A Microstructural Dry Snow Metamorphism Model Applicable to Equi-Temperature and Temperature Gradient Environments

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Abstract: Dry snow metamorphism has traditionally been classified by the thermal gradient encountered in the snowpack. Snow experiencing a predominantly equi-temperature environment develops different microstructure than snow that is subjected to a temperature gradient. As such, previous research has evaluated snow metamorphism based upon select thermal gradient dependent processes, when in reality, there is a continuum of physical processes simultaneously contributing to metamorphism. In previous research, a discrete temperature gradient transition between the two thermal environments has been used to activate separate morphological analyses. The current research focuses on a unifying approach to dry snow metamorphism that is applicable to generalized thermal environments. The movement of heat and mass is not prescribed, but is allowed to develop naturally through modeling of physical processes. Equi-temperature, transition to kinetic growth, and kinetic growth are considered with this model. Density, grain size, bond size, and temperature dependencies are each examined in an equi-temperature metamorphism environment. The same physical model is then used to define a smooth transition between equi-temperature and temperature gradient environments. Microstructural and environmental parameters that influence the transition to kinetic growth are examined. The correlation with established trends and experiments in each environment is excellent. The microstructural model is a new tool capable of evaluating metamorphism for a broad range of microstructural parameters and thermal environments.

Keywords: snow and ice, temperature gradient, kinetic growth, snow crystal growth, snow crystal structure, snow metamorphism

Introduction

Snow is a unique granular material. From the time it touches the earth until it either transitions to liquid (melts) or to vapor (sublimates), the snow microstructure is continually changing in a process called metamorphism. The time-varying microstructural quantities result in nonlinear material responses, making the study, understanding, and prediction of snow metamorphism vital to nearly all areas of snow science. The critical dependence of snow properties on microstructure makes metamorphism an extremely important area of study.

Two categories of metamorphism are classically discussed, depending upon the thermal environment. In a snowpack where the temperature is nearly uniform, metamorphism is termed "equi-temperature". If a significant temperature gradient is applied (frequently found in alpine snow), then "temperature gradient" metamorphism results. Traditionally, each of these conditions has been treated as separate and distinct since each results in a unique microstructure (Sommerfeld and LaChapelle, 1970). Use of the temperature environment to describe the metamorphic process is not universally accepted. In fact, the categorization of metamorphism has resulted in much discussion and debate. Colbeck (1980, 1982, 1983a) used crystal forms and driving forces to describe metamorphism. The current research reported here does not require a distinction between the different types of metamorphism, rather it uses physical processes common to both. The resulting unified approach makes the discussion somewhat obsolete and irrelevant.

In the absence of a macroscopic temperature gradient, ice particles are observed to sinter by growing the bonds between the individual grains. This sintering process is commonly referred to as equi-temperature metamorphism. Colbeck (1980) correctly pointed out that truly equi-temperature metamorphism is impossible for any process involving phase change. Heat must flow for phase

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change to occur, thereby requiring microscopic temperature gradients. Colbeck (1980) introduced the term "radius-of-curvature" metamorphism due to the curvature differences behind this process. The resulting microstructure is commonly referred to as equilibrium form, rounds, or equi-temperature.

In seasonal snow, it is common for snowpack temperature gradients to develop, resulting in "temperature gradient" or "kinetic growth" metamorphism. The combination of heat stored in the ground over the summer months and geothermal warming keep the layer near the ground close to 0°C for most of the winter season (McClung and Schaerer, 1993), yet the upper surface of the snowpack is subjected to diurnal temperature fluctuations. The diffusion of water vapor through the interstitial pore space changes the nature of metamorphism significantly. A temperature gradient (and resulting vapor pressure gradient) in the pore produces unique snow morphologies. As the temperature gradient increases, the snow microstructure can change from smooth rounded grains with smooth interconnections to large, highly faceted, angular crystals with large surrounding pore spaces. These crystal forms are often referred to as facets, temperature gradient metamorphism forms, kinetic forms, recrystallized snow, and depth hoar.

