A THERMOMECHANICAL FINITE ELEMENT FRAMEWORK FOR THE SIMULATION OF SELECTIVE LASER MELTING PROCESSES VIA PHASE TRANSFORMATION MODELS

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1. Introduction

Selective Laser Melting (SLM) is a technique belonging to additive manufacturing, a processing technique in contrast to the traditional material removal or casting technologies, which displays a great potential for industrial applications. Using the SLM process, a full dense metallic part with complex geometry can be produced directly and incrementally. The workpiece is manufactured using a high thermal energy source, e.g. a laser beam, to melt the metallic powder. Thus, the respective part undergoes a solid-liquid and subsequently a liquid-solid phase transformation which together result in high eigenstresses. To optimize the process parameters, the thermal, mechanical and metallurgical process has to be predicted. Thus, a finite element simulation using an appropriate model able to capture the constitutive material behaviour and the process itself is necessary. There are various models, as e.g. [6], which mostly focus on the temperature evolution, while using temperature-dependent material properties. In this contribution, the material modelling framework is adopted from solid-solid phase transformation simulation of shape memory alloys, cf. [1] and applied to the modelling of the different material states during the SLM process – powder, molten and re-solidified – as phase changes.

2. Thermomechanical framework

A fully coupled thermomechanical model is used to capture the temperature evolution and the process-induced eigenstresses. The linearised strain measure ε is applied, which is considered appropriate for the moderate strains occurring during SLM. The finite element simulation is based on the balance of linear momentum and the energy equation,

$$(1) \qquad \nabla \cdot \boldsymbol{\sigma} + \boldsymbol{b} = 0 \,,$$

$$(2) \qquad -\nabla \cdot \boldsymbol{q} + r + \mathcal{D}_{\mathrm{mech}} + \theta \, \partial_\theta [\, \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \mathcal{D}_{\mathrm{mech}} \,] - \widetilde{c} \, \dot{\theta} = 0 \,.$$

In these equations, $\boldsymbol{\sigma}$ describes the stress tensor, $\boldsymbol{b}$ is the body force, $\boldsymbol{q}$ represents the heat flux vector, r denotes the externally supplied heat, $\mathcal{D}_{\mathrm{mech}}$ symbolizes the mechanical dissipation, θ is the temperature and $\widetilde{c} := -\theta \, \partial_{\theta\theta}^2 \psi$ defines the effective specific heat capacity.

3. Constitutive framework

A mechanical material model based on fundamental constitutive models for each phase of the material, namely powder, molten and re-solidified, is used in this contribution. Adapting the framework provided in e.g. [1], the constitutive behaviour of each phase is modelled via phase energy densities ψ_i which consist of a mechanical and a caloric part. The constitutive model for the case of coexisting phases is obtained via a mixture rule

$$(3) \qquad \bar{\psi} = \sum_{i=1}^{n_{\mathrm{ph}}} \xi_i \, \psi_i(\boldsymbol{\varepsilon}_i) \,,$$

where ξ_i describes the volume fraction and $\boldsymbol{\varepsilon}_i$ the total strain of the respective phase i. The range of the volume fractions is restricted by $\sum_{i=1}^{n} \xi_i = 1$ and $0 \leq \xi_i \leq 1$. An additive decomposition of elastic and inelastic strains is applied, where the only inelastic contribution considered is thermal strains in the re-solidified phase. With

this at hand, the temperature-induced change of the material's composition is obtained via energy minimisation of (3) resulting in

$$(4) \qquad\qquad \psi^{\mathrm{rel}} = \min_{\varepsilon_i, \xi_i} \left\{ \bar{\psi} \right\}$$

subject to

$$(5) \qquad\qquad r_\varepsilon = \varepsilon - \sum_{i=1}^{n} \xi_i \, \varepsilon_i = 0 \ .$$

Thus, the relaxed energy density is obtained by the minimisation of the averaged energy density w.r.t. the total strains in each phase and the volume fractions. With this at hand, an explicit formulation for the optimal strains within the respective phase can be calculated. An additional constraint $\dot{\xi}_{\mathrm{pow}} \leq 0$ needs to be taken into account, as the rate of the powder fraction $\dot{\xi}_{\mathrm{pow}}$ can only decrease. The minimisation problem with the inequality constraints is treated via the Karush-Kuhn-Tucker approach to calculate the respective volume fractions. Accordingly, the thermal model has to be adapted. A standard linear heat expansion model is used w.r.t. the irreversible strains in the re-solidified phase, whereas a classic isotropic Fourier ansatz is made for the heat conduction model. Thus, an averaged heat conduction and the effective specific heat capacity is used. Altogether, this establishes a physically well-motivated material model, where the different states of the material, namely powder, molten, and re-solidified, are captured as single phases with respective volume fractions.

4. Implementation and numerical examples

The constitutive framework is implemented into the commercial finite element software Abaqus. Here, the fully coupled thermal-stress analysis is used which is based on the weak forms of (1) and (2). Then, the previously explained constitutive material model is defined as an user material in the subroutine *UMAT*. For the implementation further numerical reformulations are necessary. The Karush-Kuhn-Tucker constraints are rewritten by the Fischer-Burmeister nonlinear complementarity functions as established in [3], see also [1], [5]. Thus, the determination of the volume fractions of the respective phases is possible via standard Newton-type algorithms. In addition to the update of the volume fractions which are saved as internal state variables, the algorithmic tangent and the stress update have to be defined within the routine. Finally, a model of the SLM process itself has to be developed. Therefore, a layer is built up with the help of (de-)activated elements which Abaqus enables by the interaction *Model Change*. This method has been established in [4] and is also used by e.g. [6]. Furthermore, an additional subroutine is applied to model a moving volumetric heat source representing the laser beam. For further information on Abaqus the interested reader is referred to [2]. In a final step, the commercial simulation software is used to generate representative small-scale examples using the aforementioned constitutive framework and process model. This allows the generation of – at the present state of investigation – qualitatively accurate predictions of the evolution of the material states and temperature, as well as the simulation of process-induced eigenstresses and the workpiece's final geometry.

References

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