The Spectral Ice Habit Prediction System (SHIPS). Part II: Simulation of Nucleation and Depositional Growth of Polycrystals

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(Manuscript received 5 September 2007, in final form 9 February 2008)

Abstract

This paper proposes a framework to predict polycrystals along with hexagonal monocrystals in a cloud-resolving model and discusses validity of the scheme and physical processes important for habit distribution by implementing 2D cloud-resolving simulations of an orographic winter storm. The vapor depositional growth is simulated based on a habit frequency map constructed in the laboratory and based on a predicted growth history under evolving atmospheric conditions. Differences brought by predicting polycrystals in spatial distribution were apparent, and sedimentation of polycrystals from middle and upper levels was significant. The immersion freezing process appeared to be a key process resulting in the creation of planar polycrystals, while the homogeneous freezing process was found important for columnar and irregular polycrystals. The ice nuclei (IN) concentration was shown to affect habit distribution by changing the supersaturation, tendency of the freezing nucleation processes, and sedimentation. Preliminary comparison of simulated habit distributions and frequencies with observations indicates usefulness of the framework for polycrystals. Implications of these modeling studies on the needs of future observational campaigns are discussed.

1. Introduction

Polycrystals and irregular crystals existing alongside hexagonal crystals have been recognized in the literature since the modern observation of ice crystals began about 50 years ago (e.g., Nakaya 1954). It is known that orographic wave clouds and cirrus clouds are dominated by bullet rosettes and other polycrystals. Baker and Lawson (2006) used a cloud particle imager (CPI) to analyze 17 orographic wave clouds and reported that the dominant crystal type by mass in most wave clouds is the rosette shape that includes pristine bullet rosettes, mixed-habit rosettes, rosettes with sideplanes, and platelike polycrystals. Similarly, Lawson et al. (2006a) showed that mixed-habit rosettes and platelike polycrystals constitute over 50% of the surface area and mass of ice particles with maximum dimension $D > 50 \mu m$ and inferred that homogeneous and heterogeneous freezing processes similar to wave clouds occur in cirrus clouds. Irregular particles including polycrystals in altostratus clouds associated with winter orographic storms were also reported. Rauber (1987) studied 17 wintertime storm systems over the mountains of northwestern Colorado and found that irregular particles (I1, I2, I4, S1, S2, S3) accounted for 70% of the number concentration on the ground while dendrites accounted for 20% even though 72%–77% of samples were rimed. Rauber (1987) noted that the dominant habits (irregular particles) observed on the ground for cloud-top temperatures colder than $-20^\circ C$ are different from those (pristine crystals) in the cloud due to the wide range of ambient conditions that ice crystals would experience. During a snow storm over Cascade Mountain, Woods et al. (2005) reported the assemblage of plates at $T < -20^\circ C$.

Korolev et al. (2000) diagnosed ice crystal habits of cloud particle images taken with a Particle Measuring System Optical Array Probe during flights through stratiform clouds whose temperature ranged from $-45^\circ C$ to $0^\circ C$. According to Korolev et al., the frequency of irregular particles is more than 60% over the temperature range for $D > 125 \mu m$ and it tends to increase with decreasing temperature. The high frequency of irregular crystals at $T < -20^\circ C$ is supported by the laboratory experiments of Bailey and Hallett (2004a, hereafter...
BHQ04a). Aircraft measurements of the boundary layer, multilayer, and cirrus clouds over the Arctic by Korolev and Isaac (1999) had approximately 3% pristine crystals with irregular-shaped crystals prevailing. In the Antarctic the frequency of blowing snow on the ground is higher in the winter due to the stronger wind speed (Lawson et al. 2006b). However, if one excludes the blowing snow and irregular crystals associated with it, the habits observed on the ground appear to be diamond dusts with frequency ~95% in the winter and up to 60% in the summer with rosette-shaped polycrystals or precipitating snow grain accounting for the rest of the frequency (Walden et al. 2003; Lawson et al. 2006b).