Several theories have been developed that adequately explain the physics of snow sintering in an equi-temperature environment and faceted grain development in the presence of a temperature gradient. To date, no one has presented a unified theory of metamorphism that includes detailed microstructure yet is not restricted by the temperature environment. In fact, Arons and Colbeck (1995) comment "we still lack a model that integrates fundamental elements of geometry and the transfer of sensible and latent heat in a physically sound inductive model". The objective of this research is to develop a unifying dry snow microstructure metamorphism theory that accounts for important physical parameters and processes yet is applicable in general thermal environments. The approach will transition smoothly between isothermal and temperature gradient conditions.

1. Model Development

The approach begins with the definition of simple microstructural parameters. Conservation of heat and mass are then defined with phase change thermodynamics as a coupling constraint. The resulting non-linear coupled differential equations are solved numerically by finite difference techniques. The development is only briefly summarized here with the details available in Miller (2002).

1.1 Equilibrium Form Geometry

A simple grain and neck geometry is used for the rounded form of snow. To model the ice geometry, some simplifications are made. First, the grains for this morphology are assumed to be spherical. There may be several different sized grains, but the equilibrium forms are modeled as perfectly round. A universally accepted intergranular neck definition does not exist. Therefore, smooth concave necks spanning either side of crystal bonds are used to make the interparticle connections. Edens (1997) developed a stereological approach defining the grain-neck transition where the surface curvature reverses sign. Geometric definitions used here are similar to Brown et al. (1999). The pore sizes are defined based on the grain/neck sizes and snow density. While the detailed arrangement of grains and necks is complex, some simplifications are made. For snow in an isothermal environment, it is assumed that the material is macroscopically isotropic, ie, the microstructure does not depend upon the observation direction. When a temperature gradient is applied, metamorphism can result in directionally oriented microstructure. During long exposure to significant temperature gradients, channels or mesopores develop parallel to the temperature gradient. Ice chains may also develop with large, striated, faceted grains appearing. Due to this preferred orientation, it is assumed that the snow geometric properties are symmetric with respect to an axis of rotation about the temperature gradient, making the problem transversely isotropic. Symmetry is assumed in any plane perpendicular to the temperature gradient. To model equi-temperature and temperature gradient environments, a microscopic geometry is used by linking a large number of ice spheres and necks together. The configuration of two grains and one neck is given in Figure 1. Any number of grains and necks may be defined.

1.2 Theoretical Development

Before the governing equations can be developed, there are several assumptions that are made:

1. *Heat conduction in the pore space can be neglected, so that only heat flow through the ice network is considered.* This is a common assumption given the fact that the thermal conductivity of saturated vapor at cold temperatures is two orders of magnitude smaller than the thermal conductivity of pure ice (Incropera and DeWitt,1985).

2. *Saturated vapor, for a given temperature, exists everywhere in the pore spaces.* Even though no measurements of relative humidity in pore spaces have been published, this is a classic assumption given the large surface area of the ice available to interact with the pore.

3. *The vapor saturated pore may be treated as an ideal gas.* This is a common thermodynamic assumption for low pressure water vapor applications. The snowpack absolute pressure should be very close to atmospheric.

4. *The primary mass transport mechanism is vapor diffusion through the pore.* As discussed in chapter 1, substantial research has shown convection to be a significant mass transport mechanism under very select conditions. In general, convection is neglected for metamorphism modeling. Other diffusion mechanisms associated with the ice, such as lattice, surface, and grain boundary, are considered small and neglected in the primary development.

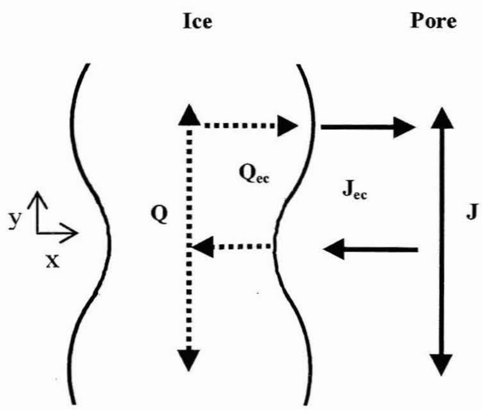


Figure 1. Heat and mass flows during metamorphism. Q represents the heat flow through the ice network, Q_{ec} is the heat flow from evaporation or condensation, J is the mass flow in the pore, J_{ec} is the mass flow from evaporation or condensation.

