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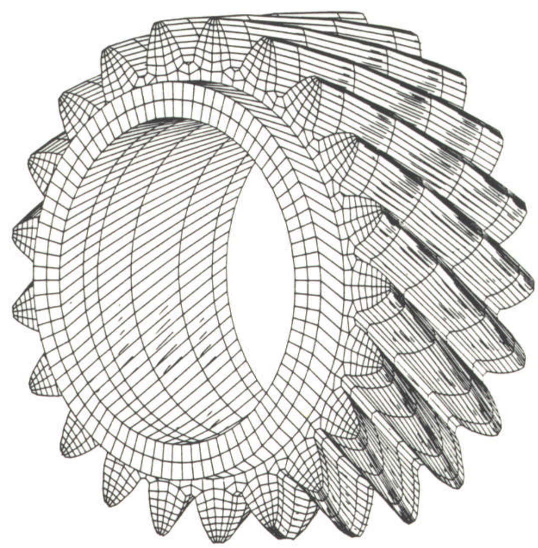

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Development of a Carburizing and Quenching Simulation Tool: Program Overview 349

W. Dowling, Jr., Ford Motor Co., Dearborn, Michigan
T. Pattok, National Center for Manufacturing Sciences, Ann Arbor, Michigan
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Development of a Carburizing and Quenching Simulation Tool: Determination of Heat Transfer Boundary Conditions in Salt 357

D. Shick, The Torrington Co., Torrington, Connecticut
D. Chenoweth, Sandia National Laboratory, Livermore, California
N. Palle, C. Mack, W. Copple, Ford Motor Co., Dearborn, Michigan
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H. Walton, The Torrington Company, Rutherfordton, North Carolina
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Development of a Carburizing and Quenching Simulation Tool: A Material Model for Carburizing Steels Undergoing Phase Transformations 367

D. Bammann, V. Prantil, A. Kumar, J. Lathrop, D. Mosher, M. Callabresi, Sandia National Laboratory, Livermore, California
H.-J. Jou, M. Lusk, G. Krauss, Colorado School of Mines, Golden, Colorado
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B. Dowling, Ford Motor Co., Dearborn, Michigan
D. Shick, The Torrington Company, Torrington, Connecticut
D. Nikkel, Lawrence Livrmore National Laboratory, Livermore, California

Development of a Carburizing and Quenching Simulation Tool: Numerical Simulations of the Rings and Gears 377

C. Anderson, P. Goldman, P. Rangaswamy, Los Alamos National Laboratory, Los Alamos, New Mexico
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Development of a Carburizing and Quenching Simulation Tool: A Material Model for Carburizing Steels Undergoing Phase Transformations

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Abstract

Properly accounting for the coupling between the thermal, mechanical, and microstructural aspects of the heat treatment and quenching of metal alloys is crucial in developing an accurate material characterization. In the austenitic, low carbon steels of interest in this work, the phase transformations often induce additional macroscopic plasticity which can have substantial effects on both residual stresses and distortions.

The modeling strategy adopted here couples differential equations for phase evolution with a multiphase macroscopic state variable material model. The kinetic rate equations for each product phase are derived using a thermodynamic formulation and fit to experimental data. Contrary to classical modeling of transformation plasticity, the material model used is based on mixture theory wherein we track the behavior of individual phases. Phase interactions are accounted for by introducing an internal stress that models both the macroscopic multiphase behavior and effects driven by the transformation. The form of the internal stress is based on discrete, micromechanical simulations of the response of a transforming representative volume.

The kinetics model is fit and tested using time temperature transformation (TTT) and continuous cooling transformation (CCT) data, and by studying the influence of stress on the kinetics through compression and tension experiments. The transformation plasticity and multiphase composite behavior predicted by the material model is validated by dilatometry and fixed volume fraction mechanical tests performed on a representative low carbon steel alloy. Finally, the model is exercised in large scale finite element simulations to capture the stress response and predict distortions during quenching of disks and long, annular cylinders.

FOR MANY APPLICATIONS IN MATERIALS PROCESSING, the thermal and mechanical response are coupled with evolution of the underlying material microstructure. This coupling is evident in heat treatment, quenching and welding of a large class of metal alloys which undergo phase transformations that alter the constitutive response of the material. When modeling this coupled material response, calculation of the residual stresses and subsequent distortion are often of primary importance. Microstructural phase transformations often have substantial effects on these global facets of the material behavior. In particular, two features at the microscopic level have direct effects on the macroscopic response. The volume difference associated with the phase change imparts a purely dilatational deformation. In addition, deviatoric straining will accompany the phase change in the presence of any macroscopic deviatoric stress field. This additional strain can have substantial effects on residual stresses and distortions.