Ice crystal habits affect both shortwave- and longwave radiative transfer directly and indirectly. The radiative forcing of clouds is one of the largest uncertainties in the global climate model. Macke et al. (1998) analyzed size distributions taken from cirrus clouds and showed that the different assumptions of crystal habits led to a significant variability of scattering properties as those from the sampled size distributions themselves. Liu et al. (2003) simulated cirrus clouds with a cloud-resolving model (CRM) and radiative transfer model for warm and cold soundings. They showed that the IR heating rate is more sensitive to habits than the solar heating rate because habits affect capacitance for the vapor deposition process and resulting microphysical properties of the cloud.

In addition to the larger capacitance, polycrystals are potentially important because of their interaction with other hydrometeors. Rauber (1987) suggested that the spatial dendrites with rimed cores and large planar dendrites were responsible for aggregation initiation due to the large differential fall speed between them and horizontal fluctuations in the large dendrite motion.

One way to study radiative impacts of clouds and precipitation or to improve remote sensing application is to simulate realistic ice crystal habits and types of ice particles with a framework where dynamics, radiative response, and microphysical processes can interact and be consistent with each other. One such framework is the use of a cloud-resolving model. However, none of the CRMs have simulated monocrystals and polycrystals together with all ice microphysical processes. Prediction is at most limited to the hexagonal habits, namely plates, dendrites, and columns (e.g., Lynn et al. 2005; Straka and Mansell 2005). Liu et al. (2003) simulated bullet rosettes as a pristine crystal category with a two-moment bulk water parameterization.

In order to reflect the complexity of ice crystal habits in the real atmosphere, this study demonstrates the simulation of nucleation and vapor deposition processes of polycrystals based on current knowledge of habit location and frequency with a cloud-resolving model. This study hopes to shed light on the roles of immersion and homogeneous freezing processes, concentration of ice nuclei (IN) for the formation and growth of monocrystals and polycrystals, and the roles of sedimentation on habit frequency observed at local points. The next section describes the framework to simulate polycrystals with the Spectral Habit Prediction System (SHIPS) (Hashino and Tripoli 2007, hereafter HT07). In section 3 the experiment design and model setup for 2D cloud-resolving simulations of an orographic snow storm are described. The results are discussed in section 4. The methodology and parameterizations used are discussed in section 5. The conclusions and future prospects are given in section 6.

2. Framework to simulate polycrystals with SHIPS

a. Brief description of SHIPS

The main concept of SHIPS is to evolve properties of ice particles in the Eulerian dynamic model continuously in such a way that the ambient conditions along the trajectory of ice particles are reflected in the evolving particle properties. The distribution of ice particles is divided into mass bins where each mass bin represents average habit and type of ice particles given the mass range. SHIPS introduces particle property variables (PPVs) that contain information on the physical structure of evolved ice particles contained in a bin. Currently, mass content components, length variable components, and volume variable components are considered. Mass content components include rime mass, aggregation mass, ice crystal mass, and melt mass. They are integrated based on the respective physical processes that ice particles are experiencing. Length variable components include lengths along the a axis, c axis, and dendritic arm. The maximum dimension of ice particles is predicted as a volume variable component.

Readers are referred to HT07 for a more detailed explanation of the scheme.

The philosophy guiding the simulation of vapor deposition process is to grow the lengths of ice crystals along the crystallographic directions based on a physical model determined empirically or analytically when available. HT07 presented simulations of the three axis lengths of hexagonal monocrystals using the inherent growth ratio approach of Chen and Lamb (1994, hereafter CL94) with a CRM, the University of Wisconsin Nonhydrostatic Modeling System (UWNMS) (Tripoli 1992). It showed that the advection and sedimentation of ice crystals affect distribution of habits significantly.
The following describes a methodology to include prediction of polycrystals into SHIPS.

b. Habit diagram and frequency

The habit diagram has been constructed by many authors (e.g., Magono and Lee 1966) for $T \leq -40^\circ$C. However, the frequency of the habits given temperature, $T$, and moisture (or ice supersaturation, $s_i$) is limited in the literature. BH04a constructed the habit diagram for $-70^\circ \leq T \leq -20^\circ$C along with the frequency of occurrence for a set of $T$ and $s_i$. As shown by Kumai (1982) and BH04a, habits are dependent on both $T$ and $s_i$ at $T > -20^\circ$C, and significant frequency is distributed among plates, columns, and polycrystals for certain pairs of $T$ and $s_i$. On the other hand, $T$ has a larger influence on habits than $s_i$ at $T > -20^\circ$C, and either planar or columnar monocrystals tend to have a dominant frequency for a given $T$.

