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Improved thermodynamic treatment of vacancy-mediated diffusion and creep

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ABSTRACT

Approximately a decade ago a new concept to describe the kinetics of one-phase solid state systems evolving by diffusion and activity of vacancies has been published by the authors. The concept is based on the Onsager-Ziegler Thermodynamic Extremal Principle (TEP). In course of the last decade several improvements and corrections have been performed, which justify an overworking of the concept. A short introduction of the TEP is followed by a detail investigation of the Gibbs energy and its rate as well as of dissipation and dissipation function due to multicomponent diffusion process coupled with vacancy activity provoking swelling/shrinkage and creep and thus internal stress state development. The application of TEP allows an exact derivation of driving forces for the coupled processes. The Manning theory of diffusion is applied and the derivation of evolution equations for all system parameters (site fractions, swelling/shrinkage and creep strain tensor) is provided.

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1. Introduction and motivation

During the last more than one decade the Thermodynamic Extremal Principle (TEP) has been applied to derive the leading equations for diffusion taking into account.

- multicomponent system,
- vacancy mediated diffusion accounting for intensities of sources/sinks for generation/annihilation of vacancies varying from zero to infinity,
- role of stress state by accounting for hydrostatic stress as well as stress deviator,
- role of (sharp) interfaces between individual phases accounted by so-called jump condition for chemical potentials and fluxes,
- diffusion along lines and surfaces and contact conditions at their junctions.

As representative examples the following papers are listed, see, e.g. Refs. [1–6], denoted later as “previous papers”. The reader finds references to important contributions, together with some details with respect to the a/m topics, of the second half of the last century in Ref. [6]. In the last decade some weak points in the derivation of leading equations for diffusion were detected both by the authors and their group as well as by other researchers. These shortcomings have been recognized and repaired. The first motivation for this paper is to re-investigate these weak points mainly due to the fact that they were reported on several places. A complete theory with corrected weak points is now presented. We have tried to avoid a too general and complicated treatment and consider the internal strain (and stress) state development due to vacancy activity (their generation/annihilation and short-range motion between jogs at dislocations) as a separate process interacting with diffusion.

As second motivation a reply to the much stronger criticism is given, namely that the TEP does not hold or is useless. Here we refer to the next section of this paper. The argument of “being false” stems mainly from the phase-field community. As representative sources for the phase field method see, e.g., [7,8]. However, bridging the gap between the TEP and the phase-field method is possible and is, indeed, not very complicated. Both concepts work with thermodynamic forces and fluxes related in a linear form. Both concepts start with a proper definition and selection of the energy terms. McDowell motivated some years ago to write a corresponding paper demonstrating the relation of both concepts as well as their applicability on simple examples, see the Acta mater. paper [9].

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As third motivation can be considered that all thermodynamic equations are formulated in the actual configuration fixed to the lattice and they can be related to a space (laboratory)-fixed coordinate system. A number of various specific reference systems and concepts are still used, see, e.g., Anderson and Ågren [10], Paul et al. [11] and the Polish group [12,13]. We do not want to criticize the works of our colleagues, but we are of the opinion that just one laboratory fixed coordinate system and just one actual configuration fixed to the lattice are the best selection for the description of the system and physical processes in it. Respective relations of the descriptions can be taken from standard continuum mechanics, see, e.g., [14,15].

2. The Thermodynamic Extremal Principle (TEP)

2.1. Introduction to the TEP

With respect to the history of this principle we refer to Onsager, 1931, Ziegler, 1963 and the overview in Acta mater [16] with the corresponding references. Concerning a material system we distinguish external variables X_i, i=1,...,n_{ext} from the set $\{X\}$ and internal (sometimes denoted as hidden) variables x_i, i=1,...,n_{int} from the set $\{x\}$. With respect to this determination we refer to the classical literature of continuum mechanics and thermodynamics, e.g. Truesdell and Toupin [17] and Coleman and Gurtin [18], concluding that only the rates of the internal variables appear in the dissipation, see below. We denote the material time derivative (rate) of a quantity, e.g. u, by a dot as $\dot{u}$.

An illustrative example of internal variables $\{x\}$, definitions, derivations and according details can be found in Ref. [6]. In the paper a representative volume element (RVE) of a multicomponent system is considered with the volume W in the actual configuration. The RVE is supposed to be a sufficiently small part of the system, so that it can be considered as a homogeneous one, but it is also large enough to allow a statistical approach.

