Constitutive modeling of metastable austenitic stainless steel

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ABSTRACT: A stress-update algorithm is developed for austenitic metastable steels which undergo phase evolution during deformation. The material initially comprises only the soft and ductile austenite phase which due to the phenomenon of mechanically induced martensitic transformation, transforms completely to the hard and brittle martensite. A mean-field homogenization algorithm is developed that can predict the mechanical response of the composite material during transformation. Furthermore, a physically based transformation model is developed that predicts the amount of transformation during deformation.

KEYWORDS: TRIP, martensitic transformation

1 INTRODUCTION

Metastable steels combine exceptional mechanical properties such as high strength and high formability, thanks to the deformation induced martensitic transformation phenomenon. This behavior has been first reported by Angel [1] and after that many studies have focused determining the underlying physics as well as simulating the complex mechanical behavior. The complexity of the mechanical behavior arises on one hand due to the contrast of the mechanical properties of the constituent phases and on the other due to the interaction between mechanical response and the phase transformation mechanism.

The material initially is completely of the austenite phase which is metastable at room temperature meaning that it doesn't have enough natural driving force to transform to a stable phase. With the help of externally applied mechanical energy however, the material gains enough driving force to overcome the energy barrier and transforms into the stable martensite phase. Austenite is a soft and ductile phase whereas martensite is hard and brittle. During the transformation therefore, the material is a metal-matrix composite with a soft matrix and hard inclusions. Therefore, to predict the mechanical response a homogenization algorithm is necessary.

In this study a stress-driven transformation model is built that predicts the transformation as function of the stress that is resolved in the material. There are many models in literature that are based on the theory of strain-induced transformation which was proposed and formulated by Olson and Cohen [5]. However, in this material the effect of strain seems to be overtaken by the effect of stress [6].

A mean-field homogenization model is built that uses an incremental formulation to predict the average stress and strain fields of the matrix and the inclusion during deformation. Similar procedures that are used by Doghri [2] are utilized with a large deformation theory.

2 TRANSFORMATION

The transformation model is based on Magee's theory of martensitic transformation under stress [4]. The mechanical driving force supplied to the material is calculated as a distribution due to the random orientation of individual grains and therefore crystallographic systems on which martensite can transform, i.e. martensitic variants. In an fcc to bcc transformation Wechsler et.al. [8] calculated 24 different martensitic variants in a single grain. Under stress due to the deformation associated with the transformation each variant results in a different mechanical work. Naturally, there will be a selection of the favored variants during transformation, which will yield a net strain throughout the material in macroscale. This net strain is the so-called TRIP strain.

For the material under consideration, the habit planes and the shear directions of the transformation are calculated as $\mathbf{n}=\{0.178\ 0.608\ 0.774\}$ and $\mathbf{s}=<-0.046\ -0.156\ 0.159>$. The associated deformation gradient with each variant is given as

$\mathbf{F}_i^{tr} = \mathbf{I} + \mathbf{s}_i \otimes \mathbf{n}_i$. The work per unit volume calculated by the large deformation theory is given as $U_i = \boldsymbol{\sigma} \cdot \mathbf{n}_i \cdot \mathbf{s}_i$. Furthermore, it is possible to calculate the theoretical maximum driving force that can be attained under a certain stress state as $U^{max} = \text{eig}(\boldsymbol{\sigma}) \cdot \text{eig}\big(\frac{1}{2}(\mathbf{s} \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{s})\big)$.

The base variants can be rotated a number of times randomly to simulate a polycrystal material with no texture. This results in a distribution of the driving force in the material rather than a single value. It is assumed that the energy barrier that the material has to overcome to transform is constant. This barrier physically represents the resistance of the matrix to elastic deformation and the surface energy required to create an interface.

During proportional loading therefore, with increasing stress the number of grains that have enough driving force to transform will increase and this will cause the material to gradually transform into martensite. The results of this simulation is given in figure 1 [6].