Because the mechanisms for formation of polycrystalline structures of ice crystals are only qualitatively known in literature, this study uses habit frequency constructed by laboratory experiments to generate polycrystals and also to allow formation of multiple habits given $T$ and $s_i$. As shown by Kumai (1982) and BH04a, habits are dependent on both $T$ and $s_i$. The hexagonal plates have moderate frequency in low $s_i$ ($s_i < 20\%$) over a wide temperature range, while columnar crystals were often observed below $T \leq -40^\circ$C with moderate and high $s_i$. The polycrystals are associated with high excess vapor density and they appear to prevail for $-45^\circ \leq T \leq -20^\circ$C. The frequency for columnar polycrystals (bullet rosettes) and planar polycrystals (side-planes, overlapping parallel plates, and crossed plates are included from BH04a’s data) given the occurrence of polycrystals is shown in Figs. 1d,e. The columnar polycrystals and planar polycrystals appear to be separated by the boundary $T = -40^\circ$C.

The habit frequency actually depends on the property of ice nuclei (Bailey and Hallett 2002). This study only uses the frequency data for soda-lime glass whose composition is close to the most prevalent IN (BH04a). If one wants to simulate ice formation by artificial precipitation, one would need the habit frequency for the IN that are present or sprayed in the volume.

c. Prognostic variables and diagnosis

This study introduces three PPVs to identify polycrystalline habits in addition to hexagonal monocrystals (Fig. 2). New predicted variables added to SHIPS are the coordinates of center of gravity of a polycrystal, $a_g$ and $c_g$, and number of extra crystalline structures added to a hexagonal monocrystal, $n_{exem}$. The coordinates, $a_g$ and $c_g$, are defined from the center of a monocrystal in the usual sense. The underlying assumption is that com-
components are hexagonal monocrystals themselves and they are all identical and symmetric. Some examples of the possible assemblages are shown in Figs. 3a–f for the conceptual model of a bullet rosette with four branches (C2a), a sideplane (S1), radiating assemblage of plates (P7a), overlapping parallel plates [(opps) in BH04a], crossed plates (cp in BH04a), and the scalelike sideplane (S2). This study categorizes Fig. 3a as the columnar polycrystals and Figs. 3b–e as the planar polycrystals. The crossed plates would have the same center of gravity as a monocrystal, but this study categorizes the habit into the planar polycrystals. The scalelike sideplane (Fig. 3f) is one example where the coordinates of the center of gravity cannot be defined uniquely from the hexagonal crystal. Those having characteristics between the columnar and planar polycrystals are called irregular polycrystals.

During the nucleation period where the maximum dimension of an ice crystal, \( D \), is less than 20 \( \mu m \), all polycrystals are initialized to have a set of characteristic \( a_g \) and \( c_g \) and non-zero \( n_{exice} \). The columnar and planar polycrystals are assumed to have \((a_g/a, c_g/c, n_{exice}) = (0, 1, 1)\), a square in Fig. 2, and \((a_g/a, c_g/c, n_{exice}) = (1, 0, 1)\), a triangle, respectively, so that they show the distinct characteristic in the parameter space. The irregular polycrystals are assumed to be in the middle of those two crystals indicated with a cross: \((a_g/a, c_g/c, n_{exice}) = (0.5, 0.5, 1)\). The monocrystals are initialized with \((a_g/a, c_g/c, n_{exice}) = (0, 0, 0)\), shown by a circle.

