which can be used to simulate the moving heat source on a mesoscale, where the source term is modeled with the well-known Goldak model [1]. Furthermore, a layer-by-layer thermomechanical model is implemented to simulate the material response on a macroscale to provide results on the component level. Finally, the inherent
strain method is implemented and applied to make a first qualitative evaluation of this 'simplified' approach.

The different functionality is implemented in MAGMASOFT® as an add-on to the integrated stress solver, MAGMAstress. The governing equations for the thermal and mechanical problems are discretized and integrated with standard linear hexagonal finite elements. All material data are temperature dependent. For the thermal solver it is possible to model convection and radiation on the outer surfaces. The constitutive law for the mechanical simulation is a standard time independent plasticity formulation, which is used during the printing process. During heat treatment a unified creep formulation is used to include time and rate effects at elevated temperature to model the stress relaxation.

Different parts from small academic size up to a large structural part from the automotive sector are simulated on different scales to evaluate the application of the integrated modeling approach. The results are compared to measurements which were performed during the evaluation of the implementation plus some comparison to findings in literature.

2. Mesoscale – moving heat source

On the mesoscale, each single laser path is simulated in detail. The energy distribution is described by a Goldak heat source model, see figure 1. The source term is directly used in the thermal simulation, where the laser parameters and the process conditions determine the moving heat source size and location. The state and temperature dependencies of the material data is taken into account to have a reasonable description of the variation in thermo-physical and mechanical properties of the powder and the solid material. For the presented results the state of the material is changed from powder to solid when the temperature is exceeding the solidus temperature. For the powder state the thermal conductivity and the surface emissivity are significantly reduced [2, 3], and the elements are not mechanically activated. For this type of simulation it means, that a new layer of powder material is activated in the thermal domain, when the re-coater has distributed the powder. The mechanical domain is dynamically growing inside the layer when the local temperature exceeds the solidus temperature and the thermal strain integration starts when the temperature drops below solidus again.

Figure 1. (a) Goldak’s double-ellipsoidal heat source model, (b) temperature distribution around the moving source term, (c) typical scanning paths and (d) temperature distribution in a patch while being built.

The results from mesoscale simulations can be useful to analyze various local effects of hatching strategies and laser parameters and the influence on temperature and stress distributions. However, due to the moving heat source and the narrow heat affected zone a fine mesh and fine time resolution are required to analyze detailed information on very small length scales. If the focus is mainly on macroscale deformations and residual stresses it is unrealistic to resolve the details of the moving heat source even on smaller parts. To perform large scale simulations on macroscale it is often necessary to switch to a layer-by-layer strategy, where heated layers or layers of predefined inherent strain components are activated in the calculation domain step by step. The advantage of such approaches is obviously a
significantly reduced calculation time due to the simplified description of the actual process, where the moving heat source is replaced by the activation of one or several full layers. Two quite different layer-by-layer approaches will be evaluated in the paper:

1. The inherent strain method, which is a pure mechanical model.
2. The thermo-mechanical method, where the thermal simulation is based on releasing the energy from the laser in one or several layers, followed by a mechanical simulation where the thermal strain is based on the simulated temperature distributions.

Measurements of deformation and stresses from two parts will be used to validate the two layer-by-layer approaches.

The heat transfer equation is solved on both mesoscale and macroscale in the thermomechanical case

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x_i} \left( k \frac{\partial T}{\partial x_i} \right) + \dot{Q}$$  \hspace{1cm} (1)

where $\rho$ is the density, $c_p$ is the specific heat capacity, $T$ the temperature and $\dot{Q}$ the source term.

The static equilibrium equations are solved in all cases, with either the thermal strain or the inherent strain components as the main load input, it should be noticed that for the inherent strain approach the thermal strain is part of the inherent strain components

$$\sigma_{ij,i} + p_j = 0$$  \hspace{1cm} (2)

where $\sigma_{ij}$ is the stress tensor and $p_j$ is the volumetric force vector.

