"A Variational Approach to Mechano-Chemical Problems"

Gabriela Venturini
Ph.D. student, Graduate Aeronautical Laboratories - California Institute of Technology

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Abstract: The response that materials exhibit macroscopically reflects the mechanics of the underlying microscopic processes. The willingness to incorporate microscopic physics to improve existing material models seems therefore natural. The objective of this work is to obtain effective thermodynamic potentials (that will become the tool to calculate material properties and to describe the evolution of the system) while circumventing the treatment of all microscopic (atomistic) degrees of freedom. Restricting ourselves to the study of multi-species crystalline materials at finite temperature, the idea is to account for the energy contained in the thermal oscillations and for the contribution of different atomic components without the knowledge of the instantaneous velocity of such vibrations or the specific identity of each atom within the system. Interatomic interactions result from processes on subatomic scales, which this model is not addressing. Therefore we use semi-empirical interatomic potentials, e.g. Embedded Atom Method, as constitutive relations to describe the interaction among species. Equilibrium properties are found by minimizing a certain effective thermodynamic potential (the Helmholtz free energy for closed system and the Grand Canonical potential for open systems at finite temperature) built upon the Max-Entropy approach proposed by Kulkarni et al. for thermo-mechanical problems. The validity of this mechano-chemical extension has been tested against experimentally obtained equilibrium properties. The model is able to capture with reasonable accuracy the variation of elastic constants and segregation profile with composition and temperature in binary alloys, among other properties.

Kinetic processes are treated by recasting the coupled mechano-chemical problem in a variational setting. To this end, we have identified a new joint-functional whose stationary points provide the field equations and the boundary conditions describing the system's evolution, i.e. linear momentum and mass balance for each component in a solid held at constant temperature. This represents an extension of the work done by Yang et al. for thermo-mechanical problems. The time-discretized version of this functional reduces the rate problem to a sequence of incremental problems with variational structure. This structure uniquely determines the coupling between mechanics and diffusion. In other words, there is no need for additional constitutive equations relating the chemical potential with the concentration field or the stress state of the lattice. Moreover, that relationship cannot be specified a priori, but is an output of the simulation. The ultimate goal of this work is the development of a framework to model slow processes, such as corrosion or segregation of impurities where the evolution occurs over time-windows that are intractable for the existing atomistic or atomistic-informed models.


Bio: Gabriela Venturini is a Ph.D. student working with Prof. Michael Ortiz at the California Institute of Technology. Her research interests lie within the broad field of computational solid mechanics, with a particular focus on problems involving multiscale modeling of solids. She received an Engineering Diploma in Chemical Engineering in 2004 from the University of Buenos Aires, Argentina. After moving to the US in 2005, she became a graduate student at Caltech, where she obtained her M.S. in Aeronautics in 2006, and her Subject Minor in Chemistry in 2009. Prior to joining Caltech she worked at the University of Buenos Aires and the Tenaris Siderca Center for Industrial Research. In addition, during her Ph.D. studies, she spent two summers at Livermore National Laboratory.