The Level Set Method for solid-solid phase transformations

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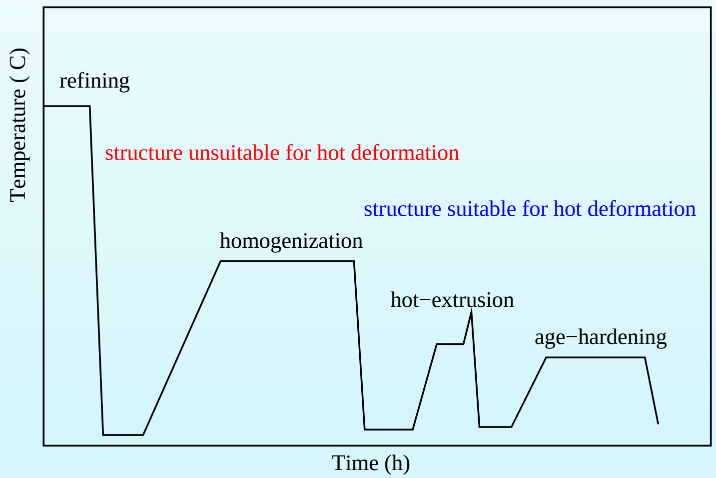
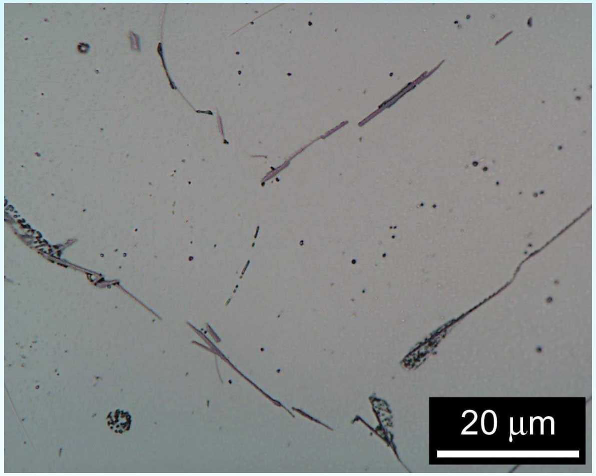
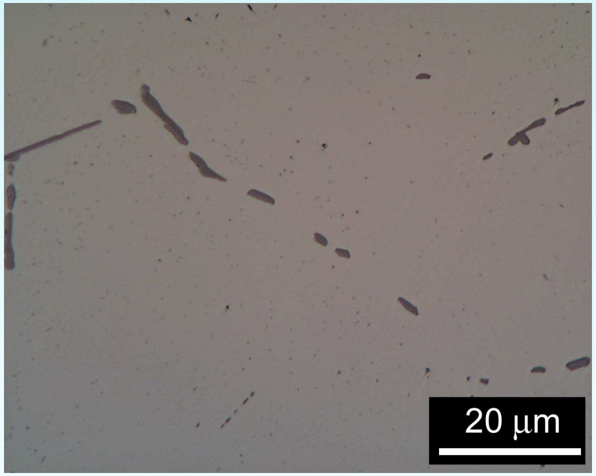
Technological background

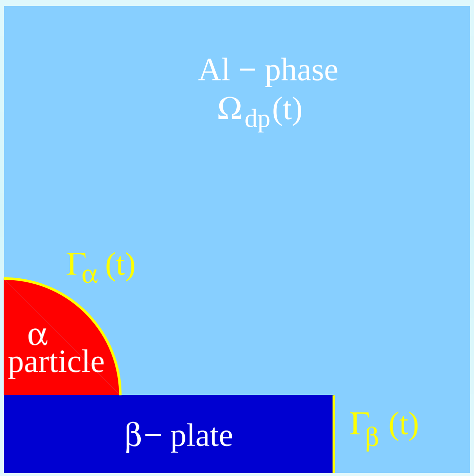






Aim of the project

Vector Stefan models for homogenization of Aluminum alloys



Diffusion of several components:

$$\frac{\partial c_i}{\partial t} = \sum_{j=1}^{n} D_{ij} \Delta c_j \quad \Omega_{dp}(t)$$

Displacement of the interface(s):

$$(c_i^{part} - c_i^{sol}) v_n^{\alpha} = \sum_{j=1}^{n} D_{ij} \frac{\partial c_i}{\partial n_\alpha} \quad \Gamma_\alpha(t)$$

$$(c_i^{part} - c_i^{sol}) v_n^{\beta} = \sum_{j=1}^{n} D_{ij} \frac{\partial c_i}{\partial n_\beta} \quad \Gamma_\beta(t)$$

