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S06 Multiphysics problems

List of abstracts

ID 54: *Electric field impact during modelling of thermoablation in multilayer breast model with tumor* (poster) – M. Paruch

ID 100: *Computational prediction of micro-crack and porosity induced changes in electrical conductivity* – A. Menzel, T. Kaiser

ID 133: *Overview on solid mechanics and digital computers* – A. Szekeres

ID 196: *Modeling of concrete corrosion, incliuding corrosion products - electric curent intensity relation* – K. Yurkova, T. Krykowski

ID 209: *Spline-based multi-field computations of optimized silicon electrodes* – M. Werner, K. Weinberg

ID 232: *Phase-field study of interfacial and elastic energy effects on microstructure evolution in Al alloys* – R. Chafle, A. Safi, E. Mathew, J. Herrnring, B. Klusemann

ID 273: *Effects of multistable configurations in extremely soft magnetorheological elastomers* – M. Rambausek, M. Neunteufel, J. Schöberl

ID 287: *Application of deep learning methods for efficient multi-scale modeling of solid-state batteries going under degradation* – S. Rezaei, A. Asheri, M. Fatihdoost, B. Xu

ID 293: *Phase field models for multi-physics problems: applications to hydrogen embrittlement and Li-Ion battery degradation* (keynote) – E. Martinez-Paneda

ID 298: *Modelling of chemo-mechanical processes in energy storage materials* – M. Poluektov, Ł. Figiel

ELECTRIC FIELD IMPACT DURING MODELLING OF THERMOABLATION IN MULTILAYER BREAST MODEL WITH TUMOR

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In oncology, hyperthermia is understood as a planned, controlled technique of heating cancerous changes to destroy their cells or stop their growth. During the hyperthermia, the tissue is typically exposed to a temperature in the range of 40-45°C, the exception is thermoablation, during which the temperatures reach much higher values. Thermoablation is characterized using high temperatures up to 90°C. The therapy consists of inducing coagulation necrosis in an area that is heated to very high temperatures.

In the case of electric field impact, mathematical modelling consists of solving a coupled problem, and, more specifically, analysis of electro-thermal coupling, in which the electric field is described by means of the Laplace equation. A tissue model is selected for the mathematical description of heat transfer, namely the classic Pennes model (the most used mathematical model describing the process of heat transfer in living organisms, on a macro scale, which is commonly used in particular to predict temperature changes during hyperthermia, or hypothermia treatments, i.e., broadly understood thermotherapy.

The coupling of these two problems takes place by means of the weak formulation, which consists of considering the source function resulting from the interaction of the electric field in the Pennes equation. Therefore, it is important to correctly describe how the electromagnetic field interacts with biological tissue. In the full Maxwell's equations, electric and magnetic fields are coupled, so it requires complex numerical calculations. Because the radiofrequency ablation method uses low frequencies, to determine the intensity of the electric field the simplification known as the quasistatic approach can be taken into account. Besides determining the temperature field in the biological tissue affected by the tumor and subjected to external thermal action, it is also necessary to estimate the degree of tissue destruction under the influence of high temperature. In the literature, we can find relations describing the relationship between temperature and perfusion, as well as between perfusion and tissue destruction. One such method is to determine the value of the Arrhenius integral.

For numerical calculations, a multi-layered (muscle, glandular layer, fat) breast geometric model is prepared. Among the various configurations, the following types of models can be distinguished: extremely dense (ED), heterogeneously dense (HD), scattered fibro-glandular (SFG), and predominantly fatty (PF).

In order to solve the equations describing the potential of electric and temperature fields, the finite element method is applied using commercial software MSC MARC/MENTAT ver. 2021.2 (64-bit).

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COMPUTATIONAL PREDICTION OF MICRO-CRACK AND POROSITY INDUCED CHANGES IN ELECTRICAL CONDUCTIVITY

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Defects, such as micro-cracks and porosity on the one hand and dislocations and grain boundaries on the other, induce changes in effective electrical conductivity in metallic materials; cf. [1]. The long term goal of using a modelling and simulation based approach to predict such defects in the context of an inverse analysis motivates the elaboration of an electromechanically coupled multiscale formulation for electrical conductors; cf. [2,3]. The particular homogenisation (FE2) framework is introduced by analogy with related coupled problems such as thermomechanics or mechanics of dielectrics, i.e. extended Hill-Mandel energy equivalence conditions need to be accounted for, but addresses electric conduction. The specific applications studied based on this computational multiscale formulation place emphasis on the influence of deformation-induced cracks (in thin films) and the influence of an experimentally generated porosity, both in particular elaborating the electric conductivity. Comparison of experimental data with computationally predicted response shows that the homogenisation framework appropriately captures micro-crack and porosity-induced changes in electrical conductivity.

