A Thermomechanical Description of Materials with Internal Variables in the Process of Phase Transitions

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Summary: A continuum mechanical description is presented for thermoplastic materials in the process of solid-solid phase transition. The material is assumed to be characterized by three different internal state variables: two internal variables which specify the crystallographic structural change during the plastic deformation, and a set of scalar internal variables which describes the extent of phase transition. Applying Edelen's decomposition theorem, the plastic quantities are determined from the dissipation potential, while the elastic quantities are specified by the internal energy. The explicit form of the flow rule and the evolutional equations for the internal variables are derived. The constitutive equations for the stress and the entropy are obtained in rate-type. It is shown that the continuous cooling transformation (C-C-T) diagram and the isothermal time-temperature-transformation (T-T-T) diagram could be derived from the theory developed here. The infinitesimal case is discussed in detail.

Eine thermomechanische Beschreibung von Materialien mit inneren Variablen beim Phasenübergang

Übersicht: Eine kontinuumsmechanische Darstellung für thermoplastische Stoffe während eines Phasenübergangs wird gegeben. Das Material wird mit Hilfe von verschiedenen Zustandsvariablen charakterisiert: zwei Variablen, die kristallographische Änderungen während der plastischen Deformation angeben und ein Satz von Variablen, welche den Umfang des Phasenübergangs beschreiben. Stoffgleichungen werden hergeleitet. Außerdem wird gezeigt, daß C-C-T- und T-T-Diagramme aus der entwickelten Theorie hergeleitet werden könnten.

1 Introduction

Phase transition of materials is one of the most interesting phenomena in the field of material science. The related topics extend from quantum mechanics to thermochemistry, and also from ferromagnetic dielectrics to carbon steels [1-10].

The phenomena have been discussed extensively not only from the point of physics but also from the point of thermodynamics and of continuum mechanics. Among the works, Landau's theory of the second order phase transition [5, 10], which is based on the consideration of statistical physics, seems to be one of the prominent starting points in the continuum mechanical study of phase transitions. One could also list the study of Enz [11, 12], who formulated the displacive transitions of the thermoelastic solids in order to discuss the soft phonon mode of lattice vibration. Recently Murdoch [13] carried out a continuum mechanical study on the phase transition for elastic materials. He regarded the material as a mixture of the two separate phases, and demonstrated that the classical results for the liquid-gas and the solid-solid transitions could be derived by tracing the method in modern continuum mechanics.

In the process of the second order phase transition, the so-called long-range order which measures the extent of phase transition, plays a very important role [5, 7]. From the continuum mechanical point of view this parameter could be interpreted as an internal state variable which specifies the position of the system in the range from the initial state to the final state [14]. It likely corresponds, for example, to the extent of reaction in the theory of reacting media or the volume fraction in the theory of mixtures [15]. This suggests that the phase transitions might be described by means of the internal state variable theory in the continuum mechanics [14, 16].

Generally speaking, the phase equilibrium condition of the solid-solid transition is so severe that the material inevitably reacts over its elastic limit [17]. And the plastic deformation of the material is always a very important factor to expect the mechanical response of materials after the phase transitions [3, 18].

In this study a continuum mechanical description is presented for thermoplastic materials in the process of solid-solid phase transition. The material is assumed to be characterized by three different internal state variables: two internal state variables which specify the crystallographic structural change during the plastic deformation [19, 20], and a set of scalar internal state variables which describes the extent of phase transition. The present theory has, therefore, a close similarity with the theory of reacting media [15]. Applying Edelen's decomposition theorem [21, 22] the dissipative or plastic quantities are determined from the dissipation potential, while the elastic quantities are specified, as usual, by the internal energy. The explicit form of the flow rule and the evolutional equations for the internal state variables are obtained by means of the Legendre transformation. This enables us to derive the rate-type constitutive equations for the stress and the entropy.

In order to show how the theory works in practice, some topics are discussed in the last section. First of all, it is shown that the expression of the continuous cooling transformation (C-C-T) diagram as well as of the isothermal time-temperature-transformation (T-T-T) diagram [23] can be derived from the theory developed here. Then the theory is reduced to the case of infinitesimal deformation with isotropy. The constitutive equations and the governing equations are written down explicitly.

2 Preliminaries

Consider a thermoplastic body in three-dimensional space, the motion of which we write

$$\mathbf{x} = \mathbf{x}(\mathbf{X}, t), \tag{2.1}$$

where X and x stand for the position vectors in the reference and the current configurations, respectively, while t means the time. The deformation gradient F is then defined by

$$\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}, \quad \det \mathbf{F} > 0.$$
(2.2)

As usual we shall use in this study the terms, the material point and its position in the reference configuration, without distinction.

Let us next assume that at any instant of deformation there exists an intermediate configuration which would be attained if a deformed material element could be unstressed elastically [24-26]. The material point X which occupies a position x in the current configuration, is transformed under such a process to a position χ in the intermediate configuration. Since the elastic deformation gradient corresponding to this transformation may be defined by

$${}_{B}\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{\chi}}, \qquad (2.3)$$

the chain-rule permits us to decompose the deformation gradient **F** into the elastic part ${}_{E}\mathbf{F}$ and the plastic part ${}_{P}\mathbf{F} \equiv \partial \mathbf{\chi}/\partial \mathbf{X}$ as follows:

$$\mathbf{F} = {}_{\boldsymbol{E}} \mathbf{F} \cdot {}_{\boldsymbol{P}} \mathbf{F}, \qquad (2.4)$$

where, and throughout this study, the prefix E represents the elastic part, while P indicates the plastic part. In the sequel, we employ the following notation:

$$[\mathbf{A} \cdot \mathbf{B}] \dots_{ij} \dots \equiv A \dots_{ik} B_{kj} \dots, \quad [\mathbf{A} : \mathbf{B}] \dots_{ij} \dots \equiv A \dots_{ikl} B_{klj} \dots,$$

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and grad and Grad mean the gradient with respect to x and χ , respectively, while div and Div are the divergence with respect to x and χ , respectively. The suffixes T and -1 stand for the transpose and the inverse. The superposed dot denotes the material time derivative.

