

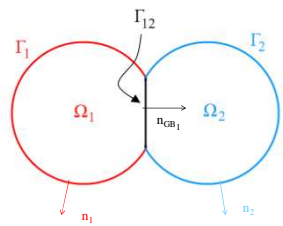
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Context

- Sinterability of powders for nuclear fuel pellets is of major importance for fuel fabrication, to this aim a sub-granular model is under development
- In the framework of the modelling of sintering on a sub-granular scale, a densification law has been derived in the case of two grains. Predictions from these laws are commented.

Model description



1. Elastic behaviour at each time step:
 Displacement field computation with Von Neumann Boundary conditions: Laplace law

For Γ_1 and Γ_2 free surfaces: $\bar{\sigma}(\vec{n}) \cdot \vec{n} = -p_{gaz} - 2\gamma_{SV}k_{SV}$ with σ the stress tensor, \vec{n} the outer normal, γ_{SV} the Solid/Vapor surface energy and k_{SV} the local mean curvature.

For Γ_{12} grain boundary: $\bar{\sigma}_1(\vec{n}_1) \cdot \vec{n}_1 = \bar{\sigma}_2(\vec{n}_1) \cdot \vec{n}_1 - 2\gamma_b k_b$

2. Chemical potential μ with a mechanical origin:
 $\mu = -\frac{1}{3}tr(\sigma) - \frac{1}{2}\Theta(\sigma : s : \sigma)$ with s the compliance matrix

3. Onsager first law: mass flow

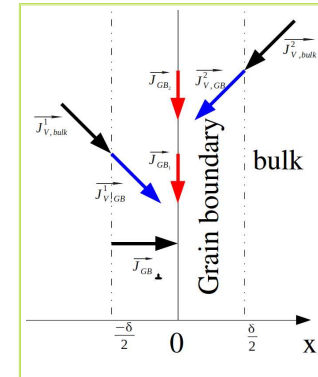
Bulk, free surface and grain boundary fluxes: $\vec{J} = -L\vec{\nabla}\left(\frac{\mu}{T}\right)$

4. Onsager second law: interface movements

Normal speed V_{int} of interfaces \rightarrow irreversible mass flow

$$\iint_S \rho V_{int} \cdot \vec{n} dS = M \iint_S \left(\left(\vec{j}_{GB1}^1 + \vec{j}_{GB1}^2 \right) \cdot \vec{n} + \text{div}_S \left(\vec{j}_{GB}^1 - \vec{j}_{GB}^2 + \left(\delta \left(\vec{j}_{GB1}^1 - \vec{j}_{GB1}^2 \right) \vec{t} \right) \right) \right) dS$$

Local Fick's second law



It has been shown that if \dot{V}_1 is the total mass of matter (or quasi-incompressible volume) produced along the grain boundary by grain 1 per time unit in direction of grain 2

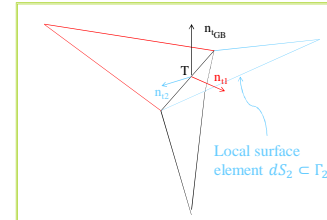
$$\dot{V}_1 = -\Omega \int_{\Sigma_{GB}} \left(\vec{j}_{GB}^1 \cdot \vec{n}^1 + \text{div}_S(\vec{j}_{GB}^1 + (\delta \vec{j}_{GB}^1 \vec{t})) \right) dS$$

\dot{V}_1 total mass of matter (or quasi-incompressible volume) produced along the grain boundary by grain 1 per time unit in direction of grain 2

In the same way for the other side:

$$\dot{V}_2 = -\Omega \int_{\Sigma_{GB}} \left(\vec{j}_{GB}^2 \cdot \vec{n}^2 + \text{div}_S(\vec{j}_{GB}^2 + (\delta \vec{j}_{GB}^2 \vec{t})) \right) dS$$

Kirchhoff's current law (KCL)



At triple point T: $\vec{j}_{S1} \cdot \vec{n}_{t1} = -\vec{j}_{GB1} \cdot \vec{n}_{t1}$ with \vec{n}_{t1} the normal to the triple edge tangent with surface 1
 So that if \vec{j}_{V1} can be neglected and Ostrogradski relation is used :

$$\dot{V}_1 = \Omega \oint_{\Gamma_{12}} \vec{j}_{S1} \cdot \vec{n}_{t1} dl$$

$$\vec{j}_{S1} = -L\vec{\nabla}_S\left(\frac{\mu}{T}\right) \text{ with } \mu \text{ the chemical potential}$$

Densification rate

The shrinkage of two grains reads: $\dot{h} = \frac{1}{2A_{GB}}(\dot{V}_1 + \dot{V}_2)$ with A_{GB} the area of the grain boundary

Model predictions for densification

➤ **A consequence of Kirchoff Current Law**
 The shrinkage rate depends only on the shape of the free surfaces in the vicinity of the triple line,

For rigid grains ($\mu_{bulk} = \mu_0$), the chemical potential at a surface can be expressed without solving any mechanical Partial Differential Equations:

$$\mu = \mu_{bulk} + \Omega \left\{ \gamma_S \left[\frac{1}{R_1} + \frac{1}{R_2} \right] + \frac{1}{R_1} \frac{\partial^2 \gamma_S}{\partial^2 n_1} + \frac{1}{R_2} \frac{\partial^2 \gamma_S}{\partial^2 n_2} \right\}$$

➤ **A consequence of the surface chemical potential expression:**
 For spherical rigid grains ($R_1=R_2$ =sphere radius) $\vec{\nabla}_S \frac{1}{R} = \vec{0}$ diffusion along free surfaces can only occur if the material is non-isotropic, i.e.: $\frac{\partial^2 \gamma_S}{\partial^2 n_i} \neq 0$

For rigid grains, absence of diffusion perpendicular to the grain boundary ($\vec{j}_{GB^\perp} = \vec{0}$) i.e. with only grain boundary and surface diffusion the shrinkage rate would be zero: $\dot{h} = 0$

The latter conclusions are changed when grains are no more considered as rigid but for instance as elastic at a given time (quasi-static step) during the sintering process ($\mu_{bulk} = f(\sigma) \neq \mu_0$).

Conclusions

- The mechanical model developed can be a useful tool for the study of impact of initial grain morphology upon sintering
- Non obvious consequences of the mechanical part of the chemical potential upon grain shrinkage rate can be discussed