Time independent plasticity is used for the building process as the constitutive description, with the $J_2$ von Mises yielding condition

$$f = \sigma_e^2 - \sigma_y^2 = 0, \text{with } \sigma_y = \sigma_y(\varepsilon^{pl}_e, T) \text{ and } \sigma_e = \sqrt{3}J_2$$  \hspace{1cm} (3)

Using the consistency condition to determine the load step

$$\dot{f} = \frac{\partial f}{\partial \varepsilon^{pl}_e} \dot{\varepsilon}^{pl}_e + \frac{\partial f}{\partial T} \dot{T} = 0$$  \hspace{1cm} (4)

where $f$ is the yield function, $\sigma_e$ the von Mises stress, $\sigma_y$ the yield stress and $\varepsilon^{pl}_e$ the effective plastic strain used as hardening the parameter.

A Unified creep formulation is used for the heat treatment simulation to include the time effects in the results

$$\dot{\varepsilon}_{ij} = A \exp \left( \frac{-Q}{RT} \right) \left( \frac{\sigma_e}{\sigma_{ref}} \right)^m n_{ij}$$  \hspace{1cm} (5)

where $A$ is a reference strain rate, $Q$ the activation energy, $R$ the gas constant, $T$ the absolute temperature, $\sigma_{ref}$ the hardening stress, $m$ the strain rate sensitivity exponent and $n_{ij}$ is the outwards normal to the yield surface. For heat treatment the inelastic strain tensor makes a contribution to the well-known strain decomposition.

$$\varepsilon_{ij}^{tot} = \varepsilon_{ij}^{el} + \varepsilon_{ij}^{in} + \delta_{ij} \varepsilon^{th}$$  \hspace{1cm} (6)

3. The inherent strain method

The inherent strain method is a well-known approach for numerical modeling of deformation and stress in the field of classical welding, [4]. The method distributes measured or modelled permanent strain in a simplified macroscopic calculation, including the loading from the moving heat source.

For the finite element method, the inherent strain components are added to the elastic strain tensor in the strain decomposition equation

$$\varepsilon_{ij}^{tot} = \varepsilon_{ij}^{el} + \varepsilon_{ij}^{inh}$$  \hspace{1cm} (7)

with three non-zero normal components $\varepsilon_{ij}^{inh} = \delta_{ij} \varepsilon_{ij}^{el}$

Inserting this in Hooke’s law yields the standard expression for the stress tensor
\[
\sigma_{ij} = \frac{E}{1 + \nu} \left\{ \varepsilon_{ij}^{tot} - \delta_{ij} \varepsilon^{*}_{kk} + \delta_{ij} \frac{\nu}{1 - 2\nu} (\varepsilon_{kk}^{tot} - \varepsilon^{*}_{kk}) \right\}
\]

In addition to the inherent strain components, the usual inelastic strain tensor is included in the implementation.

3.1. U-profile
To validate the application of the inherent strain method on simple geometries, two AlSi10Mg U-profiles were built on a GE M2 machine and then simulated. The distance between the legs of the U-profile was 4mm and 8mm, respectively. Again two inherent strain simulations were performed assuming the inherent strain components to be -1.3\%, which is estimated from earlier work on the mesoscale.

![Figure 2](image)

**Figure 2.** Comparison between the numerical results and the optical measurements for a 4mm and 8mm U-profile. (a) The simulation results and (b) the measurements. \(\Delta d\) is the deviation in measured displacement and the un-deformed geometry.

The results from the inherent strain method show same trends as the measurements. The deviation, \(\Delta d\), between the measured displacement and the un-deformed geometry of the U-profile after machining, increases for the increased distance between the legs from approximately +1.0mm to +1.2mm. The main reason for the bending is the elastic spring-back during machining, when the residual stress state is released. Stresses mainly build up in the top layers of the U-profile when the final layers are printed and contract.

4. The thermomechanical layer-by-layer method
The layer-by-layer inherent strain method is based on a selective mapping of results from mesoscale to macroscale, where the choice of mapping becomes critical for the accuracy of the results. For complicated parts the definition and selection of the inherent strain components might not be so clear and the consequence could be a lack in quality in the prediction of deformations and stresses. Furthermore, the inherent strain approach does not include a thermal simulation on macro scale, which of course saves some calculation time, but it also means that it is not possible to evaluate the temperature related effects like the cooling conditions from support structure and powder leading to e.g. critical locations of hot spots.