As the result of the decomposition proposed for F, the deformation velocity tensor

$$\mathbf{L} = \dot{\mathbf{F}} \cdot \mathbf{F}^{-1} \tag{2.5}$$

is also decomposed as

$$\mathbf{L} = {}_{B}\mathbf{L} + {}_{B}\mathbf{F} \cdot {}_{P}\mathbf{L} \cdot {}_{B}\mathbf{F},$$
(2.6)

where the elastic and the plastic parts of the deformation velocity tensor, $_{E}\mathbf{L}$ and $_{P}\mathbf{L}$, respectively, are defined as

$${}_{E}\mathbf{L} \equiv {}_{E}\dot{\mathbf{F}} \cdot {}_{E}\overset{-1}{\mathbf{F}}, \qquad {}_{P}\mathbf{L} \equiv {}_{P}\dot{\mathbf{F}} \cdot {}_{P}\overset{-1}{\mathbf{F}}.$$
(2.7)

We also define the strain tensor $_{E}\mathbf{E}$ by

$${}_{E}\mathbf{E} \equiv 1/2({}_{E}\mathbf{C}-1) \quad \text{with} \quad {}_{E}\mathbf{C} \equiv {}_{E}\mathbf{F}^{T} \cdot {}_{E}\mathbf{F}, \tag{2.8}$$

where 1 stands for the unit tensor of the second rank. The strain tensor $_{E}E$ turns out to be the Green strain tensor

$$\mathbf{E} = 1/2(\mathbf{F}^T \cdot \mathbf{F} - \mathbf{1}), \tag{2.9}$$

while the tensor ${}_{E}\dot{\mathbf{E}}$ is the stretching tensor

$$\mathbf{D} \equiv 1/2(\mathbf{L} + \mathbf{L}^T), \tag{2.10}$$

when the deformation is limited within the elastic range, hence the prefix E on E in $(2.8)_1$ is reasonable.

For later use we write here a formula, which is derived from (2.6), and will play an important role in the following discussion:

$$\bar{\mathbf{D}} = {}_{E} \dot{\mathbf{E}} + {}_{P} \bar{\mathbf{D}}, \qquad (2.11)$$

where $\overline{\mathbf{D}}$ and $_{P}\overline{\mathbf{D}}$ are given by

$$\overline{\mathbf{D}} \equiv {}_{E}\mathbf{F}^{T} \cdot \mathbf{D} \cdot {}_{E}\mathbf{F}, \qquad {}_{P}\overline{\mathbf{D}} = 1/2[{}_{E}\mathbf{C} \cdot {}_{P}\mathbf{L} + ({}_{E}\mathbf{C} \cdot {}_{P}\mathbf{L})^{T}].$$
(2.12)

This expression states that the stretching tensor can also be decomposed in the intermediate configuration.

Corresponding to the decomposition in the kinematical quantities, we propose the entropy density η be also written as [27]

$$\eta = {}_{E}\eta + {}_{P}\eta. \tag{2.13}$$

As the thermodynamic state variables which describe the thermodynamic state of the materials treated here, we employ the following set of variables:

$$\hat{\mathbf{j}} = ({}_{E}\mathbf{E}, {}_{E}\eta, \mathbf{g}, \boldsymbol{\pi}, \boldsymbol{\pi}, \boldsymbol{\xi}), \tag{2.14}$$

where g stands for the material temperature gradient determined from the temperature gradient in the current configuration, grad θ , by

$$\mathbf{g} \equiv {}_{E}\mathbf{F}^{T} \cdot \operatorname{grad} \theta$$
.

Similarly, π is the material version of a symmetric second order tensor in the current configuration, $\overline{\pi}$, i.e.

$$\boldsymbol{\pi} \equiv {}_{E}\mathbf{F}^{T} \cdot \boldsymbol{\overline{\pi}} \cdot {}_{E}\mathbf{F}.$$

The tensor π and the scalar π are introduced as the internal state variables in order to specify the internal crystallographic structure of the materials [19, 20]. Of course, the internal structure of the materials may be characterized not only by π and π alone but also by more internal state variables of the same order as well as of the higher order tensors. This does, however, not produce any essential change in the following formulation.

The quantity $\boldsymbol{\xi}$ represents a set of the scalar internal variables which characterize the extent of phase transition [15, 18]. When the phase transition among N + 1 phases is discussed, $\boldsymbol{\xi}$ may be composed of the volume or mass fractions of any N components. In the present study, however, $\boldsymbol{\xi}$ is regarded as a set of N scalar variables without any practical physical interpretations.

We note here that the variables that constitute \hat{j} are all invariant with respect to any rigid rotations in the sense of modern continuum mechanics [28].

3 Consequence of Clausius-Duhem Inequality

The equation of energy balance is written in the current configuration as

$$\varrho \dot{U} - \mathbf{T} : \mathbf{L} + \operatorname{div} \mathbf{q} - \varrho \sigma = 0, \tag{3.1}$$

where T, q and σ denote the Cauchy stress tensor, the heat flux vector and the heat production term, respectively, while ϱ is the density. As is proposed in the preceding section, the internal energy U is specified by the state variable \hat{j} , i.e.

$$U = U(\hat{j}). \tag{3.2}$$

From (3.1) we can derive an alternative version of the energy equation in the intermediate configuration. The result reads

$$\varrho_{\mathbf{0}}\dot{U} - \mathbf{K} :_{E}\dot{\mathbf{E}} - \mathbf{K} :_{P}\overline{\mathbf{D}} + \text{Div }\mathbf{Q} - \varrho_{\mathbf{0}}\sigma = 0, \qquad (3.3)$$

where the second Piola-Kirchhoff stress tensor and the material heat flux vector are introduced through the definitions

$$\mathbf{K} \equiv (\varrho_0/\varrho) \stackrel{-1}{_{B}\mathbf{F}} \cdot \mathbf{T} \cdot (\stackrel{-1}{_{B}\mathbf{F}})^{T},$$

$$\mathbf{Q} \equiv (\varrho_0/\varrho) \stackrel{-1}{_{B}\mathbf{F}} \cdot \mathbf{q}.$$
(3.3a)

In the above equations, the density in the intermediate configuration, $\overline{\varrho}$, has already been replaced by the density in the reference configuration, ϱ_0 , since the relation

$$\det \mathbf{F} = (\det_{E} \mathbf{F}) \cdot (\det_{P} \mathbf{F}) = (\bar{\varrho}/\varrho) \det_{P} \mathbf{F} = \varrho_{0}/\varrho$$

which is derived from (2.4) and the balance of mass, implies $\bar{\varrho} = \varrho_0$, provided that the incompressibility condition of the plastic deformation, det $_{P}F = 1$, is assumed.

