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Hashin–Shtrikman type mean field model for the two-scale simulation of the thermomechanical processing of steel

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Thermomechanical treatment of steel plays an important role in production, e.g., hot stamping. To capture the complex polymorphic material behavior of steel under thermal and mechanical loads, the usual approach in literature is to use a macroscopic phenomenological ansatz. In contrast, the aim of this work is to establish a more physically based two-scale model taking the material behavior of the different phases on the micro scale into account. The scale transition from macro scale to micro scale is performed by a nonlinear localization method of Hashin–Shtrikman type, which is based on a phase-wise constant stress polarization. The thermomechanical constitutive law is determined by both the phase transformation on micro scale and the temperature-dependent mechanical behavior of each phase. The mechanical behavior is based on a thermodynamical approach, i.e. introduction of a Helmholtz free energy for each phase and use of potential relations gained from the Clausius–Duhem (CD) inequality. The temperature-affected diffusionless evolution of the microstructure is modeled by both a Koistinen–Marburger (KM) consistent rate law and a suggested nonlinear extension of the KM model. The suggested transformation model leads to a better agreement with experimental results compared to the usually used approaches. The Johnson–Mehl–Avrami–Kolmogorov (JMAK) model is chosen to describe the diffusion driven phase transformation. After a parameter identification of the steel 42CrMo4 and a validation of the thermomechanical coupling, the influence of the latent heat, the transformation strain occurring during phase transformation, and the additional parameter arising in the homogenization scheme on the macroscopic behavior is investigated.

1. Introduction

Thermomechanical processes play an important role in the industrial manufacturing of steel components, e.g., forming of sheet metals. The polymorphic property of steel provides a huge amount of possibilities to influence the desired mechanical behavior of final parts. In this context, the process chain of hot stamping, well overviewed by Karbasian and Tekkaya (2010), delivers components with an optimized strength-weight ratio ensuring an enhanced occupant safety and fuel consumption of cars. The rise of this process procedure in the eighties and the gain of importance in automotive industries have led to a demand on constitutive models to be able to perform efficient and accurate simulations. In particular, for further use in, e.g.,

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crash simulations, the properties of the final parts have to be predicted precisely. The final properties of polymorphic steel components are determined by the microstructure, which is evolving during the thermomechanical process referred to as phase transformation. Regions of equal chemical composition and mechanical properties are referred to as phases. In this work and in the context of hot stamping, the phases austenite, ferrite, pearlite, bainite, and martensite are distinguished.

Due to the fact that this work is considered to be a preliminary-stage for the simulation of the hot stamping process, it competes with thermomechanical models which either have been applied or are applicable to simulate the hot stamping process. The works in the context of hot stamping (see, e.g., Ackerström et al., 2007; Bok et al., 2014; Durrenberger et al., 2009; Hochholdinger et al., 2011) use a phenomenological approach by modeling the yield stress with a semi-empirical as well as physically based ansatz for the strain rate and temperature dependent yield stress (see, e.g., Hoff, 1954; Johnson and Cook, 1983; Nemat-Nasser, 1999). The microstructure and the properties of the phases are taken into account by both the volume fraction and by the mixture rule applied on the yield surfaces of the different phases, respectively (see, e.g., Ackerström et al., 2007; Caseiro et al., 2011; Kim et al., 2005; Wolff et al., 2008). In the cited works, however, the thermoelastic properties of the bulk are assumed to be independent of the phases. Indeed, the experimental results for, e.g., the steel 42CrMo4, show a deviation of the Youngs's modulus of the ferritic phase from the austenitic phase of about 60% at a temperature of 1000 K, at which an austenitic-ferritic mixture can be present. For the same steel, the thermal expansion coefficient of austenite differs from the martensitic phase up to about 80% (Miokovic, 2005). To reduce such discrepancies, some authors (see, e.g., De Oliveira et al., 2010; Wolff et al., 2008) introduced, additionally, a mixture law for the thermoelastic behavior of the bulk. Thus, the thermoelastic properties of all phases in the microstructure are taken into account in a simple way. In contrast to the usual works concerning the hot stamping process, the latter cited authors set up a thermodynamic framework for the description of the constitutive behavior by introducing a Helmholtz free energy in a small deformation context. This procedure results in a thermodynamically consistent material model under suitable conditions. Noteworthy is the use of phenomenological approaches or of first-order bounds for the consideration of different phase behaviors in the cited works.