Previous attempts to model the effects of phase transformations have met with mixed success. Empirical methods of incorporating a temperature dependent yield strength to simulate a phase change does not account for the volume change or any additional plasticity [1,2]. Mimicking the phase change with large changes in the thermal expansion coefficient can capture the effects of the spherical volume change, but not the microplasticity that accompanies them [1,3,4]. Calculations which account for the dilatational volume change explicitly, but not the microscopic deviatoric strains exhibit discrepancies with measured residual stresses [5,6]. For problems that are predominantly deformation driven or exhibit large kinematic constraints, the predicted stresses can be substantially in error. Simulations both with and without account for this augmented plasticity indicate that neglecting this effect can result in residual stresses that are incorrect in sign and magnitude [1,7,8]. Because transformation strains are accounted for locally, their effect on modeling global distortions and residual stresses will, in general, be problem dependent [3,7]. The severity of constraints on the global level or inhomogeneity of the transformation locally may determine, in part, the effect of the transformation phenomenon in any particular application. The thermal and mechanical boundary conditions can, therefore, play a significant role in determining the relative importance of incorporating transformation plasticity in the analysis of a global boundary value problem.

We begin with a brief description of phase transformation plasticity and the phenomenology of its dependence on stress and transformation kinetics. Based on the form of these previous descriptions, we motivate a formalism for incorporating these effects by explicitly defining the microscopic stress field that drives this additional plastic straining. To illustrate this approach, we extend a previously developed two-phase system [9] to account for five phases. We review how this multiphase state variable constitutive formulation naturally accounts for the stress dependent microstraining by considering discrete micromechanical simulations of the phase transformation by Saeedvafa and Asaro [10]. Comparisons with the discrete model indicate that the volume fraction dependence can be captured well by the multiphase state variable framework. We then address the details of extending this model to account for more than two phases.

The state variable model is joined with a new approach to simulating phase transformation kinetics recently proposed by Lusk, Krauss and Jou [11]. Here an earlier version of the model is extended to track multiple phases. Finally, we use this model to analyze the stress response during quenching of an idealized, long annular cylinder and a hollow dilatometer specimen, commenting on the effects of incorporating the phase transformation phenomenon for global boundary value problems.

Transformation Plasticity

When alloys undergo a solid state phase change, the volume difference between the crystal structures causes microscopic plastic flow as the transformation proceeds. In the absence of a far field stress, this strain field has no deviatoric part on average. There is, thus, no net contribution to the macroscopic plastic flow. In the presence of a deviatoric stress field, however, the straining from the volume misfit exhibits a deviatoric part proportional to the surrounding stress. This effect was described by Greenwood and Johnson [12] for applied stresses well below the yield strength of the weaker phase. There is evidence to indicate that under extreme cooling rates where a purely martensitic structure forms, the resulting platelet microstructure induces an additional shear deformation in the presence of an applied stress [13]. This imparts an inherent directionality to the response. For simplicity, we consider only the Greenwood-Johnson mechanism here. An extensive theoretical treatment of transformation plasticity has been described by Leblond, Mottet and Devaux [14,15]. Leblond, Devaux and Devaux [16,17] provide a mathematical overview wherein the transformation plastic strain rate is given by

$$\dot{\boldsymbol{\varepsilon}}^{TR} = \frac{K}{\Sigma_y}\left(\frac{\Delta V}{\mathrm{V}}\right)\Psi(\Phi)\,\dot{\Phi}\boldsymbol{\sigma}' \qquad (1)$$

The transformation plastic strain rate is proportional to the applied stress deviator, $\boldsymbol{\sigma}'$, the rate of change of volume fraction, $\dot{\Phi}$, the volume misfit, $\Delta V/V$, and is inversely proportional to the yield strength of the weaker phase, Σ_y. While variations on equation (1) have met with some success, recent discrete micromechanical simulations of the transformation under applied stress indicate that the proportionality of this strain rate on stress is not strictly linear over a broad range of stresses [10]. In addition, the dependence on volume fraction reported by Saeedvafa and Asaro [10] has shed light on the particular form of the function $\Psi(\Phi)$.

As described by Leblond, Mottet, Devaux and Devaux [18], the additional macroscopic straining might not seem to be of the same nature as ordinary plasticity owing to its dependence on the transformation rate. However, assuming ordinary plasticity operates on the microscopic level of individual phases and consistently averaging to the macrolevel, the continuum behavior exhibits an additional plastic straining whose rate is proportional to the rate of evolution of the product phase. Therefore, macroscopic transformation plasticity is a manifestation of microscopic ordinary plasticity [18]. What is interesting is that the transformation plastic strain rate is proportional to the deviatoric stress, not the deviatoric stress rate [1]. As such, it closely resembles the phenomenological form of flow laws for state variable descriptions of viscoplasticity. This dependence has interesting implications because it indicates that the additional plasticity can be modeled by a state variable formulation. We do this by defining a macroscopic stress which is a local average of the microscopic stress field acting between particles of different phases. To motivate this interaction stress, we appeal to the notion of an internal stress as a measure of material structure.