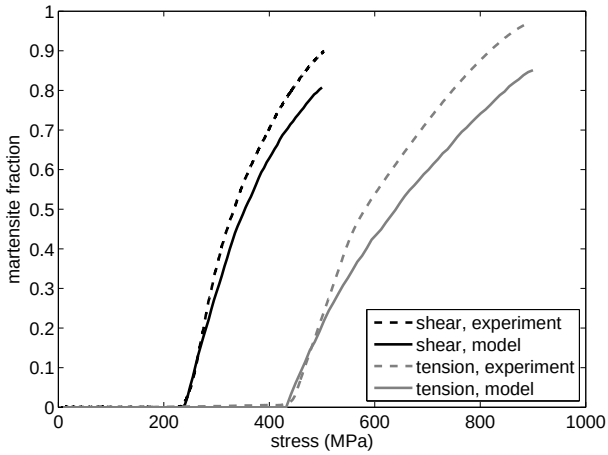

Figure 1: Comparison of the Magee theory results with experimental results for the shear and tension tests.

On figure 1 it is clear that this model can capture the basic mechanisms of transformation. However, to utilize in the constitutive model, a smooth function is desirable. Therefore, the following function is introduced to approximate the Magee model. The function gets the stress tensor as input and returns the amount of martensite that would form.

$$f = 1 - \left[1 + (r-1)\left(\frac{U^{max}}{\Delta G_{cr} + C}\right)^m\right]^{\frac{1}{1-r}} \qquad (1)$$

where, f is the volume fraction of martensite, ΔG_{cr} is the critical energy barrier, C, m and r are constant that determine the shape of the curve.

3 HOMOGENIZATION

The homogenization models discussed further on are based on Eshelby's solution of the inclusion problem [3]. In this solutionm, the strain concentration due to a single inhomogeneity in an infinitely long matrix is determined exactly.

$$\boldsymbol{\epsilon}_1 = \mathcal{H} : \boldsymbol{\epsilon}_0, \quad \mathcal{H} = \left[\mathcal{S} : (\mathcal{C}_0^{-1} : \mathcal{C}_1 - \mathcal{I}) + \mathcal{I}\right]^{-1} \qquad (2)$$

where, ϵ_1 and ϵ_0 are the strain in the inhomogeneity and the matrix, $\mathcal{C}_1$ and $\mathcal{C}_0$ are the elasticity tensors of the inhomogeneity and the matrix, $\mathcal{S}$ is the Eshelby tensor and $\mathcal{H}$ is Eshelby's strain concentration tensor.

In the composite material however, the exact solution is not applicable since the matrix and the inhomogeneity have finite volumes. Therefore, the fields in the phases are represented by the averaged quantities and the mixture rule holds.

$$\begin{aligned} \langle \mathbf{D} \rangle &= f\langle \mathbf{D}_1 \rangle + (1-f)\langle \mathbf{D}_0 \rangle \\ \langle \overset{\triangledown}{\boldsymbol{\sigma}} \rangle &= f\langle \overset{\triangledown}{\boldsymbol{\sigma}}_1 \rangle + (1-f)\langle \overset{\triangledown}{\boldsymbol{\sigma}}_0 \rangle \end{aligned} \qquad (3)$$

Additionally, the elastic theory is generalized to elasto-plastic cases by replacing the elastic moduli with elasto-plastic moduli of the phases and the individual phases are assumed to behave with their own respective constitutive behavior.

$$\langle \overset{\triangledown}{\boldsymbol{\sigma}}_1 \rangle = \mathcal{C}_1^t : \langle \mathbf{D}_1 \rangle, \quad \langle \overset{\triangledown}{\boldsymbol{\sigma}}_0 \rangle = \mathcal{C}_0^t : \langle \mathbf{D}_0 \rangle \qquad (4)$$

Working with the averages, Eshelby's strain concentration tensor needs to be replaced with a tensor that relates the average fields to each other.

$$\langle \mathbf{D}_1 \rangle = \mathcal{A} : \langle \mathbf{D}_0 \rangle \qquad (5)$$

However, it is clear that some assumptions have to be made to achieve this. There are different algorithms which differ with this choice of assumptions.