5. *Liquid water in the snow is not considered.* Solid ice and water vapor are the only phases of water considered for dry snow.

Figure 1 shows graphically the heat and mass fluxes available given the geometry and assumptions discussed. Mass can diffuse vertically through the pore spaces as well as to and from the ice surface during phase changes. Heat can flow vertically through the ice network as well as to or from the ice surface due to the latent heat exchange associated with phase change.

The first consideration is the movement of vapor in the pore spaces. The mass conservation equation with mass sources/sinks from phase change is given by

$$\frac{\partial \rho}{\partial t} + \vec{\underline{\nabla}} \cdot (\underline{J}) = MS \tag{1}$$

where ρ is the vapor density (kg/m^3), J is the molecular flux vector (kg/(sm^2)), and and MS is the mass supply or sink from phase change (kg/m^{3}s). MS is given by

$$MS = J_{ec} \frac{A_{ec}}{V_{pore}} \tag{2}$$

where A_{ec} is the surface are undergoing phase change (m^2) and V_{pore} is the volume of the pore (m^3). If the vapor is treated as an ideal gas and using the differential form of the Clausius-Clapeyron relationship, Fick's Law for vapor diffusion may be expressed as

$$\underline{J} = -D\frac{PL}{R^2T^3}\vec{\underline{\nabla}}T = \frac{-D}{RT}\vec{\underline{\nabla}}P \tag{3}$$

where D is the water vapor diffusion coefficient in air (m^2/s), R is the water vapor gas constant (J/(kgK)), T is the pore temperature (K), L is the water latent heat of sublimation (J/kg), and P is the pore pressure (Pa). If equations (1), (2), and (3) are combined, a non-linear differential equation that is coupled to the ice through phase change (MS) results.

Heat conduction through the ice is considered next. Energy conservation in the ice accounting for the latent heat associated with phase change leaves

$$\frac{d^2\theta}{dy^2} + \frac{1}{A}\frac{dA}{dy}\frac{d\theta}{dy} = \frac{HS}{kA} \tag{4}$$

where k is the ice thermal conductivity (W/mK), A is the cross sectional area for heat diffusion (m^2), and θ is the ice temperature (K), and HS is a heat source term that is coupled to the pore through the phase change at the boundary. HS is given by

$$HS = J_{ec} L \frac{dA_{ec}}{dy}. \quad (5)$$

The heat conduction and mass conservation equations are coupled through the phase change flux, J_{ec}. This flux results from a vapor pressure gradient between the ice surface and the surrounding pore. The vapor pressure over the ice surface is corrected for temperature and curvature (Adams and Brown, 1983; Gubler, 1985). The phase change vapor flux is given by

$$Jec = \frac{-D}{RT}\frac{dP_v}{dx}. \quad (6)$$

Phase change is controlled by the local heat transfer at the vapor/ice interface. Heat must flow to or from the interface to either add or remove latent heat. The heat balance at the interface can be expressed as

$$-k_{ice}\frac{d\theta}{dx} + k_{pore}\frac{dT}{dx} = J_{ec} L. \quad (7)$$

In equation (7), the difference in conducted heat between the ice and pore is the latent heat. The phase change temperature appears in the gradients in equation (7).

The mass conservation equation, energy conservation equation, and phase change constraints result in three non-linear differential equations that are coupled through the phase change flux, J_{ec}. The equations are solved numerically after the ice and pore network are discretized into elements and nodes (nodes shown in Figure 2). Finite difference equations are developed for each of the differential equations. The resulting systems of equations are solved using various iterative numeric techniques. The details of the solution are found in Miller (2002).