By taking a similar procedure, the Clausius-Duhem inequality in the current configuration

$$\varrho\dot{\eta} - \varrho \, \frac{\sigma}{\theta} + \operatorname{div}\left(\frac{\mathbf{q}}{\theta}\right) \ge 0$$
(3.4)

is transformed to the formula in the intermediate configuration:

$$\left(\frac{1}{\varrho_0} \mathbf{K} - U_{_{E}\mathbf{E}} \right) : {}_{E}\dot{\mathbf{E}} + (\theta - U_{_{E}\eta}) {}_{E}\dot{\eta} - U_{\mathbf{g}} \cdot \dot{\mathbf{g}} + \frac{1}{\varrho_0} \mathbf{K} : {}_{P}\overline{\mathbf{D}} + \theta {}_{P}\dot{\eta} - U_{\boldsymbol{\pi}} : \dot{\boldsymbol{\pi}} - U_{_{\boldsymbol{\pi}}}\dot{\boldsymbol{\pi}} - U_{\boldsymbol{\xi}} \cdot \dot{\boldsymbol{\xi}} - \frac{1}{\varrho_0 \theta} \mathbf{Q} \cdot \text{Gard } \theta \ge 0,$$

$$(3.5)$$

where we have used (3.2). The partial differentiation of U is denoted by the suffix, i.e.

$$U_{_E\!\mathbf{E}} \equiv \partial U/\partial_E \mathbf{E}, \ \ U_{\mathbf{g}} = \partial U/\partial \mathbf{g}, \ \ \mathrm{etc.}$$

The same way of writing is also employed for Φ , Γ , $\overline{\Gamma}$, A and k in the later discussions.

When a standard argument of the type employed by Coleman and Curtin [14] is used in (3.5), we are led to the following results:

$$U = U(\mathbf{j}), \quad \mathbf{j} = ({}_{E}\mathbf{E}, {}_{E}\eta, \boldsymbol{\pi}, \boldsymbol{\pi}, \boldsymbol{\xi}),$$

$$\frac{1}{\varrho_{0}}\mathbf{K} = U_{{}_{E}\mathbf{E}}, \qquad \theta = U_{{}_{E}\eta},$$

$$\mathscr{D}(\mathbf{W}, \mathbf{J}) = \mathbf{W} * \mathbf{J} \ge 0 \quad \text{with} \quad \mathscr{D}(\mathbf{W}, 0) = 0,$$
(3.6)

where the ordered sets in the (N + 17)-dimensional space E^{N+17} , W and J, are introduced by

$$\mathbf{W} = \left(\mathbf{K}, \theta, \mathbf{\Pi}, \Pi, \boldsymbol{\xi}, -\frac{1}{\theta} \mathbf{Q}\right), \tag{3.7}$$

 $\mathbf{J} \equiv ({}_{P}\mathbf{D}, \varrho_{0P}\dot{\eta}, \boldsymbol{\pi}, \dot{\boldsymbol{\pi}}, \mathbf{A}, \operatorname{Grad} \boldsymbol{\theta}),$

together with

$$\mathbf{\Pi} = -\varrho_0 U_{\mathbf{\pi}}, \quad \Pi = -\varrho_0 U_{\mathbf{\pi}}, \quad \mathbf{A} = -\varrho_0 U_{\mathbf{\xi}}. \tag{3.8}$$

The operation W * J in (3.6), means the inner product in E^{N+17} defined by

$$\mathbf{W} * \mathbf{J} \equiv \mathbf{A} : \mathbf{a} + Bb + \mathbf{C} : c + Dd + \mathbf{E} \cdot \mathbf{e} + \mathbf{F} \cdot \mathbf{f}$$
(3.9)

for any $B, D, b, d \in E^1$, $\mathbf{F}, \mathbf{f} \in E^3$, $\mathbf{A}, \mathbf{C}, \mathbf{a}, \mathbf{c} \in E^6$ and $\mathbf{E}, \mathbf{e} \in E^N$.

It is not meaningless to point out here that W and J in $(3.6)_5$ are called the generalized force and the generalized flux, respectively, in the irreversible thermodynamics [29].

Inequality $(3.6)_5$ states that the entropy production has a minimum at $\mathbf{J} = 0$. If we assume \mathbf{W} being at least of class C^1 with respect to \mathbf{J} , this minimum is analytic, and hence, $\mathbf{W} = 0$ for $\mathbf{J} = 0$, which means that the force vanishes whenever the corresponding flux vanishes.

Combination of (3.3) with (3.6) yields an alternative version of the energy equation:

$$\varrho_{0}\theta\dot{\eta} + \operatorname{Div}\mathbf{Q} - \varrho_{0}\sigma - \left(\mathscr{D} + \frac{1}{\theta}\mathbf{Q}\cdot\operatorname{Grad}\theta\right) = 0$$
(3.10)

which will be used later.

4 Constitutive Equations for the Plastic Parts

Let us assume that the constitutive equations for the plastic quantities W take the form

$$\mathbf{W} = \mathbf{W}(\mathbf{J}; \mathbf{j}), \tag{4.1}$$

where, as was explained in the preceding section, W is at least of class C^1 in J. Following the decomposition theorem by Edelen [21, 22], we can write the explicit form of (4.1) as

$$\mathbf{W} = \boldsymbol{\varphi}_{\mathbf{J}}(\mathbf{J}; \mathbf{j}) + \mathbf{U}(\mathbf{J}; \mathbf{j}), \tag{4.2}$$

where the anomaly term U(J; j) has the following property:

$$\mathbf{J} * \mathbf{U} = 0, \qquad \mathbf{U}(0; \mathbf{j}) = 0 \ \forall \ \mathbf{j}.$$

$$(4.3)$$

In the following discussion, we restrict ourselves to the case in which

$$\mathbf{U} = \mathbf{0}.\tag{4.4}$$

The scalar function $\Phi(\mathbf{J}; \mathbf{j})$, which is called the dissipation potential, is of class C^2 in \mathbf{J} , and is given as a solution of the differential inequality

$$\mathcal{D} = \Phi_{\mathbf{J}} * \mathbf{J} \ge 0. \tag{4.5}$$

This is solved to be

$$\Phi(\mathbf{J};\mathbf{j}) = h(\mathbf{j}) + \int_{0}^{\infty} \mathscr{D}(\mathbf{W};\lambda\mathbf{J}) \frac{\mathrm{d}\lambda}{\lambda}, \qquad (4.6)$$

where $h(\mathbf{j})$ is an arbitrary, physically irrelevant function.