3.1 Mori-Tanaka

In the Mori-Tanaka algorithm, the strain concentration tensor is assumed to be equal to that of Eshelby's. This assumption reduces to that of low volume fraction of inclusions since the far field strain in Eshelby theory is now replaced with the matrix strain.

3.2 Self Consistent

In the self-consistent algorithm both phases are treated as inclusions in the composite material, in other words the far field strain is replaced with the strain of the composite.

$$\mathcal{A} = (1-f)(\mathcal{I} - f\mathcal{H}_1)^{-1} : \mathcal{H}_1 \tag{6}$$

where, $\mathcal{H}_1 = \left[\mathcal{S} : (\mathcal{C}^{t^{-1}} : \mathcal{C}_1^t - \mathcal{I}) + \mathcal{I}\right]^{-1}$. This algorithm is theoretically more accurate than the Mori-Tanaka algorithm however it is intrinsically non-linear and hence expensive.

3.3 Double-Inclusion

In the double-inclusion model [2] the Mori-Tanaka algorithm is applied twice in opposite directions and the resulting strain concentration tensors are interpolated with respect to the volume fraction of the inclusions. This way the efficiency of the MT method is taken towards higher volume fractions. The resulting strain concentration tensor is:

$$\mathcal{A} = \left[(1-\phi)\mathcal{H}_0^{-1} + \phi\mathcal{H}_1^{-1}\right]^{-1} \tag{7}$$

where, $\mathcal{H}_i = \left[\mathcal{S} : (\mathcal{C}_j^{t^{-1}} : \mathcal{C}_i^t - \mathcal{I}) + \mathcal{I}\right]^{-1}$ and ϕ is the interpolation function.

The accuracy of the double-inclusion algorithm is found to be very sensitive to the interpolation function used. Two different functions have been tested, the one originally suggested by Lielens [2], $\phi_1 = f(1+f)/2$ and a new one created phenomenologically, $\phi_2 = d_1/(1+e^{-(f-c_1)c_2}) - d_2$.

3.4 Comparison of algorithms

The above algorithms are tested on an elastic material with an inhomogeneity inside. The inhomogeneity is chosen to be spherical in shape to result in an isotropic Eshelby tensor and the elastic moduli of the phases are chosen to have a large contrast. This simulates the case when the soft phase is plastically flowing while the hard inclusion is still elastic. The results are shown on figure 2.

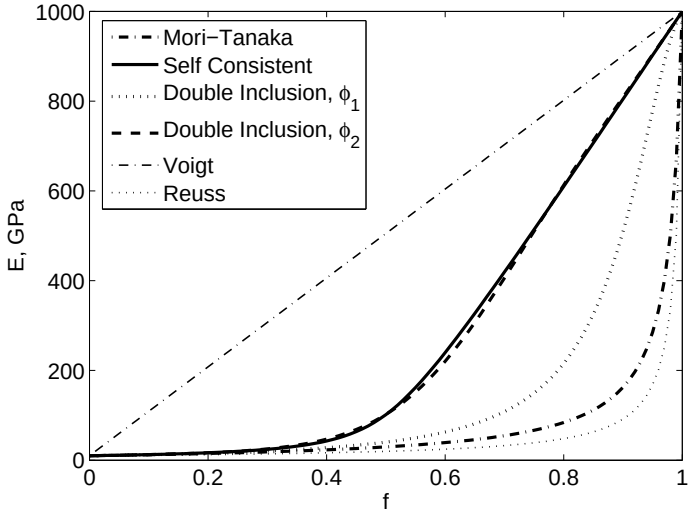

Figure 2: Comparison of the homogenization algorithms during the elastic deformation of a composite material.