To include the thermal simulation on macroscale without simulating the moving heat source, it is proposed in literature to release the energy in bigger regions at the same time, see e.g. [5] for a more detailed description or [6] for an alternative approach. The obtained thermo-mechanical hatch-by-hatch, patch-by-patch or layer-by-layer (often with multiple layers combined) approaches offer a simplified thermal solution, which can also be used as input for a subsequent mechanical simulation. The price to pay is the loss in details of the thermal load. However, for the suggested thermo-mechanical layer-by-
layer approach, the energy is flashed in one or several layers, consistent with the power of the laser. The
time of energy release is estimated from the process conditions to ensure a reasonable peak temperature
in the layer, which resembles the peak temperature of the mesoscale simulation of the moving heat
source.

The delivered energy from the laser in one layer is estimated from the build time and the effective
power of the laser
\[ E = P \cdot \eta \cdot \frac{A}{h \cdot v} \quad \text{and} \quad t_{\text{flash}} = \frac{L_{\text{spot}}}{v} \]
where \( P \) is the power of the laser, \( \eta \) effective absorptivity of the laser, \( A \) the area of the layer, \( h \) the hatch
distance and \( v \) the laser velocity.

If the source term used in the thermal simulation would be based on the full time it takes to build a
layer, the energy density would be very small and the peak temperature in the layer would be too low.
It is therefore proposed to flash the total energy for one layer in the same time it takes the laser spot to
pass a generic material point. A similar suggestion is presented in [5].

Figure 3. (a) Illustration of a time line for the moving heat source and for the release of energy layer-
by-layer. (b) The time interval for releasing the energy is estimated from the spot size and the
velocity of the laser.

In this way it is possible to get a peak temperature in one layer which is similar to the peak temperature
in the moving heat source calculation on mesoscale. The main reason for using this approach is to ensure
thermal gradients between the layers, which are similar to the gradients in the mesoscale simulation.
This is of course important for the mechanical simulation where the thermal gradients govern the
mechanical response of the material. Nevertheless, when several layers are flashed at the same time it is
typically necessary to scale up the time to allow energy to conduct away and reduce the peak temperature
to a reasonable level.

4.1. Bridge example
The thermomechanical layer-by-layer method is applied on a bridge example to compare the residual
stress results to the measurements presented in a recent publication from [7]. A uniform mesh with
element size 0.225mm is used and each powder layer in the simulation is based on 10 physical powder
layers. The laser energy is flashed in 0.33ms followed by approximately 15s of cooling. The time
corresponds well to the process time for building and distributing powder for the 10 physical layers.

Figure 4. Dimensions of the bridge example [7].

The material is Ti-6Al-4V and temperature dependent properties were used for the simulations
similar to the data presented in the publication. Three simulations were performed, two identical thermal
layer-by-layer simulations with different integration of the thermal strain in the powder and one
simulation based on the inherent strain method using -2% for the inherent strain components. The
activation of elements in the mechanical macroscale model is different from the activation of elements in the mesoscale model. In the mesoscale model the elements become active in the mechanical simulation when the material switches from powder to solid. In the macroscale model the elements are activated in a layer-wise manner in both the thermal and the mechanical models. The immediate activation in the mechanical simulation leaves a choice of thermal strain integration in the powder during heating. In the first simulation thermal strain is integrated in the powder during heating, while in the second simulation it is assumed that the powder does not build up thermal strain as a solid and the integration of thermal strain is only performed during cooling. The measured residual normal stress components are presented in figure 5 together with the results from the 3 simulations.

Figure 5. (a) Measurements, [7], (b) and (c) thermomechanical simulation, without and with thermal strain in the powder while heating, respectively and (d) the inherent strain method.