An Internal State Variable Model. Internal state variable models have been utilized previously to describe the response of single phase metals over large temperature and strain rate ranges and have been formulated in a manner consistent with the kinematics of large deformation elastic-plastic response [19]. In these types of models the free energy and the stress are assumed to depend on the elastic strain, the temperature, the strain rate, and the current values of internal variables that are introduced to describe the state of the material. Generally, the state variables are associated with underlying micro-mechanisms that are assumed to dominate the macroscopic response for a range of temperatures and strain rates. Isotropic mechanisms are characterized by scalar variables while directional effects are modeled with tensorial variables. For example, scalar variables could be introduced to represent dislocation substructures such as subgrain diameter, dislocation density for high temperature creep, or porosity for plastic deformation controlled growth of voids. Tensor variables could be identified with texture or grain orientation for problems involving large strain and moderate temperature, or may be required to adequately describe the high temperature response of a material in which diffusional controlled growth of voids along grain boundaries is the dominant mechanism. At the macroscopic level, the introduction of these variables results in the prediction of strain rate history and temperature history dependent material response. This type of response cannot be predicted with classic equation of state type models in which the stress is assumed to be a unique function of the plastic strain, the temperature and the strain rate independent of the history of loading.

An example of this type of model has been proposed by Bammann [19] and utilized in the finite element analysis of several types of boundary value problems, including welding and quenching analyses. In this particular model, a tensor variable, $\boldsymbol{\alpha}$, and a scalar variable, κ, were introduced and evolution equations proposed for each. The evolution of both state variables is cast into a familiar hardening minus recovery format. Both dynamic and thermal recovery terms were proposed for the variables. The dynamic recovery was motivated from dislocation cross slip that operates on the same time scale as dislocation glide. For this reason, no additional rate dependence results from this recovery term. The thermal recovery term is related to the diffusional process of vacancy assisted climb. Because this process operates on a much slower time scale, a strong rate dependence is predicted at higher temperatures where this term becomes dominant.

The tensor variable, $\boldsymbol{\alpha}$, often referred to as the backstress or the kinematic hardening variable, represents a short transient and results in a smoother "knee" in the transition from elastic to elastic-plastic response in a uniaxial stress-strain curve. What is more important, this variable controls the unloading response and is critical in welding or quenching problems during the cooling cycle of the problem. It is termed a short transient in that the variable hardens rapidly and saturates to a constant steady state value over a very short period of time during a monotonic loading at constant temperature and strain rate. This saturation value is maintained until the rate, temperature or loading path changes and the process repeats. This variable is responsible for the apparent material softening upon unloading termed the Bauschinger effect. The importance of the variable $\boldsymbol{\alpha}$ in the prediction of residual stresses in welding problems was detailed in [20]. The scalar variable, κ, is an isotropic hardening variable that predicts no change in flow stress upon reverse loading. This variable captures long transients and is responsible for the prediction of continued hardening at large strains. Unlike $\boldsymbol{\alpha}$, once steady state has been reached under constant conditions, this variable is not affected by a change in loading. As an example, the model prediction for various strain rates and temperatures for 304L stainless steel is depicted in Figure 1. The response is dominated by dynamic recovery at lower temperatures where the rate dependence is weak. The effects of thermal recovery become significant at higher temperatures where the rate dependence is strong.

In Figure 2 the model prediction is compared with uniaxial compression tests that involve a significant change in temperature. Two specimens were loaded, one at 20C to a strain of nearly 0.5 and the other at 800C to a strain of 0.23. This specimen was unloaded and quenched rapidly. Once the specimen had cooled, it was reloaded at 20C. If the stress was a unique function of temperature and plastic strain, the flow stress upon reload would have been identical to the 20C specimen at that strain. As shown in Figure 2, this is not the case. Rather, there is a strong temperature history effect upon reload that is adequately captured by the state variable model.

