



Numerical simulation of coarsening in binary solder alloys



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ARTICLE INFO

Article history:

Received 20 November 2013
 Received in revised form 6 June 2014
 Accepted 7 June 2014
 Available online 25 July 2014

Keywords:

Cahn–Larché system
 Phase separation
 Adaptive finite elements
 Schur–Newton multigrid

ABSTRACT

Coarsening in solder alloys is a widely accepted indicator for possible failure of joints in electronic devices. Based on the well-established Cahn–Larché model with logarithmic chemical energy density (Dreyer and Müller, 2001) [20], we present a computational framework for the efficient and reliable simulation of coarsening in binary alloys. Main features are adaptive mesh refinement based on hierarchical error estimates, fast and reliable algebraic solution by multigrid and Schur–Newton multigrid methods, and the quantification of the coarsening speed by the temporal growth of mean phase radii. We provide a detailed description and a numerical assessment of the algorithm and its different components, together with a practical application to a eutectic AgCu brazing alloy.

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1. Introduction

The life span of electronic devices strongly depends on the reliability of solder joints connecting the different components. As voids and cracks typically develop at phase boundaries, a well-known source of failure is thermomechanically induced phase separation in solder alloys, often called coarsening. Though there is good knowledge about the coarsening of classical tin–lead solders, such alloys are intended to be significantly reduced worldwide and are even banned in the European Union since 2006, in order to avoid the distribution of lead by electronic waste. The investigation of environmentally friendly substitutes based both on experiments and numerical simulation is still underway.

About ten years ago, Dreyer and Müller [20] utilized the framework of stress-induced diffusion [15] to derive meanwhile well-established Cahn–Larché models for thermomechanically induced phase separation of binary solder alloys. Such models consist of a Cahn–Hilliard system, accounting for spinodal decomposition and Ostwald ripening, coupled with an elasticity equation that represents thermomechanical interaction. In the Cahn–Hilliard system, both theoretical considerations [30,31] and practical reasoning [9,10,55] suggest a chemical energy density of logarithmic type.

The singular behavior of logarithmic chemical energy densities turned out to be one of the major challenges of Cahn–Larché systems both in analysis and numerical approximation. First existence and uniqueness results were obtained by Garcke [24–26], who also investigated sharp interface limits. Related results for a viscous

Cahn–Larché system were obtained by Bonetti et al. [11]. Upper bounds for time-averaged coarsening rates, i.e. for the average speed of demixing of the alloy, have been provided by Novick-Cohen et al. [57,58] in absence of mechanical effects, i.e. for the pure Cahn–Hilliard system. These results extend earlier work of Kohn and Otto [48] for a quartic chemical energy density.

Numerical simulations with Cahn–Larché systems are facing both locally small mesh sizes, as required by the spatial resolution of the diffuse interface, and the algebraic solution of corresponding large-scale systems with logarithmic nonlinearity occurring in each time step. First qualitative numerical studies of Garcke et al. [28] utilize local adaptive mesh refinement, accounting for the diffuse interface, and, in order to enable algebraic solution by standard Newton methods, content themselves with a quartic chemical energy density. An accompanying paper contains the convergence analysis of the underlying implicit Euler discretization in time and finite element discretization in space [29]. Later, Merkle [53] aimed at quantitative results based on physical data. However, still lacking for a suitable algebraic solver, he used smooth spline interpolations instead of the logarithmic chemical energy density. Recent numerical simulations of coarsening in a eutectic AgCu alloy by Anders and Weinberg [1] suffer from a severe under-resolution of the diffuse interface.