After advecting PPVs between mass bins and spatial grid cells, \((a_g/a, c_g/c, n_{exice})\) of a mass bin changes with time and takes any combination of values in the parameter space. This study simply assumes the ice particle is a monocrystal, if \( n_{exice} < 0.5 \), and otherwise is a polycrystal. The particles are diagnosed as planar (columnar) polycrystals if \( a_g/a \geq c_g/c + 0.5 \) \((c_g/c \geq a_g/a + 0.5)\) (Fig. 2). Then, the region between those boundaries is taken to be irregular polycrystals. As a result this study identifies five crystal habits from six PPVs: two monocrystal habits and three polycrystalline habits. Dendritic arm lengths are predicted for each habit, as defined in HT07, and the growth of dendritic arms for columns and columnar polycrystals can be thought of as the growth of plates on the basal facets of columns.

For now we assume the number of extra crystalline structure \( n_{exice} = 1 \) for the polycrystals because \( n_{exice} \) is not quantitatively known in literature. The bullet rosettes commonly have two to four bullets in a laboratory setting with a maximum multiplicity reached around \( T = -50^\circ C \) (BH04a), while the number of different crystalline structures for planar polycrystals are, in general, not known. Furthermore, it is not clear that \( n_{exice} \) is a continuous function of \( T \) and \( s_i \). In this study \( n_{exice} = 1 \) is treated as an indication of polycrystals rather than as the actual number of extra crystalline structures. No geometrical length for polycrystals is predicted due to lack of information on the growth along the crystallographic directions. Instead, we diagnose the maximum dimension by using empirical mass–diameter relationships. The planar polycrystals are diagnosed by the sideplanes (S1) of Mitchell et al. (1990), the columnar polycrystals by bullet rosettes model with four branches of Chiruta and Wang (2003), and other irregular polycrystals by aggregates of sideplanes, bullets, and columns (S3) of Mitchell et al. (1990).

There is still only one mass variable for an ice crystal: mass component of ice crystal, \( m_P \). The mass growth is calculated based on the diagnosed habit. Three axis lengths of a hexagonal crystal are always changed according to mass growth whether or not the diagnosed habit is polycrystalline. This way the mass component of ice crystal and \( a \)-axis, \( c \)-axis, and \( d \)-axis (dendritic arm) lengths are continuous and consistent with the predicted mass component of the ice crystal.

d. Growth rate calculation

This study uses a capacitance approach to simulate mass growth of hexagonal monocrystals and polycrystals. The capacitance of hexagonal monocrystals is modeled as a spheroid following CL94’s treatment, and Chiruta and Wang (2003) is used for columnar polycrystals. Other polycrystal capacitances are modeled
with a spheroid assuming a semiaxis ratio of 0.25. As for the growth rate of length of hexagonal monocrystals the inherent growth approach of CL94 is extended to \( T \leq -20^\circ C \). The inherent growth ratio \( \Gamma \) is a temperature-dependent parameter to describe the growth rate of \( a \) and \( c \) axis lengths: \( \frac{dc}{da} = \Gamma(T)\frac{c}{a} \). Figure 4 shows extended \( \Gamma \) for \( T = -20^\circ C \) in which two curves divert at \( T = -20^\circ C \) for columnar and planar growth regimes. BH04a states \( 2 < c/a < 4 \) at \( T = -42^\circ C \) under 13\% < \( s_i \) < 25\% and 3 < \( c/a \) < 6 at \( T = -60^\circ C \) under 10\% < \( s_i \) < 15\%. Thus, \( \Gamma \) for the columnar regime was tuned so that the axis ratio of simulated single particle reaches 2.7 and 5 at \( T = -40^\circ C \) and \(-60^\circ C\), respectively, under \( s_i = 30\% \) after 60 min of depositional growth. There are no alternative measurements of growth along the \( a \) and \( c \) axes or \( c = \eta a^6 (\Gamma = \beta) \) in \( T \leq -30^\circ C \) at this moment. The ventilation coefficients are calculated with a formula for idealized ice crystals in Pruppacher and Klett (1997) except that the one for bullet rosettes is calculated by Liu et al.’s (2003) formula.

