

A snow isothermal metamorphism model applicable on microtomographic images

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Context – importance of a good knowledge of the snowpack



Context – snowpack properties are changing with time



Context – need of microscale observations



Context – X-ray microtomography to obtain 3D images



Brzoska et al, 1999; Flin et al 2003; Schneebeli and Sokratov 2004; Chen and Baker, 2010; Srivastava et al, 2010; Calonne et al, 2011; Loewe et al, 2011; Pinzer et al, 2012; Hammonds et al, 2015; Krol and Loewe, 2016; Ishimoto et al, 2018; Letcher et al, 2021; Robledano et al, 2023; Bouvet et al, 2023... Access geometrical and physical properties

Context – Several types of grains and metamorphism regimes



Context – Isothermal metamorphism



Equations – Physical modelling

Sublimation-deposition process: without diffusion, convection and settling of grains

Mechanism: Hertz-Knudsen equation

$$v_n = \alpha v_{\rm kin} \frac{\rho_{vs}^{\rm amb} - \rho_{vs}^{\Gamma}}{\rho_{vs}^{\Gamma}} \quad \text{on } \Gamma$$

with
$$v_{\rm kin} = \frac{\rho_{vs}^{\rm ref}}{\rho_i} \sqrt{\frac{k^2}{2\pi}}$$

$$\begin{array}{c|c}
 & R = 1/C \\
 & V_{n} \\
 & V_{n} \\
 & Air \\
 & \sqrt{\frac{kT}{2\pi m}} \\
\end{array}$$
Interface velocity

 ρ_{vs}^{Γ} : saturation vapor density on the ice-air interface

Deposition coefficient α : probability that a water vapor molecule is incorporated into the ice phase. Today still poorly quantified!

Belongs to [0, 1] and depends at least on temperature T.

Driving force: Kelvin's (or Gibbs-Thomson) law

on
$$\Gamma$$
 $\rho_{vs}^{\text{amb}} = \rho_{vs}^{\text{ref}} e^{2d_0 C^{\text{amb}}}$

C: local curvature C_{amb} : integrated curvature on whole interface d_0 : capillary length << 1

 $\rho_{vs}^{\Gamma} = \rho_{vs}^{\text{ref}} e^{2d_0C}$

→ $v_n = 2d_0 \alpha v_{kin} (C_{amb} - C)$ Typical case of volume preserving curvature flow

Equations – Phase-field modelling: Bretin et al (2019)

Application of classical phase-field equation to the case of isothermal metamorphism:

$$\frac{\partial u}{\partial t}(x,t) = d_0 \alpha v_{\rm kin} \left(\Delta u(x,t) - \frac{1}{\varepsilon^2} W'(u) \right)$$



Following Bretin et al (2019), the canonical dimensionless equation can be written:

$$\frac{\partial \tilde{u}}{\partial \tilde{t}} \left(\tilde{x}, \tilde{t} \right) = \Delta \tilde{u} \left(\tilde{x}, \tilde{t} \right) - \frac{1}{\tilde{\epsilon}^2} W' + \tilde{\mu} \frac{1}{\tilde{\epsilon}} \sqrt{2W(\tilde{u}, \tilde{t})}$$
Where: $\tilde{t} = \frac{t \alpha v_{\text{kin}} d_0}{d_x^2}, \quad \tilde{x} = \frac{x}{d_x}, \quad \tilde{\epsilon} = \frac{\epsilon}{d_x}$
And $\tilde{\mu}$ is a Lagrange multiplier verifying: $\tilde{\mu} = \frac{1}{\tilde{\epsilon}} \frac{\int_{\Omega} W'(\tilde{u}, \tilde{t}) d\tilde{x}}{\int_{\Omega} \sqrt{2W(\tilde{u}, \tilde{t})} d\tilde{x}}$

Bretin et al, 2019: Phase-field modelling and computing for a large number of phases, Elie Bretin, Roland Denis, Jacques-Olivier Lachaud and Edouard Oudet, ESAIM: M2AN, 53 3 (2019) 805-832, DOI: <u>https://doi.org/10.1051/m2an/2018075</u>

28 h of equi-temperature experiment at -7°C



Experimental result











Model calibration:

Link between the non-dimensional time \tilde{t} and the physical time t:



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Link between the non-dimensional time \tilde{t} and the physical time t:



Model evaluation:

Evaluation of α using an independent experimental series of isothermal metamorphism at -2°C (Hagenmuller et al, 2019).



Simulation of isothermal metamorphism at -2°C.



→ Good agreement between simulated and experimental microstructural parameters.

Model predictions: snow microstructures at -2°C









Conclusions:

- Application of a 3D phase-field model developed for curvature flow with mass conservation
- The model is applicable on tomographic images, and gives consistent results for the isothermal metamorphism of snow
- It allowed calibrating the deposition coefficient α at -2°C, and this result has been confirmed by an independent time series
- → Better understanding of the physical mechanisms involved

Perspectives:

- At the beginning of the simulation: elongated grains are disconnected by curvature effects. How modeling their mechanical rearrangement?
- Extension to wet snow metamorphism (add another phase)
- Extension to Temperature Gradient metamorphism (add crystal growth effects, thermal field computation...)
- → Suggestions are welcome!



An attempt to simulate the grain rearrangement





An attempt to simulate the grain rearrangement

Densification caused by the breaking of the necks

Evaporation-condensation \rightarrow densification

Established principle in Material Sciences: the evaporation-condensation mechanism happens without any densification