20th European Mechanics of Materials Conference - EMMC20
Florence, Italy | May 27th-29th, 2026
www.emmc20.unifi.it

On the chemo-thermo-mechanics of constrained reactive mixtures of solids.

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Paper ID: 350
Symposium S10: Coupled problems in material mechanics

Abstract

Building upon the classical chemo-mechanical theory of Larch{\'e} and Cahn for equilibrium, numerous studies have investigated the transport of species in solids, with or without trapping phenomena. In most applications --- such as the swelling of hydrogels, hydrogen embrittlement in metals, and the transport of lithium or sodium in battery electrodes --- the formation of a new phase or compound can be directly associated with the concentration of the diffusing species. In the present work, we focus on the formation of solid mixtures made of multiple compounds, each characterized by its own volumetric expansion coefficient. Such a scenario arises, for instance, during the sodiation of tin anodes, in several mechanobiological applications, and in case hardening of metals, among other systems. The theoretical framework developed herein elucidates and differentiates the concepts of phases and flowing species, while establishing rigorous connections between them. The classical Larch{\'e} and Cahn chemo-mechanical framework is naturally recovered as a particular case of the proposed formulation.

Keywords:

Chemo-thermo-mechanics Finite strains Mechanobiology Mixtures of reactive solids