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The complete expression of the plastic quantities W is now available in the form

$$\begin{split} \mathbf{K} &= \boldsymbol{\Phi}_{p\mathbf{\overline{D}}}, \qquad \boldsymbol{\theta} = \boldsymbol{\Phi}_{\boldsymbol{\theta} \circ p \boldsymbol{\overline{\eta}}}, \\ \mathbf{\Pi} &= \boldsymbol{\Phi}_{\mathbf{\pi}}, \qquad \boldsymbol{\Pi} = \boldsymbol{\Phi}_{\mathbf{\pi}}, \\ \dot{\boldsymbol{\xi}} &= \boldsymbol{\Phi}_{\mathbf{A}}, \qquad -\frac{1}{\theta} \, \mathbf{Q} = \boldsymbol{\Phi}_{\text{Grad}\theta}. \end{split}$$
(4.7)

For later convenience, we employ the following ordered sets:

$$\begin{split} \tilde{\mathbf{W}} &= (\mathbf{K}, \theta, \mathbf{\Pi}, \Pi), \\ \tilde{\mathbf{W}} &= \left(\dot{\mathbf{\xi}}, -\frac{1}{\theta} \mathbf{Q} \right), \\ \tilde{\mathbf{J}} &= \left({}_{P} \overline{\mathbf{D}}, \ \varrho_{0P} \dot{\eta}, \ \dot{\boldsymbol{\pi}}, \dot{\boldsymbol{\pi}} \right), \\ \tilde{\mathbf{J}} &\equiv (\mathbf{A}, \operatorname{Grad} \theta). \end{split}$$

$$(4.8)$$

The constitutive equation (4.7) is then rewritten as

$$\begin{split} \tilde{\mathbf{W}} &= \boldsymbol{\varPhi}_{\tilde{\mathbf{J}}}(\tilde{\mathbf{J}}, \tilde{\mathbf{J}}; \mathbf{j}), \\ \tilde{\mathbf{W}} &= \boldsymbol{\varPhi}_{\widetilde{\mathbf{J}}}(\tilde{\mathbf{J}}, \tilde{\mathbf{J}}; \mathbf{j}), \end{split}$$
(4.9)

and the inequality $(3.6)_5$ takes the form

$$\mathscr{D} = \mathbf{W} * \mathbf{J} = \mathbf{\tilde{W}} * \mathbf{\tilde{J}} + \mathbf{\tilde{W}} * \mathbf{\tilde{\tilde{J}}} \ge 0.$$
(4.10)

In the above equation, every symbol * means the inner product but in different dimensional spaces. The definition of the last two inner products can, although it is not written explicitly, be understood from (3.9) and (4.8).

Let us assume that the plastic deformation is characterized by the dissipation potential

$$\Phi(\mathbf{J};\mathbf{j}) = \tilde{\Phi}(\tilde{\mathbf{J}};\mathbf{j}) + \tilde{\tilde{\Phi}}(\tilde{\mathbf{J}};\mathbf{j}), \tag{4.11}$$

where the first part of the potential, $\tilde{\Phi}(\mathbf{J}; \mathbf{j})$, is proposed to be homogeneous of order one in \mathbf{J} ; i.e.

$$ilde{\Phi}(\lambda ilde{\mathbf{J}}\,;\,\mathbf{j}) = \lambda ilde{\Phi}(ilde{\mathbf{J}}\,;\,\mathbf{j}) \quad \forall \, \lambda > 0. aga{4.12}$$

Then, Euler's theorem states that

$$\tilde{\Phi}_{\tilde{\mathbf{j}}} * \tilde{\mathbf{J}} = \tilde{\Phi} \tag{4.13}$$

holds.

Differentiating (4.13) with respect to $\tilde{\mathbf{J}}$, we obtain

 $\tilde{\Phi}_{\tilde{1}\tilde{1}} * \tilde{\mathbf{J}} = \mathbf{0}. \tag{4.14}$

For this to hold for all \hat{J} ,

$$\det\left(\tilde{\boldsymbol{\Phi}}_{\tilde{\mathbf{j}}\tilde{\mathbf{j}}}\right) = 0 \tag{4.15}$$

must be satisfied for all $\tilde{\mathbf{J}} \neq 0$. Provided that

$$\operatorname{rank}\left(\tilde{\Phi}_{\tilde{\mathbf{J}}\tilde{\mathbf{J}}}\right) = \dim\left(\tilde{\mathbf{J}}\right) - 1,\tag{4.16}$$

this suggests the existence of a scalar function $\overline{\Gamma}(\mathbf{\tilde{W}};\mathbf{j})$ which has the property [30]

 $\overline{\Gamma} = 0$ if $\mathbf{J} \neq 0$.

