A numerical method for finite-strain mechanochemistry with chemical reaction fronts treated as immersed boundaries

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Chemical reactions, such as oxidation or lithiation, in solid bodies lead to large volumetric expansions of the materials and thereby lead to the emergence of mechanical stresses, which, in turn, affect the rates of the chemical reactions. In recent years, there has been an immense growth of models that describe mechanochemical processes, e.g. [1-3]. Some of these models focus on describing the influence of mechanical stresses on the kinetics of chemical reactions that take place at a surface (a chemical reaction front) inside a solid body. The reaction front moves due to the consumption of the diffusive reactant, which is supplied to the reaction front by the diffusion process, while the velocity of the front is also affected by the stresses. Thus, the problem is described by the coupled mechanical and diffusion equations, where one of the boundary conditions is enforced at the moving reaction front, the velocity of which depends on the solution of both equations.

From the computational point of view, when the standard finite-element method (FEM) is applied to problems of mechanochemistry, the geometry should be remeshed each time the reaction front moves, see e.g. [4]. This leads to accumulation of the numerical error and excessive computations. An alternative way of treating such problems is a computational method that allows the interface (the reaction front) to cut through the elements and to move independently of the mesh. In this talk, a rigorous formulation of such numerical method is presented.

The numerical formulation of the problem consists of the mechanical and diffusion parts, and the part related to the movement of the reaction front. In the mechanical part of the problem, the force equilibrium and the displacement continuity conditions at the reaction front are enforced weakly using a Nitsche-like method. The total potential energy is formulated, from which the weak form of the problem is derived. Afterwards, the finite-element formulation of the problem on a non-conforming mesh is obtained. Up to now, this type of approach has only been applied to problems in linear elasticity [5]. In this talk, the method is derived for the case of large deformations and arbitrary constitutive behaviour of materials. It is demonstrated that the proposed implementation of the method has the same convergence rate with respect to the mesh size as the standard FEM. The diffusion part of the problem is also solved on a finite-element mesh, which is non-conforming to the reaction front. In addition, a novel numerical algorithm for the movement of the points of the chemical reaction front is proposed.

Several case studies of the chemical reactions in solid hyperelastic bodies are presented to illustrate the robustness of the method. The developed method can easily be applied to the bodies of complex geometry and microstructure, such as silicon-based anodes in Li-ion batteries, which undergo stress-affected chemical reactions, and thus the method can be useful for designing anodes in future Li-ion batteries.

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