Generally, the results from the three simulations are quite similar and overall the agreement to the measurements is also quite good. The compression zone in the z component matches quite well with the measurements and the outer tensile zones in all 3 directions are overall in good agreement in size and location. It is interesting to see that even the inherent strain method predicts similar stress levels as the layer-by-layer thermomechanical simulation and the measurements, even by assuming the simple uniform inherent strain components.

It is furthermore interesting to notice the similar results for the two layer-by-layer thermomechanical simulations, where the thermal strain in the powder is only integrated during heating in the first simulation. However, by having a closer look at the sequence of the added layers, it is seen that in the case where no thermal strain is integrated in the powder, the powder is stretched by the solid material below when it is heated. The stretching of the powder leads to accumulated plastic strain in the powder, which to a certain extent corresponds to the thermal expansion which is integrated in the powder in the first simulation. The plastic stretching of the powder in the second simulation leads to a quite different level of residual plastic strain in the two simulations. But having the different thermal strain level and the general strain decomposition in mind it is interesting to see how the stress levels nevertheless are quite similar.

\[
\varepsilon_{ij}^{\text{tot}} = \varepsilon_{ij}^{\text{el}} + \varepsilon_{ij}^{\text{pl}} + \delta_{ij} \varepsilon_{ij}^{\text{th}} \tag{10}
\]
5. Heat treatment

High thermal gradients during the building process often lead to high stress levels, which increase the risk of cracks and deformations during machining and service loading. Heat treatment is a useful way of relaxing the stress level in addition to optimize the mechanical properties. To analyze the effect of heat treatment it is possible to simulate the stress relief at elevated temperature. A unified creep model is applied during a 4 hours heat treatment process at 650 °C followed by an air cooling step.

![Figure 7. Stress relaxation in the bridge example during heat treatment.](image)

The stress level is relaxed from a peak level of approximately 800 MPa at the end of building to approx. 200 MPa at the elevated temperature level. After cooling to room temperature the stress level increases to a peak level of 300 MPa. With the implemented functionality it is possible to quantitatively see the effect of different heat treatment temperature and time levels.

6. Automotive structural part

3D printing of large structural parts is possible even though it is slow and expensive compared to conventional production. However, for prototyping and small series it is becoming interesting to evaluate the process on even large automotive parts. To show the current state in printing large structural aluminum parts an experimental shock tower from the research project CustoMat3D is shown below. The main focus of the project has been to develop new aluminum alloys for additive manufacturing, with high fatigue strength, which should be suitable for load carrying automotive components, like the topology optimized demonstrator part.

To challenge the implemented model the part is simulated. Similar to the production the part is split in two, see figure 8 below. The two simulation domains include the support structure highlighted in yellow and the base plate in dark grey. The mesh is uniform with 2mm side length. The support structure is included in the simulation. The material data corresponds to the AlSi10Mg alloy at room temperature, with uniform inherent strain components equal to -1.3%.

![Figure 8. Shock tower simulation domains.](image)

The presented results are based on the inherent strain method. The results are obtained in approximately 8 hours for the small part and 16 hours for the large part. Both simulations were...
performed on 32 cores. The approach makes it possible to check and make relative comparisons of different designs and support structures in a reasonable calculation time.

![Figure 8: Topology optimized shock tower; (a) real part, (b) build setup of part 1, (c) build setup of part 2 and (d) the simulation results of the two parts using the inherent strain method.](image)

7. Conclusions
Simulation of 3D metal printing and the post treatment steps has a growing interest in research and industry due to the wide application of the process. A general thermomechanical approach has been implemented to model the moving heat source on mesoscale and a layer-by-layer approach on macro scale. The inherent strain method has been implemented as well to test the possibility to obtain sufficiently accurate results for this simplified approach.

Results have been compared to measurements for different parts. For the considered examples it was possible to get good agreement for both the residual stresses before machining and deformations after machining. The integrated modeling of printing and heat treatment made it possible to predict and analyze the stress relaxation at elevated temperature.

Finally, it was possible to simulate the stress level in large structural automotive parts in reasonable simulation times to make it realistic to check different designs and process conditions.

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