Modeling Heat and Mass Transfer in Snow at a Microstructural Level using a Phase-Field Approach – First Results

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ABSTRACT

Snow is a highly porous medium consisting of an ice matrix and porous space containing water vapor. With time, snow undergoes metamorphism as heat flow and interface effects induce mass flow and thus profoundly change the microstructure. We present a phase-field model to solve the coupled heat and mass transport problem including phase-change processes in an evolving ice-pore network. The model considers mass fluxes that are induced by temperature gradients in the snow as well as by curvature effects. We applied the model to 2D sections of X-ray micro-tomography images of snow to study the interplay between heat flow, mass transport, and evolving snow microstructure.

Keywords: snow, metamorphism, modeling, phase field

INTRODUCTION

Snow is a highly porous medium consisting of an ice matrix and porous space containing water vapor. With time, snow undergoes metamorphism and its microstructure evolves. There is a strong interaction between the snow microstructure and snow pack properties. Understanding snow metamorphism is thus crucial for predicting mechanical properties used in avalanche forecasting, chemical composition associated with the interpretation of ice cores data, or thermophysical properties important for modeling the energy balance of snow-covered landscapes. The link between heat transport and metamorphism is particularly strong. On the one hand, heat flow through snow induces mass flow and thus an evolution of the ice-pore network; on the other hand, the microstructure influences heat flow as heat transport is governed by conduction in the ice and pores as well as phase change processes and water vapor transport in the pore space (Fig. 1).

Snow metamorphism is often parametrized with respect to grain and bond sizes and forms. However, questions remain with respect to the range of validity of parametrizations and, more fundamentally, the relative importance of the processes governing metamorphsim. Recently, computed X-ray micro-tomography emerged as a tool to observe snow metamorphism at a microstructural scale (Schneebeli and Sokratov, 2004). A numerical model operating at similar length scales and based on fundamental physics is highly desirable to study metamorphism in detail. A first attempt in this direction by (Christon *et al*., 1994) used an adaptive finite element method which did not allow for topological changes. This limits the computations to artificial ice lattices or short time scales and might be the reason why such an approach was never pursued.

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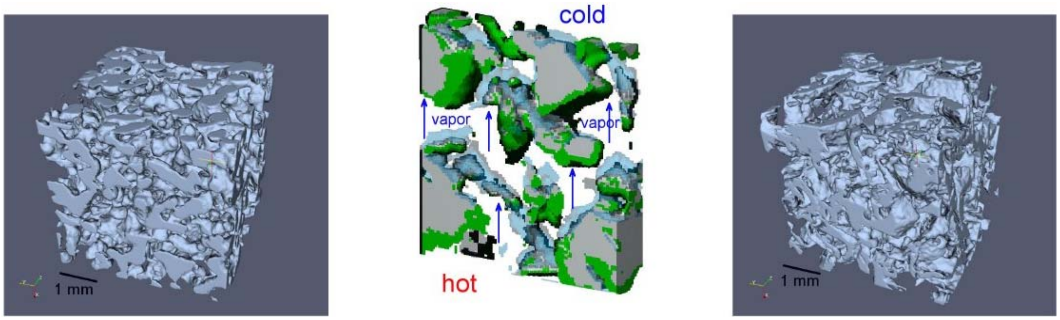

Figure 1. Metamorphing snow imaged by X-ray micro-tomography: New snow (left) evolves towards a coarser and more faceted structure (right) when submitted to a temperature gradient (here $\nabla T \cong 50\,\mathrm{K/m}, T \cong -3.4\,^{\circ}\mathrm{C}$, time 10 days). Due to the temperature gradient, a water vapor gradient arises in the pore space that drives mass flow (center; blue represents sublimated, green freshly condensated ice during one day).

PHASE FIELD MODELING

Phase field models treat multi-phase systems with complicated interface conditions by tackling the problem continuously, inclusive of the interfacial region (Fig. 2). This continuous variation across the interface is realized using an order parameter, the phase field function ϕ, which describes the phases thermodynamically. We suppose $\phi = 1$ in ice, $\phi = -1$ in air, and $-1 < \phi < 1$ represents the ice-air interface.

