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On the Singularity of the Leblond Model for TRIP and Its Influence on Numerical Calculations

Michael Wolff and Michael Böhm

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Transformation-induced plasticity (TRIP) in steel may be a cause of distortion of workpieces. Therefore, it is necessary to study this phenomenon to develop knowledge for the simulation of production processes (e.g., for heat treatment). The well-known Leblond model for TRIP becomes formally singular when the phase fraction *p* of the forming phase is zero. Usually, this singularity is avoided by changing the model via a cutoff procedure. This article addresses those conditions in which the singularity is formally removable and the output differences of the noncutoff and the cutoff models. Depending on the thresholds used for the cutoff functions, it turns out that the differences might be of an essential magnitude. Moreover, for constant temperature and stress, these differences turn up regardless of what phase transition law for *p* is used.

Keywords Leblond model, nonisothermal phase transformation singularity, transformation-induced plasticity

1. Introduction and Motivation

Phase transformations in steel under nonzero deviatoric stress yield a permanent volume-preserving deformation, even if the von Mises (macro) stress does not achieve the yield stress. This phenomenon is called transformation-induced plasticity (TRIP) and cannot be described by classic plasticity. In the case of the formation of one phase (e.g., pearlite from austenite), TRIP can be taken into account by an additional (linearized) strain tensor $\varepsilon_{\text{TRIP}}$. The corresponding Franitza-Mitter-Leblond proposal in the incremental form is (Ref 1-6):

$$\frac{d}{dt}\varepsilon_{\text{TRIP}}(t) = \frac{3}{2}\kappa[\theta(t), \sigma^*(t)]\,\sigma^*(t)\frac{d}{dt}\Phi[p(t)] \qquad \text{(Eq 1)}$$

where θ is the temperature, σ^* is the deviator of the stress tensor σ, $\kappa > 0$ is the Greenwood-Johnson parameter possibly depending on θ and σ^*, Φ is the saturation function, p is the volume fraction of the forming phase, and $t \geq 0$ is the time.

Further, Φ is assumed to be a monotonic differentiable function on [0, 1] with:

$$\Phi(0) = 0 \text{ and } \Phi(1) = 1 \qquad \text{(Eq 2)}$$

There are several proposals (Ref 4) for Φ, partially based on experiments, partially derived from theoretical considerations, like the one due to Leblond et al. (Ref 2), which uses:

$$\Phi(p) := p[1 - \ln(p)], \text{ for } p \in [0,1] \text{ and } \Phi(0) := 0 \qquad \text{(Eq 3)}$$

Michael Wolff and **Michael Böhn,** Zentrum für Technomathematik, FB3, Universität Bremen, PB330440, D28334 Brenen, Germany. Contact e-mail: mwolff@math.uni-bremen.de, mbohm@math.uni-bremen.de.

From Eq 1 and 3, the Leblond model for TRIP is obtained in its integral form, which is often used in calculations (Ref 7):

$$\varepsilon_{\text{TRIP}}(t) = \frac{3}{2}\int_0^t \kappa[\theta(s), \sigma^*(s)]\,\sigma^*(s)\,\{-\ln[p(s)]\}\frac{d}{ds}p(s)\,ds \qquad \text{(Eq 4)}$$

Due to the logarithm, the integrand in Eq 4 has a singularity at $p = 0$. Other proposals for Φ (Ref 4) do not lead to such singularities, and so the model, Eq 4, is used.

For the sake of brevity, in Eq 4 corrections for larger stresses (Ref 2) are omitted, and it should be noted that inclusion of these stresses would not cause any additional mathematical problems in the discussion. For the same reason, any

Nomenclature	
$\varepsilon_{\text{TRIP}}$	strain tensor due to TRIP
t	time
θ	temperature
σ, σ^*	stress tensor and its deviator, respectively
κ	Greenwood-Johnson parameter of TRIP
Φ	saturation function of TRIP
p	volume fraction of the forming phase
$\varepsilon_{\text{TRIP},\delta}$	TRIP strain obtained via a cutoff procedure
δ	cutoff threshold
H	Heaviside function
n, τ	Johnson-Mehl-Avrami parameters for isothermal phase transformations
g	function taking into account nonisothermal phase transformation
f	function taking into account stress-dependent phase transformation
μ	temperature dependent function in a special transformation law (Ref 8)
$\hat{\theta}$	integral average of the temperature (Ref 10)
α	positive constant (Ref 10)
θ_{ms}	martensite-start temperature
c	positive constant (Ref 11)
$E(\delta)$	relative error when using a cutoff procedure

dependence of ε_{TRIP}, θ, σ*, and p on spatial coordinates is ignored.

