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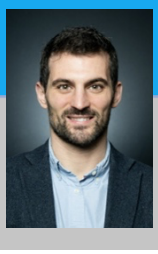
Applied Mechanics

Battery INNOVATION CLUSTER

Phase-field models for multi-physics problems: applications to hydrogen embrittlement and Li-Ion battery degradation



Prof. Emilio Martinez-Pañeda

Department of Engineering Science. University of Oxford

July 29, 2024 | 10.30 am – 12.00 pm (PDT)

Location: CEME 2202

Abstract

Phase-field methods have gained remarkable popularity in recent years, becoming the de facto tool for simulating complex interfacial problems: from fracture mechanics to corrosion to microstructural evolution. Complex topological changes such as the division or merging of interfaces can be readily captured. For example, in the context of fracture mechanics, this enables predicting complex phenomena such as tortuous crack trajectories, crack branching, crack merging and crack nucleation from arbitrary locations. Moreover, phase field approaches are well-suited to open new modelling horizons in multi-physics problems as the phase field evolution law can be readily combined with equations describing various coupled physical phenomena. In this talk, I will review the fundamentals of phase field modelling and present some of our recent work in developing new phase field formulations for coupled chemo-mechanical problems of notable technological relevance; namely, hydrogen embrittlement and Li-Ion battery degradation. Hydrogen is being hailed as the energy vector of the future but has a dark side; metals experience a dramatic drop in ductility and fracture resistance in the presence of hydrogen (of up to 90%). This phenomenon, termed hydrogen embrittlement, continues to challenge scientists and engineers and constitutes a major threat to the development of a hydrogen infrastructure. I will show how mechanistic multi-physics phase field formulations can be used to accurately predict hydrogen assisted failures in laboratory experiments and real-scale applications. Similarly, I will discuss how phase field-based deformation-diffusion-fracture models can be used to gain insight into Li-Ion battery degradation and to predict cracking at the microstructural, particle and electrode levels. Moreover, I will show how the phase field paradigm can be used to model voiding in the Li metal anode of all-solid-state batteries, mapping the conditions that prevent dendrite nucleation and enabling an all-solid-state battery breakthrough.

Bio

Prof Emilio Martinez-Paneda is an Associate Professor at the University of Oxford. Prior to joining Oxford, he was a Reader (Associate Professor) at Imperial College London, where he led an interdisciplinary research group from 2019 to 2023 (2019: Lecturer, 2021: Senior Lecturer, 2023: Reader). Before that, he was an 1851 Research Fellow at the University of Cambridge. Prof Emilio Martinez-Paneda's research spans a wide range of challenges lying at the interface between mechanics and other disciplines such as biology, geology, chemistry and materials science. He has been the PI on over 5M GBP of funding in the past five years (ERC Starting Grant, UKRI) and his work has been recognized through multiple awards, including the 2021 UK Young Engineer of the Year (Royal Academy of Engineering), the 2022 Imperial College President's Medal for Excellence in Research, and the 2021 Gustavo Colonnetti Medal (RILEM).