3. Equi-temperature Results

During snow metamorphism, several microstructural parameters direct metamorphic trends. Traditionally, grain size has been the primary time varying parameter considered. Grains are the most readily visible structure when examining snow. In addition to grain size, the interconnecting neck size has recently been recognized as an equally important feature. As with grains, bonds and necks influence nearly all physical attributes such as strength, stability, thermal properties, optical properties, elastic response, inelastic response etc. The broad influence of grains and their interconnections requires that their interactions be included in any reasonable metamorphism theory. In the current research, bonds, necks, and grains have been described and are an integral part of the theory. While the absolute sizes of grains and bonds are important, their relative size is commonly used to describe the level of bonding or maturity of metamorphism. The bond to grain ratio is the ratio of the bond size to the grain radius. During the metamorphism of equal sized grains in an equi-temperature environment, several parameters such as grain geometry, intergranular neck geometry, pore geometry, density, and temperature influence the rate and nature of metamorphism. The influence of several parameters is examined by defining a baseline configuration, given in Table 1. Grain size, bond size, density and temperature are then independently varied to see the sensitivity of metamorphism to each.

Grain Sizes	r_g=0.125, 0.5, 1.0 mm
Ratio	0.4
Snow Density	150 kg/m^3
Temperature	-5°C

Table 1. Equi-temperature metamorphism study parameters.

Figure 2 pictorially represents the heat and vapor flux paths that result from this analysis. Small vapor pressure gradients between nodes result in vapor flux from the convex surfaces, to the pore, through the pore, and onto the concave necks. The local temperature gradient in the pore was typically on the order of 0.05 °C/m to initiate and maintain the metamorphism. While this temperature gradient appears very small, metamorphism in a macroscopically isothermal environment could not commence without it.

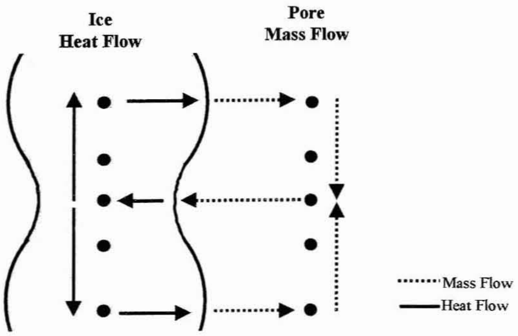
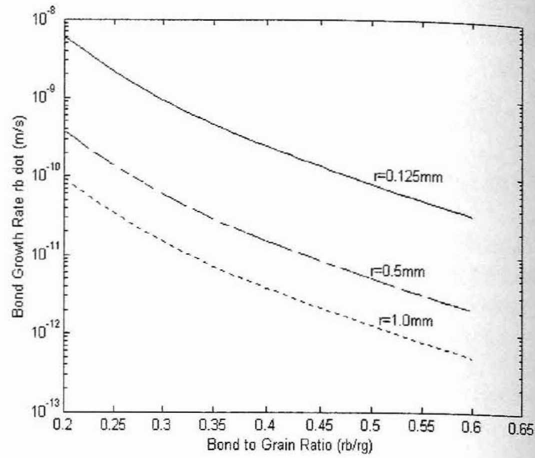


Figure 2. Heat and mass flow during metamorphism in equi-temperature conditions. Nodes for numerical solution are shown in the ice and pore.

The vapor and heat flow depicted in Figure 2 result from the following process. The convex grain surface curvature creates a vapor pressure gradient between the ice surface and pore. Vapor sublimates from the surface and becomes a vapor source, causing vapor to diffuse to the pore node. As vapor is added at the node, the temperature increases slightly, creating a gradient to the neighboring nodes. Vapor diffuses in the pore toward the necks thereby increasing the vapor pressure at this node. A vapor pressure gradient therefore develops between the pore node and the concave neck surface, causing vapor to diffuse toward the neck. Vapor is allowed to condense and release the associated latent heat to the ice neck's central node. This slightly raises the neck nodal temperature resulting in heat conduction to the neighboring nodes. At the central grain node, heat is removed thereby providing the latent heat of sublimation required, and the cycle is complete. The geometry is updated as time integration proceeds by adding or removing mass from ice elements.