If \( D < 20 \mu m \) and \( T \leq -20^\circ C \), the growth regime that the ice crystal takes at a given temperature and moisture is determined by using the corresponding cumulative relative frequency of habits and random number generator. First, the growth regime is chosen from polycrystalline, columnar, and planar hexagonal regimes and then, if it is polycrystalline, another random number determines if it is columnar or planar polycrystals. Furthermore, if it is polycrystalline, another random number drawing determines the growth regime for a hexagonal monocrystal. In other words, small ice crystals can grow with a different growth mode from the habit diagnosed at the beginning of the time step. At \( T > -20^\circ C \), polycrystals are assumed not to form. Once the maximum dimension is greater than 20 \( \mu m \), the ice crystal is assumed to follow the growth of the diagnosed habit at the beginning of a time step.

c. Bin shifting of polycrystal variables

After calculating mass growth and growth of the axis length for the representative hydrometeor in a bin (see section 4 of HT07 for details), the polycrystalline property of ice particles in the shifted bin is calculated as follows: as explained above, the three parameters \((a_g', c_g', n_{exice}^g)\) for the ice crystals in a shifted bin are only initialized when ice crystals are small \((D < 20 \mu m)\) based on the growth regime: \((a_g', c_g', n_{exice}^g) = (0, c', 1)\) for columnar polycrystals, \((a_g', c_g', n_{exice}^g) = (a', 0, 1)\) for planar polycrystals, \((a_g', c_g', n_{exice}^g) = (0.5a', 0.5c', 1)\) for irregular polycrystals, and \((a_g', c_g', n_{exice}^g) = (0, 0, 0)\) for monocrystals. The variables \( a' \) and \( c' \) are the \( a \) and \( c \) axis lengths of a hexagonal monocrystal in a shifted bin and calculated with \( \delta a \) and \( \delta c \) obtained from Eqs. (41)–(44) of CL94. For \( D \geq 20 \mu m \),

\[
\begin{align*}
    a_g' &= a_g + r_a \delta a \\
    c_g' &= c_g + r_c \delta c,
\end{align*}
\]

Fig. 3. Conceptual models of center of gravity for polycrystals: (a) bullet rosette, (b) sideplane, (c) assemblage of plates, (d) overlapping parallel plates, (e) crossed plates, and (f) scalelike sideplane.

Fig. 4. Extended inherent growth ratios for columnar and planar growth for \( T \leq -20^\circ C \).
where \( r_a = 1.0 \) and \( r_c = 0.0 \) for planar polycrystals, \( r_a = 0.0 \) and \( r_c = 1.0 \) for columnar polycrystals, \( r_a = 0.5 \) and \( r_c = 0.5 \) for irregular polycrystals, and \( r_a = 0.0 \) and \( r_c = 0.0 \) for monocrystals.

The number of extra crystalline structures in a shifted bin, \( n_{\text{exice}} \), is also initialized according to the growth regime if \( D < 20 \mu m \). For \( D \geq 20 \mu m \), it stays the same as the dynamically advected number, that is, \( n_{\text{exice}} = n_{\text{exice}} \).

The coordinates of center of gravity are transferred between mass bins as concentration-weighted cubic lengths in the same way as other length variable components. The number of extra crystalline structures is weighted by concentration.

### f. Terminal velocity

The general formula of Bohm (1992) is used in this study as done in HT07. For polycrystals, the aspect ratio \( \alpha \) is assumed to be 0.25. The area ratio \( q_{\text{rat}} \) for bullet rosettes is calculated with Chiruta and Wang’s (2003) geometric model, and those for other polycrystals are calculated by substituting predicted bulk crystal density into Heymsfield et al.’s (2002) formula for S1.