To avoid an experimentally observed overestimation for small values by Eq 3, Leblond et al. (Ref 2) introduced a cutoff procedure in the following way:

$$\varepsilon_{TRIP,\delta} = \frac{3}{2}\int_0^t \kappa[\theta(s), \sigma^*(s)]\sigma^*(s)\{-\ln[p(s)]\}\frac{d}{ds}p(s)\, H[p(s)-\delta]\, ds \qquad \text{(Eq 5)}$$

where H is the Heaviside function and δ is a threshold value between 0 and 1. Clearly, in Eq 5 the above-mentioned singularity is also avoided. This cutoff procedure is discussed in section 4.1.

To use Eq 4 or 5, a transformation law for p in Eq 4 is needed. Some possible examples are noted below, and the interested reader is referred to Böhm et al. (Ref 8) for a survey.

1.1 Example 1: Diffusive Transformation, Generally Nonisothermal (Ref 9, 10)

The phase fraction $p = p(t)$ is determined by the nonzero solution of a modified JMA differential equation (for a complete transformation):

$$\frac{d}{dt}p(t) = [1-p(t)]\frac{n[\theta(t)]}{\tau[\theta(t)]}\{-\ln[1-p(t)]\}^{\frac{n[\theta(t)]-1}{n[\theta(t)]}} \cdot \left\{1 - g[\theta(t)]\frac{d}{dt}\theta(t)\right\} f[\sigma(t)] \qquad \text{(Eq 6)}$$

with the initial value:

$$p(0) = 0 \qquad \text{(Eq 7)}$$

where n and τ are parameters obtained for the isothermal transformation, g is a correcting function for the nonisothermal transformation (see Ref 9 and 10), and f represents a correcting function for the stress-dependent transformation with $f(0) = 1$ (Ref 5 and 6 for details).

1.2 Example 2

Here are alternative differential equations for $p = p(t)$, nonisothermal transformations (Ref 8, 11, 12):

$$\frac{d}{dt}p(t) = [1-p(t)]\,\mu[\theta(t)] \qquad \text{(Eq 8)}$$

where μ is continuous, $\mu(s) \geq 0$ and $\mu(\theta_0) > 0$.

1.3 Example 3

A modification of Eq 6 for nonisothermal transformations involving temperature averages is

$$\frac{d}{dt}p(t) = [1-p(t)]\frac{n(\hat{\theta})}{\tau(\hat{\theta})}\{-\ln[1-p(t)]\}^{\frac{n(\hat{\theta})-1}{n(\hat{\theta})}} f[\sigma(t)] \qquad \text{(Eq 9)}$$

where the current temperature $\theta(t)$ is substituted by its integral average:

$$\theta(t) := \alpha(1-e^{-\alpha t})^{-1}\int_0^t \theta(s)\, e^{-\alpha(t-s)} ds \qquad \text{(Eq 10)}$$

for $t > 0$, where $\hat{\theta}(0) := \theta(0)$, n, and τ are as shown in Eq 6, and $\alpha > 0$ is a parameter that has to be determined by experiments (Ref 8 for details and Ref 11 for some validation based on dilatometer data). The use of the average temperature instead of its current value takes into account the influence of the history of the temperature.

1.4 Example 4

In the case of the formation of martensite, the Koistinen-Marburger formula is

$$p(\theta) = 1 - e^{-(\theta_{ms}-\theta)/c} \qquad \text{(Eq 11)}$$

where c is a positive constant. Assuming that θ is smaller than the martensite-starting temperature θ_{ms}, Eq 11 expresses the amount of martensite formed from pure austenite when cooling to θ. Because the martensite transformation occurs very quickly, the value $p(\theta)$ is assumed to equal the current one (i.e., $p(t)$) (Ref 8 for a discussion). So Eq 11 evolves into Eq 12 by differentiation with respect to t:

$$\frac{d}{dt}p(t) = -[1-p(t)]\frac{1}{c}\frac{d}{dt}\theta(t) \qquad \text{(Eq 12)}$$

with Eq 7 and assuming $\theta_{ms} = \theta(0)$ and also a strong cooling, that is, $d/dt\,\theta(t) < 0$.

