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A multi-phase model for transformation plasticity using thermodynamics-based metallurgical algorithm

Junyan Ni[a], Xiaowei Wang[b,c,*], Jianming Gong[b,c], Magd Abdel Wahab[d,e,*]

[a] Department of Electrical energy, metals, mechanical constructions and systems, Faculty of Engineering and Architecture, Ghent University, Belgium
[b] School of Mechanical and Power Engineering, Nanjing Tech University, Nanjing 210000, China
[c] Jiangsu Key Lab of Design and Manufacture of Extreme Pressure Equipment, Nanjing 210000, China
[d] Institute of Research and Development, Duy Tan University, 03 Quang Trung, Da Nang, Viet Nam
[e] Soete Laboratory, Faculty of Engineering and Architecture, Ghent University, Ghent 9000, Belgium

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ABSTRACT

The current work is aimed at establishing a flexible thermo-metallo-mechanical finite element (FE) model for steels. The flexibility is improved in the metallurgical analysis by adopting a thermodynamics-based algorithm, in which only the chemical composition and the thermal history are needed. On the other hand, the transformation plastic constitutive equations are extended for consideration of multi-phase transformation. An explicit consistent tangent modulus is derived for model implementation. The microstructural results are coupled with the constitutive equations using utility and user subroutines in the FE commercial software ABAQUS to create the complete model. The transformation kinematic and strain evolution equations are first validated using experimental data from the literature. The effect of the cut-off function on the transformation plasticity model is discussed. The discrepancy found at the initial stage of strain evolution is explained from a metallurgical point of view. The proposed model is further applied to a multi-pass welding process of more than twenty thermal cycles. A good agreement is observed in comparison between the metallurgical graphs and the predicted microstructural distribution. The result of stress distribution is improved by including the transformation plasticity in simulation. The influence of the cut-off function is analyzed again by comparing the X-ray measurements of stresses at external surface with the predicted ones.

1. Introduction

The evaluation of residual stresses resulted from thermal processes, such as welding, high temperature forming and quenching, is crucial to the subsequent application of the components and the structures [1–3]. During those processes, the microstructure is unavoidably modified, leading to plastic deformation even as the load is much smaller than the yield stress. This phenomenon is known as transformation plasticity, which has been already formulated in a system of constitutive equations [4,5]. The significant effect of the microstructural evolution on the final dimension and geometry of mechanical parts was investigated in a FE simulation of quenching process [1]. Similarly, Lee et al. [2] performed a FE analysis to show the important role of phase transformation in improving mechanical properties and moderating dimensional change of hot press formed metal sheet. Hamelin et al. [6] investigated the effect of heat input on residual stress distributions in a single pass welding process by considering phase transformation. A priori term, instead of the one derived from the micromechanical analysis [5], was adopted in their thermo-elasto-plastic FE model [6]. Jiang et al. [7] followed a similar approach to analyse the material behaviour during phase transformation, in which the prediction was compared to the neutron diffraction measurement.

In this sense, the metallurgical analysis, which tracks the phase development in a specific process, is of particular importance to the complete simulation model. Among various algorithms, the Johnson-Mehl-Avrami-Kolmogorov (JMAK) equation is the most frequently used one. Kang and Im [1] used the JMAK equation to simulate the diffusional transformation. The same equation was used in modelling of hot press forming process and steel heat treatment [2,8]. The JMAK equation was originally developed for isothermal transformation. For non-isothermal condition, the continuous cooling curve is discretised as small isothermal time steps, and the law of additivity was adopted to determine the transformation start point [6]. The martensitic transformation was often calculated by the Koistinen-Marburger (KM) relationship [9]. Alternatively, the Olson-Cohen (OC) relationship was adopted by Sierra and Nemes [10] to investigate the effects of martensitic

* Corresponding author at: School of Mechanical and Power Engineering, Nanjing Tech University, Nanjing 210000, China.
E-mail addresses: xwwang@njtech.edu.cn (X. Wang), magd.abdelwahab@ugent.be (M.A. Wahab).

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Nomenclature

Transformation kinetics

$\overline{D}$	Prior austenite grain size
$\overline{L}$	Mean linear intercept for an equiaxed grain structure
M_o^*	The mobility of the grain boundary
Q_{app}	Apparent energy required for grain growth
n_r	Magnitude of the resistance due to the precipitate
τ_i	Incubation time
τ_f	Transformation finish time
n_p	Number of the phases
V	Representative volume
V_i^{e}	Extended volume of ith phase
V_i	Real volume of ith phase
z_i	Volume fraction of ith phase
I_i	Nucleation rate per unit area of ith phase
$A_{j,k,\,y}$	Changing rate of area intersected with the plane at y in jth phase, which nucleates at time $t=k\mathrm{d}\tau$
O_{B}	Area of the grain boundary
$O_{j,y}^{\text{e}}$	Extended area of jth phase intersected at y
$O_{j,y}$	Area of jth phase intersected at y
η_j	Ratio of growth rate between the parallel and the normal directions in jth phase
ζ_j	Thickening rate of jth phase
$\Delta F_{\max}$	Maximum molar free energy change required for nucleation
u	Volume of bainitic platelet
ΔF_N	Experimentally fitted energy for nucleation
μ_X^j	Molar free energy of X in jth phase
a_X^j	Activity of X in jth phase
$\Delta F^{\gamma\to\alpha'}$	Difference of molar free energy when nucleus of product phase inherits the same carbon concentration of parent phase

