A variational thermodynamic framework for modelling non-equilibrium diffusion processes and their coupling with plasticity

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ABSTRACT

Diffusion effects of various kinds can significantly affect the mechanical behaviour of many materials. For example, diffusion of moisture (for soils) or of other chemical species (for metallic alloys) at the microscale, or evolution of phase transformations, can influence the (visco-)plastic behaviour at the macroscale.

Most thermodynamic models of diffusion, coupled or not with mechanics, rely on the assumption of a local equilibrium, i.e. a well defined relation between a local chemical potential and concentration of the considered species. Dissipative processes are then necessarily related to diffusion. Although this assumption is valid in many practical cases, it can be put under scrutiny when characteristic times at the macroscale be come small enough to be comparable to characteristic times of the microscale. This situation can be encountered upon fast (mechanical, thermal, or chemical) loading at the macroscale, but also for complex, highly heterogeneous microstructures. The assumption of local equilibrium should then be reconsidered, and constitutive models constructed allowing for nonunique relation between concentration and chemcal potential.

For example, such a model has been proposed in [1], which defines a non-equilibrium chemical potential. When coupled to plasticity, it allows to reproduce experimentally observed behaviours in Li-ion batteries' electrodes, with coupling effects between Li-ion flow and development of plastic strains.

In this paper, we propose first a variational formulation of the model proposed in [1], extending the framework proposed in [2]. This framework allows to formulate coupled boundary-value problems as optimization of a scalar functional, endowing the formulation with nice mathematical properties (such as symmetry, ...).

Next, we motivate the occurrence of non-equilibrium effects at the macroscale by an analysis of a heterogeneous representative volume element in which constituents locally obey equilibrium constitutive relations., This analysis both justifies some of our assumptions in the formulation of the acroscopic model, and allow to calibrate some of the material constants introduced in the non-equilibrium constitutive relations.

REFERENCES

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