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NUMERICAL STUDIES OF KINETICS AND STABILITY OF CHEMICAL REACTION FRONTS IN SOLIDS

A. Morozov[1], M.Poluektov[2], A.B. Freidin[3], Ł. Figiel[2], and W.H. Müller[1]

[1] Berlin Institute of Technology, Str. des 17. Juni 135, Berlin 10623, Germany, morozov@tu-berlin.de, wolfgang.h.mueller@tu-berlin.de

[2] International Institute for Nanocomposites Manufacturing, University of Warwick, Coventry CV4 7AL, UK, m.poluektov@warwick.ac.uk, l.w.figiel@warwick.ac.uk

[3] Institute for Problems in Mechanical Engineering of the Russian Academy of Sciences, 61 Bolshoy, V.O., St.Petersburg 199178, Russia, alexander.freidin@gmail.com

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This work focuses on modeling kinetics and analyzing the stability of chemical reaction fronts in solids. We consider a localized reaction between diffusing and elastic solid constituents. The reaction is accompanied by a chemical transformation that produces internal stresses, which, together with external stresses, affect the reaction front propagation, see [1] and references therein. Chemo-mechanical coupling is modeled based on a chemical affinity tensor.

The propagating front can be either stable or unstable. For the propagating planar interface, we perform an analytical stability check. We consider the interface stable if the imposed perturbations decay due to the interface kinetic equation and unstable otherwise. For more complicated cases the front propagation and the stability analysis have to be performed numerically. Two different numerical approaches are used and compared. First, the standard finite-element method with an additional remeshing algorithm to resolve the moving inter-phase boundary [2]. The second approach is based on CutFEM, which was recently adapted for the problems of chemo-mechanics [3]. This approach allows the reaction front to cut through the elements and move independently of the finite-element mesh. In this work, various geometrical configurations and loading scenarios are considered, and the emphasis is made on the stability of the propagating interface.

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