In this paper, we present a computational framework for the efficient and reliable simulation of coarsening in binary alloys. A semi-implicit Euler scheme provides the decomposition into a Cahn–Hilliard system and an elasticity equation. We analyze existence and uniqueness of the resulting spatial problems. Spatial discretization is performed by adaptive finite elements, based on a posteriori error estimation. More precisely, we first determine an initial grid which is as coarse as possible but as fine as necessary

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to detect the basic structure of the unknown diffuse interface. From this grid, we compute a corresponding approximation, which is then used to automatically detect regions with large errors by hierarchical a posteriori error estimation [38]. After local refinement in these regions the solve/refinement process is repeated until the unknown diffuse interface is resolved sufficiently well. Careful assembling by high-order quadrature rules instead of mass lumping provides mass conservation, even for temporally varying grids [33, p. 42, Section 6.2]. Recent Schur–Newton solvers [32,33,36,37,34] allow for an efficient and reliable solution of the occurring large-scale algebraic systems with logarithmic nonlinearity without any regularization but with linear multigrid efficiency. These methods exploit the reformulation of the algebraic saddle-point systems in terms of convex minimization problems to which gradient-like descent methods can be applied. In order to provide direct compatibility with experimental results, the coarsening speed is quantified by the temporal growth of the *mean phase radius* [9] rather than the inverse of interfacial energy [28,48].

In our numerical experiments, we observed optimal convergence rates of the adaptive finite element discretization and local mesh independence both of the Schur–Newton method and of a classical multigrid solver for the elasticity problem. Equilibrium concentrations are reproduced up to 0.04% inside the phases and mass is preserved up to $1.9 \cdot 10^{-9}\%$ after 2000 time steps. Coarsening is enhanced by increasing influence of thermomechanical stress, as expected. In quantitative simulations, the temporal growth of the mean phase radius seems to strongly depend on the selection of the chemical free energy. More precisely, replacing a chemical free energy of logarithmic type by a smooth polynomial interpolate (cf., e.g., Merkle [53]), turned out to slow down the coarsening dynamics significantly (cf. Fig. 6 in Subsection 6.3 below).

As a practical application, we present the simulation of coarsening in a eutectic AgCu brazing alloy. In agreement with experimental results, we found only minor influence of mechanical interactions for this alloy.

In light of extensive literature on modeling, analysis, numerical analysis, and fast numerical solution of multicomponent alloys and Cahn–Hilliard systems (cf., e.g., [10,22,23,40,43,46,47]) an extension of our actual computational framework to multicomponent alloys is subject of current research.

2. Mathematical modeling of binary solder alloys

2.1. Generalized Cahn–Larché equations

We consider the local mass concentrations c_A, c_B of the two constituents A and B of some binary alloy in a bounded domain $\Omega \subset \mathbb{R}^d, d = 1, 2, 3$. As concentrations satisfy the pointwise constraints $c_A, c_B \geq 0$ and $c_A + c_B = 1$, we can eliminate c_B and reduce our considerations to the single concentration variable $c = c_A \in [0, 1]$. Introducing the displacement field \mathbf{u} and the corresponding linearized strain $\varepsilon(\mathbf{u}) = \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$ we consider the generalized Ginzburg–Landau free energy

$$\mathcal{E}(c, \mathbf{u}) = \int_{\Omega} \frac{1}{2} \Gamma(c) \nabla c \cdot \nabla c + \Psi(c) + \mathcal{W}(c, \varepsilon(\mathbf{u})) \, dx - \int_{\partial \Omega} \mathbf{u} \cdot \mathbf{g} \, ds. \quad (1)$$

Here, the interfacial energy term $\Gamma(c) \nabla c \cdot \nabla c$ penalizes large concentration gradients and involves the concentration-dependent symmetric, positive definite matrix $\Gamma(c) \in \mathbb{R}^{d \times d}$. A most simple choice is $\Gamma(c) = \gamma(c) \text{Id}$, where Id denotes the identity matrix in $\mathbb{R}^{d \times d}$ and

$$\gamma(c) = c \gamma_A + (1 - c) \gamma_B \quad (2)$$

relies on linear interpolation of constant parameters γ_A, γ_B associated with the pure constituents A, B , respectively. The double-well potential Ψ represents the chemical energy density and drives the uphill diffusion in the separation process towards the equilibrium concentrations. Chemical energy densities of logarithmic type are suggested both by theoretical and practical considerations [20,30,31]. To fix the ideas, we consider the Margules ansatz [10]