[1] T. Kaiser, M.J. Cordill, C. Kirchlechner, A. Menzel. Electric and mechanical behaviour of metal thin films with deformation-induced cracks predicted by computational homogenisation. International Journal of Fracture, 231:223-242, 2021.
[2] T. Kaiser, A. Menzel. An electro-mechanically coupled computational multiscale formulation for electrical conductors. Archive of Applied Mechanics, 91:1509-1526, 2021.
[3] T. Kaiser, A. Menzel. A finite deformation electro-mechanically coupled computational multiscale formulation for electrical conductors. Acta Mechanica, 232:3939-3956, 2021.

OVERVIEW ON SOLID MECHANICS AND DIGITAL COMPUTERS

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The presentation displays my activity and the socalled results in the fields of solid mechanics (SM) and digital computers. This expression sounds funny, but in the early 1960s it was not clear, at least in Hungary, that the digital or analog computers will be the future. The speech consists of five main chapters.

First, the beginning including my MSc thesis (1963), the early works as an R&D engineer of a big electrical factory and a part time job researcher of TU Budapest. My dr. techn. thesis was based on this. (In the presentation I will refer to the publications, too).

Second, I am going to show in a flowchart the milestones of a long researcher carrier, that led to the Budapest Center of Thermo-Hygro-Mechanics (BCoTHM).

Third, this part is based on my presentations given during the previous SolMech Conferences. I am going to emphasize not only my Polish cooperating partners, but also the international character (Finnish, Estonian, American, Bulgarian, Israeli, Hungarian, Indian, Ukrainian, etc.) of the BCoTHM.

Fourth, this chapter is devoted to my Polish friends (partners), to the cooperation with them and to the rich outcome. E.g. Richard Hetnarski and Martin Ostoja-Starzewski from America, Bogdan Maruszewski from Poznan, Witold Kosinski and Marek Sklodowski from Warsaw, Radek Iwankiewicz from South-Africa and Hamburg.

The fifth chapter contains different specialties. During my visiting professorship at Oulu Uni (Finland, 1993) I gave a course on continuum-mechanics (CM) in the frame of the international school on CAME (Computer Aided Mechanical Engineering). Later (in 1995) I returned as visiting researcher, that was the time of the start of my THM, that became an independent issue of SM and an international school with center in Budapest (BCoTHM).

During my visit at the Virginia Tech (USA, 1994) I gave a course on Thermal Stresses (TS) and returning to Hungary later a course on basic Thermomechanics(TM). It became a basic course of different faculties at BUTE.

There were several international series of conferences organized by me as a principal organizer, mainly on SM. E.g. Finno-Ugric Days of Mechanics (FUDoM: 1995, 98, 2001, 05, 09, 13), Continuum Physics and Engineering Application (CPEA: 2007, 10, 13), Conference on TS: 2011.

As a peculiarity I would mention my first study trip to Warsaw (1971). It was my first personal meeting with the world-famous Polish mechanics. For us in Hungary that time Warsaw and the IPPT were the Mekka of mechanics!

Similarly, my first international conference in Varna (1973), where I met Witold Nowacki and Juri Engelbrecht. Nowacki gave me the good advise: journal and research institute of mechanics needed to the faster development. With Juri we built up a lifelong friendship and he and our works became one of the strongest leg of the BCoTHM. The fruits of this cooperation are dozens of publications, e.g. my candidate of science thesis.

Finally, I am going to display how the thermodynamics developed in the frame of SM and through several steps, i.e. SM -> TS -> TM -> THM -> TMOM (e.g. BTHM) (thermo-multi object-mechanics, bioTHM), we arrived to an independent part of SM, similarly to CMM.