The first study examines metamorphism as the bond to grain size ratio is varied. Figure 3 shows the variation of grain decay and bond growth with bond to grain radii ratio. As the bond to grain ratio increases from 0.2 to 0.6, the bond growth rate decreases by two orders of magnitude for each grain size. The reduction in surface curvature, increase in neck length, neck surface area, and neck volume during metamorphism combine to reduce the growth rate with increasing bond size. An analogous process is taking place during grain radius reduction. The sintering rate decreases dramatically with increased bonding, a simple well understood yet important result (Hobbs and Mason, 1964; Maeno and Eblnuma, 1983). Observations have shown that snow sinters very rapidly initially, then decreases



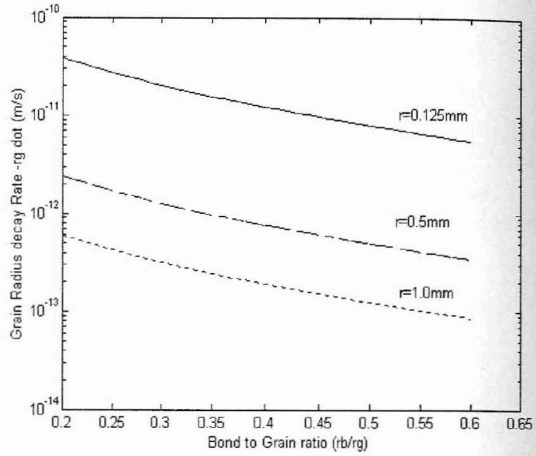


Figure 3. Bond growth and grain decay rates vs bond to grain ratio. T=-5°C, ρ=150 kg/m^3

dramatically in time. As the bonds grow, the vapor pressure gradient decreases as the neck radius of curvature decreases. It is evident from Figure 3 why very large bond ratios are rarely, if ever, observed in seasonal snow.

Using the parameters in Table 1 but now varying temperature, Figure 4 shows the grain decay rate and bond growth rate for snow comprised of equally sized grains in an equi-temperature environment. As expected, the metamorphic rates are sensitive to temperature. The bond growth rate decreases by a factor of approximately 8 for all three grain sizes as the temperature is lowered from 0 to –20 °C, confirming another well established experimental metamorphic trend (Hobbs and Mason, 1964). As previously discussed, microstructural temperature gradients do develop in the pore and ice, but here the average macroscopic temperature is varied.

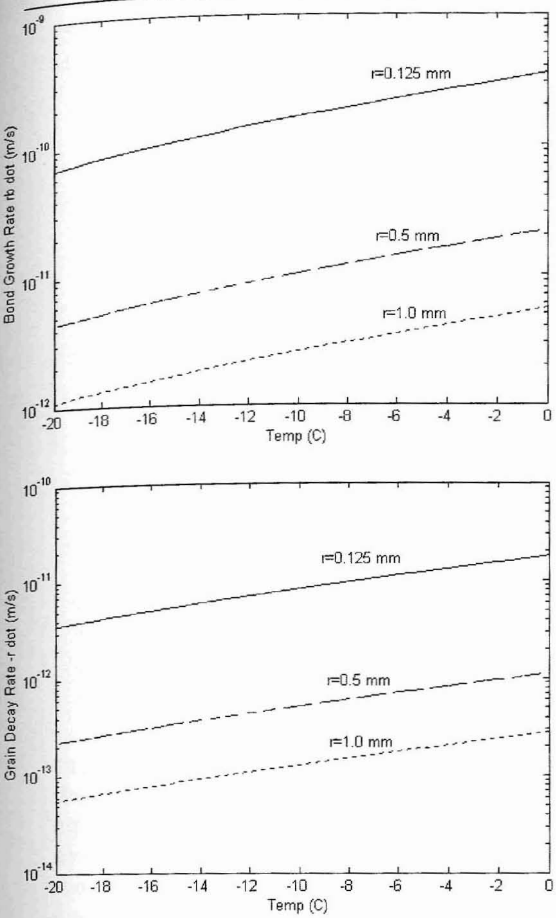


Figure 4. Bond growth and grain decay rates vs temperature. ρ=150 kg/m^3, bond/grain ratio=0.4