For multiphase materials, additional complications arise in predicting the material response. In particular, the effects of phase transformation induced plastic strain must be included. As a steel is cooled from above the austenization temperature, a solid state phase transformation occurs. Which phase forms depends upon the temperature and the cooling rate. In general, these product phases are larger in volume and harder than the surrounding austenite. As austenite transforms to one of several product phases, a volumetric strain develops in the austenite. In the presence of any deviatoric far field stress, this will be accompanied by a deviatoric component of strain. Since the product phases are generally stronger, this results in a *forward*

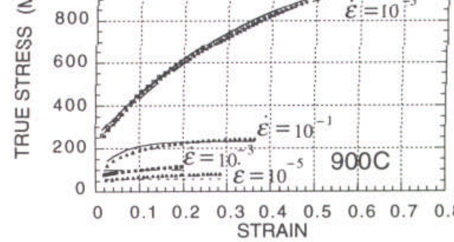

Figure 1. Model prediction for 304L stainless steel tension tests

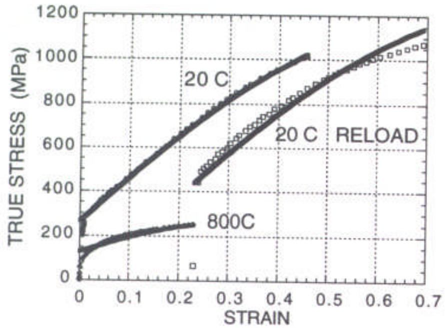

Figure 2. Model prediction of compression tests and compression reload demonstrating temperature history effects

stress, $\pi^{(i)}$ (i=1), in the austenite, resulting in an apparent softening of the material, as discussed previously. Similarly, a *backward* stress, $\pi^{(i)}$ (i=2,5), is created in each of the product phases, where $i = 1-5$ denotes austenite, pearlite, ferrite, bainite, and martensite respectively. This stress field is a true, tensorial backstress that must be subtracted from the applied stress to get the glide resistance to macroscopic plastic flow. It is proportional to the volume fraction of hard particles to first order [21]. Introducing such a backstress in the yield condition and flow rule provides a natural way to model the apparent yield drop and additional plasticity characteristic of transforming alloys.

To generalize the state variable model for multiphase materials, we assume that each point of the continuum can be occupied simultaneously by all phases. Each phase is modeled by the single phase state variable model with rate and temperature dependence as described above. Then the material response can be modeled with as much complexity or simplicity as required, since the model reduces to rate independent bilinear response with an appropriate choice of parameters. We denote the current configuration deviatoric Cauchy stress in each phase by $\boldsymbol{\sigma}'^{i}$. We assume a classic volume fraction weighted rule of mixtures, such that the total deviatoric Cauchy stress, $\boldsymbol{\sigma}'$, is given by

$$\boldsymbol{\sigma}' = \sum_i \Phi_i \boldsymbol{\sigma}'^{(i)} \;\; ; \;\; \sum_i \Phi_i = 1. \tag{2}$$

where Φ_i represents the volume fraction of each respective phase, subject to the constraint that the sum of the volume fractions of phases present must equal one. We assume a hypoelastic relation for each phase that is consistent with an assumption of linear elasticity giving

$$\overset{\circ}{\boldsymbol{\sigma}}'^{(i)} = 2\mu \boldsymbol{D}'^{(i)}_e + \frac{\dot{\mu}}{\mu}\boldsymbol{\sigma}'^{(i)} \tag{3}$$

where $\boldsymbol{D}'^{(i)}_e$ is the elastic symmetric part of the deviatoric velocity gradient, and μ is the temperature dependent shear modulus, assumed to be the same for all phases. In our initial implementation we neglect the effect of the term related to the time rate of change of the shear modulus. Elastic deformation rates are defined as the difference between the total deformation rate and the sum of the thermal, $\boldsymbol{D}'^{(i)}_{th}$, and the inelastic, $\boldsymbol{D}'^{(i)}_p$, contributions in each phase

$$\boldsymbol{D}'^{(i)}_e = \boldsymbol{D}' - \boldsymbol{D}'^{(i)}_p - \boldsymbol{D}'^{(i)}_{th} \;. \tag{4}$$

In equation (3), $\circ$ denotes the convective derivative of the Cauchy stress defined by

$$\overset{\circ}{\sigma}^{(i)} = \dot{\sigma}^{(i)} - W_e^{(i)}\sigma^{(i)} + \sigma^{(i)}W_e^{(i)} \tag{5}$$

where $\boldsymbol{W}_e^{(i)}$ is the skew part of the elastic velocity gradient for each respective phase given by

$$\boldsymbol{W}_e^{(i)} = \boldsymbol{W} - \boldsymbol{W}_p^{(i)} \;. \tag{6}$$

For the present purposes we choose a Jaumann derivative and all $\boldsymbol{W}_p^{(i)} = 0$.