In hot stamping, the transformation induced plasticity effect, abbreviated by TRIP, plays an important role. The TRIP effect takes place in the case of a phase transformation under external load. There are two effects causing non classical plasticity: the Magee and the Greenwood–Johnson (GJ) mechanism. While the Magee mechanism represents an orientation effect of the grains on the microstructure, the GJ mechanism considers the micromechanical plastic strains arising in the parent phase. For a detailed discussion see, e.g., Papatriantafillou et al. (2006) or Taleb and Sidoroff (2003). In the works concerning hot stamping, apart from the mixture rule for the overall yield surface, the influence of the phase transformation on the stress development is taken into account just by the GJ mechanism. The Magee effect is usually neglected. The inverse relation, i.e. the stress dependence of the phase transformation as it is considered in the context of shape memory alloys (see, e.g., Wang et al., 2008; Yu et al., 2014), is neglected. In this work, neither of those effects, i.e. the influence of the stress on the phase transformation and TRIP effect, are taken into account. However, once the hot stamping is to be simulated, the considered model can be extended.

The phase transformation is subclassified into two effects: the diffusion driven and the diffusionless transformation. For modeling the diffusion driven microstructure evolution during thermomechanical processes, mainly two models are used: the Kirkaldy–Venugopalan (KV) (Ackerström et al., 2007; Bok et al., 2014; Lee and Lee, 2008) and the Johnson–Mehl–Avrami–Kolmogorov (JMAK) model (Caseiro et al., 2011; Lee et al., 2009; De Oliveira et al., 2010). While the KV model is based on fitting of empirical equations to published time-temperature-transformation (TTT) diagrams, the JMAK approach is derived by use of the extended volume approach. For the modeling of the diffusionless phase transformation, Koistinen and Marburger (1959) proposed an exponential model for the determination of the martensitic volume fraction depending on the undercooling below the martensite formation start temperature. The model is referred to as Koistinen–Marburger (KM) model. For further discussion see, e.g., Kirkaldy and Venugopalan (1983), Lee et al. (2010), Starink (2001), and Todinov (1998) with respect to diffusion driven transformation, and Koistinen and Marburger (1959) as well as Christian (2002) with respect to diffusionless transformation. Another approach to phase transformation based on energetic considerations, i.e. the derivation of expressions for driving forces and activation energies, has been proposed by, e.g., Kubler et al. (2011), Levitas (1998), and Mahnken et al. (2015). For further discussion please refer to these references.

In the context of a finite deformation formulation of the constitutive law, Hallberg et al. (2007) suggested a monolithic thermodynamically derived model taking the austenitic and the martensitic phase into account. Furthermore, Hallberg et al. (2007) assumed a phase independent elastic and plastic bulk behavior. Both Hallberg et al. (2010) and Mahnken et al. (2012) extended and modified this model. The latter authors suggested a multi-phase extension with a focus on the bainitic phase transformation.

In contrast to the models proposed so far in the context of hot stamping or modeling of thermomechanical processes, the model suggested in this work is based on the following approaches:

- For each phase, a Helmholtz free energy is introduced separately with its own thermo-elasto-plastic parameter set. With the Clausius–Duhem inequality and the principle of maximum dissipation of plasticity, thermodynamically consistent thermomechanical constitutive equations for each phase are formulated.
- The nonlinear isotropic hardening of each phase is modeled by a temperature dependent Voce type law.