Front Propagation of Chemical Processes with Stress Assistance in Deformable Solids

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Abstract

We take into account the front of a chemical reaction that is aided by stress spreading through a deformable material that is experiencing a localized chemical reaction involving solid and gas components. Diffusion of the gas component through the changed solid material sustains the process. The internal strains caused by the chemical reaction's transformation strain have an impact on the reaction's front kinetics. We propose a kinetic equation based on the idea of the chemical affinity tensor that describes how the front velocity depends on the chemical affinity tensor's normal component. We use the propagation of a planar chemical reaction front in an elastic plate that is being subjected to uniaxial compression or tension as an example. We show how the reaction could be blocked by tensions at the reaction front, a locking effect. We thoroughly investigate the relationship between chemical reaction front velocity, locking effect and external loading.

Keywords: Chemical reaction; Deformable; Diffusion; Chemical affinity; Propagation

Introduction

Both basic and practical researches are still very interested in the relationships between chemical reactions and deformation and fracture processes. As an illustration, silicon oxidation has been crucial to the advancement of silicon integrated circuit technology. The lifespan of micron scale MEMS components composed of polycrystalline silicon thin films is governed by the stress assist oxide layer development. The mechanisms of metal hydride production used in hydrogen storage applications serve as another illustration of the drivers for thorough mechano chemistry modelling. The diffusion of the gas constituent through the changed material supports the oxidation of silicon and the absorption of hydrogen and the chemical reaction occurs at the reaction front that separates the two solid components. Deal and Grove proposed one of the earliest and most important models describing these interactions. The application of this one dimensional, stress free model was for the formation of films on flat surfaces. The difference between the kinetics of oxide films produced on nonplanar substrates and planar substrates was then discovered. Marcus and Sheng noticed slowed oxidation growth at silicon trench convex and concave corners. In a series of tests, Kao, et al. investigated the oxidation of cylindrical silicon structures. It was shown that acute curves slowly down the oxidation of curved silicon surfaces and that concave structures are more severely affected than convex ones. These observations have led to the conclusion that internal tensions produced during the oxidation process have an impact on oxidation behaviour.

Description

Huang, Jaccodine and Butler investigated the impact of outside pressures it was demonstrated that compressive forces slowed down oxidation whereas external tensile strains accelerated it. Mihalyi, Jaccodine and Delph conducted additional experimental tests for silicon strips in four points bending in an oxidizing atmosphere. The findings of this series of studies showed that while the effect of tensile stress was unclear, applied compressive stress had a retarding effect on the formation of the oxide layer. Yen and Hwu demonstrated that the tensile stress significantly increases the oxidation rate while looking at the impact of external stress on silicon wafer oxidation.

By extending the Deal Grove model to two dimensional stress dependent models, a number of models have been constructed to

explain microscopic oxidation behaviour. These models proposed surface reaction rate, oxidant diffusivity and oxide viscosity as stress dependent oxidation parameters to account for the impacts of stress. The initial models made the assumption that the reaction front's hydrostatic and normal stresses had the greatest influence on the parameters. Then, models with shear stress dependent viscosity were developed. The concordance between theoretical conclusions and experimental data on the oxidation kinetics supported the parameter selection for the models. Take note of the heuristic introduction of the parameter dependences on stresses. In this study, we attempt to describe the impact of stress using the concept of chemical affinity. This idea, which served as the basis for the rational thermodynamic theory of phase transformations and chemical reactions, was first proposed by Gibbs in 1948 and de Donde in 1936. Combining the chemical potentials of the substances (constituents) involved in the transformation yielded the expression of the chemical affinity. The reaction rate was calculated using a kinetic equation that took the chemical affinity acting as a thermodynamic force into account. It was discovered in the latter half of the twentieth century that the orientation of the border with respect to the stress and isotropy axes affects the phase equilibrium at the interphase boundary in a deformable solid. This led to the realization that in the case of solid phases, the chemical potential is to be a tensor. Phase equilibrium at the interphase boundary and the kinetics of the interface were determined by the normal components of the chemical potential tensors of the phases, according to the derivations, which demonstrated that the chemical potential tensor was equal to the Eshelby energy momentum tensor divided by the referential mass density. Rusanov and Rusanov the tensorial character of the chemical potential and the chemical affinity were also covered. The chemical affinity tensor was then deduced for both the case of nonlinear elastic solid constituents and for any arbitrary solid constituent as a combination of Eshelby stress tensors of solid constituents and a chemical potential of a gas constituent.

Conclusion

We developed an approach to modeling stress assist chemical reactions between solid and gas constituents basing on the chemical affinity tensor and its specification for linear elastic solid constituents. We emphasize that neither derivations of the expression of the chemical affinity tensor nor the accepted kinetic equation for the reaction front propagation are dependent on the constitutive equations of solid constituents.