With a physical motivation similar to dispersion hardening, $\pi^{(i)}$ are long range internal stresses acting in the different phases of the composite alloy. This type of approach was taken by Freed, Raj and Walker [22] in modeling hard and soft regions of a polycrystalline material as first proposed by Kocks [23]. By approximating compatibility of relative hard and soft regions of the multiphase alloy, a self-consistent type scheme was used here to motivate an evolution equation for the internal stresses that is consistent with the mixture theory. The resultant stress rates are proportional to the temperature-dependent shear modulus and volume fraction rates of change,

$$\begin{aligned}\dot{\pi}^{(i)} = C\mu \left[\left(\frac{\Delta V}{V}\right)^{(i)} \frac{\dot{\Phi}_i}{\Phi_i} - \sum_i \dot{\Phi}_i \left(\frac{\Delta V}{V}\right)^{(i)}\right] \\ + \frac{\dot{\Phi}_i}{\Phi_i}\left(\pi^1 - \pi^{(i)}\right)\end{aligned} \tag{7}$$

Consistent with a mixture theory, the interaction terms in the evolution law are proportional to the stress difference with the virgin austenitic phase, ensuring that the sum of internal stresses is self-equilibrating.

In addition to the long range forward and backward internal stress fields which act between the phases, we assume the existence of two short range internal stress fields $\boldsymbol{\alpha}^{(i)}$ and $\boldsymbol{\kappa}^{(i)}$, which act locally within each phase. We then define the net stress acting in each phase, as,

$$\boldsymbol{\xi}^{(i)} = \boldsymbol{\sigma}'^{(i)} - \boldsymbol{\alpha}^{(i)} - \boldsymbol{\kappa}^{(i)} - \boldsymbol{\pi}^{(i)} \;. \tag{8}$$

Now, we impose specific assumptions concerning the directionality of the stresses $\boldsymbol{\pi}^{(i)}$ and $\boldsymbol{\kappa}^{(i)}$. In particular we postulate that they act in the direction of the Cauchy stress minus the short range stress, $\boldsymbol{\alpha}^{(i)}$, in each phase,

$$\boldsymbol{\pi}^{(i)} = \pi^{(i)} \frac{\boldsymbol{\sigma}'^{(i)} - \boldsymbol{\alpha}^{(i)}}{\left|\boldsymbol{\sigma}'^{(i)} - \boldsymbol{\alpha}^{(i)}\right|} \qquad \boldsymbol{\kappa}^{(i)} = \kappa^{(i)} \frac{\boldsymbol{\sigma}'^{(i)} - \boldsymbol{\alpha}^{(i)}}{\left|\boldsymbol{\sigma}'^{(i)} - \boldsymbol{\alpha}^{(i)}\right|} \quad (9)$$

The effective stresses acting to cause plastic flow in each phase are then given by

$$\left|\xi^{(i)}\right| = \left|\boldsymbol{\sigma}'^{(i)} - \boldsymbol{\alpha}^{(i)}\right| - \kappa^{(i)} - \pi^{(i)}, \quad (10)$$

where $\kappa^{(i)}$ are the scalar internal variables acting in each phase as discussed above. The plastic flow rule is chosen to have a strong nonlinear dependence upon the deviatoric stress

$$\boldsymbol{D}_P^{(i)} = f^{(i)}(\theta)\sinh\left\{\frac{\left|\xi^{(i)}\right| - Y^{(i)}(\theta)}{V^{(i)}(\theta)(1+N(C))}\right\}\frac{\boldsymbol{\sigma}'^{(i)} - \boldsymbol{\alpha}^{(i)}}{|\boldsymbol{\sigma}'^{(i)} - \boldsymbol{\alpha}^{(i)}|}, \quad (11)$$

where $f(\theta)$ and $V(\theta)$ describe a rate dependence of the yield stress at constant temperature and $N(C)$ describes the yield increase with increasing carbon content, C. Tensor variables, $\boldsymbol{\alpha}^{(i)}$, and scalar variables, $\kappa^{(i)}$, have been introduced to describe the deformed state of each phase as described previously for a single phase material [18]. The evolution of these variables is defined for each phase by

$$\begin{aligned} \dot{\kappa}^{(i)} &= H^{(i)}(\theta, C)\left|\boldsymbol{D}_P^{(i)}\right| - \left\{R_s^{(i)}(\theta) + R_D^{(i)}(\theta)\left|\boldsymbol{D}_P^{(i)}\right|\right\}\left|\kappa^{(i)}\right|\kappa^{(i)} \\ \dot{\boldsymbol{\alpha}}^{(i)} &= h^{(i)}(\theta, C)\boldsymbol{D}_P^{(i)} - \left\{r_s^{(i)}(\theta) + r_D^{(i)}(\theta)\left|\boldsymbol{D}_P^{(i)}\right|\right\}\left|\boldsymbol{\alpha}^{(i)}\right|\boldsymbol{\alpha}^{(i)} . \end{aligned} \quad (12,13)$$

The fit to the carbon dependent data reported by Sjöström [21] is shown in Figure 3.