The binary model in 2D

$$\frac{\partial c}{\partial t}(x,y,t) = D\Delta c(x,y,t) \quad (x,y) \in \Omega_{dp}(t),\ 0 < t < T$$

$$c(x,y,t) = c^{sol} \quad (x,y) \in \Gamma(t),\ 0 < t < T$$

$$c(x,y,t) = c^{part} \quad (x,y) \in \Omega_{p}(t),\ 0 < t < T$$

$$\frac{\partial c}{\partial n}(x,y,t) = 0 \quad (x,y) \in \partial\Omega,\ 0 < t < T$$

$$(c^{part} - c^{sol})v_n(x,y,t) = D\frac{\partial c}{\partial n}(x,y,t), \quad (x,y) \in \Gamma(t),\ 0 < t < T$$

Properties

Existence of similarity solutions

Growth problem unstable (Mullins & Sekerka, *JAP '63*)

$$r(t,\theta,\varphi) = R(t) + \delta(t) Y_{lm}(\theta,\varphi)$$

$$\frac{d\delta}{dt} > 0 \iff R > R_c(l) = \left[\frac{(l+1)(l+2)}{2} + 1\right] R^*$$

The Level Set Method

The level set function: ϕ continuous s.t.

$$\phi(x,y,t)=0 \iff (x,y)\in\Gamma(t),\ \forall t>0.$$

Displacement of the interface:

$$\frac{\partial\phi}{\partial t}+\mathbf{V}\cdot\nabla\phi=0 \qquad \Omega$$

$\mathbf{V}$ continuous extension of $\mathbf{v}=\frac{D}{c^{part}-c^{sol}}\nabla c$ onto Ω

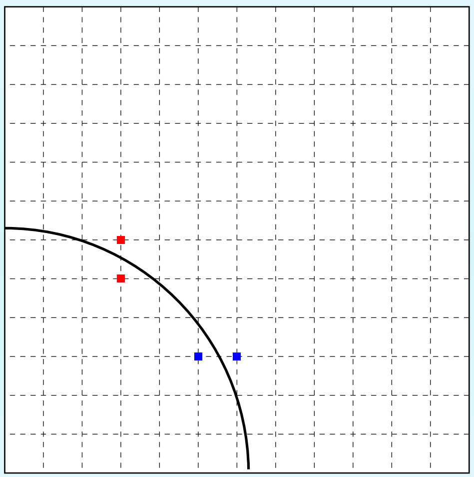
Reinitialization of the level set:

$$\frac{\partial\phi}{\partial\tau}=\mathrm{Sign}(\phi^0)\Big(1-|\nabla\phi|\Big)$$

Outline of the algorithm

1. Find the velocity $\mathbf{V}$ from c^n, ϕ^n
2. Update the level set $\rightarrow \phi^{n+1}$
3. Reinitialize ϕ^{n+1} (Russo & Smereka, *JCP '00*)
4. Solve diffusion equation where $\phi^{n+1} > 0$
5. Go to 1

Fully FD approach



Interface velocity $\mathbf{v} = \lambda \nabla c = (v_1, v_2)^t$

Suppose $\phi_{i-1j} < 0$ and $\phi_{ij} > 0$

$$v_1 = \frac{D}{c^{part} - c^{sol}} \frac{\partial c}{\partial x} \approx \frac{D}{c^{part} - c^{sol}} \frac{c_{ij} - c^{sol}}{r_{ij} \Delta x}$$

with $r_{ij} = \frac{\phi_{ij}}{\phi_{ij} - \phi_{i-1j}}$

Continuous extension $\mathbf{V}$:

$$\frac{\partial V_1}{\partial \tau} + \mathrm{Sign}\left(\phi \frac{\partial \phi}{\partial x}\right) \frac{\partial V_1}{\partial x} = 0 \qquad \Omega$$

$$V_1(x, y, \tau) = v_1(x, y, \tau) \qquad \Gamma$$

Fully FD approach, cont.

Diffusion equation:

$$\frac{c_{ij}^{n+1}-c_{ij}^{n}}{\Delta t^n} = D\left(\frac{c_{i-1j}^{n+1}-2c_{ij}^{n+1}+c_{i+1j}^{n+1}}{\Delta x^2} + \frac{c_{ij-1}^{n+1}-2c_{ij}^{n+1}+c_{ij+1}^{n+1}}{\Delta y^2}\right)$$

Near the interface:

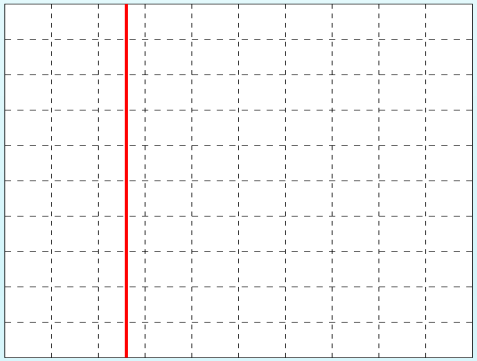
$$\frac{c_{ij}^{n+1}-c_{ij}^{n}}{\Delta t^n} = D\left(LPx'' c^{n+1} + LPy'' c^{n+1}\right)$$