The snow density in Table 1 is now varied while holding the temperature and bond ratio fixed for all three grain sizes. The ice geometry is fixed for a particular problem and the pore sizes are varied with density. As the density increases, the size of the pore space for vapor movement decreases. Figure 5 shows the variation of bond growth rate and grain decay rate with density. Metamorphism in an equi-temperature environment appears to be relatively insensitive to variations in density. The bond growth rate changes are generally less than 20% over a large range of densities. Grain decay rate changes with density are slightly larger, but still small compared to bond size and temperature affects.

This result may seem surprising, but upon further thought and investigation, is logical. During vapor metamorphism in an equi-temperature environment, it is believed that vapor moves the very short distance from grains to neighboring necks (Kingery, 1960; Hobbs and Mason, 1964; Maeno and Eblnuma, 1983). As the vapor leaves the grain surface, diffuses through the pore, and condenses on the neck, the size of the pore is not a limiting parameter due to the local vapor movement. Given a specific ice geometry, the diffusion distance between grains and necks does not vary substantially with density, only the pore size changes. Since the pore size decreases with increased density, the pore's vapor storage capability decreases, slightly decreasing the metamorphic rate. The size of the pore is not the critical factor in this metamorphic regime. In the extremely dense snow where the pore becomes very small, pore size could become a limiting factor. For common snow densities less than 450 kg/m^3, density is not significantly limiting local vapor transfer between grains and necks.

In order for this result to be valid, most of the vapor leaving a grain should deposit on neighboring necks. If this were not the case, the pore would either supply vapor or remove vapor locally through diffusion. If significant diffusion to or away from neck and grain localities existed, the pore size would influence metamorphic rates. When a temperature

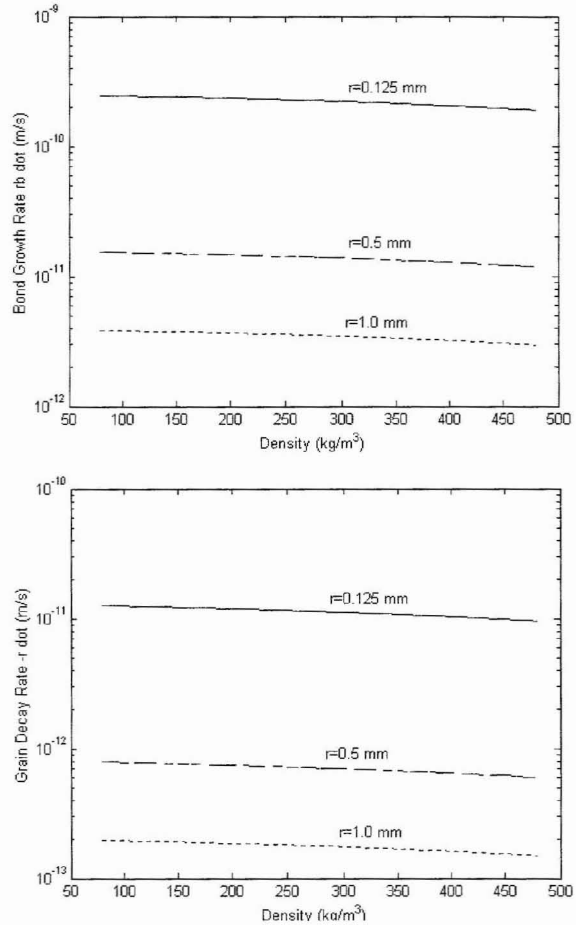


Figure 5. Bond growth and grain decay rates vs temperature. T=-5°C, bond/grain ratio=0.4

gradient is applied, the density (pore size) will become a significant factor. The mass leaving the grains and the mass arriving at the necks were compared to see if a mass balance exists. While not presented here, a mass balance between the grains and surrounding necks was very good, supporting the local mass transfer.

