

Univ. Prof. Dr. rer. nat. Wolfgang H. MÜLLER

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Fakultät V – Institut für Mechanik

Lehrstuhl für Kontinuumsmechanik und Materialtheorie (LKM)

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Ankündigung eines Gastvortrages

im Rahmen des Mechanik Seminars

zum Thema

On the kinetics of chemical reaction fronts in elastic solids

Ort: **Technische Universität Berlin, Gebäude MS,
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Gastdozent:

Ph.D. Elena N. Vilchevskaya

Institute for Problems in Mechanical Engineering

Russian Academy of Sciences (IPME RAS), St.Petersburg, Russia

Abstract:

We consider a stress-assisted chemical reaction front propagation implying a reaction like the silicon oxidation within the frameworks of the concept of configurational (driving) forces. We suppose that the reaction is localized at the front that divides two solid constituents and sustained and controlled by the diffusion of the gas constituent through the transformed material.

We also assume that the gas diffusion is not affected by strains and does not produce additional strains in the solid phases. We obtain an expression of the entropy production due to the reaction front propagation and, as a result, derive the formula of the chemical affinity tensor as a combination of Eshelby stress tensors of the solid constituents and a chemical potential of a gas constituent. In a linear thermodynamic approach a velocity of the reaction front is proportional to a normal component of the chemical affinity tensor which depends on stresses and the gas constituent concentration. We say that the gas concentration is at equilibrium c_{eq} at the reaction front if, given temperature, front position and stresses, the normal component of the chemical affinity is equal to zero. Since the concentration c_{eq} depends on stresses, the stresses can accelerate or lock the reaction front propagation.

An axially-symmetric mechano-chemistry problem is considered as a model problem. For a given transformation strain we show that in the absence of external stresses the reaction rate in the case of a convex surface is greater than in the case of non-convex surface. The growth of the oxide layer leads to an increase of equilibrium concentration in the case of the hole, which in turn may lock the reaction. An externally applied pressure renders the reaction possible at all thicknesses of an oxide layer but a further pressure increase may lead to a total locking of the reaction. This effect is a consequence of the non-monotonic dependence of c_{eq} on the pressure. In contrast, in the case of a cylinder, the growth of the oxide layer decreases the equilibrium concentration, which in turn promotes the propagation of the chemical reaction front.