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Now we can conclude that there exists such an inverse transformation of $(4.9)_1$ that

$$\mathbf{\tilde{J}} = \begin{cases} \Lambda \overline{\Gamma}_{\widetilde{\mathbf{W}}}(\widetilde{\mathbf{W}}; \mathbf{j}) \ \forall \ \widetilde{\mathbf{W}} | \ \overline{\Gamma} = 0, \\ 0 \qquad \forall \ \widetilde{\mathbf{W}} | \ \overline{\Gamma} \neq 0, \end{cases}$$
(4.16)

where Λ is a multiplier to be determined. Without loss of generality we put such additional assumption for the scalar function $\overline{\Gamma}$ introduced above that

$$\overline{\Gamma}_{\widetilde{\mathbf{W}}} \neq 0 \quad ext{while} \quad \overline{\Gamma} = 0.$$

Equations (4.9), (4.10) and (4.13), together with (4.11), combine to yield a formula for \mathscr{D} in the form

$$\mathscr{D} = \tilde{\varPhi}(\tilde{\mathbf{J}}; \mathbf{j}) + \tilde{\varPhi}_{\widetilde{\mathbf{J}}}(\tilde{\overline{\mathbf{J}}}; \mathbf{j}) * \tilde{\mathbf{J}} \ge 0.$$
 (4.17)

We could show that under the condition considered this implied

$$\tilde{\varPhi}(\mathbf{\tilde{j}};\mathbf{j}) \ge 0 \quad ext{and} \quad \tilde{\varPhi}_{\mathbf{\tilde{j}}}(\mathbf{\tilde{\tilde{j}}};\mathbf{j}) * \mathbf{\tilde{\tilde{j}}} \ge 0.$$

$$(4.18)$$

Equations (4.13) and (4.18)_i ensure $\tilde{\Phi} = 0$ only at $\tilde{\mathbf{J}} = 0$, otherwise $\tilde{\Phi} > 0$. Then, the inverse transformation (4.16) can be rewritten as

$$\tilde{\mathbf{J}} = \begin{cases}
\Lambda \overline{\Gamma}_{\widetilde{\mathbf{W}}} & \text{if } \overline{\Gamma} = 0 \text{ and } \Lambda \ge 0, \\
0 & \text{if } \overline{\Gamma} < 0,
\end{cases}$$
(4.19)

where the condition $\overline{\Gamma} \neq 0$ has been replaced by $\overline{\Gamma} < 0$ without any loss of generality. The multiplier Λ is determined from the condition $\widehat{\Gamma} = 0$.

If the one-one correspondence of the constitutive equations for the elastic processes $(3.6)_{3,4}$ is taken into account, the dependence on the ordered set $(\tilde{W}; j)$ may be replaced by the dependence on

$$\boldsymbol{\omega} \equiv (\mathbf{K}, \theta, \boldsymbol{\pi}, \pi)$$
 and $\boldsymbol{\xi}$.

We can, therefore, introduce a new scalar function, the so-called yield function in the theory of plasticity, through the relation

$$\Gamma(\mathbf{W};\mathbf{j}) = \Gamma(\boldsymbol{\omega},\boldsymbol{\xi}). \tag{4.20}$$

It was proved that the yield surface $\Gamma = 0$ is a convex surface in the stress space. The form of the yield function might be further restricted, provided that the pressure-insensitivity of the plastic deformation is taken into account.

Equation (4.20) gives us an alternative expression of the constitutive equation (4.19) in the form,

$$\mathbf{\tilde{J}} = \begin{cases}
\Delta \Gamma_{\mathbf{\omega}} & \text{if } \Gamma = 0 \text{ and } \Lambda \ge 0, \\
0 & \text{if } \Gamma < 0,
\end{cases}$$
(4.21)

which is called the flow rule in the ordinary theory of plasticity. With the multiplier Λ determined from

$$\Gamma(\mathbf{W};\mathbf{j})=\dot{\Gamma}(\boldsymbol{\omega},\boldsymbol{\xi})=0,$$

<u>.</u>

the constitutive equation $\mathbf{\tilde{J}}=\boldsymbol{\varDelta \Gamma _{\boldsymbol{\omega}}}$ can be written explicitly as

$$P \mathbf{\overline{D}} = G(\Gamma_{\mathbf{K}} \otimes \Gamma_{\mathbf{K}}) : \dot{\mathbf{K}} + G(\Gamma_{\mathbf{K}}\Gamma_{\theta}) \dot{\theta} + G(\Gamma_{\mathbf{K}} \otimes \Gamma_{\mathbf{\xi}}) \cdot \dot{\mathbf{\xi}},$$

$$\varrho_{0P} \dot{\eta} = G(\Gamma_{\theta}\Gamma_{\mathbf{K}}) : \dot{\mathbf{K}} + G(\Gamma_{\theta}\Gamma_{\theta}) \dot{\theta} + G(\Gamma_{\theta}\Gamma_{\mathbf{\xi}}) \cdot \dot{\mathbf{\xi}},$$

$$\dot{\pi} = G(\Gamma_{\pi} \otimes \Gamma_{\mathbf{K}}) : \dot{\mathbf{K}} + G(\Gamma_{\pi}\Gamma_{\theta}) \dot{\theta} + G(\Gamma_{\pi} \otimes \Gamma_{\mathbf{\xi}}) \cdot \dot{\mathbf{\xi}},$$

$$\dot{\pi} = G(\Gamma_{\pi}\Gamma_{\mathbf{K}}) : \dot{\mathbf{K}} + G(\Gamma_{\pi}\Gamma_{\theta}) \dot{\theta} + G(\Gamma_{\pi}\Gamma_{\mathbf{\xi}}) \cdot \dot{\mathbf{\xi}},$$
(4.22)

where

$$G \equiv -[\Gamma_{\pi} \colon \Gamma_{\pi} + \Gamma_{\pi} \Gamma_{\pi}]^{-1}, \qquad (4.22a)$$

and the symbol \otimes stands for the tensor product.

Equations (4.22) and (4.9)₂ constitute a full set of constitutive equations for the thermoplastic process. The last two equations of (4.22) and the first equation of (4.9)₂ or (4.7)₅ are called the evolutional equations [14, 16], which specify the growth of the internal state variables π , π and ξ , respectively. The second equation of (4.9)₂ or (4.7)₆ may be regarded as the constitutive equation of the heat flux **Q**.

In summarizing, the thermoplastic materials in the process of phase transition can be completely described by $(3.6)_{3,4}$, (4.22) and $(4.9)_2$. The behavior of the material is, therefore, specified through the internal energy U and the dissipation potential Φ . The former characterizes the elastic process and the latter the plastic process. In this theory, a part of Φ , $\tilde{\Phi}$ which determines \tilde{W} , is shown to be replaced by the yield function Γ . This will be explained in practice in Section 6.