### 3. Model setup and experiment design

As described in HT07, SHIPS has been installed into a cloud-resolving model, UWNMS. The case study that SHIPS is validated against is a winter orographic snowstorm observed 13–14 December 2001 during the second Improvement of Microphysical Parameterization through Observational Verification Experiment (IMPROVE-2) campaign (see Woods et al. 2005 for synoptic and microphysical observations). Most of the model setups for the two-dimensional idealized simulation are the same as HT07 except for the following few points: cloud condensation nuclei (CCN) are modeled not to be affected by microphysical prediction, namely by nucleation of cloud droplets and evaporation of hydrometeors. On the other hand, the nucleation scavenging processes (deposition–condensation freezing and contact freezing nucleation processes) and evaporation process are modeled to change concentration and mass content of IN. In the dynamics model the threshold mass content for each mass bin can be defined to remove insignificant mass content and thus to avoid consuming computational time on the advection of insignificant mass content in the model. HT07 set the threshold mass content to \( 10^{-6} \) of the mixing ratio of water species. By eliminating slow-growing small ice particles in the low and middle levels (especially those nucleated by depositional nucleation), effects of sedimentation of ice crystals nucleated at the initial stage showed up more clearly. This study uses the threshold of \( 10^{-12} \) to keep track of those small crystals in the dynamics model in order to see the effect of vapor competition. HT07 diagnosed the aggregation mass component from total mass and the other mass components. This study predicts the aggregation mass component to avoid any production of the component caused by nonlinear operators and truncation errors in numerical schemes for dynamics.

Eight experiments are carried out as listed in Table 1. S-HCH simulates only monocrystals with the CL94 inherent growth parameterization extended to \( T \leq -20°C \) and habit frequency approach, while S-PCH simulates polycrystals in addition to the monocrystals. Those are implemented with the threshold for mass contents, as done in HT07, to investigate the sedimentation effect of polycrystals. In addition to the deposition–condensation freezing, immersion freezing, and contact freezing processes, the homogeneous freezing process was simulated in PCH, PCHH, PCL, and PCLH. The parameterization of Heymsfield and Milsheevich (1993) for pure water was used in this study.

### Table 1. List of sensitivity experiments. The experiments with FH produce hexagonal monocrystals by contact, immersion, and homogeneous freezing processes. Ice nuclei (IN) concentration is set to 230 or 1 L⁻¹. The experiments with H in mass limit focus on sedimentation of relatively large ice particles, while those with L retain all nucleated small ice particles. Only S-HCH does not predict polycrystals at all. The experiments with NF do not simulate immersion and homogeneous freezing processes.

<table>
<thead>
<tr>
<th>Expt</th>
<th>Immersion freezing</th>
<th>Homogeneous freezing</th>
<th>Formation of polycrystals by freezing</th>
<th>IN concentration (L⁻¹)</th>
<th>Mass limit</th>
<th>Polycrystal prediction</th>
</tr>
</thead>
<tbody>
<tr>
<td>S-HCH</td>
<td>On</td>
<td>Off</td>
<td>FH</td>
<td>230</td>
<td>H</td>
<td>No</td>
</tr>
<tr>
<td>S-PCH</td>
<td>On</td>
<td>Off</td>
<td>Yes</td>
<td>230</td>
<td>H</td>
<td>Yes</td>
</tr>
<tr>
<td>PCH</td>
<td>On</td>
<td>On</td>
<td>Yes</td>
<td>230</td>
<td>L</td>
<td>Yes</td>
</tr>
<tr>
<td>PCHH</td>
<td>On</td>
<td>On</td>
<td>FH</td>
<td>230</td>
<td>L</td>
<td>Yes</td>
</tr>
<tr>
<td>PCL</td>
<td>On</td>
<td>On</td>
<td>Yes</td>
<td>1</td>
<td>L</td>
<td>Yes</td>
</tr>
<tr>
<td>PCLH</td>
<td>Off</td>
<td>Off</td>
<td>HF</td>
<td>1</td>
<td>L</td>
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<tr>
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<td>Off</td>
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<tr>
<td>PCLN</td>
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<td>Off</td>
<td>NF</td>
<td>1</td>
<td>L</td>
<td>Yes</td>
</tr>
</tbody>
</table>
PCH and PCL are assumed to form polycrystals through the four nucleation processes based on the habit frequency, whereas PCHH and PCLH only form hexagonal monocrystals from the contact, immersion, and homogeneous freezing processes. The sensitivity of polycrystal formation to the freezing nucleation processes is discussed by comparison between them. PCH and PCHH (PCL and PCLH) have IN concentration, \( N_{\text{IN}} \), of 230 L\(^{-1}\) (1 L\(^{-1}\)) to investigate the sensitivity of habit distribution and vapor depositional growth to \( N_{\text{IN}} \). PCHN and PCLN do not simulate immersion and homogeneous freezing processes.