The results so far have used equally sized grains. While not presented here, the model did demonstrate the growth of large grains at the expense of small.

4. Transition to Kinetic Growth

The transition between the smooth rounded growth forms common in an equi-temperature environment and the sharp faceted forms found in a temperature gradient environment has not been studied extensively. Most research surrounding this transition is experimental. It is commonly believed that the critical temperature gradient for faceted growth is around 10-20°C/m (Akitaya, 1974; Armstrong, 1980; Colbeck, 1983a, 1983b) or greater than 25°C/m (Marbouty, 1980). It is recognized that this transition is a function of density, pore size, grain size, and temperature (Colbeck, 1983b), but little analytical work has been done to show the relative importance of each. It is recognized that low density snow transitions at a lower temperature gradient than higher density snow, but microstructurally based analytical approaches explaining this phenomenon are lacking. The current approach may be used to study this transition and various parameters influencing the transition. First, a definition of kinetic growth transition temperature gradient is required.

There is clearly no agreed upon point where equilibrium forms dominate and then suddenly faceted forms appear. A smooth transition based on physical constraints is desired instead of relying on incomplete empirical data. Grains cannot grow in a kinetic form when they are decaying, as may be the case in an equi-temperature environment. When a temperature gradient is applied, vapor diffuses in the pore, and heat conducts through the ice. As the temperature gradient increases, the grain decay rate decreases, and the neck growth rate increases due to the excess vapor pressure of the pore. Kinetic growth processes are allowed to begin when the temperature gradient is sufficient to transition the grains from decay to growth.

For this study, the temperature gradient where a "majority" of the grains start to grow is defined as the onset or transition temperature gradient for kinetic growth. One can think of the equi-temperature and temperature gradient processes commencing simultaneously in both environments, but which is predominant when? In an equi-temperature environment, the excess vapor pressure is negative resulting in a negative kinetic growth velocity. When the kinetic growth velocity is negative, that process is inactive when the grain is decaying, resulting in no kinetic growth. The smooth rounded forms are allowed to develop as previously described. As the temperature gradient increases to the point where grains begin to grow, this is the first opportunity for kinetic growth. Near the transition temperature gradient, the smooth and faceted forms may be equally viable, resulting in combined morphologies. Mixed rounded and kinetic forms are rare, but have been observed (Colbeck, 1982; 1983a). As the temperature gradient continues to increase, the grain growth due to kinetic metamorphism becomes predominant. The model includes both, and allows each to commence as required. Figure 6 gives a pictorial representation of this process and the definition of the transition temperature gradient. As the temperature gradient increases, the flux leaving the grains decreases. At the transition temperature gradient, the grains begin to grow.

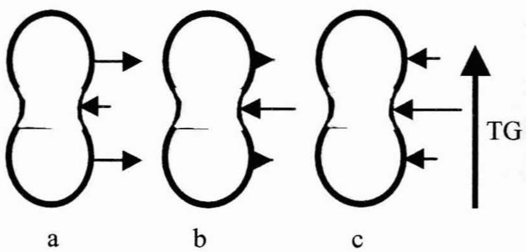


Figure 6. Vapor flux definition of temperature gradient at onset of kinetic growth. (a) TG=0, Equi-temperature vapor fluxes. (b) TG>0, TG less than onset of kinetic growth. (c) TG>0, TG at onset of kinetic growth

The transition from grain decay to grain growth is shown for three grain sizes as a function of the applied temperature gradient in Figure 7. As the temperature gradient increases, the grain growth rate increases. The onset of kinetic growth is clearly visible as the grain radial growth rate transitions from negative to positive. Throughout the temperature gradient range, the changes are smooth and continuous. Previous models required a discrete transition as new physical models were required. Also, kinetic growth transitions have generally been based on the 10°C/m criteria, with little or no regard to any physical parameters that may effect that value. Since the temperature gradient shown did not exceed

25°C/m, the 0.5mm grains did not yet reach their kinetic growth transition.