5 Rate-Type Constitutive Equations for K and η

A set of rate-type constitutive equations for **K** and η is derived in this section. We first differentiate $(3.6)_{3,4}$ with respect to time. Assuming that the elastic deformation is not influenced by the plastic deformation [31], i.e.

$$\begin{split} U_{_{B}\mathbf{E}\boldsymbol{\pi}} &= 0, \qquad U_{_{E}\mathbf{E}\boldsymbol{\pi}} = 0, \\ U_{_{E}\eta\boldsymbol{\pi}} &= 0, \qquad U_{_{R}\eta\boldsymbol{\pi}} = 0, \end{split} \tag{5.1}$$

we get the following formulas:

$$\dot{\mathbf{K}} = \boldsymbol{\Delta} : {}_{\mathcal{B}} \dot{\mathbf{E}} + \boldsymbol{\Theta} \dot{\boldsymbol{\theta}} + {}_{\mathbf{K}} \boldsymbol{\Xi} \cdot \dot{\boldsymbol{\xi}},$$

$${}_{\mathcal{B}} \dot{\boldsymbol{\eta}} = -\frac{1}{\varrho_0} \boldsymbol{\Theta} : {}_{\mathcal{B}} \dot{\mathbf{E}} + \frac{1}{\varrho_0} c \dot{\boldsymbol{\theta}} + {}_{\eta} \boldsymbol{\Xi} \cdot \dot{\boldsymbol{\xi}},$$
(5.2)

where we have introduced the material tensors defined by

$$\begin{split} \mathbf{\Delta} &= \varrho_0 [U_{_{E}\mathbf{E}_{E}\mathbf{E}} - (U_{_{E^{\eta}E^{\eta}}})^{-1} (U_{_{E}\mathbf{E}_{E^{\eta}}} \otimes U_{_{E^{\eta}E}\mathbf{E}})], \\ \mathbf{\Theta} &= \varrho_0 (U_{_{E^{\eta}E^{\eta}}})^{-1} U_{_{E}\mathbf{E}_{E^{\eta}}}, \\ \mathbf{K} \mathbf{\Xi} &= (U_{_{E^{\eta}E^{\eta}}})^{-1} (U_{_{E}\mathbf{E}_{E^{\eta}}} \otimes \mathbf{A}_{_{E^{\eta}}}) - \mathbf{A}_{_{E}\mathbf{E}}, \\ c &= \varrho_0 (U_{_{E^{\eta}E^{\eta}}})^{-1}, \\ \eta \mathbf{\Xi} &= \frac{1}{\varrho_0} (U_{_{E^{\eta}E^{\eta}}})^{-1} \mathbf{A}_{_{E^{\eta}}}. \end{split}$$
(5.2a)

The tensors Δ and Θ correspond to the elastic moduli tensor and the thermoelastic moduli tensor, while c has the dimension of the specific heat when divided by the temperature.

With the use of (2.11) and $(4.22)_{1,2}$ together with (5.2), we arrive at the final rate-type constitutive equations for **K** and η :

$$\begin{split} \dot{\mathbf{K}} &= \tilde{\mathbf{\Delta}} : \mathbf{\bar{D}} + \mathbf{\tilde{\Theta}} \dot{\theta} + \mathbf{K} \mathbf{\tilde{\Xi}} \cdot \mathbf{\dot{\xi}}, \\ \dot{\eta} &= -\frac{1}{\varrho_0} \mathbf{\tilde{\Theta}} : \mathbf{\bar{D}} + \frac{1}{\varrho_0} \mathbf{\tilde{c}} \dot{\theta} + \mathbf{\eta} \mathbf{\tilde{\Xi}} \cdot \mathbf{\dot{\xi}}, \end{split}$$
(5.3)

where we have defined the material tensors by

$$\begin{split} \tilde{\boldsymbol{\Delta}} &\equiv \boldsymbol{\Delta} - g(\boldsymbol{\Delta} \colon \boldsymbol{\Gamma}_{\mathbf{K}}) \otimes (\boldsymbol{\Gamma}_{\mathbf{K}} \colon \boldsymbol{\Delta}), \\ \tilde{\boldsymbol{\Theta}} &\equiv \boldsymbol{\Theta} - g(\boldsymbol{\Delta} \colon \boldsymbol{\Gamma}_{\mathbf{K}}) \left(\boldsymbol{\Gamma}_{\boldsymbol{\theta}} + \boldsymbol{\Gamma}_{\mathbf{K}} \colon \boldsymbol{\Theta} \right), \end{split}$$
(5.3a)

$$\begin{split} \mathbf{\tilde{E}} &= \mathbf{K} \mathbf{\Xi} - g(\mathbf{\Delta} \colon \Gamma_{\mathbf{K}}) \otimes (\Gamma_{\mathbf{\xi}} + \Gamma_{\mathbf{K}} \colon \mathbf{K} \mathbf{\Xi}), \\ \tilde{c} &= c + g(\Gamma_{\theta} + \mathbf{\Theta} \colon \Gamma_{\mathbf{K}})^{2}, \\ \eta \tilde{\mathbf{\Xi}} &= \eta \mathbf{\Xi} + \frac{1}{\rho_{0}} g(\Gamma_{\theta} + \mathbf{\Theta} \colon \Gamma_{\mathbf{K}}) (\Gamma_{\mathbf{\xi}} + \Gamma_{\mathbf{K}} \colon \mathbf{K} \mathbf{\Xi}), \end{split}$$
(5.3a)

with

$$g \equiv [\Gamma_{\mathbf{K}} : \Delta : \Gamma_{\mathbf{K}} - G^{-1}]^{-1}.$$
(5.3b)

In closing this section, we give a brief scheme for solving the boundary-value problems. The quantities estimated in the intermediate configuration can always be transformed to their version in the current configuration by means of, for example, (3.3a). The same is possible for the rate quantities, such as $\dot{\mathbf{K}}$, although the transformation formulas are somewhat complicated in this case. We could, therefore, derive a set of governing equations for the displacement and the temperature in the current configuration, i.e. the equation of motion and the heat conduction equation. In fact, they might be given in rate or incremental form.

6 Some Comments and Consequences

In this section, the general theory developed in the preceding sections is explained in detail on some topics.

