Computational methods for modelling interface kinetics in solids

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ABSTRACT

There is a wide range of problems in solid mechanics that involve non-stationary interfaces. These problems include, for example, classical stress-induced solid-solid phase transitions and chemo-mechanics with localised chemical reaction fronts. Kinetics of such interfaces is governed by configurational forces [1], which depend on mechanical stresses and deformations, which, in turn, depend on the interface position. Furthermore, phase-transforming materials often involve multi-physics processes. For example, twin boundaries in magnetic shape memory alloys are affected both by mechanical stresses and by magnetic field; chemical reaction fronts in oxides are affected both by mechanical stresses and by oxygen diffusion. Finally, these materials often undergo large deformations during transformations; therefore, the non-linear mechanical behaviour must be considered.

From the mathematical point of view, the considered problems are represented by systems of PDEs with discontinuities across time-dependent interfaces, velocity of which depend on the solution of the PDEs. During the past decades, a large variety of computational methods emerged in attempts to solve efficiently such problems. Most methods can be classified into two groups: the diffuse-interface methods, such as the phase-field method, and the sharp-interface methods. The latter category includes the boundary integral method, the standard FEM with finite-element mesh conforming to the interface and with remeshing each time the interface moves, and the fictitious-domain methods, where the mesh is static and the interfaces cut through the elements. Such methods include XFEM/GFEM [2], DE-FEM [3], CutFEM [4] and others.

The aim of this mini-symposium is to combine recent developments in computational methods for modelling kinetics of time-dependent interfaces. The topics will include both the diffuse-interface and the sharp-interface methods, with a specific emphasis devoted to the comparison of these frameworks and to the analysis of advantages and disadvantages of individual approaches. Furthermore, the mini-symposium will discuss tailoring of the methods for phase-transforming materials involving multi-physics processes and thereby requiring the solution of coupled PDEs, which, in general, are non-linear.

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