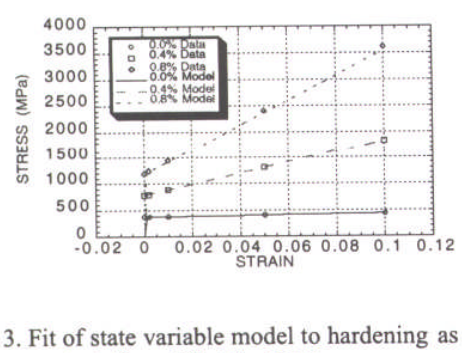

Figure 3. Fit of state variable model to hardening as a function of carbon content (from Sjöström [21]).

Multiphase Transformation Kinetics

A fundamental balance principle is used to model phase transformation kinetics at a volume fraction relevant for a broad range of industrial steels. This micro balance provides differential equations for transformation kinetics which couple naturally to the differential equations governing the mechanical and thermal aspects of a given process [24,25]. Avrami-type kinetics as well as the Koistinen-Marburger equation have been shown to result from special classes of energy and mobility functions [11]. An illustrative example using a 5140 alloy demonstrates how time-temperature-transformation (TTT) and continuous cooling transformation (CCT) curves can be generated using a particularly simple energy function. The formulation of this theory is discussed in [11] for a single product phase, but the interest here is in modeling the possibly competitive development of ferrite, pearlite, bainite and martensite. For ease of identification, we replaace the numericqal indices with latin indices and let the volume fraction of austenite, ferrite, pearlite, bainite and martensite be denoted by Φ_a, Φ_f, Φ_p, Φ_b and Φ_m respectively. Let the temperature be given by θ and the carbon concentration by C. Then a set of global balance postulates and constitutive restrictions result in the following system of equations for phase evolution:

$$\begin{aligned} \frac{d\Phi_f}{dt} &= v_f(C,\theta)\Phi_f^{\alpha f}\Phi_a^{\beta f}\left\{\Phi_{f,final}(C,\theta) - \Phi_f\right\}, \Phi_f(0) = 0.0001 \\ \frac{d\Phi_p}{dt} &= v_p(C,\theta)\Phi_p^{\alpha p}\Phi_a^{\beta p}, \qquad \Phi_p(0) = 0.0001 \\ \frac{d\Phi_b}{dt} &= v_b(C,\theta)\Phi_b^{\alpha b}\Phi_a^{\beta b}, \qquad \Phi_b(0) = 0.0001 \\ \frac{d\Phi_m}{d\theta} &= \begin{cases} 0, & \Phi_m(0) = 0.0001 \;\; \theta > M_s(C) \\ -v_m(C,\theta)\Phi_m^{\alpha m}\Phi_a^{\beta m}, & \Phi_m(0) = 0.0001 ; \theta < M_s(C) \end{cases} \end{aligned} \quad (14)$$

where equation $(2)_2$ becomes,

$$\Phi_a = \left(1 - \Phi_f - \Phi_p - \Phi_b - \Phi_m\right) \quad (15)$$

and where the functions $v_f(C,\theta)$, $v_b(C,\theta)$, $v_p(C,\theta)$ and $v_m(C,\theta)$ as well as the constants α_f, α_p, α_b, α_m, β_f, β_b, β_p and β_m are material dependent quantities that are determined from TTT quench data. These equations can be fully coupled to the thermomechanical equations, but are solved using a predetermined thermal profile in the present work.

The thermal transformation strains were modeled as follows. The thermal strain for austenite, E_A, and an arbitrary product phase, E_P, are taken to be linear and cubic functions of temperature, respectively, with the coefficients in these polynomials themselves being quadratic functions of the carbon concentration. The transformation strain, E_P^X, for this product phase is then given by

$$E_P^X = \frac{E_P - E_A}{1 + E_A} \qquad (16)$$

This modeling approach has been used successfully to predict CCT curves for a 6150 steel [11] and is applied here to predict CCT curves for a 5140 steel. While the goal of this project is not to generate CCT curves, such a task represents a check on model performance. TTT data generated using Minitech software [26] was used to fit the model parameters. We designed and used a differential fitting routine to accomplish this so that analytic solutions were not required for the kinetic equations. The TTT fit for all phases is shown in Figure 4. The model was then used under an assumption of exponential cooling to generate the CCT curves of Figure 5, where they are compared with the curves generated using Minitech. While only the total product volume fraction is plotted, it should be noted that the volume fraction of each phase is determined for all times.

