29th Nordic Seminar on Computational Mechanics
NSCM-29
R. Larsson (Ed.)
2016

MODELLING ELECTROMECHANICAL COUPLING ON INTERFACES IN METAL-POLYMER NANOCOMPOSITES NSCM-29

JANA WILMERS*, ANDREW T. MCBRIDE† AND SWANTJE BARGMANN‡

*Institute of Materials Research, Materials Mechanics
Helmholtz-Zentrum Geesthacht
Max-Planck-Straße 1, 21502 Geesthacht, Germany
e-mail: jana.wilmers@hzg.de, web page: http://www.hzg.de/materials_modelling

†Infrastructure and Environment, School of Engineering
University of Glasgow
Glasgow G12 8QQ, United Kingdom
e-mail: andrew.mcbride@glasgow.ac.uk - Web page:
http://www.gla.ac.uk/schools/engineering/

‡Chair of Solid Mechanics, School of Mechanical Engineering and Safety Engineering
University of Wuppertal
Gaussstraße 20, 42119 Wuppertal, Germany
e-mail: bargmann@uni-wuppertal.de - Web page: www.mechanics.uni-wuppertal.de

Key words: Nanocomposites, Interfaces, Multiphysics Coupling, Micromechanics

1 INTRODUCTION

Actuators and sensors that utilise the electromechanically coupled behaviour of materials are important elements of numerous technical applications. Electromechanical coupling arises from different physical processes in the material, e.g., charge re-orientation or surface modification. One example of a functional material like that are nanoporous metals which, due to their unique structure, have an exceptionally high surface-to-volume ratio and, thus, react sensitively to any electrically induced surface modification.

The build-up of surface charges in response to an applied potential and the electroadsorption of electrolyte ions induces stresses in the metal surface that result in a macroscopic deformation of the material. Thus, when filled with a dry electrolyte, nanoporous metals are promising sensor and actuator materials with a wide range of possible application fields.

Such nanoscale composite actuators exhibit actuation behaviour that is a superposition of the multiphysically coupled behaviour of the bulk polymeric electrolyte and the electromechanical coupling arising due to the interface modification as described above.

Table 1: Governing equations

	bulk	interface
linear momentum	$\rho_0 \ddot{\boldsymbol{u}} = \operatorname{Div} \boldsymbol{P} + \boldsymbol{B}$	$\overline{\rho}_0 \ddot{\overline{\boldsymbol{u}}} = \overline{\operatorname{Div}}\, \overline{\boldsymbol{P}} + \overline{\boldsymbol{B}} + [\![\boldsymbol{P}]\!] \cdot \overline{\boldsymbol{N}}$
Gauß's law	$0 = -\operatorname{Div} \boldsymbol{D} + q_0^f$	$0 = -\overline{\operatorname{Div}}\, \overline{\boldsymbol{D}} + \overline{\operatorname{Div}}\, \overline{\boldsymbol{N}} \left[\boldsymbol{D} \cdot \boldsymbol{N}\right] + \overline{q}_0^f - [\![\boldsymbol{D}]\!] \cdot \overline{\boldsymbol{N}}$
diffusion	$\dot{c}_0 = -\operatorname{Div} \boldsymbol{J} + W$	$\dot{\overline{c}}_0 = -\overline{\operatorname{Div}}\, \overline{\boldsymbol{J}} + \overline{W} - [\![\boldsymbol{J}]\!] \cdot \overline{\boldsymbol{N}}$

Computational modelling of the composite material is, therefore, not only important to describe and predict the actuation behaviour but allows insights into the interaction of the actuation mechanisms and physical processes at play that are inaccessible from experiments.

2 MODEL

In this work[1], a thermodynamically consistent continuum model for the chemoelectromechanically coupled behaviour of nanoscale composites is proposed. This model couples large deformations with electrostatics and mass transport as the transport of ions in an electric field and their interaction with the polymer network is responsible for the actuation behaviour of dry electrolytes.

To account for the dominant effects of the metal-polymer interface that cannot be captured by classic continuum theories, an extension of surface elasticity theory[2] is developed that allows to describe the multiphysical coupling on the interface.

The electroactive nanocomposite is modelled here as a body consisting of three physical domains that exhibit considerably different physical behaviours, namely the metal, the polymer, and the metal-polymer interface. The different material behaviours and coupling mechanisms arising in each of the three domains are modelled by endowing each domain with its own, unique properties and constitutive description.

For both, the bulk and the interface, the governing equations as presented in Table 1 are derived from fundamental balance principles. In Table 1, an overbar denotes an interface property. The mass density, charge density and the ion concentration are denoted by ρ_0, q_0^f and c_0, respectively, while $\boldsymbol{P}$ is the first Piola-Kirchhoff stress tensor, $\boldsymbol{B}$ is the vector of body forces, $\boldsymbol{D}$ is the electric displacement field and $\boldsymbol{J}$ and W denote ion fluxes and sources, respectively. Jumps of the bulk quantities over the interface are denoted by $[\![\bullet]\!]$. With these governing equations and suitable constitutive relations, the coupling between mass transport, electrostatics and deformation is fully described by the proposed model.

In contrast to previously published models of electroactive composites, this framework describes the interaction of the different phenomena and physical fields at the interface and is able to take into account pure interface effects such as the stresses induced by electroadsorption and the build-up of an interface charge. Furthermore, the coupling between bulk and interface as visible in space charge regions close to the metal-polymer interface is accounted for in the proposed model, thus, capturing the significant effect the

presence of an interface has on the overall composite behaviour.

To solve the highly non-linear and strongly coupled system of equations, the finite element method is applied within an in-house finite element code. Here, special attention has to be paid not only to the representation of the interface and its embedment within the volume mesh, but especially to the mapping of bulk information to the interface. This mapping is necessary to account for the coupling of interface properties to bulk values such as jumps in the fields over the interface or the ion concentration.

The strongly coupled system is solved monolithically, that is all coupled effects and interactions between the equations are taken into account and no simplifying assumptions about the coupled nature are made.

With this code, numerical studies are carried out that elucidate the capabilities of the proposed model and are used to study the influence of interface effects. Furthermore, numerical simulations are used to investigate the different coupling mechanisms and their interaction with each other, thus, providing valuable insight into the functionality of electroactive nanocomposites.

ACKNOWLEDGEMENT

We gratefully acknowledge financial support from the German Research Foundation (DFG) via SFB 986 "M^3", project B6.

REFERENCES

[1] Wilmers, J., McBride, A. & Bargmann, S. Interface elasticity effects in polymer-filled nanoporous metals. under review (2016).

[2] McBride, A., Javili, A., Steinmann, P. & Bargmann, S. Geometrically nonlinear continuum thermomechanics with surface energies coupled to diffusion. *Journal of the Mechanics and Physics of Solids* **59**, 2116–2133 (2011).