MODELING OF CONCRETE CORROSION, INCLIUDING CORROSION PRODUCTS - ELECTRIC CURENT INTENSITY RELATION

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The often used approach to the experimental assessment of the propagation of corrosion processes in reinforced concrete elements are tests of accelerated corrosion of reinforcement. The undoubted advantage of this type of approach to evaluation the propagation time of the width of the cracks in reinforced concrete elements is the rate of the progress of the phenomenon. The disadvantage is the dependence of corrosion products formed in the electrode reaction on the current density. In the case of accelerated corrosion tests, even in a situation of very high initial current density, the value of this parameter decreases because of tightening of the corrosion products on the rod perimeter. There is a gradual increase in the electrical resistance of the system and a decrease in current intensity, which affects the diverse chemical composition of formed corrosion products. From the point of view of mechanical interactions, due to the varied increase in the volume of corrosion products, the rate of propagation of damage in the concrete cover is changed.
The paper presents the analysis of the impact of corrosion products on the time of cracking of the cover of the reinforced concrete element. The function describing the time-varying chemical composition of corrosion products were determined by approximation of experimental results obtained from the literature for variable current densities in the range of 50 to 300 microA/cm^2. Calculations were made for test elements, which consider both the uniform distribution of corrosion products on the surface of the reinforcement as well as for those in which corrosion of the reinforcement occurs only on parts of the bar cross-section. The results obtained for the case of uniform corrosion were compared with the results of experimental studies. Calculations were made for both elastic and plastic concrete models with degradation as well as microplane models with gradient regularization.

SPLINE-BASED MULTI-FIELD COMPUTATIONS OF OPTIMIZED SILICON ELECTRODES

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The politics in Europe forces to set the focus on renewable energy sources, such as wind, water, solar, biomass, and geothermal. In the case of solar energy, the converted energy need to be stored, e.g., by photovoltaic. There are various individual technical solutions on the market, but Lithium-ion batteries (LiB) have become established.

LiB are one of the highest gravimetric energy density storage systems with high efficiency and long service life, even with intensive use. A LiB's construction consists of two electrodes (e.g., silicon and LiCoO2), a separator in between (e.g., polyolefin), and an electrolytic solution (e.g., LiPF6 salt).

Charging and discharging of a LiB's electrode result from particle exchange between the anode material and the electrolyte - and often lead to particle swelling of 300%. In addition, multiple physical processes (such as ion flux and diffusion, electrical and thermal conduction, and others) influence the overall process at the electrode. Theoretical modeling of the underlying multi-physics coupling is achieved through the constitutive relations, obtained within a consistent thermodynamic framework based on the definition of the free energy density.

Most of the existing approaches account for small deformations and linear elasticity, but silicon-electrode developments require to account for considerable volumetric changes. Our current approach is characterized by finite kinematics under the assumption of the locality of deformation. Accordingly, the deformation gradient is multiplicatively decomposed into elastic and inelastic parts and treated as a concentration-dependent quantity. We illustrate the features of the model by means of selected examples, showing that chemo-mechanical interaction affects the equilibrium concentrations of the phases.

Such multi-physics problems' modeling involves higher-order differential equations, which cannot be directly solved with standard finite element methods. B-splines as finite element basis functions provide the required continuity and smoothness. Moreover, finding the optimum design of the LiB anode is a challenge, which addresses the competitive task of maximizing conductivity on the one hand and mechanical robustness on the other hand - and also the meshing itself is not trivial either. We also study several examples for several optimized silicon particles using a spline-based description for the geometry.

PHASE-FIELD STUDY OF INTERFACIAL AND ELASTIC ENERGY EFFECTS ON MICROSTRUCTURE EVOLUTION IN AL ALLOYS

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In recent years, Al alloys have attracted considerable interest due to their outstanding strength to weight ratio, qualifying them as cutting-edge candidates for aerospace applications. The addition of Li to the well-studied Al-Cu system decreases the density and introduces a broad range of precipitates that contribute to the material's dispersion strengthening. Due to the severe implications in weldability, Al-Cu-Li alloys are challenging to handle in fusion-based processes. Hence, solid-state processes are applicable where the peak process temperatures are kept below the bulk melting point of the alloy being processed. The Al-Cu-Li alloys display high tensile strength, improved high cycle fatigue and fatigue crack growth resistance. The Cu/Li ratio mainly controls the mechanical properties as it determines the thermodynamic equilibria of the phases and the precipitation sequence. The size, frequency and morphology of these precipitates depend on thermodynamics and diffusion kinetics.