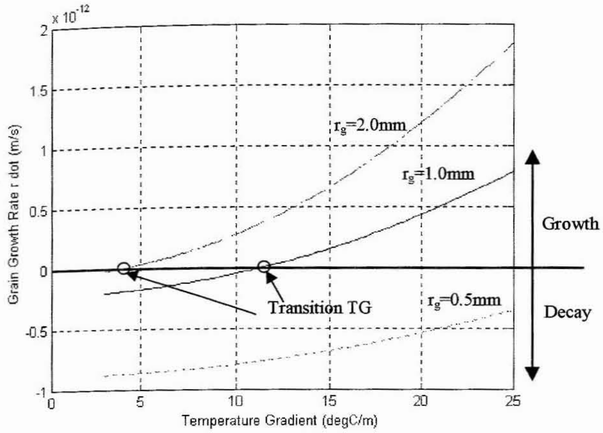


Figure 7. Grain growth rate vs temperature gradient. The smooth transition to kinetic growth is shown. T=-3°C, ρ=150 kg/m^3, r_b/r_g=0.4.

In a temperature gradient environment, the size of the pore spaces, and therefore the density, should be a major factor in the onset of kinetic growth. It is commonly accepted that lower density snow (larger pore spaces) is much more likely to show kinetic growth with a smaller temperature gradient. In addition to the pore size for vapor transport, large faceted crystals need sufficient space to grow. Marbouty (1980) showed an increase in the grain size with decreasing density when subjected to a temperature gradient sufficient for kinetic growth. He also showed a kinetic growth upper limit density of 350 kg/m^3, above which kinetic growth was not observed even under large temperature gradients. In higher density snow, Marbouty found the lack of pore space obstructs crystal growth. The crystals became sharp, but failed to grow appreciably in size. These crystals formed under large temperature gradients and dense conditions were referred to as "hard" depth hoar (Akitaya, 1974). Figure 8 shows the onset of kinetic growth as a function of grain size and density. As expected, the onset of kinetic growth is a strong function of density. As the density decreases, the larger pore spaces allow for easier vapor movement, resulting in a lower onset temperature gradient.

Using this model, the onset of kinetic growth was strongly influenced by bond to grain ratio, but relatively insensitive to temperature. Grain size and density were the significant parameters determining the onset of kinetic growth.

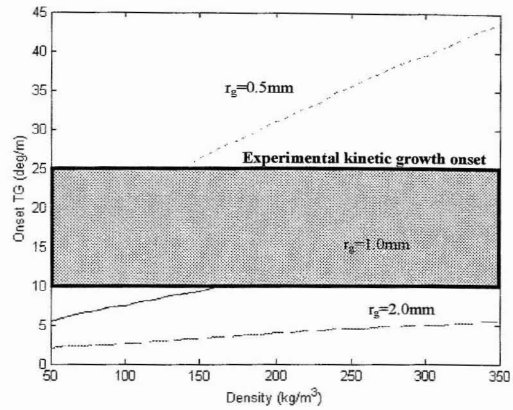


Figure 8. Onset temperature gradient for kinetic growth vs density, T=-3°C, r_b/r_g=0.5. Boxed region represents experimental temperature gradient required for kinetic growth.

The model does include a kinetic growth module that is used to examine crystal growth after the transition temperature gradient is achieved. The details and results of that module are given in Adams and Miller (2002).

5. Conclusions

The current effort uses simple microstructural configurations and fundamental physical processes to simulate dry snow metamorphism unlimited by the thermal environment. The model is useful for examining the sensitivity of several parameters in metamorphism. Sintering in an equi-temperature environment was examined and various sensitivities were discussed. The transition to kinetic growth was defined and studied. The model provides a very flexible tool for examining metamorphism at a microstructural level. Numerous parameters may be simultaneously examined in a complex environment.

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