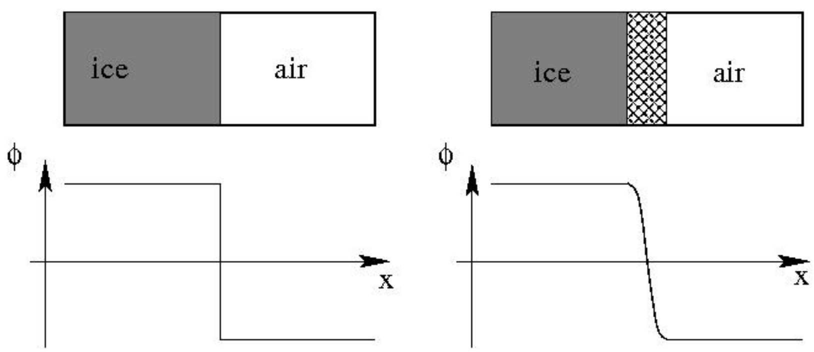

Figure 2. Sharp interface (left) and diffuse interface (right) with the phase field function ϕ.

In a classical formulation the basic equations have to be written for each medium and the interface boundary conditions must be explicitly tracked. In diffuse-interface theory the basic equations, with supplementary phase field terms, are deduced from a free energy functional for the whole system and interface conditions do not occur. In fact, they are replaced by a partial differential equation for the phase field. Phase field methods are widely used to model the formation of complex microstructures during solidification processes and we refer to (Boettinger *et al.*, 2002) for an overview.

SNOW METAMORPHISM PHASE-FIELD MODEL

Snow metamorphism under an imposed temperature gradient is governed by heat and mass conservation laws, with possible phase change at ice-air interfaces. In the diffuse interface approach, we use the phase field function ϕ to continuously express the physical parameters, defining for example the heat conductivity by

$$\kappa(\phi) = \kappa_i \frac{1+\phi}{2} + \kappa_a \frac{1-\phi}{2},$$

where κ_i and κ_a are the heat conductivities of ice and air, respectively. Analogous definitions for the specific heat capacity $\rho c_p(\phi)$ and the chemical diffusion coefficient D can be defined, where for the latter we set $D_i = 0$ and $D_a = D_v$ the diffusion coefficient of water vapor in dry air. Moreover, we suppose the ice density ρ_i constant, denote by ρ_v the water vapor concentration in the air and define a continuous water concentration, in the ice equal to the density, as

$$\rho(\phi) = \rho_i \frac{1+\phi}{2} + \rho_v \frac{1-\phi}{2}.$$

We denote the equilibrium water vapor concentration in air by $\rho_{veq}(T)$ and suppose that the continuous equilibrium water concentration, respectively density, is given by

$$\rho_{eq}(\phi, T) = \rho_i \frac{1+\phi}{2} + \rho_{veq}(T) \frac{1-\phi}{2}.$$

We choose now a reference temperature T_0, set $\rho_{veq}^0 = \rho_{veq}(T_0)$ and define a dimensionless chemical potential by

$$u = \frac{\rho(\phi) - \rho_{eq}(\phi, T_0)}{\rho_{veq}^0}.$$

Note that u is constant through an equilibrium interface at a given temperature T and denote the constant $u_{eq}(T)$.

With the above hypothesis and notations the snow metamorphism model reads

$$\tau \frac{\partial \phi}{\partial t} = W^2 \nabla^2 \phi + \phi - \phi^3 + \lambda \frac{\rho_{veq}^o}{\rho_i} (u - u_{eq}(T))(1 - \phi^2)^2,$$

$$\rho c_p(\phi) \frac{\partial T}{\partial t} = \nabla(\kappa(\phi) \nabla T) + \frac{L_{sv} \rho_i}{2} \frac{\partial \phi}{\partial t},$$

$$\frac{\partial u}{\partial t} = \nabla(D(\phi) \nabla u) - \frac{\rho_i}{\rho_{veq}^0} \frac{1}{2} \frac{\partial \phi}{\partial t},$$

where W is the interface thickness, τ is the phase field relaxation time, λ is a coupling constant which determines the capillary length, and L_{sv} denotes the latent heat of sublimation.

One problem when simulating snow metamorphism using the above equations is the large time scale, since the ice matrix migration velocity is of order μm/h. Fortunately, since diffusion of heat and of water vapor in the pore space is fast, we can assume metamorphism to be quasi-steady, i.e., the temperature and water vapor concentration fields are supposed to be steady. This fact can be exploited to scale up the interface velocity.

FIRST RESULTS

We discretized the phase field model by finite differences and applied it to a 2D section of an X-ray micro-tomography image of natural snow. We extracted a 3 voxel (60 μm) thick section from the tomography image (Fig. 3) and combined it into one plane to obtain the computational domain of size $2 \times 4\,\text{mm}$. Note that, even though we combined several slices, the ice-matrix was still not fully connected in the 2D space (see Fig. 4) and the simulations can thus not be completely representative of the 3D situation.