With the preceding as an introduction, the purpose of this article is to answer two questions:

- Under which conditions on the parameters n and τ does the integral in Eq 4 exist despite the singularity at $p = 0$?
- In cases in which the answer in 1 is affirmative: What is the relative error made by substituting Eq 4 with Eq 5? And how does the error depend on the choice of the transformation law (e.g., examples 1 to 4)?

2. Some Formal Mathematical Assumptions

Some assumptions are needed in the subsequent discussion:

$$\sigma, \theta, \frac{d}{dt}\theta, \kappa, n(\theta), \tau(\theta), f \text{ and } g \text{ are continuous with} \qquad \text{(Eq 13)}$$

$$n(\xi) > 0, \text{ there is some } \tau_o > 0, \text{ such that: } \tau(\xi) \geq \tau_o \text{ for all } \xi \geq 0 \qquad \text{(Eq 14)}$$

3. Results

3.1 Theorem 1

The assumptions in Eq 6, 13, 14, and:

$$n(\theta_o) > 1, \text{ with } \theta_o = \theta(0) \text{ corresponding to } p(0) = 0 \quad \text{(Eq 15)}$$

imply that

$$\lim_{s \to 0} \ln[p(s)] \frac{d}{ds} p(s) = 0 \quad \text{(Eq 16)}$$

Therefore, the singularity of the integrand in Eq 4 is removable, and the integral in Eq 4 exists, that is,

$$\left| \int_0^t \kappa[\theta(s), \sigma^*(s)]\, \sigma^*(s) \{-\ln[p(s)]\} \frac{d}{ds} p(s)\, ds \right| < +\infty \text{ for all } t \geq 0 \quad (17)$$

3.1.1 Proof. Because $[-\ln(1 - p)] \approx p$ for small p (>0), the insertion of Eq 6 into Eq 4 shows that the essential term governing the behavior near $p = 0$ (i.e., near $s = 0$) is:

$$\{-\ln[p(s)]\} p(s)^{\frac{n[\theta(s)]-1}{n[\theta(s)]}} \quad \text{(Eq 18)}$$

The continuity of n yields numbers $s_0 > 0$ and n_0 with $1 < n_0 < n(\theta_0)$ and

$$n_o < n[\theta(s)] \leq n_o + 1 \text{ for } 0 < s \leq s_o \quad \text{(Eq 19)}$$

This implies for Eq 18:

$$0 < \{-\ln[p(s)]\}\, p(s)^{\frac{n[\theta(s)]-1}{n[\theta(s)]}} \leq \{-\ln[p(s)]\}\, p(s)^{\frac{n_o-1}{n_o+1}} \text{ for } 0 < s \leq s_o \quad \text{(Eq 20)}$$

Because $[(n_o - 1)/(n_o + 1) > 0]$, the rest follows from standard properties of logarithms.

Equation 15 corresponds to the observation that the diffusive phase transformations start with a zero rate (i.e., at the beginning of the transformation its p-curve has a horizontal tangent). Based on experiments with 100Cr6 steel, Dalgic and Löwisch (Ref 13) obtained $n > 1$ for pearlitic and bainitic transformations. In the study by Hunkel et al. (Ref 9), values of n between 0 and 1 can be found.

3.2 Remark 2

Assume only Eq 13 and 14. Then, inserting Eq 6 into Eq 4, one obtains:

$$\lim_{s \to 0} \{-\ln[p(s)]\} \frac{d}{ds} p(s) = +\infty \quad \text{(Eq 21)}$$

but the integral in Eq 4 exists (i.e., Eq 17 is still valid).

The proof of the validity of Eq 17 and 21 also carries over to example 3: replacing Eq 6 by Eq 9 and 10. Example 2 is covered by the preceding remark by using Eq 8 instead of Eq 6 (i.e., one has Eq 21).