The Gibbs energy G of the RVE is a function G=$G(\{X\},\{x\})$ including some, often time-independent, material parameters. The rate $\dot{G}$ follows as

$$\dot{G} = \sum_{i=1}^{n_{\mathrm{ext}}} \frac{\partial G}{\partial X_i}\dot{X}_i + \sum_{i=1}^{n_{\mathrm{int}}} \frac{\partial G}{\partial x_i}\dot{x}_i, \tag{1}$$

and the dissipation $D = D(\{X\},\{x\},\{\dot{x}\})$ in the system is defined as

$$D = -\sum_{i=1}^{n_{\mathrm{int}}} \frac{\partial G}{\partial x_i}\dot{x}_i = -\sum_{i=1}^{n_{\mathrm{int}}} \frac{\partial \dot{G}}{\partial \dot{x}_i}\dot{x}_i = W\sum_{i=1}^{n_{\mathrm{int}}} f_{\dot{x},i}\dot{x}_i, \tag{2}$$

The equation for the dissipation stems from the combination of the equations for the entropy production and the energy balance in rate form, including the (material) time derivative of the Gibbs energy G. To assure the entropy production to be positive, all terms multiplied by the rates of the external variables must disappear. Finally the dissipation consists only of the rates of the internal variables multiplied by the according force terms. This fact can mathematically be expressed in the following context by simple writing “keeping the external variables as fixed (in the variational procedure)”. For a detailed derivation we refer here to Sect. 2, Thermodynamic Processes, in Coleman and Gurtin [18]. The quantities $f_{\dot{x}}, i = -(1/W)\partial G/\partial x_i = -(1/W)\partial \dot{G}/\partial \dot{x}_i$ are denoted as thermodynamic forces being conjugated to $\dot{x}_i$ as the rates of internal variables, which may represent one of the possible sets of kinetic variables of the system.

Furthermore, we assign a dissipation function $Q = Q(\{X\},\{x\},\{\dot{x}\})$ being a non-negative function such that

$$Q = D. \tag{3}$$

The function Q is assumed as homogeneous function of order l in $\dot{x}_i$ (in the actual case l=2), accounts for the kinetic material parameters (e.g. diffusion coefficients) and structure parameters (e.g. grain structure) of the system and does not involve any thermodynamic forces $f_{\dot{x},i}$, i, for more details we refer to the overview [16] in Acta mater. We do not deal with other types of description of the dissipation mechanisms as the Onsager-Casimir case [19,20], or some other types of dissipation favouring the introduction of a so-called dissipation potential, see the treatment of rate independent processes by Glitzky and Mielke [21] and the recent study by Goddard [22].

2.2. Formulation of the TEP in rates of internal variables

The TEP states that the dissipation D assumes a maximum subjected to the constraint (3). Also further constraints with respect to the rates of internal variables (e.g. mass balances etc.) can be met. With no further constraints the corresponding Lagrangian follows using Eqs. (2) and (3) as

$$\mathfrak{L} = D - \lambda(Q - D) \tag{4}$$

with λ being a Lagrange multiplier. Maximizing of $\mathfrak{L}$ with respect to the rates $\dot{x}_i$ of internal variables provides the following relation between the thermodynamic forces $f_{\dot{x},i}$ and the kinetic parameters $\dot{x}_i$ as

$$Wf_{\dot{x},i} = \frac{Q}{\sum_{j=1}^{n_{\mathrm{int}}} \frac{\partial Q}{\partial \dot{x}_j}\dot{x}_j}\frac{\partial Q}{\partial \dot{x}_i}. \tag{5}$$

Since Q is supposed to be a homogeneous function in $\dot{x}_i$ of order l, thus $\sum_{j=1}^{n_{\mathrm{int}}} \frac{\partial Q}{\partial \dot{x}_j}\dot{x}_j = lQ$, and consequently

$$Wf_{\dot{x},i} = \frac{1}{l}\frac{\partial Q}{\partial \dot{x}_i}. \tag{6}$$

As one needs finally the evolution equations for $\dot{x}_i$, it is necessary to invert Eq. (6). If Q is a quadratic function in $\dot{x}_i$ (l=2), having the form $Q = \sum_{i=1}^{n_{\mathrm{int}}}\sum_{j=1}^{n_{\mathrm{int}}} U_{ij}(\{X\},\{x\})\dot{x}_i\dot{x}_j$ with U_{ij} being a positive-definite matrix involving material and structure parameters, then Eq. (6) yields

$$\dot{x}_i = W\sum_{j=1}^{n_{\mathrm{int}}} U_{ij}^{-1} f_{\dot{x},j}. \tag{7}$$

The following aspects are important:

(i) The TEP can be understood as a “strong” form of the second law of thermodynamics. The second law of thermodynamics allows an infinite number of paths of the system with positive dissipation function D. The TEP selects only that one corresponding to the constrained maximum of dissipation function D. The TEP is not a “Law of Physics” but a “Selection Principle”. It provides finally evolution equations for the rates $\dot{x}_i$ of internal parameters. We use the “classical” formulation of the TEP by employing the dissipation D (i.e. the entropy production multiplied by the temperature) and a dissipation function Q but not a dissipation potential as applied by Onsager. Our concept follows exactly the TEP as introduced by Ziegler, see Sect. 2.1. With respect to all the details concerning the TEP we refer to our overview paper [16] in Acta mater.

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