6.1 C-C-T and T-T-T diagrams [23]

As a general expression of the evolutional equation for ξ , we proposed in (4.7)₅ and (4.11) the following form:

$$\dot{\boldsymbol{\xi}} = \boldsymbol{\varPhi}_{\boldsymbol{A}}(\boldsymbol{J}; \boldsymbol{j}) = \boldsymbol{\varPhi}_{\boldsymbol{A}}(\widetilde{\boldsymbol{J}}; \boldsymbol{j}). \tag{6.1}$$

In this subsection, let us limit our attention to the case in which the dissipation potential be further restricted to

$$\begin{split} \varPhi(\mathbf{J};\mathbf{j}) &= \tilde{\varPhi}(\mathbf{\tilde{J}};\mathbf{j}) + \tilde{\varPhi}(\mathbf{\tilde{J}};\mathbf{j}) \\ &= \tilde{\varPhi}(\mathbf{\tilde{J}};\mathbf{j}) + \mathbf{\varrho}\tilde{\varPhi}(\operatorname{Grad}\theta;\mathbf{j}) + \mathbf{\xi}\tilde{\varPhi}(\mathbf{A};\mathbf{j}). \end{split}$$
(6.2)

Each part of the potential should of course be chosen so as to be compatible with (4.18.) We assume that this is the case in the following discussion. The evolutional equation (6.1) thus reduces to

$$\dot{\boldsymbol{\xi}} = \boldsymbol{\Phi}_{\mathbf{A}} = \boldsymbol{\xi} \boldsymbol{\tilde{\Phi}}_{\mathbf{A}}(\mathbf{A}; \mathbf{j}). \tag{6.3}$$

In order to proceed further, let us suppose the case in which the deformation of materials has no effect on the progress of phase transition, and then, the far right-side of (6.3) may be expressed as

$$\dot{\boldsymbol{\xi}} = \boldsymbol{\xi} \widetilde{\boldsymbol{\Phi}}_{\mathbf{A}}(\mathbf{A}; \mathbf{j}) = \widetilde{\boldsymbol{M}}(\boldsymbol{\xi}) \cdot \mathbf{N}(\boldsymbol{\theta}).$$
(6.4)

We emphasize that this type of evolutional equation for $\boldsymbol{\xi}$ has a sound experimental background [18]. Equation (6.4) could be integrated for an arbitrary uniform temperature history $\theta(t)$ from $(t, \boldsymbol{\xi}) = (0, \boldsymbol{\xi}_0)$ to an arbitrary generic point $(t, \boldsymbol{\xi})$, where $\boldsymbol{\xi}_0 \equiv \boldsymbol{\xi}|_{t=t_0}$. The result reads

$$\int_{\xi_0}^{\xi} \mathbf{M}(\xi) \cdot \mathrm{d}\xi = \int_0^t \mathbf{N}(\theta(t)) \,\mathrm{d}t.$$
(6.5)

This equation suggests the existence of an expression for the extent of phase transition $\boldsymbol{\xi}$ that

$$\boldsymbol{\xi} = \boldsymbol{M}(t). \tag{6.6}$$

Equation (6.6) corresponds to the continuous cooling transformation (C-C-T) diagram which is studied in detail in metallurgy. In order to clear the situation discussed, let us consider a process

of constant cooling rate; $\theta(t) = \vartheta t + \vartheta_0$ with the constants ϑ and ϑ_0 . Equation (6.6) could now be written as

$$\boldsymbol{\xi} = \widetilde{\mathbf{M}}(t; \theta, \vartheta). \tag{6.7}$$

When (6.7) is plotted in the $\theta - t$ plane with ϑ as a parameter and $\boldsymbol{\xi}$ as the parameters along the curves, the diagram obtained is no other than a C-C-T diagram.

When the temperature history is chosen so that

$$\theta(t) = \begin{cases} \frac{\vartheta - \vartheta_0}{\hat{t}} t + \vartheta_0; 0 \le t < \hat{t} \\ \vartheta \qquad ; t \ge \hat{t} \end{cases}$$
(6.8)

for the given temperatures ϑ and ϑ_0 , and (6.5) is estimated for sufficient small values of \hat{t} , a formula for $\boldsymbol{\xi}$ derived, which could be written as

$$\boldsymbol{\xi} = \hat{\mathbf{M}}(t; \vartheta), \tag{6.9}$$

corresponds to the isothermal time-temperature-transformation (T-T-T) diagram.

Returning to (6.1), the equation could be said to specify the progress of the phase transition which is strongly influenced by the elasto-plastic deformation of the materials. Therefore, the C-C-T diagram, if it could be constructed in this case, depends on the full history that the material has been experienced before.

6.2 Constitutive Equation for **Q**

The constitutive equation for the heat flux $(4.7)_6$ reduces to

$$\mathbf{Q} = -\mathbf{\varkappa} \cdot \operatorname{Grad} \theta, \tag{6.10}$$

if the potential $_{\mathbf{Q}}\tilde{\Phi}(\operatorname{Grad} \theta; \mathbf{j})$ in $(6.2)_2$ is chosen with a positive definite tensor of the second rank $\boldsymbol{\varkappa}$ in the form

$${}_{\mathbf{q}}\widetilde{\widetilde{\Phi}}(\operatorname{Grad}\,\theta;\mathbf{j}) = \frac{1}{\theta}\,\mathbf{\varkappa}:(\operatorname{Grad}\,\theta\otimes\operatorname{Grad}\,\theta). \tag{6.11}$$

6.3 Infinitesimal Theory

In this subsection we reduce the theory to the case of infinitesimal deformation. The concrete procedure of the linearization is not discussed here since one could find a similar discussion elsewhere [31, 32].

