Seminar:

Confluence of Electrochemistry and Mechanics: From Engineering the Rechargeable Batteries to Corrosion in Extreme States

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VYKM2 Seminar Room

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Abstract

During the recent decades, the portable electronics (cell-phones, laptops, etc.) have entered the daily lifestyle, and require exponentially-increasing versatility and computational power. Hence, they demand portable electricity source necessitating the boost in terms of energy density, safety, efficiency and sustainability. On the other hand, the ever-increasing need for harnessing the green renewable energy as a potential replacement of the pollutant fossil fuels for applications such as electric vehicles, requires their capture and management via stationary smart infrastructures. The electrochemical systems, such as rechargeable batteries are the prominent answer for the in above-mentioned applications. Therefore, while the exploitation of new high-energy density materials/composites for high-power applications is unavoidable, herein we delve into the engineering of the advanced electrochemical devices (batteries) and phenomena (corrosion) as well as their coupling with the mechanics at the interfaces, by performing multi-physics modeling and electrochemical experiments as the following:

• ***Dendrites:*** Understanding the key components driving the ionic motion and formation of the growing destructive microstructures, we devise and investigate new charging methodologies to shorten and minimize them, either by real-time tuning of the charging forms, or spectral variation in the environmental parameters. In particular, noting the significant spatiotemporal scale gap between the experiments ($\sim mm, \sim ms$) and typical MD simulations ($\sim nm, \sim fs$), we develop a new coarse-grained (CG) predictive model which is extendable to experimental regimes. Such model which passes up the information from the lower-scale atomistic interactions provides possibility of the affordable simulation for the formation of dendritic micros-structures. (Fig. 1).

• ***Corrosion:*** We develop a diffusion-reaction framework, coupled with external stress field during the non-stoichiometric equilibrium to address the state of corrosion of the material. The established

model anticipates the mechanical failure during the prolonged oxidation and extreme temperatures, both before (Fig. 2) and after (Fig. 3) the fracture and formation of cracks.

• ***Composites:*** We will establish percolation-based frameworks to analyze and enhance the electrical and thermal conductivities of the $2D$ (thin) and $3D$ (thick) binary polymer composites with inclusion of fillers with higher conductivity. In broader sense, we additionally develop percolation-based efficacy measure for fiber-reinforced concrete in flexural loading and establish computational tool for capturing the rheological properties (i.e. viscosity) of super absorbent-filled concrete. As well, using percolation tools, we develop geometric-based percolation framework for estimating the size distribution of aggregates, traditionally performed via sieve experiments.

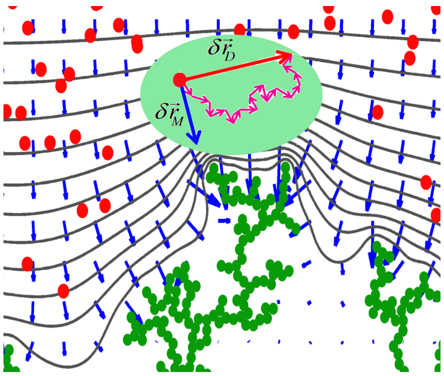

Figure 1: Dendritic evolution with representative ionic transport parameters and respective vector fields.

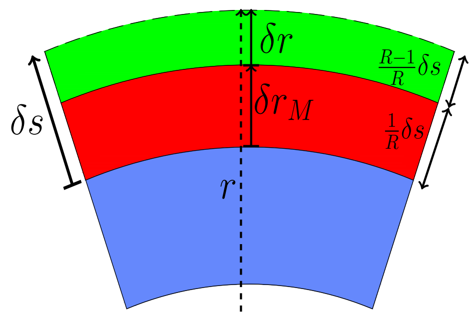

Figure 2: Quantifying the misfit stress due to swelling, during the corrosion on the curved surface, (blue: metal, red: oxide, green: swelling)

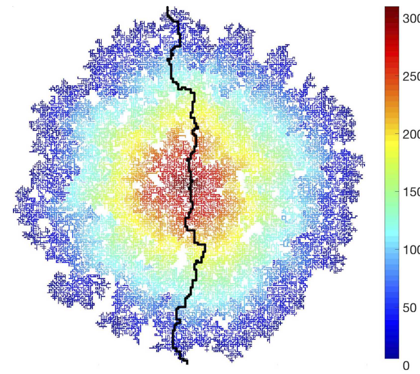

Figure 3: The shortest crack pathway via center-initiated *bond percolation*.

Bio:

Asghar Aryanfar received the B.S. in Civil and Mechanical Engineering (double major, *top* 2%) from Sharif University of Technology, Tehran, Iran in 2009 and the M.S. and Ph.D. degrees in Mechanical Engineering from California Institute of Technology, in 2010 and 2015, respectively. He is currently Assistant Professor of Mechanical Engineering at American University of Beirut ($2019-$present). Prior to current position, he was visiting faculty at Caltech ($2018 - 2019$) as well as lecturer at Faculty of Engineering at Bahçeşehir University ($2016 - 2019$). Before then, he was Postdoctoral Associate at University of California, Los Angeles (UCLA) ($2015 - 2016$). Aryanfar's research has been in the application of multi-physics modeling and experimental electrochemistry into engineering of the energy storage and conversion devices, materials and and exploitation of their interfacial phenomena. Particularly, his research on safety of high-energy rechargeable batteries has appeared as the Cover image of the Journal of Chemical Physics [link] and he has been interviewed in CNN for his 1^{st} prize winning invention of novel wastewater treatment system [link] from the *Gates Foundation*. Current projects are the material/interfacial physics and include analysis and design of state-of-the-art sustainable rechargeable lithium metal batteries and prediction of heterogeneous cracking behavior for electrolytic membranes exposed to extreme temperature/pressure.