Constitutive formulation

α_i	Expansion coefficient of ith phase
$\boldsymbol{\varepsilon}$	Macroscopic strain tensor
$\boldsymbol{\varepsilon}^e$	Elastic strain tensor
$\boldsymbol{\varepsilon}^{thm}$	Thermo-metallurgical strain tensor
$\boldsymbol{\varepsilon}^p$	Plastic strain tensor
$\boldsymbol{\varepsilon}^{tp}$	Transformation plastic strain tensor
$\boldsymbol{\varepsilon}_{\Sigma}^{cp}$	Classical plastic strain due to the stress variation
$\boldsymbol{\varepsilon}_{T}^{cp}$	Classical plastic strain due to the temperature variation
$\boldsymbol{\varepsilon}_{m+1}^{e\ \text{trial}}$	Elastic trial strain tensor at time $t=t_{m+1}$
$\Delta\boldsymbol{\varepsilon}$	Strain increment between t_m and t_{m+1}
$\boldsymbol{\varepsilon}_m^e$	Elastic strain tensor solved at time $t=t_m$
$\boldsymbol{\Sigma}$	Macroscopic stress tensor
$\boldsymbol{\Sigma}_{m+1}^{\text{trial}}$	Macroscopic trial stress tensor at time $t=t_{m+1}$
$\boldsymbol{\Sigma}_{m+1}$	Macroscopic stress tensor at time $t=t_{m+1}$
$\mathbf{S}$	Macroscopic stress deviator
$\mathbf{S}_{m+1}$	Macroscopic stress deviator at time $t=t_{m+1}$
Σ^{eq}	Macroscopic equivalent stress
Σ^y	Macroscopic yield stress
D^e	Elasticity tensor
D_{m+1}^e	Elasticity tensor at time $t=t_{m+1}$
σ_i^y	Yield stress of ith phase
ε_i^{eq}	Equivalent strain of ith phase
$\boldsymbol{\varepsilon}_i^{th}$	Thermal strain of ith phase
ε_i^{eff}	Parameter for effect of strain hardening in ith phase
θ_i	Memory coefficient of ith phase
ε^{pt}	Axial strain component
γ^{pt}	Shear strain component

transformation rate and stress state on the material behaviour. Leblond and Devaux [11] expressed a generalized function in terms of the equilibrium volume fraction and the characteristic time, which was able to predict all product phases and has been already integrated in the commercial software SYSWELD. However, all the mentioned metallurgical models need to be calibrated before implementation. The transformation coefficients in JMAK equation should be adjusted according to the time-temperature-transformation (TTT) diagram for specific steel. Similarly, the continuous cooling transformation (CCT) is required to determine the temperature-dependent parameters in Leblond's transformation model [11]. As a result, none of the models is able to work independently of metallurgical diagrams. Comparably, a series of incremental functions that treat the transformation parameters empirically [12] were implemented to simulate the microstructural evolution during welding [13], but some discrepancies were found in prediction of CCT diagram and transformation kinetics [14]. Similar empirical treatment was also found in the calculation of transformation start temperatures [2]. Instead, a thermodynamics-based algorithm, in which the transformation start temperatures were determined by equilibrating chemical potentials, was proposed by Bhadeshia et al. [15–18]. The growth of phases in the reconstructive transformation was modelled as pile-up of material layers controlled by carbon diffusion function, resembling the real growth mechanism [18]. However, due to its complexity, this model has not been implemented for calculation of transformation plasticity yet.

With respect to the mechanical analysis, several efforts have been devoted to improve or to simplify the model and its implementation. A numerical homogenization based on a unit cell of 10^3 elements was proposed to obtain the dependence of the hardening modulus on the volume fraction of the product phase, where the elements belonging to the product phase were stochastically distributed [19]. The global yield condition was always satisfied during phase transformation, which was different from the two-fold framework proposed by Lelond [5]. Later, Mahnken et al. [20] developed a macroscopic model for multi-phase transformation. The constitutive equations were implemented by multiplicative decomposition of the deformation gradient. Lee et al. [21] proposed another model for multi-phase transformation based on the constitutive functions of the single phase transformation plasticity [5], in which all the product phases were equilibrated as a volume of hard phase. The implicit procedure was implemented through an approximate numerically determined consistent tangent modulus [21]. Bok et al. [22] adopted a combined implicit-explicit simulation for hot forming process, in which a modified Johnson-Cook law was used to calculate the yield stress of each individual phase. Similarly, a meso-model in which each phase followed its own constitutive law was proposed to allow any type of non-linearly mixed material behavior [23]. Taleb and Sidoroff [24] noticed that a singularity in the description of transformation plasticity occurs when the volume fractions of transformation products tend to be zero. Originally, a cut-off value was used to avoid this problem [4]. An in-depth analysis was employed by considering elasticity in both product and parent phases rather than neglecting elasticity in parent phase [24]. As a result, a cut-off function that depends on both single phase and overall material properties arose naturally from the derivation. The effect of this function was discussed in cases of uniaxial and multi-axial loading tests, but its influence on a specific manufacturing process has not been presented. Recently, an improved microscopic model was developed by separately calculating the deviatoric and volumetric parts of strain increment due to phase transformation [25]. Unlike the treatment of product phases as an equivalent hard phase, the transformation-related strain increments were analysed individually. The singularity was overcome by allowing a minimal volume of product phase as it nucleated, but the determination of this minimal value was not described.

Combining the two aspects discussed above, an attempt is made in the present paper to establish a more flexible thermo-metallo-mechanical model based on the mentioned metallurgical algorithm