We employ the dissipation potential written by $(6.2)_2$. The yield function might have the following form, provided that the absence of the Bauschinger effect is assumed:

$$\Gamma = \mathbf{K} : \mathbf{\Gamma} : \mathbf{K} - 1 = 0,$$

$$\mathbf{\Gamma} = \mathbf{\Gamma}(\hat{\boldsymbol{\omega}}, \boldsymbol{\xi}), \quad \hat{\boldsymbol{\omega}} \equiv (\boldsymbol{\theta}, \boldsymbol{\pi}, \boldsymbol{\pi}),$$
(6.12)

where the material tensor Γ has the same symmetry properties as the elastic moduli tensor Δ . It is worth noting here that according to the linearization \mathbf{K}, π and $\mathbf{\overline{D}}$ coincide with their

alternative version in the current configuration, i.e. $\mathbf{T}, \overline{\boldsymbol{\pi}}$ and \mathbf{D} , respectively. If the pressure-insensitivity of the plastic deformation is taken into account, the yield function (6.12) is shown to be expressed as [33]

$$\Gamma = \mathbf{K}^* : \mathbf{\Gamma} : \mathbf{K}^* - 1 = 0,$$

$$\mathbf{K}^* = \mathbf{K} - \frac{1}{3} \mathbf{1} \text{ tr } \mathbf{K},$$
(6.13)

together with

$$1: \mathbf{\Gamma} = \mathbf{\Gamma}: 1 = 0$$

In order to proceed further we assume that the material tensors are isotropic, and hence can be written as

$$\begin{aligned}
\Delta_{ijkl} &= \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}), \\
\mathbf{\Theta}_{ij} &= a \delta_{ij}, \\
\mathbf{K} \mathbf{\Xi}_{ijk} &= b_k \delta_{ij}, \\
\Gamma_{ijkl} &= \alpha \delta_{ij} \delta_{kl} + \beta (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}).
\end{aligned}$$
(6.14)

The material constants λ , μ , α , **b**, α and β are in general functions of $\hat{\boldsymbol{\omega}}$ and $\boldsymbol{\xi}$. Equation (6.14)₃ states that the phase transitions discussed here exhibit only the isotropic change in kinematics. Combination of (6.13)₁ and (6.14)₄ leads to

$$\Gamma = \frac{1}{2} \mathbf{K}^* : \mathbf{K}^* - k = 0,$$

$$k(\hat{\boldsymbol{\omega}}, \boldsymbol{\xi}) \equiv \frac{1}{4\beta},$$
(6.15)

which is no other than von Mises' yield condition generalized to our context.

The rate-type constitutive equations for \varkappa and η are now reduced to

$$\dot{\mathbf{K}} = \lambda \mathbf{1} \text{ tr } \mathbf{D} + 2\mu \mathbf{D} + a\mathbf{1}\dot{\theta} + (\mathbf{1} \otimes \mathbf{b}) \cdot \dot{\boldsymbol{\xi}} - 2\mu g(2\mu \mathbf{K}^*; \mathbf{D} - k_{\theta}\dot{\theta} - k\boldsymbol{\xi} \cdot \dot{\boldsymbol{\xi}}) \mathbf{K}^*,$$

$$\dot{\eta} = -\frac{1}{\varrho_0} a \text{ tr } \mathbf{D} + \frac{1}{\varrho_0} c\dot{\theta} + {}_{\eta} \mathbf{\Xi} \cdot \dot{\boldsymbol{\xi}} - \frac{1}{\varrho_0} gk_{\theta}(2\mu \mathbf{K}^*; \mathbf{D} - k_{\theta}\dot{\theta} - k\boldsymbol{\xi} \cdot \dot{\boldsymbol{\xi}}).$$

$$(6.16)$$

From $(6.16)_1$ we can derive the formula

$$\operatorname{tr} \mathbf{D} = \frac{1}{3\lambda + 2\mu} \operatorname{tr} \dot{\mathbf{K}} - \frac{3a}{3\lambda + 2\mu} \dot{\theta} - \frac{3}{3\lambda + 2\mu} \mathbf{b} \cdot \dot{\boldsymbol{\xi}}.$$
(6.17)

Integrating this from t = 0 to t along the path under the condition of stress-free, i.e. $\mathbf{K} = 0$, we obtain

$$\int_{0}^{t} \operatorname{tr} \mathbf{D} \, dt = -\int_{0}^{t} \frac{3a}{3\lambda + 2\mu} \, \dot{\theta} \, \mathrm{d}t - \int_{0}^{t} \frac{3}{3\lambda + 2\mu} \, \mathbf{b} \cdot \dot{\mathbf{\xi}} \, \mathrm{d}t.$$
(6.18)

Relation (6.18), which is often called the dilatation curve [18] once plotted \int_{0}^{1} tr **D** dt vs. θ , reveals that the change in volume, the term on the left-hand side, is composed of the thermal expansion, the first term on the right-hand side, and the expansion due to the phase transition, the second term. The relation also suggests that the material tensor **b** could be determined experimentally from the dilatation curves, provided that the evolutional equation for $\boldsymbol{\xi}$ is explicitly given.

The heat conduction equation follows from the energy equation (3.10) along with (4.22), (6.15) and (6.16) in the form

$$\boldsymbol{\varkappa}: \operatorname{grad} \operatorname{grad} T - \hat{c}\dot{T} - \varrho_0 \hat{\sigma} = -\theta_0 a \operatorname{tr} \mathbf{D} + 2\mu g \tilde{k} \mathbf{K}^*: \mathbf{D}, \qquad (6.19)$$

with

$$\begin{split} \hat{c} &\equiv \theta_0 c - g \tilde{k} k_T, \\ \hat{\sigma} &\equiv \sigma + \frac{1}{\varrho_0} \left(\varrho_0 \theta_{0,\eta} \Xi + \mathbf{A} - g \tilde{k} k_{\Xi} \right) \cdot \dot{\Xi}, \\ \tilde{k} &\equiv 2k - 2\theta_0 k_T - \pi \colon k_\pi - \pi k_\pi, \end{split}$$
(6.19a)

where the constitutive equation for the heat flux (6.10) was employed, while θ_0 and T stand for the reference uniform temperature and the excess temperature above it, respectively, i.e.

$$T = \theta - \theta_0. \tag{6.20}$$

The excess temperature T is assumed to be small compared to θ_0 , i.e. $|T/\theta_0| \ll 1$.

The second part of $(6.19a)_{1,2}$ and the second term on the right-hand side of (6.19) come from the assumption (2.13). Among the terms, the second part of $(6.19a)_2$ represents the heat production due to the phase transitions, i.e. the latent heat.

The heat conduction equation (6.19) need be supplemented by the equation of motion, which reads under the assumptions considered here

$$\varrho_0 \ddot{\mathbf{x}} = \operatorname{div} \mathbf{K} + \varrho_0 \mathbf{f}, \tag{6.21}$$

in order to complete the governing equations for the displacement and the temperature fields.

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