We subjected the snow sample to a vertical temperature gradient of $\nabla T = 200\,\text{K/m}$ and observed the heat and mass fluxes and the evolution of the ice-matrix (Fig. 4).

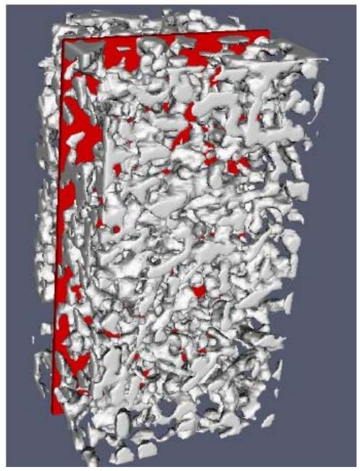

Figure 3. Construction of 2D computational domain.by extracting and combining three slices of an X-ray micro-tomography image of snow.

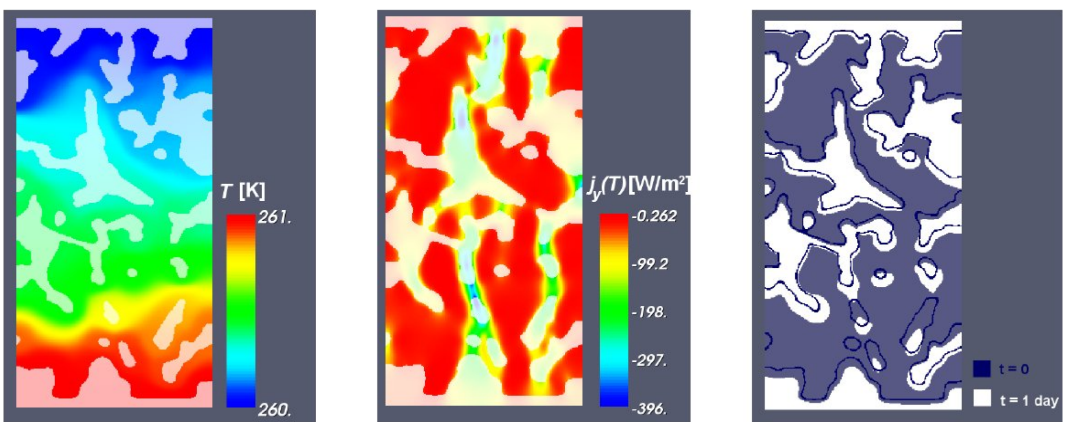

Figure 4. Phase field computation on a 2D slice of tomographed snow: A vertical temperature gradient was imposed, the ice matrix is shown in overlayed white. Temperature distribution (left), heat fluxes (center), and ice matrix after one day compared to the initial condition (right).

The temperature distribution is considerably disturbed from a linear one, due to the different heat conductivities of ice and air (Fig. 4, left). Even though the ice matrix is not fully connected, we observe that the heat fluxes concentrate along the ice structure (Fig. 4, center). Moreover, strong inhomogeneities in the heat fluxes in the pore space are observed, leading consequently to similar inhomogeneities in the induced water vapor fluxes. Such effects have also to be expected in 3D. Using the phase field function ϕ, we can easily follow the microstructural evolution including topological changes and identify regions where the ice matrix sublimates or regions of crystal growth (Fig. 4, right).

CONCLUSION

We present a phase field model to simulate temperature gradient driven snow metamorphism at the microstructural level. The model considers heat and mass fluxes through the intricate ice-pore network forming snow and includes sublimation and condensation at the ice-air interfaces. Water vapor transport is, for the conditions presented here, mainly governed by the temperature gradients arising within the pore space, but the phase field model also handles implicitly any curvature effects. The model readily assimilates structural initial conditions from snow X-ray micro-tomography measurements, albeit for the moment its implementation is two-dimensional.

One major advantage of this diffuse interface approach is that it implicitly handles any topological changes. Moreover, it's extension to three spatial dimensions is straight forward and the only additional difficulties arise from higher computational times.

The model will be validated using simplified geometries from (Christon *et al.*, 1994) and direct comparison to tomography measurements. A future challenge will be the extension of the model to allow for anisotropic crystal growth, which is necessary to simulate the growth of faceted ice crystals and depth hoar formation.

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