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Phase separation in solder alloys

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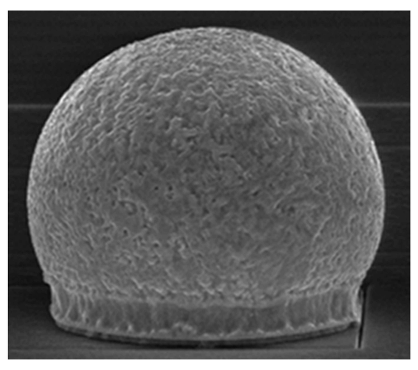
Introduction

Cahn-Hilliard equation

- 4th order diffusion equation
- C^1 continuity of the shape functions required

Application to an eutectic Sn-Pb alloy

- Phase separation using real world data
- 3D computational modeling of the large scale system



Cahn-Hilliard equation

Formulation of the problem [1]

- Diffusion equation

$$\frac{\partial c}{\partial t} = \nabla \cdot (\boldsymbol{M}\nabla\mu), \quad \boldsymbol{M} = M(c)\boldsymbol{D}$$

- Strong form

$$\frac{\partial c}{\partial t} = \nabla \cdot (\boldsymbol{M}(c)\nabla(\partial_c \Psi^{\text{con}}(c) - \lambda\Delta c))$$

$$c = g \quad \text{on} \quad \Gamma_u \times [0, \mathcal{T}]$$
$$\boldsymbol{M}\nabla\mu \cdot \boldsymbol{n} = s \quad \text{on} \quad \Gamma_s \times [0, \mathcal{T}]$$
$$\nabla c \cdot \boldsymbol{n} = 0 \quad \text{on} \quad \Gamma$$

- Weak form

$$\int_{\mathcal{B}_0} \frac{\partial c}{\partial t}\varphi \, \mathrm{d}V = -\int_{\mathcal{B}_0} M(c)\,[\partial_c^2\Psi^{\text{con}}]\nabla c\boldsymbol{D}^{\mathrm{T}}\nabla\varphi \, \mathrm{d}V - \int_{\mathcal{B}_0} \lambda\Delta c[\partial_c M]\nabla c\boldsymbol{D}^{\mathrm{T}}\nabla\varphi \, \mathrm{d}V - \int_{\mathcal{B}_0} M(c)\,\lambda\Delta c\boldsymbol{D}^{\mathrm{T}} : \nabla \otimes \nabla\varphi \, \mathrm{d}V$$

Computational modeling

Discretization [2]

- Isogeometric Analysis (IGA)

$$\varphi^h = \sum_{A\in\omega} R^A q_A \quad \text{and} \quad c^h = \sum_{A\in\omega} R^A c_A$$

- Multivariate NURBS shape functions

$$R^A = \frac{N_{\mathrm{i},p}(\xi)M_{\mathrm{j},q}(\eta)L_{\mathrm{t},r}(\zeta)w_{\hat{\mathrm{i}},\hat{\mathrm{j}},\hat{\mathrm{t}}}}{\sum_{\hat{\mathrm{i}}=1}^{n}\sum_{\hat{\mathrm{j}}=1}^{m}\sum_{\hat{\mathrm{t}}=1}^{l} N_{\hat{\mathrm{i}},p}(\xi)M_{\hat{\mathrm{j}},q}(\eta)L_{\hat{\mathrm{t}},r}(\zeta)w_{\hat{\mathrm{i}},\hat{\mathrm{j}},\hat{\mathrm{t}}}}$$

- B-Splines – Cox-de Boor relation

$$N_{\mathrm{i},p} = \frac{\xi - \xi_{\mathrm{i}}}{\xi_{\mathrm{i}+p} - \xi_{\mathrm{i}}} N_{\mathrm{i},p-1}(\xi) + \frac{\xi_{\mathrm{i}+p+1} - \xi}{\xi_{\mathrm{i}+p+1} - \xi_{\mathrm{i}+1}} N_{\mathrm{i}+1,p-1}(\xi)$$

where

$$N_{\mathrm{i},0}(\xi) = \begin{cases} 1 & \text{if } \xi_{\mathrm{i}} \le \xi < \xi_{\mathrm{i}+1} \\ 0 & \text{otherwise} \end{cases}$$

- Implicit Crank-Nicholson scheme in time

$$[0, \mathcal{T}] = \bigcup_{n=0}^{n_t-1} I_n, \quad \Delta t = t_{n+1} - t_n$$

Sn-Pb Solder Alloy

Experimental data for eutectic Sn-Pb solder [3]

