A coupled model of transport-reaction-mechanics with trapping. Part I - small strain analysis.

Salvadori A., McMeeking R., Grazioli D., Magri M.

PII: S0022-5096(17)31106-7
DOI: 10.1016/j.jmps.2018.02.006
Reference: MPS 3280

To appear in: *Journal of the Mechanics and Physics of Solids*

Received date: 9 December 2017
Revised date: 15 February 2018
Accepted date: 15 February 2018

Please cite this article as: Salvadori A., McMeeking R., Grazioli D., Magri M., A coupled model of transport-reaction-mechanics with trapping. Part I - small strain analysis., *Journal of the Mechanics and Physics of Solids* (2018), doi: 10.1016/j.jmps.2018.02.006

A coupled model of transport-reaction-mechanics with trapping. Part I - small strain analysis.

Salvadori A.[1,2], McMeeking R.[3,4,5], Grazioli D.[1,6], Magri M.[1]

[1] DICATAM - Dipartimento di Ingegneria Civile, Architettura, Territorio, Ambiente e di Matematica
Università di Brescia, via Branze 43, 25123 Brescia, Italy

[2] Department of Aerospace and Mechanical Engineering,
Center for Shock Wave-processing of Advanced Reactive Materials,
University of Notre Dame, Notre Dame, Indiana.

[3] Materials and Mechanical Engineering Departments, University of California,
Santa Barbara CA 93106, USA

[4] School of Engineering, University of Aberdeen, King's College, Aberdeen AB24 3UE, UK

[5] Leibniz Institute for New Materials, Campus D2 2, Saarbruecken, Germany

[6] Faculty of Civil Engineering and Geosciences, Delft University of Technology,
P.O. Box 5048, 2600 GA Delft, The Netherlands

February 17, 2018

Abstract

A fully coupled model for mass and heat transport, mechanics, and chemical reactions with trapping is proposed. It is rooted in non-equilibrium rational thermodynamics and assumes that displacements and strains are small. Balance laws for mass, linear and angular momentum, energy, and entropy are stated. Thermodynamic restrictions are identified, based on an additive strain decomposition and on the definition of the Helmholtz free energy. Constitutive theory and chemical kinetics are studied in order to finally write the governing equations for the multi-physics problem. The field equations are solved numerically with the finite element method, stemming from a three-fields variational formulation. Three case-studies on vacancies redistribution in metals, hydrogen embrittlement, and the charge-discharge of active particles in Li-ion batteries demonstrate the features and the potential of the proposed model.

1 Introduction

Several multi-disciplinary applications involve mass transport - driven by diffusion, migration or both - coupled with chemo-thermo-mechanics. In many cases, only a fraction of the total available mass of mobile species is effectively transported, whereas a significant counterpart remains immobilized by specific phenomena occuring concurrently with transport, i.e. trapping. Some examples clarify this concept.

One example is when metals are exposed to hydrogen gas, typically in storage tanks, and H atoms diffuse within the crystalline structure of the metal [1, 2, 3, 4, 5, 6, 7, 8]. H is found then not only in interstitial lattice sites, but also in defects such as vacancies, dislocations, grain boundaries, second-phase particle boundaries, and voids. Since such trapping of H in defects is energetically favorable, the mean residence time of diffusing hydrogen atoms is significantly longer in defects than in interstitial lattice sites. Furthermore, hydrogen free defects are filled very rapidly.

In electrochemical energy storage the fundamental mechanism of charge-discharge is the motion of ions between two electrodes. Particularly in Li-ion batteries, insertion of ions in active particles often alters the crystal structure of the particle itself, leading to a core-shell configuration with one segment, e.g. the shell in the case of insertion, rich in lithium with a sharp interface that separates it from a pristine inner core [9, 10, 11, 12, 13, 14]. Formation of chemical bonds between guest and host atoms allows alloying of lithium ions with the host matrix, transforming its initial crystal structure. Either fully reversible or not upon