

PHYSICS, CHEMISTRY AND MECHANICS ARE GROWING TOGETHER - THE ROLE OF NONEQUILIBRIUM THERMODYNAMICS

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1. Introduction

Materials are rather complex systems described by a number of characteristic parameters (CPs), conservation laws and phenomenological equations, together with boundary and contact conditions. All these relations are engaged to simulate the development of the material system, mostly under simplified conditions. The extraction of the time evolution of the CPs from the solution is often impossible. Therefore, we start with the Thermodynamic Extremal Principle (TEP), proposed by Onsager in 1931 for heat conduction and 1945 for diffusion, which allows a direct derivation of the evolution equations for CPs in the case of slow processes at elevated temperatures, e.g. diffusive processes, dealing with linear non-equilibrium thermodynamics.

2. The Thermodynamical Extremal Principle (TEP)

The TEP is outlined shortly as following, for details see e.g. [1]. We have CPs denoted as $q_i, (i=1, \dots, N)$, e.g. concentrations etc., and their rates \dot{q}_i . The total Gibbs energy of the system is supposed to be $G(q_1, \dots, q_N)$ with its rate $\dot{G} = \sum_{i=1}^N (\partial G / \partial q_i) \dot{q}_i$. Linear constraints exist in the form

$C_k = \sum_{i=1}^N a_{ik} \dot{q}_i = 0, k=1, \dots, m$. We define a dissipation Q_h as a positive homogeneous function of the $\dot{q}_1, \dots, \dot{q}_N, h$ with h being the order homogeneity. This dissipation function Q_h reflects the power generated by the evolution of the internal variables. We look now for a maximum of Q_h constrained by $\dot{Q}_h + G = 0$ and the constraints $C_k = 0, i=1, \dots, m$. The result are evolution equations for the \dot{q}_i as

$$(1) \quad \sum_{j=1}^N U_{ij} \dot{q}_j + \sum_{k=1}^m a_{ik} \beta_k = -\frac{\partial G}{\partial q_i}, i=1, \dots, N,$$

if Q_h is a quadratic function $\sum_{i,j=1}^N U_{ij} (q_1, \dots, q_N) \dot{q}_i \dot{q}_j$. The β_k are Lagrange multipliers.

It is interesting to note that the TEP may be equivalent to the minimization of $\dot{G} + \Delta(q_1, \dots, q_N; \dot{q}_1, \dots, \dot{q}_N)$ with Δ being a dissipation potential for a wide class of functions as shown by Hackl and Fischer [2], yielding for homogeneous functions $Q_h = h\Delta$.

3. Application of the TEP

The first application of TEP is demonstrated on grain coarsening both with grain boundary motion and additionally diffusion in the matrix in the case of coarsening of precipitates, for details see [3]. If the grain radii are chosen as those parameters, the application of the TEP reproduces Hillert's classical evolution equations for the radii of individual grains (multigrain concept). The observed or calculated ensemble of grains is usually classified by a grain radii distribution function involving a certain number of parameters. A new concept [4] is now represented by the direct

application of the TEP to the radii distribution function by derivation of the evolution equations for its parameters (distribution concept). The kinetics of systems with bimodal and different monomodal starting distribution functions are calculated by means of both multigrain and distribution concepts and the results of simulations are compared and discussed. The dissipation of the grain coarsening process is evaluated, and it is shown that the width of the distribution function decisively influences the coarsening kinetics.

The second application deals with a chemically driven inelastic deformation in systems with non-ideal sources and sinks for vacancies. As thermodynamic forces generalized chemical potentials including both chemical and mechanical terms appear together with an evolution law for the vacancies, [5]. As a representative example the inelastic deformation state in a Fe-Mn-C bamboo-structured wire is demonstrated in dependence on the activity of sources and sinks for vacancies at dislocation jogs in the bulk. Sources and sinks for vacancies are supposed to be ideal at grain boundaries. Fig. 1 shows the axial strain along a wire with the dimension-free length 2 and two grain boundaries ($\bar{x} = 0.5, \bar{x} = 1.5$) at a certain time instant for different jog densities ρL^2 ; details can be taken from [6].

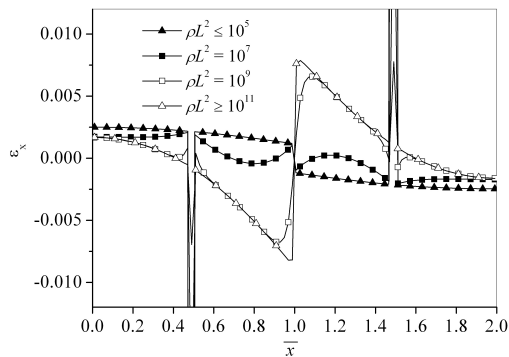


Figure 1. Chemically driven longitudinal strain in a wire.

4. References

- [1] J. Svoboda, I. Turek, F.D. Fischer (2005). Application of the Thermodynamic Extremal Principle to Modeling of Thermodynamic Processes in Material Sciences, *Phil. Mag.*, **85**, 3699-3707.
- [2] K. Hackl and F.D. Fischer (2007). On the Relation between the Principle of Maximum Dissipation and Inelastic Evolution Given by Dissipation Potentials, to be published *Proc. R. Soc. A*.
- [3] F.D. Fischer, J. Svoboda, P. Fratzl (2003). A Thermodynamical Approach to Grain Growth and Coarsening, *Phil. Mag. A*, **83**, 1075-1093.
- [4] J. Svoboda and F.D. Fischer (2007). A New Approach to Modelling of Non-Steady Grain Growth, *Acta mater.*, **55**, 4467-4474.
- [5] J. Svoboda, F.D. Fischer, P. Fratzl (2006). Diffusion and Creep in Multi-Component Alloys with Non-Ideal Sources and Sinks for Vacancies, *Acta mater.*, **54**, 3043-3053.
- [6] J. Svoboda, F.D. Fischer, E. Gamsjäger (2007). Simulation of Chemically Driven Inelastic Strain in Multi-Component Systems with Non-Ideal Sources and Sinks for Vacancies, to be published *Acta mater.*