- configurational free energy function

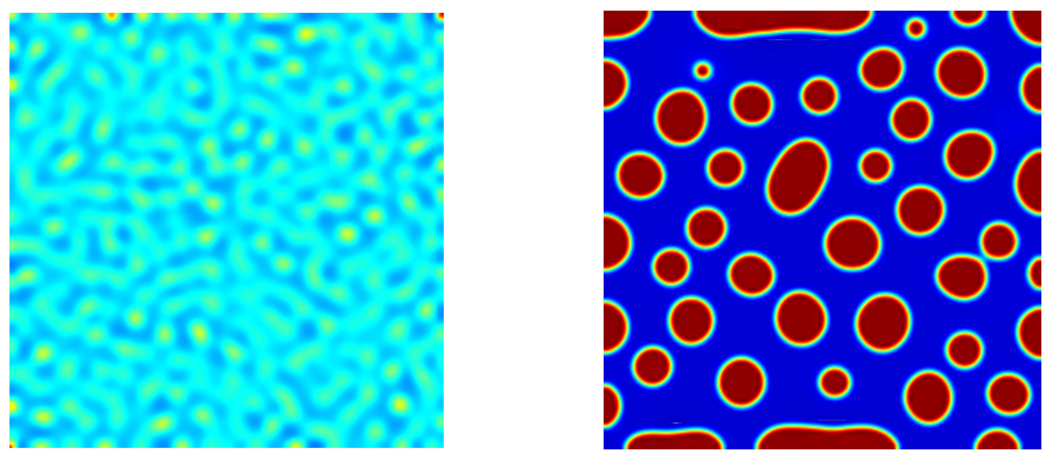
$$\Psi^{\text{con}} = g_1 c + g_2(1-c) + g_3 c\ln(c) + g_4(1-c)\ln(1-c) + g_5 c(1-c)$$

- Sn-Pb: chemical database MTDATA®

$g_1\,\left[\frac{\text{GJ}}{\text{m}^3}\right]$	$g_2\,\left[\frac{\text{GJ}}{\text{m}^3}\right]$	$g_3\,\left[\frac{\text{GJ}}{\text{m}^3}\right]$	$g_4\,\left[\frac{\text{GJ}}{\text{m}^3}\right]$	$g_5\,\left[\frac{\text{GJ}}{\text{m}^3}\right]$
−1.3527	−1.5145	0.3575	0.1585	0.8599

2D Simulation

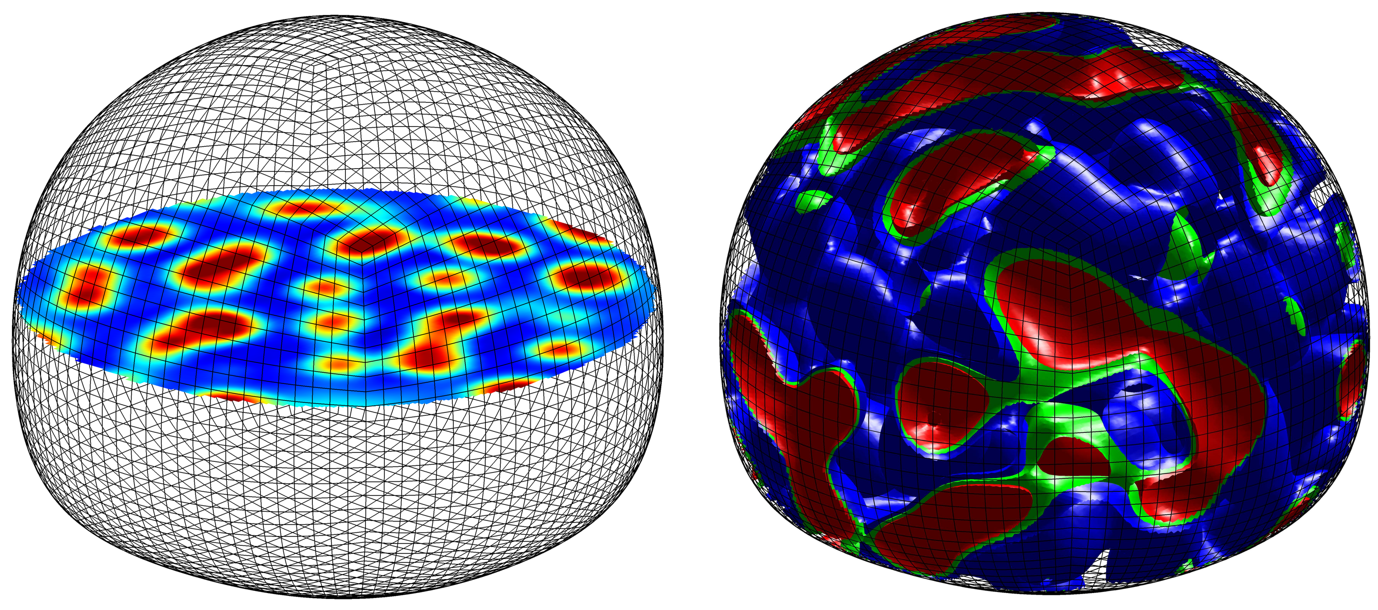
A grid of 128 × 128 nodes and 15876 elements are used to discretize the 4 μm^2 area.



The left side shows the system shortly after initialization, the right after 10 hours of aging.

3D Simulation

A grid of 28 × 28 × 28 elements is used for the simulation of a 0.5 μm ball.



Simulation results after 0.15 hours of aging are displayed.

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