Computational Materials Science 155 (2018) 541–553

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Numerical Benchmark of Phase-Field Simulations with Elastic Strains: Precipitation in the Presence of Chemo-Mechanical Coupling

Reza Darvishi Kamachali[a,b,*], Christian Schwarze[b], Mingxuan Lin[c], Martin Diehl[a], Pratheek Shanthraj[a,d], Ulrich Prahl[c,e], Ingo Steinbach[b], Dierk Raabe[a]

[a] Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany
[b] Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, 44801 Bochum, Germany
[c] Department of Ferrous Metallurgy, RWTH Aachen University, Intzestraße 1, 52072 Aachen, Germany
[d] The School of Materials, The University of Manchester, Manchester M13 9PL, UK
[e] Institut für Metallformung, Technische Universität Bergakademie Freiberg, Bernhard-von-Cotta-Straße, Germany

ARTICLE INFO

Keywords:
Phase-field modelling and simulation
Microstructure evolution
Precipitation
Diffusion
Elasticity

ABSTRACT

Phase-field studies of solid-state precipitation under strong chemo-mechanical coupling are performed and benchmarked against the existing analytical solutions. The open source software packages OpenPhase and DAMASK are used for the numerical studies. Solutions for chemical diffusion and static mechanical equilibrium are investigated individually followed by a chemo-mechanical coupling effect arising due to composition dependence of the elastic constants. The accuracy of the numerical solutions versus the analytical solutions is quantitatively discussed. For the chemical diffusion benchmark, an excellent match, with a deviation <0.1%, was obtained. For the static mechanical equilibrium benchmark Eshelby problem was considered where a deviation of 5% was observed in the normal component of the stress, while the results from the diffuse interface (OpenPhase) and sharp interface (DAMASK) models were slightly different. In the presence of the chemo-mechanical coupling, the concentration field around a static precipitate was benchmarked for different coupling coefficients. In this case, it is found that the deviation increases proportional to the coupling coefficient that represents the strength of coupling concentration and elastic constants. Finally, the interface kinetics in the presence of the considered chemo-mechanical coupling were studied using OpenPhase and a hybrid OpenPhase–DAMASK implementation, replacing the mechanical solver of OpenPhase with DAMASK's. The observed deviations in the benchmark studies are discussed to provide guidance for the use of these results in studying further phase transformation models and implementations involving diffusion, elasticity and chemo-mechanical coupling effect.

1. Introduction

Modelling and simulation has become an indispensable tool in materials science and engineering, offering tremendous potential to understand, study and design future materials. Advanced full-field simulation techniques and mean-field modelling are especially beneficial in material design to establish *processing* ↔ *microstructure* ↔ *properties* relations. In this regard, the current trend of developing multi-physics simulation tools, enhanced by cluster supercomputing and statistical analysis, enables the investigation of coupled thermo-chemo-mechanical phenomena [1–3]. Quantitative modelling and simulation of various coupled physical phenomena can be regarded as the next challenge in this context. Among several full-field approaches, the phase-field method has demonstrated its remarkable ability to treat physically sound studies [4–11]. In particular, the multi-phase-field approach [12–17] has been successfully applied to study complex microstructure evolution such as in solidification [18,19], recrystallization [20–22], particle pinning [23–25], precipitation during aging [26–30] and, grain growth on the micro- [31–35] and nano-scales [36,37]. As individual microstructure evolution mechanisms may either compete or reinforce each other, the coupling between different physical phenomena and their effects on the microstructure and phase evolution become increasingly significant. Moreover, the various nonlinear modes of interaction between different physical phenomena render the validation of the models a challenging task, as even rough estimates for kinetics and equilibrium states are often not available. To address this issue, the provision of carefully selected benchmarks—systematically derived from the

* Corresponding author at: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany.
E-mail addresses: kamachali@mpie.de, reza.darvishi@rub.de (R. Darvishi Kamachali).

https://doi.org/10.1016/j.commatsci.2018.09.011
Received 13 April 2018; Received in revised form 1 September 2018; Accepted 3 September 2018

isolated treatment of individual effects—is required to ensure (i) the accuracy of numerical solutions compared to the analytical solution for each individual effect and (ii) to specify uncertainties due to numerical techniques in a multi-physics (coupled) framework. In the current study, a set of such benchmark problems related to chemo-mechanical coupling problems and their reference solutions obtained by open source software packages OpenPhase [38,39] and DAMASK [40,41] are presented.

While most models and their implementation are (hopefully) validated and benchmarked against known solutions, these efforts are usually either not published at all or only briefly discussed as a subsection in a model presentation, that makes it difficult to readily apply benchmarks when developing or extending existing implementations. Some attempts, however, have been made to present reference benchmark solutions for materials modelling. Zhang et al. [42] and Münch [43], for instance, have benchmarked the meshing issues regarding phase-field modelling using finite element techniques. In a systematic effort, the Center for Hierarchical Materials Design (CHiMaD) and the National Institute of Standards and Technology (NIST) are developing a set of benchmark problems for phase field models [44]. The first set of these benchmarks was published in 2017 by Jokisaari et al. [45], consisting of an Ostwald ripening model and a spinodal decomposition model with different geometries of simulation domain and two different adaptive time stepping techniques. The second set of benchmarks [46] comprises a study of dendritic growth model and a multiphysics model for an elastically constrained precipitate, where the bifurcation of precipitate shape versus the L' parameter (characteristic ratio between elastic and interfacial energies [47]) is stressed. On the dendritic growth, similar benchmark studies was conducted by Karma and Rappel [48] in developing quantitative phase-field schemes for solidification studies. In this work we present and apply benchmarks on solid-state precipitation, similar to the latter benchmarks of Jokisaari et al. [46], but with a focus on a chemo-mechanical coupling effect that features cross-coupled numerical solutions for diffusion and mechanical problems.

