Thermodynamically Consistent Modeling of an Electro-chemo-thermo-mechanical System with Imperfect Interfaces

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Electro-chemo-thermo-mechanical couplings, wherein electro-chemo-thermal processes interact with mechanical deformation, govern the behavior of a wide class of multi-functional materials and devices. Typical examples are batteries and shape-morphing devices that comprise electrodes separated by (liquid or solid) electrolyte. In these systems, ionic transport, electrochemical reactions, and electric fields are intrinsically coupled with deformation, both in the bulk material and, not the least, at interfaces.

To retain maximal generality at the outset, we consider the interface as an "energetic" surface that is equipped with its own balance and constitutive equations. It is thereby tacitly assumed that the interface is "imperfect" in the sense that kinematic as well as flux variables are discontinuous across the interface. We develop a generic thermodynamically consistent framework, while restricting to small strain kinematics, that provides constraints on constitutive relations for the bulk material, as well as for the interface. A particular challenge is offered by extending Ampere's and Faraday's laws, as well as establishing the proper definition of the Poynting vector (representing the electro-magnetic power), for interfaces. The work represents an extension of previous efforts pertinent to mechanics, Javili et al. [1, 2]. As an illustration of the general framework, we consider the specific system (under isothemal conditions) of a half-cell, wafering an SEI-layer, in a battery or in a shape-morphing device.

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