MICROSTRUCTURAL SIMULATIONS WITH CAHN-HILLIARD THEORY

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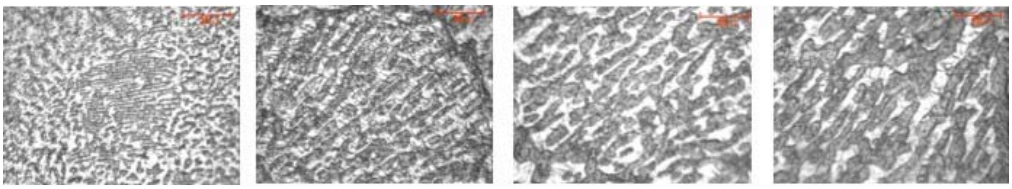
Experimental investigations show that the microstructure of solders changes over time. In order to estimate the reliability and the lifetime of microelectronics it is important to predict the rate of microstructural changes. Starting with a detailed overview on coarsening phenomena and intermetallic growth as observed in lead-free solder alloys this talk concentrates on the description of nucleation and spinodal decomposition as well as subsequent phase growth that occurs in various solder alloys below a critical temperature (cf., Fig. 1).



0 h 22 h 26 h 41 h

Fig 1. Optical micrographs showing aging of a eutectic SnPb lamella structure at 170°C [4].

An extended diffusion equation of the phase field type is presented, which can be interpreted as a generalization of the well known Cahn-Hilliard equation [1]. It reads:

$$\rho_0 \frac{\partial c}{\partial t} + \frac{\partial J_i}{\partial X_i} = 0 ,$$

where the diffusion flux J_i is given by (see [1] for a detailed description of all symbols):

$$J_i = -\rho_0 M_{ij} \frac{\partial}{\partial X_j} \left[\frac{\partial \psi_{\mathrm{conf}}}{\partial c} - 2A_{kl} \frac{\partial^2 c}{\partial X_k \partial X_l} - \frac{\partial A_{kl}}{\partial c} \frac{\partial c}{\partial X_k} \frac{\partial c}{\partial X_l} - \right.$$

$$\left. 2 \frac{\partial A_{kl}}{\partial \varepsilon_{mn}} \frac{\partial c}{\partial X_k} \frac{\partial \varepsilon_{mn}}{\partial X_l} - \frac{\partial^2 a_{kl}}{\partial \varepsilon_{op} \partial \varepsilon_{mn}} \frac{\partial \varepsilon_{op}}{\partial X_k} \frac{\partial \varepsilon_{mn}}{\partial X_l} - \frac{\partial a_{kl}}{\partial \varepsilon_{mn}} \frac{\partial^2 \varepsilon_{mn}}{\partial X_k \partial X_l} \right] . \qquad (2)$$

This equation takes diffusion of the Fickean type, surface tensions along the phase boundaries as well as local mechanical stresses into account. Moreover it represents a

nonlinear partial differential equation of 4th order that describes the temporal development of α - and β -phases in a binary alloy A-B [1,2].

Furthermore all required material parameters of the diffusion equation, i.e., the mass density of the homogeneous mixture ρ_0, the mobility M_{ij}, the Gibbs free energy density ψ_{conf} and the higher gradient coefficients $A_{kl} = \partial a_{kl} / \partial c + b_{kl}$, a_{kl} and b_{kl}) are determined either from the literature / databases, e.g. [6], or from calculations based on the embedded atom method which is suitable to describe atomic interactions in metals [3,5]. As an example the FCC-structured lead-free solder alloy AgCu is considered and the following material parameters as functions of the mass density c can be obtained ($\rho_0 = 9980.57\ \text{kg}/\text{m}^3$):

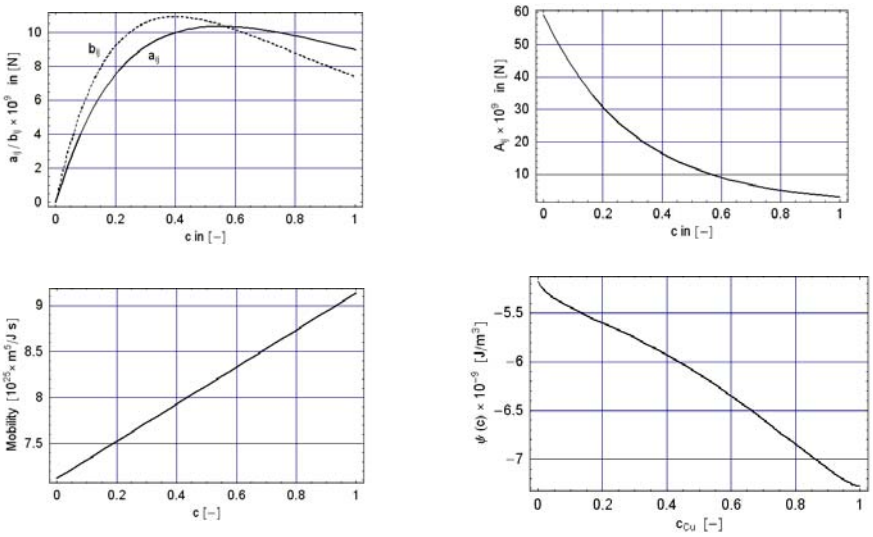


Fig. 2. The higher gradient coefficients, the mobility and the Gibbs free energy density ψ as a function of mass concentration c for AgCu at T=1000 Kelvin.

Finally we restrict to the one dimensional case and calculate the numerical solution of the extended diffusion equation to arrive at a quantitative description of temporal micromorphological development.

Altogether the following steps are performed to simulate spinodal decomposition and phase growth in the binary lead-free solder alloy AgCu, which is important to estimate the reliability, strength and lifetime of solder joints:

1. setup of all equations relevant to describe extended diffusion,
2. determination of all material parameters required for the simulation,
3. specialization to the one-dimensional case as well as its numerical solution by means of discrete Fourier transforms for spatial and partially implicit Euler schemes.

Exemplary results of the simulation are presented and compared with experimental investigations. The talk will end with a discussion on how the presented methods can be extended to also describe the growth of intermetallic compounds as observed along interfaces in lead-free solder alloys. In particular it will be discussed under which circumstances phase field theory will lead to equations of the LSW-type which were used in the papers by Kim & Tu for the prediction of IMC growth [7].

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