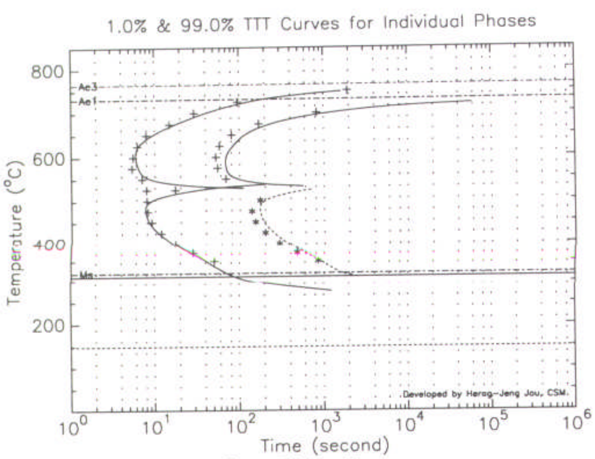

Figure 4. TTT curves for a 5140 alloy.

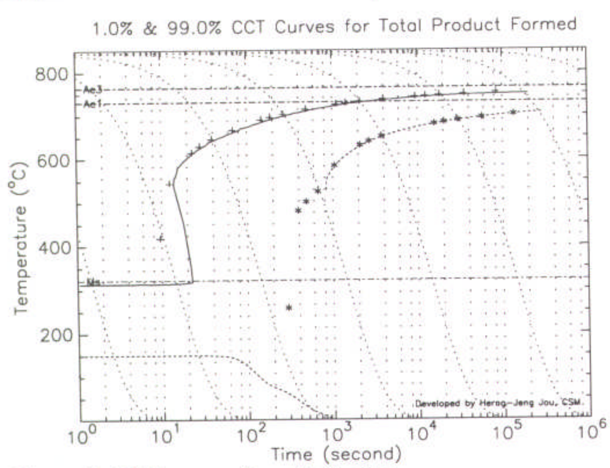

Figure 5. CCT curves for a 5140 alloy.

Model Simulations

Local Transformation Behavior. Locally, the averaged microplasticity is manifested on the continuum level as additional plastic strain whose stress dependence originates in that of the internally stressed austenitic parent phase. In our model, the stress dependence of the flow in the austenite is accounted for naturally. Figure 6 illustrates the dependence of the plastic strain rate as a function of volume fraction for cooling rates sufficiently high to produce only martensite. These curves were obtained by integrating equations (3), (7), (12) and (13) for various applied stresses. These curves illustrate the effects of the nonlinearity of the model. In addition to the obvious nonlinear stress dependence of the flow rule, these curves also reflect the nonlinear response of the state variables during the transformation. For high applied stress, the short transient $\boldsymbol{\alpha}^{(i)}$, has saturated for very small values of Φ since $\boldsymbol{\alpha}^{(i)}$ grows initially as the hyperbolic sine of the stress. Saeedvafa and Asaro [10] have recently investigated the stress dependence of the microplasticity using a numerical micromechanical approach. A comparison of the state variable prediction with the discrete simulation is depicted in Figure 7 over a broad range of applied stresses.

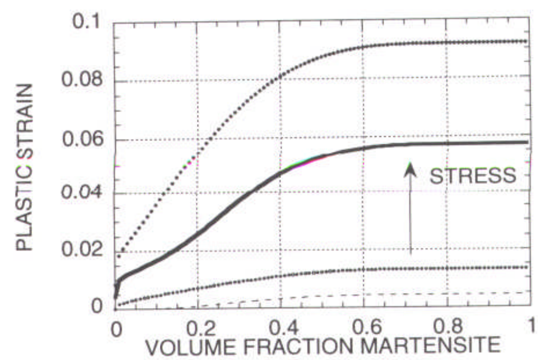

Figure 6. Dependence of transformation plastic strain on volume fraction as a function of stress.

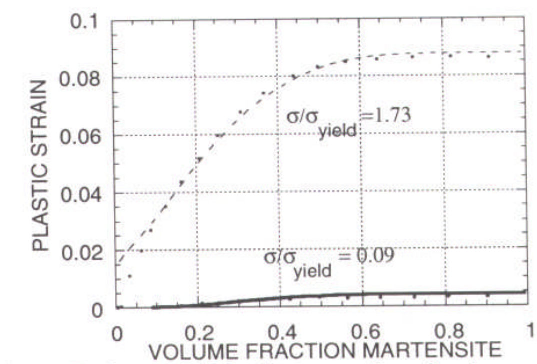

Figure 7. State variable fit to results of micromechanical simulations on a transforming representative volume.

