Workshop on ELECTROCHEMOMECHANICS AND ENGINEERING

Martedì 16 luglio 2024
Dipartimento di Ingegneria Civile, Architettura, Territorio e Ambiente e di Matematica, via Branze 43, Aula Seminari

PROGRAMMA

10.30 – 11.30
Thomas Wallmersperger (Technische Universität Dresden) – **Modeling and simulation of smart polymers under applied voltage**

11.30 – 12.30
Alessandro Leronni (University of Bath) – **Determination of the occupancy-dependent diffusivity of lithium ions in Ni-rich cathode particles via optical scattering microscopy**

12.30 – 14.30 **Pausa pranzo**

14.30 – 15.30
Massimiliano Gei (Università degli Studi di Trieste) – **Surprising actuation mechanisms in laminated soft electro-elastic elastomers**

15.30 – 16.30
Alain Boldini (New York Institute of Technology) – **Modeling soft ionic membranes with ionic liquids for smart actuators**

16.30 – 17.00 **Pausa caffè**

17.00 – 18.00
Alessandro Musesti (Università Cattolica del Sacro Cuore, Brescia) – **Mathematical modeling of activation in biological soft materials**

La partecipazione è gratuita previa iscrizione tramite email, da inviare all'indirizzo: **lorenzo.bardella@unibs.it**

Thomas Wallmersperger – **Modeling and simulation of smart polymers under applied voltage**

When modeling smart materials, different approaches with different knowledge about the underlying physical processes can be considered. For this purpose, physics-based models and phenomenological models based on experimental data are available for each level of description. The presentation will first introduce a continuum-based model to describe the behavior of polymer gels and thin polymer membranes. It is often difficult to experimentally investigate the chemo-electro-mechanical behavior of small smart polymers. Therefore, numerical simulations are performed to gain a better understanding of the chemical reactions that take place in small (interfacial) regions near the electrode/electrolyte interfaces. For the transport, diffusive and migrative ion fluxes and the distribution of the electric field are taken into account. The fully coupled electrochemical field is given by the Poisson-Nernst-Planck equations. Time-dependent numerical simulations in a finite element framework are performed using both in-house and commercial numerical tools. A black-box model is then presented, which transfers the input data to the output data. Finally, the models are compared and evaluated with regard to their practical applicability.

Alessandro Leronni – **Determination of the occupancy-dependent diffusivity of lithium ions in Ni-rich cathode particles via optical scattering microscopy**

There is the need to characterise the diffusivity of lithium ions in nickel-rich manganese cobalt oxide (NMC) cathode particles to overcome critical capacity losses in these materials. The diffusivity of lithium ions in cathode materials for lithium-ion batteries is typically determined by measuring transient and steady-state voltage changes in applied consecutive pulses of constant current followed by relaxation periods. This method is grounded upon a set of limiting assumptions and only allows one to find an overall ion diffusivity within the cathode, which could differ from the diffusivity at the single particle level. Here, optical scattering microscopy is conveniently used to monitor the spatiotemporal changes of lithium occupancy in an NMC single particle during the applied current pulses, and hence to determine the occupancy-dependent diffusivity of lithium ions within this particle. For each current pulse, the time-dependent distribution of optical intensity within the particle is obtained and converted into lithium occupancy by assuming linearity between the two. Finite element diffusion simulations, adopting a parameterised occupancy-dependent diffusivity, are performed for each pulse. The least-square method is employed to find the parameters that ensure the best agreement between theory and experiments. The obtained diffusivity is shown to increase of about 50 times as the lithium occupancy in the NMC particle reduces from 90% to 70%, confirming previous approximate estimates based on solid-state nuclear magnetic resonance.

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Massimiliano Gei – **Surprising actuation mechanisms in laminated soft electro-elastic elastomers**

The talk presents the results of two actuation problems for thin laminates composed of two soft dielectric phases. In the first one, it is shown that, by selecting properly the contrast between constituents (i.e. shear moduli and permittivity ratios), the composite may display longitudinal contraction when actuated by a voltage jump across the thickness. In particular, both rank-one and rank-two laminates are investigated. The latter performs in general better; however, guidelines on how to optimise the microstructure to limit the values of the contrast parameters at which the new 'non-conventional' mode becomes available are provided [Proc. R. Soc. A 479, 20230168]. In the second problem, the aim is to demonstrate that the incompressibility constraint customarily adopted in the literature for soft composites may lead to largely inaccurate predictions. To reach our goal, we determine the actuation response of the laminate where the softest phase admits volumetric deformation. Our results [J. Elast. 148,167–198, 2022], discussed in the light of the limit case in which the softest phase consists of vacuum, challenge the hypotheses usually assumed in the modelling of soft dielectric composites providing new insight on the coupled mechanics of hierarchical dielectric composites.

Alain Boldini – **Modeling soft ionic membranes with ionic liquids for smart actuators**

Soft ionic membranes are often regarded as ideal solutions for smart actuators in robotics and bioengineering. Most of them rely on water as a solvent, thereby limiting the adoption of these materials for in-air use due to water evaporation. To avoid the negative consequences of solvent evaporation, water is often substituted by ionic liquids. However, to date, no physics-based model can capture the complex microscopic composition of ionic membranes with ionic liquids. In this talk, I will present a theory for the mechanics and electrochemistry of ionic membranes with ionic liquids. First, I will put forward a classification of ionic membranes with ionic liquids, depending on composition. Next, I will propose a thermodynamically consistent continuum theory that describes the multi-ion migration occurring in ionic membranes with ionic liquids. I will specialize the theory to beam-like actuators and conduct parametric analyses to study the influence of physical parameters on actuation. The model helps shed light on the physics of ionic actuators, while providing indications to material scientists to improve ionic membranes and ionic liquids for transducer applications.

Alessandro Musesti – **Mathematical modeling of activation in biological soft materials**

Guided by the important example of skeletal muscle tissue, I will discuss the main techniques employed in the modelization of biological soft active materials. Considering an incompressible and transversely isotropic material in a hyperelastic setting, constitutive relations will be designed so that the model will agree on uniaxial experimental data, whenever possible.