$$\Psi(c) = \beta_0 R \theta (c \log(c) + (1 - c) \log(1 - c)) + \beta_1 (1 - c) + \beta_2 c + c(1 - c)(\beta_3 c + \beta_4 (1 - c)) \quad (3)$$

with given temperature $\theta > 0$, universal gas constant R , and material parameters $\beta_i, i = 0, \dots, 4$. Note that the choice $\beta_0 = 1/R, \beta_1 = \beta_2 = 0$ and $\beta_3 = \beta_4 = \frac{\theta c}{2}$ leads to the classical logarithmic potential

$$\Psi(c) = \frac{1}{2} \theta (c \log(c) + (1 - c) \log(1 - c)) + \frac{1}{2} \theta c (1 - c) \quad (4)$$

with critical temperature $\theta_c > \theta$.

The elastic energy density \mathcal{W} takes the form

$$\mathcal{W}(c, \varepsilon(\mathbf{u})) = \frac{1}{2} (\varepsilon(\mathbf{u}) - \bar{\varepsilon}(c)) : \sigma. \quad (5)$$

We assume Hooke's law $\sigma = \mathcal{C}(c)(\varepsilon(\mathbf{u}) - \bar{\varepsilon}(c))$ with a given, positive definite tensor $\mathcal{C}(c)$ that fulfills the usual symmetry conditions of linear elasticity [56] and given eigenstrains $\bar{\varepsilon}(c)$. Both Hooke's tensor $\mathcal{C}(c)$ and the eigenstrains $\bar{\varepsilon}(c)$ are allowed to depend on the concentration c , e.g., linearly as (2). The boundary integral term finally accounts for the prescribed boundary stress \mathbf{g} .

We postulate conservation of mass of the components of the alloy. Hence, the evolution of c is given by

$$\partial_t c = -\text{div } J \quad (6)$$

with some diffusional flux J . We assume that J is defined by

$$J = -M(c) \nabla w,$$

where $M(c)$ denotes a concentration-dependent mobility matrix and

$$w = \frac{\partial \mathcal{E}}{\partial c} = -\text{div}(\Gamma(c) \nabla c) + \frac{1}{2} \nabla c^T \Gamma'(c) \nabla c + \Psi'(c) + \frac{\partial}{\partial c} \mathcal{W}(c, \varepsilon) \quad (7)$$

is the chemical potential. Since mechanical equilibrium is expected to be attained much faster than thermodynamical equilibrium, we assume that

$$\frac{\partial \mathcal{E}}{\partial \mathbf{u}} = 0 \quad (8)$$

holds throughout the evolution. Selecting some final time $T > 0$, the above equations constitute the generalized Cahn–Larché system

$$\partial_t c - \text{div } M(c) \nabla w = 0 \quad (9a)$$

$$-\text{div}(\Gamma(c) \nabla c) + \frac{1}{2} \nabla c^T \Gamma'(c) \nabla c + \Psi'(c) + \frac{\partial}{\partial c} \mathcal{W}(c, \varepsilon(\mathbf{u})) - w = 0 \quad (9b)$$

$$\text{div}(\mathcal{C}(c)(\varepsilon(\mathbf{u}) - \bar{\varepsilon}(c))) = 0 \quad (9c)$$

on $\Omega \times [0, T]$ for the unknown concentration c , chemical potential w , and displacement \mathbf{u} . We prescribe the Neumann boundary conditions

$$\Gamma(c) \nabla c \cdot \mathbf{n} = 0, \quad \nabla w \cdot \mathbf{n} = 0, \quad \sigma \cdot \mathbf{n} = \mathbf{g} \quad \text{on } \partial \Omega \times [0, T] \quad (10)$$

with \mathbf{n} denoting the outward unit normal to $\partial \Omega$ and given boundary stress \mathbf{g} . Finally, we impose the initial condition

$$c(\cdot, 0) = c^0 \quad \text{on } \Omega. \quad (11)$$

A thermodynamical derivation of the Cahn–Larché system (9) using a higher gradient theory of mixtures was carried out by Böhme et al. [9,10].

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