The multiphase state variable model has been implemented in a user material subroutine in the finite element program ABAQUS [27] and used to simulate the time history of the evolving gauge length for a 5140 quench dilatometer specimen. The temperature and carbon dependent transformation strains and start temperatures for transformation are captured well, as shown in Figure 8.

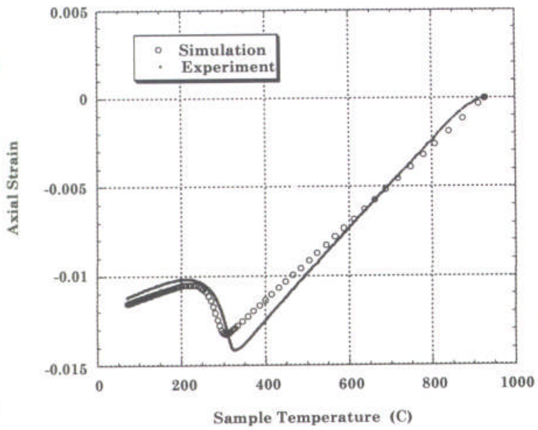

Figure 8. Quench dilatometer simulation for a 5140 alloy.

Global Transformation Behavior. The multiphase implementation in ABAQUS has been used to simulate the quenching of a long annular rod of arbitrary thickness. The rod is initially at uniform temperature, $T_a = 1073K$. The quenchant temperature, T_q, is $400K$ and the heat flux differs on inner and outer boundaries. The problem geometry is depicted in Figure 9. For long aspect ratio cylinders, the thermal response is one-dimensional. It can be computed analytically [28] and used to drive the transformation.

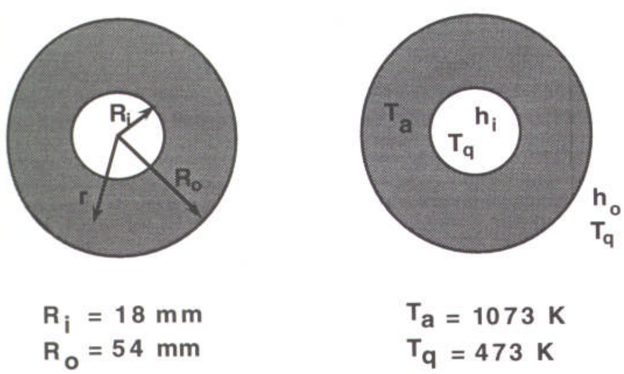

Figure 9. One-dimensional, annular rod or disk.

The corresponding radial and hoop stresses are depicted in Figure 10. Including transformation plasticity has noticeable effects on both components. The tangential stresses are increased marginally at the inner surface, but relieved just beyond the transformation front. Near the outer surface, the tangential stress changes sign while maintaining nearly the same magnitude. Radial stresses are larger, in general, and, again, change sign at the outer surface. These results indicate that local microplasticity is manifest on the global macroscopic scale in a way that can be cast in a state variable framework. A corresponding experimental program is underway to characterize a class of low alloy steels and verify the simulations over a broad range of conditions. While the qualitative trends are reasonable, the quantitative predictions will need to be revisited when sufficient experimental data are available.

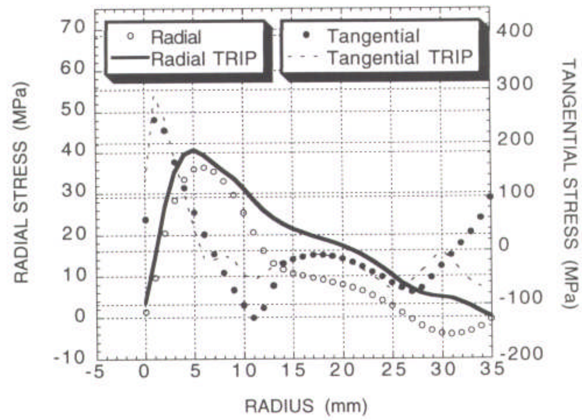

Figure 10. Radial and tangential stresses calculated with and without the effects of phase transformation.

Conclusions

An internal state variable formulation for phase transforming alloy steels is presented. We have illustrated how local transformation plasticity can be accommodated by an appropriate choice for the corresponding internal stress field acting between the phases. The state variable framework compares well with a numerical micromechanical calculation providing a discrete dependence of microscopic plasticity on volume fraction and the stress dependence attributable to a softer parent phase. The multiphase model is used to simulate the stress state of a quenched bar and show qualitative trends in the response when the transformation phenomenon is incorporated on the length scale of a global boundary value problem.

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