In this study, the quantitative influence of Cu and Li concentration on the precipitation behavior in this alloy class is investigated via a coupled Cahn-Hilliard and Allen-Cahn phase-field model discretized in a finite-element formalism. The precipitation behaviour is captured by incorporating the anisotropy in the interfacial energy and the elastic contribution to the total free energy. The model is numerically implemented using the deal.II library, thus providing efficient numerical solution schemes and an adaptive meshing algorithm that dynamically refines domains with a relatively high estimated numerical error and coarsens the regions with low error. Additionally, the phase-field method is coupled with CALPHAD framework to derive thermodynamic free energies and kinetic parameters.

EFFECTS OF MULTISTABLE CONFIGURATIONS IN EXTREMELY SOFT MAGNETORHEOLOGICAL ELASTOMERS

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The coupled magnetoelastic response of magnetorheological elastomers is well understood nowadays for composites based sufficiently stiff matrix material. However, as the matrix shear modulus becomes smaller, magnetoelasticity ceases to be a sufficiently powerful framework for the description of the macroscopic material response. Indeed, even when dissipation in the constituents is neglected, the composite apparently exhibits significant dissipation. More precisely, magnetic composites based on very soft matrix material can only store very limited amounts of elastic energy. But then, depending on the applied magnetic field, the magnetostatic field energy can locally dominate the system. This, as a consequence, allows for multiple (meta-)stable states at the microscale. By that, the composite material becomes 'magneto-pseudoelastic'. We are perfectly aware that such 'magnetodeformal shape-memory' have been documented some time ago, e.g., [1, 2]. However, we are not aware of any corresponding quantitative full-field simulations.
Our presentation features some first attempts on filling this gap. In detail, we show finite element simulations for extremely deformable magnetomechanical systems that push the limits of updated Lagrangian finite element methods in large deformation settings. For this purpose we showcase adaptive remeshing strategies for highly deformed bodies implemented with Netgen/NGSolve. By their very nature, the methods presented can be also applied to dielectric elastomers as well as to other coupled and non-coupled problems in the field of soft-matter.

[1] Nikitin L.V. and Stepanov G.V. and Mironova L.S. and Gorbunov A.I. Magnetodeformational effect and effect of shape memory in magnetoelastics. J. Magn. Magn. (2004) 272-276: 2072-2073.
[2] G. V. Stepanov, D. Y. Borin, Y. L. Raikher, P. V. Melenev and N. S. Perov. Motion of ferroparticles inside the polymeric matrix in magnetoactive elastomers. J. Phys.: Condens. Matter (2008) 20: 204121.

APPLICATION OF DEEP LEARNING METHODS FOR EFFICIENT MULTI-SCALE MODELING OF SOLID-STATE BATTERIES GOING UNDER DEGRADATION

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Lithium-ion batteries (LIB) have shown great potential in energy storage applications such as portable electronic devices and electric vehicles. Recently solid-state lithium batteries which use a solid electrolyte (SE) instead of a liquid one, as in conventional LIBs, have gained much interest. These batteries can achieve higher energy densities and have better safety conditions than the traditional ones. One aspect which hinders the application of solid-state batteries cracking in different parts and interfaces. Therefore simulations and models can be of great interest to understanding the behavior of different materials better. In this contribution, we would like to first address the microscopic modeling aspects and then show how information from the simulations at the micro-level can be transferred to the cell level.

On the other hand, the multiscale models which account for the microscale details are usually costly and inefficient. Therefore, we would like to present a simple approach based on deep learning to perform this task. It is shown how the required data for a deep learning algorithm can be obtained by means of offline simulations at the micro-scale. The network is also designed in a specific way to respect some basic thermodynamics laws. Utilizing this approach one can gain huge speed up in multiscale simulation in the multiphysics environments.