3.3 Theorem 3

Under the assumptions of Eq 7, 11, and 12, one obtains Eq 17 and 21.

3.3.1 Proof. Inserting Eq 12 and 13 into Eq 4 and substituting

$$p(s) := 1 - e^{-(\theta_{ms} - \theta(s))/c} \quad \text{(Eq 22)}$$

which leads to

$$\int_0^{p_0} [-\ln(p)] dp < +\infty \quad (\text{with } 0 < p_0 < 1) \quad \text{(Eq 23)}$$

3.4 Remark 4

All of the above results do not depend on the cooling rate, meaning that they are independent of a special behavior of θ'.

4. Quantitative Discussion

4.1 Relative Error When Using Cutoff Functions

The relative error when using Eq 5 instead of Eq 4 can be estimated for the complete transformation under constant temperature and stress. To this end, it is assumed that:

$$\theta = \text{const. and } \sigma = \text{const.} \quad \text{(Eq 24)}$$

implies that

$$\kappa = \text{const.} \quad \text{(Eq 25)}$$

It has been assumed that t_∞ is a sufficiently large time after which the transformation can be considered to be complete. Due to Eq 2 to 4, the full TRIP strain determined by Eq 4 becomes:

$$\varepsilon_{\text{TRIP}}(t_\infty) = \frac{3}{2} \kappa \sigma^* \quad \text{(Eq 26)}$$

whereas the full TRIP strain by the cutoff model (i.e., Eq 5), becomes:

$$\varepsilon_{\text{TRIP},\delta}(t_\infty) = \frac{3}{2} \kappa \sigma^* [1 - \Phi(\delta)] \quad \text{(Eq 27)}$$

Hence, the relative error $E(\delta) := \varepsilon_{\text{TRIP}}(t_\infty)^{-1} [\varepsilon_{\text{TRIP}}(t_\infty) - \varepsilon_{\text{TRIP},\delta}(t_\infty)]$ is:

$$E(\delta) = \Phi(\delta) \quad \text{(Eq 28)}$$

Note that under constant temperature and stress Eq 28 is independent of the choice of the phase transformation law provided by examples 1 to 4 (e.g., the value $\delta = 0.03$ is used by

Leblond et al. (Ref 2) and in SYSWELD). For comparison, $E(0.01)$ is calculated to obtain:

$$E(0.03) = \Phi(0.03) = 0.135 \text{ and } E(0.01) = \Phi(0.01) = 0.056 \quad \text{(Eq 30)}$$

respectively. Although $E(\delta) \to 0$ as $\delta \to 0$, this means that there is an essential relative error that cannot be neglected.

In reality, the stress is hardly constant. Large stresses that occur during heat treatment (e.g., during quenching) could increase $E(\delta)$, whereas small stresses could decrease this value.

4.2 Further Remarks

Taleb and Sidoroff (Ref 3) have proposed a threshold depending on material parameters that include, in particular, the yield stress of the parent phase. Additionally, they modified the "saturation function (Φ)," obtaining $\Phi(0) > 0$ instead of Eq 3. Estimating this threshold for 100Cr6 steel for the transformation of austenite to pearlite at 600 °C according to their approach, an approximate threshold value of 0.08 is obtained with a relative error of 0.08.

5. Conclusions

- For the diffusive transformations in examples 1 and 3, the Leblond model in Eq 4 involves a removable singularity under the assumptions of Eq 13 to 15, and the integral in Eq 4 exists.
- However, without Eq 15, as well as for a diffusive transformation in example 2, a nontrivial singularity is obtained, but the integral in Eq 4 still exists.
- The last statement is valid for martensitic transformations (example 4).
- From a purely mathematical point of view, the Leblond model in Eq 4 is applicable without a cutoff procedure. Some difficulties may occur when calculating values by numerical programs, which generally cannot deal with improper integrals. It is then necessary to adopt an appropriate program.
- Using a cutoff function, one can avoid these kinds of singularities, but essential differences are obtained. For constant temperature and stress, this last assertion does not depend on the model used for the phase transformation, if the integral in Eq 4 exists. Thus, using cutoff functions, one can obtain different models. Even different δ for $\varepsilon_{TRIP,\delta}$ in Eq 5 yield relatively large errors (Eq 30).

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