Precipitation hardening plays a critical role in enhancing mechanical properties of engineering alloys [49]. This typically includes diffusion-controlled nucleation and growth of a secondary-phase from a supersaturated matrix that is followed by a subsequent competitive ripening process. While formation of interfaces suppresses the growth, the chemical energy difference between the saturated matrix and the precipitates drives the precipitation reaction. In the solid-state, precipitation is often accompanied by transformation strains which results in stresses within and around precipitates. Depending on the local geometry and volume fraction of the precipitates, stresses can either suppress or reinforce precipitation kinetics. As a result of such long-range diffusion and elastic interaction effects, precipitation process becomes a complex, nonlinear problem [50]. Furthermore, a mutual coupling between the stress/strain and concentration fields can also influence the precipitation process that is the focus of this benchmarking study.

The chemo-mechanical coupling effects during precipitation are expected as composition gradients and strain/stress field evolve and interact at the transformation front, simultaneously. As a model system, we consider here the formation of a δ' precipitate (Al_3Li) in the binary Al-Li system in which a significant coupling effect, arising due to the composition dependence of elastic constants, was found earlier [28,29]. This kind of chemo-mechanical coupling, i.e. composition dependence of elastic constants, was indeed discovered long ago [51] but neglected until recently when its effect on the equilibrium concentration profile around a precipitate has been discussed [52] and applied for studying precipitation in NiTi shape memory alloys [27]. Similar coupling effects manifest themselves in different processes such as bainitic transformation [53], adsorption [54] and shape memory effects [27,55]. Currently, chemo-mechanical coupling effects in metals and polymers are the subject of the priority research programme, SPP1713 [56], initiated by the German Research Foundation (DFG). The current benchmark setups are thought as simple and ensured starting points for numerical studies in the broad community of researchers working on chemo-mechanics problems within and beyond the SPP1713 programme.

In this study, a systematic benchmarking approach—that is hopefully also useful for studying similar problems—is considered in which we first separate the problem of precipitation into diffusion of a second species and mechanical equilibrium, then consider the combined solution of these two problems, i.e. diffusion and mechanical equilibrium with mutual coupling [52], and finally investigate precipitate formation. In the following, the theory and modelling of chemo-mechanical coupling are presented in Section 2. The software packages OpenPhase and DAMASK and a hybrid OpenPhase–DAMASK implementation are briefly introduced in Section 3. The set-up and details of the simulations are presented in Section 4. For the diffusion problem a 1D diffusion couple with a concentration contrast is studied. For elastic equilibrium we consider an inclusion with volumetric expansion and contraction (Eshelby problem). Using these two solvers, the chemo-mechanically coupled relaxation around a static precipitate is discussed. Finally, as an application to our benchmarks, phase-field study of precipitation kinetics in the presence of chemo-mechanical coupling effects (Section 4.4) is presented. The results of the benchmarks are discussed in Section 5.

2. Theory and modelling

In this section, first a description of a chemo-mechanical effect, that is the focus of the study, is given. Then, this model is inserted into the phase-field formalism as presented in the following subsections. The free energy functional for a domain Ω can be written as

$$F\left(\phi, c, \epsilon\right) = \int_{\Omega} \left\{ f_{\text{intf}} + f_{\text{chem}} + f_{\text{elas}} + \ldots \right\} \mathrm{d}V, \tag{1}$$

where f_{intf}, f_{chem}, and f_{elas} are the interfacial, chemical and elastic free energy densities, respectively. These are the energetic contributions of interest in the current benchmark study, but further contributions can be considered in the same formalism. The evolution of a phase α is modelled in terms of the evolution of a non-conserved phase-field variable, $\phi_\alpha(x, t)$, using a generalized form of the time dependent Ginzburg-Landau equation [12,13]:

$$\dot{\phi}_\alpha = -\frac{L}{N_\phi} \sum_{\alpha=1, \alpha\neq\beta}^{N_\phi} \left(\frac{\delta F}{\delta \phi_\alpha} - \frac{\delta F}{\delta \phi_\beta} \right) \tag{2}$$

where L is the interface mobility, N_ϕ is the total number of phase-fields and δ indicates functional derivative. The phase-field variables are constrained with $\sum_{i=1}^{N_\phi} \phi_\alpha = 1$. In the absence of convection, the solute atoms redistribute in the system only through diffusion. In a closed system this results in the following continuity equation:

$$\dot{c} = -\nabla \cdot \mathbf{J} = \nabla \cdot M \nabla \frac{\delta F}{\delta c} \tag{3}$$

where c is solute concentration field, $\mathbf{J}$ is the solute flux, M the mobility of the solute atoms, and $\frac{\delta F}{\delta c}$ is the diffusional potential. Eq. (3) drives solute redistribution to reduce the spatial contrast in the total free energy, F. Here, the chemo-mechanical interaction results from a mechanical contribution to the solute flux, a scenario that extends the classical Fick's laws to consider the influence of micromechanical effects. A well-known case of such an interaction occurs when the size difference between solute and solvent atoms results in a local distortion. For a dilute solid solution this effect can be approximated by the linear rule of mixtures referred to as Vegard's law. This effect has been extensively discussed in previous studies concerning phase transformation kinetics [57–61].

A lesser known chemo-mechanical interaction phenomenon, that is considered in the current benchmark study, arises when the elastic stiffness of a material depends on its local composition. In the solid-state, the atomic bonds between the solute and solvent atoms, which are responsible for the material behaviour in the presence of a small deformation, are composition-dependent. Thus a variation in bonding strength, represented here by the elastic constants, is expected if the