PHASE FIELD MODELS FOR MULTI-PHYSICS PROBLEMS: APPLICATIONS TO HYDROGEN EMBRITTLEMENT AND LI-ION BATTERY DEGRADATION

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Phase field methods have gained remarkable popularity in recent years, becoming the de facto tool for simulating complex interfacial problems: from fracture mechanics [1] to corrosion [2] to microstructural evolution [3]. 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 [3] and real-scale applications [4]. 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 the cracking of particles and even full-size electrodes [5]. Moreover, I will show how the phase field paradigm can be used to model voiding in the Li metal anode of all-solidstate batteries, mapping the conditions that prevent dendrite nucleation and enabling an all-solid-state battery breakthrough.

References

[1] P.K. Kristensen, C.F. Niordson and E. Martinez-Paneda. An assessment of phase field fracture: crack initiation and growth. Philos. Trans. R. Soc. London, Ser. A, 379, 20210021, 2021.
[2] C. Cui, R. Ma and E. Martinez-Paneda. A phase field formulation for dissolution-driven stress corrosion cracking. J. Mech. Phys. Solids, 147, 104254, 2021.
[3] P.K. Kristensen, C.F. Niordson and E. Martinez-Paneda. A phase field model for elastic-gradient-plastic solids undergoing hydrogen embrittlement. J. Mech. Phys. Solids, 143, 104093, 2020.
[4] P.K. Kristensen, C.F. Niordson and E. Martinez-Paneda. Applications of phase field fracture in modelling hydrogen assisted failures. Theor. Appl. Fract. Mech., 110, 102837, 2020.
[5] A. Boyce, E. Martinez-Paneda, A. Wade, Y.S. Zhang, J.J. Bailey, T.M.M. Heenan, D.J.L. Brett and P.R. Shearing. Cracking predictions of lithium-ion battery electrodes by X-ray computed tomography and modelling. J. Power Sources, 526, 231119, 2022.

MODELLING OF CHEMO-MECHANICAL PROCESSES IN ENERGY STORAGE MATERIALS

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Performance enhancement of heterogeneous materials for energy storage, e.g. for Li-ion batteries, requires thorough understanding of chemo-mechanical processes occurring across various length scales. The microstructure of such materials can undergo a complex electro-chemo-thermo-mechanical cycling during battery exploitation, which e.g. involves extreme volumetric expansion of the active material during the chemical reaction. The expansion is causing mechanical stress, which, in turn, influences the kinetics of chemical reactions even up to their arrest [3]. Thus, to predict the chemo-mechanical behaviour of a multi-material battery electrode, both the multi-physics phenomena and microstructure must be taken into account.

Up to now, the major focus has been on the development of coupled mechanics-diffusion-reaction models, e.g. [4], and in particular models capturing localised chemical reactions, such as lithiation and oxidation, e.g. [1-2]. To address the multiscale nature of the electrode materials and energy storage devices, full-field homogenisation approaches have been formulated for problems of stress-affected diffusion of Li ions, e.g. [5].

In this talk, some recent developments are combined into a unified multiscale framework for modelling of energy storage materials from the micro to the meso scale. The framework considers an electrode (mesoscopic) scale and material microstructure (microscopic) scale, which are linked via a full-field homogenisation scheme. Evolution of the field quantities (deformation, concentration, extent of the reaction and temperature) is handled via a thermodynamically-consistent mechanics-diffusion-reaction-temperature theory. Within the theory, the volumetric reaction between the solid component (e.g. Si) and the mobile diffusive species (e.g. Li ions) is modelled; thus, the distinction is made between the transport process (i.e. diffusion) and the reaction (i.e. absorption of mobile species by the solid). Furthermore, at the microscopic scale, the damage and fracture of the material due to deformation is modelled using a cut-finite-element method [6].

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References
[1] ZW Cui, F Gao, JM Qu (2013) J Mech Phys Solids 61:293-310
[2] AB Freidin, EN Vilchevskaya, IK Korolev (2014) Int J Eng Sci 83:57-75
[3] K van Havenbergh, S Turner, N Marx, G van Tendeloo (2016) Energy Technol 4:1005-1012
[4] VI Levitas, H Attariani (2014) J Mech Phys Solids 69:84-111
[5] A Salvadori, D Grazioli, MGD Geers (2015) Int J Solids Struct 59:90-109
[6] M Poluektov, L Figiel (2022) Comput Methods Appl Mech Eng 388:114234