Dissolution problems: $\phi_{ij}^{n+1} > 0$ but $\phi_{ij}^{n} < 0$. Consider $t_{ij}^{*} \in (t^n, t^{n+1})$ s.t. $\phi(x_i, y_j, t_{ij}^{*}) = 0$

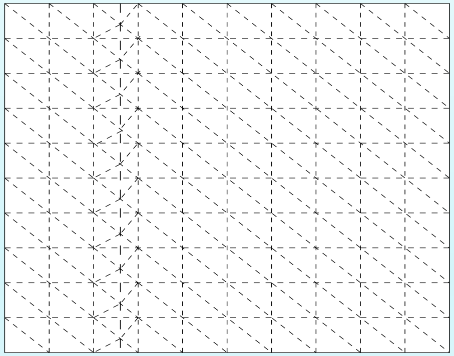
$$\Delta \tilde{t}_{ij}^{n} = t^{n+1} - t_{ij}^{*} = \Delta t^n \frac{\phi_{ij}^{n+1}}{\phi_{ij}^{n+1}-\phi_{ij}^{n}} \quad \rightarrow \quad \frac{c_{ij}^{n+1}-c^{sol}}{\Delta \tilde{t}_{ij}^{n}} = D\Delta_h c_{ij}^{n+1}$$

FD/FE approach

FE attractive → SEPRAN package



Finite Differences mesh



Finite Elements mesh (cut−cell apporach)

Interface velocity

Update of the level set

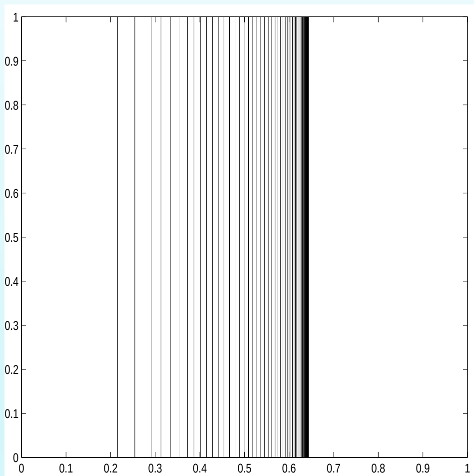
Reinitialization

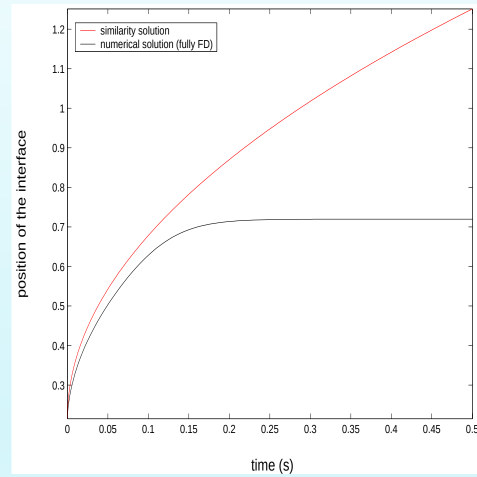
Diffusion equation

Cut-cell approach

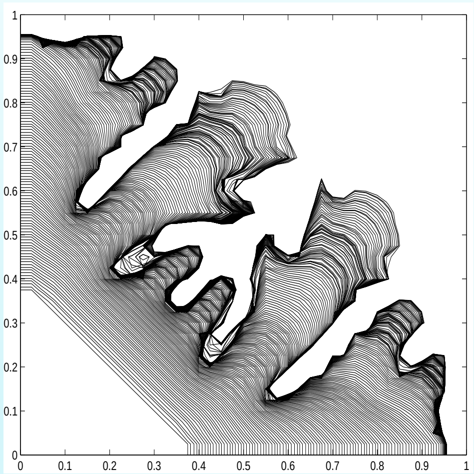
Interpolation between meshes

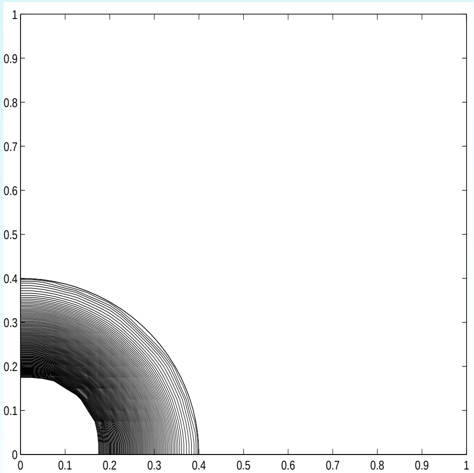
Numerical experiments





Numerical experiments





Conclusions and future work

Conclusions

Level Set Method suitable

Artificial continuous extension of the front velocity

FD approach elegant but

FE/FD approach elegant and strong numerical model

Future work

Dissolution problems included

Surface tension included

Fully FE approach