4 MODEL

The homogenization model is extended for computing evolving volume fraction of inclusions since there are other aspects associated with transformation such as transformation strain and dilution.

During transformation because of the preferred selection of the martensitic variants there is a net strain in the direction of the deviatoric part of the stress. Additionally, because of the difference in densities of the phases a volumetric expansion accompanies the transformation. Therefore, the resulting TRIP strain can be formulated as:

$$\mathbf{D}^{tr} = \dot{f}(T\mathbf{n} + \frac{\delta v}{3}\mathbf{I}) \tag{8}$$

where, T is the magnitude of the transformation strain and δv is the volume change. T and δv are natural outputs of the transformation model. T is approximated with a linear function, $T = 0.15 - 0.1f$ and δv is found to be 0.02.

When new martensite plates form in virgin austenite, to conserve local equilibrium, they must be at the stress that is equal to average stress in austenite. This assumption results in the following equation:

$$\langle\dot{\boldsymbol{\sigma}}_1\rangle = \langle\dot{\boldsymbol{\sigma}}_1\rangle + \dot{f}\big(\langle\boldsymbol{\sigma}_0\rangle - \langle\boldsymbol{\sigma}_1\rangle\big) \tag{9}$$

As a results of this equation, during transformation because of the occurrence of new plates in the microstructure the average stress in the martensite is diluted.

When all the above is implemented in a stress-update algorithm in which a deformation path is given

as input it is possible to calculate the amount of induced transformation as well as the stress that builds up in the material. Results of the model are compared to mechanical tests in figure 3. The experiment was conducted using a biaxial tester under simple shear deformation and the shear stress and martensite amount was measured [7].

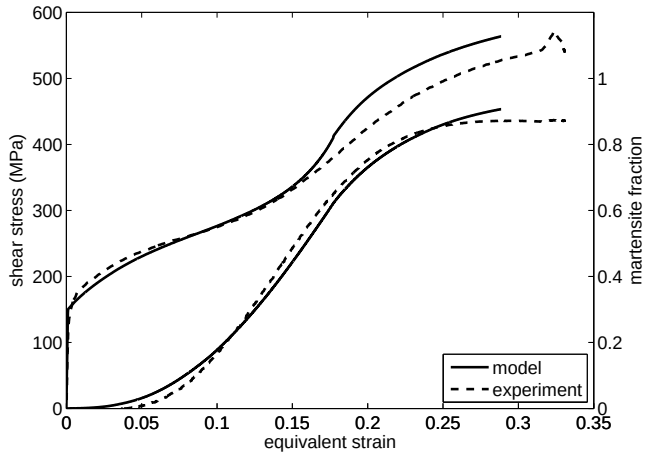

Figure 3: Stress-strain and martensite fraction results of the model compared to simple shear experiment.

5 CONCLUSION

An algorithm has been developed that predicts the amount of deformation induced martensitic transformation and homogenizes the two-phase microstructure to calculate the response of the overall material. The transformation model is stress-driven and is based on the Magee theory. The discrete meso-scale calculations for transformation are taken to the macro-scale using an analytical function derived using the maximum mechanical driving force resolved as independent variable. This function is based on physical parameters such as the critical energy barrier for transformation which is determined using mechanical tests. The resulting two-phase microstructure is then homogenized using the double-inclusion algorithm. The Mori-Tanaka algorithm is found to lack accuracy at high volume fraction of inhomogeneities while the self-consistent algorithm is found to be accurate but computationally inefficient. The double-inclusion algorithm is based on a phenomenological interpolation function but the parameters need to be tuned only once to make the results match the self-consistent results. The transformation is incorporated in the homogenization model by introduction of the transformation strain and dilution concepts. The transformation strain causes the material to soften during the deformation. The results are compared to mechanical test results and a very good correspondence is observed.

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