First, a quasi-steady state was obtained only with liquid microphysics, as was done in HT07. Then, the above experiments were started by using the quasi-steady state as initial conditions and by turning on the ice microphysics processes including ice nucleation, vapor deposition, and melting processes. Note that the time of simulation mentioned is the time after the ice microphysics processes were turned on. In the following, the horizontal distance from the west boundary in the domain is denoted with \( y \), and the altitude with \( z \).

4. Results

a. Simulated relationships between ice crystal properties

The SHIPS reproduces the known dependence of dimension and terminal velocity on the axis ratio, \( \phi = c/a \). The mass dimensional and mass terminal velocity relationships of hexagonal monocrystals at 20 min of simulation are shown for S-HCH in Fig. 5. The data points correspond to predicted properties at mean mass (representative hydrometeor) of all mass bins and grid

**Fig. 5.** Mass-dimensional and mass-terminal velocity relationships at 20 minutes of simulation for S-HCH. Each data point corresponds to property of representative hydrometeor of each mass bin of all spatial grid points. The color of the points for plates and dendrites indicate axis ratio \( \phi = c/a \) as 0.8 < \( \phi \) < 1.0: blue, 0.6 < \( \phi \) < 0.8: cyan, 0.4 < \( \phi \) < 0.6: green, 0.2 < \( \phi \) < 0.4: yellow, 0.1 < \( \phi \) < 0.2: magenta, \( \phi \) < 0.1: black. Those for columnar crystals as \( \phi < 2: \) blue, 2 < \( \phi < 4: \) cyan, 4 < \( \phi < 6: \) green, 6 < \( \phi < 8: \) yellow, 8 < \( \phi < 10: \) magenta, and 10 < \( \phi: \) black. HK87 denotes Heymsfield and Kajikawa (1987), K82 Kajikawa (1982), LH74 Locatelli and Hobbs (1974), MZP90 Mitchell et al. (1990), and M96 Mitchell (1996); Ag indicates aggregates of the habit.
cells in the domain. Note that SHIPS does not use any empirical relationships between these variables, but predicts the axis lengths of hexagonal monocrystals, thus the maximum dimension based on a vapor deposition model, and calculates the terminal velocity based on a general theory. A few empirical power laws are also plotted for comparison. It can be seen that the maximum dimension (terminal velocity) becomes large (small) with the decrease of $\phi$ given mass for planar crystals, which is expected. The opposite is true for columnar crystals. The maximum dimension predicted for plates turned out to be less than $P_{1a}$ of Mitchell (1996) and Heymsfield and Kajikawa (1987) in the mass greater than $10^{-4}$ mg. This is true for dendrites against $P_{1a}$ of Heymsfield and Kajikawa. Here $\phi$ of plates and dendrites mostly range between 0.1 and 1.0. As noted in HT07, underestimation of the thinning of planar crystals has to be resolved in the future. Some are related to ice particles formed from supercooled liquid drops and planar growth ratio $\Gamma$ in $T \leq -20^\circ C$ with $\phi$ close to 1. In turn, this resulted in a larger terminal velocity than the empirical formulas would predict. The columnar crystals show a wide range of $\phi$ from 1 to a maximum of 38. They are partially enveloped by the hexagonal columns and $N_{1a}$ of Mitchell (1996), which seems to be reasonable. Most of the columnar crystals with mass less than $10^{-4}$ mg exist at $z > 8$ km ($T < -40^\circ C$) and hardly fall, as shown later. Polycrystals follow the mass-dimensional relationships specified with empirical equations and the terminal velocities calculated with Bohm’s general formula agree with empirical relationships well.

b. Habit distributions with and without polycrystals and the effect of sedimentation

The differences in predicted habit distributions with and without polycrystals and sedimentation of the habits in middle and upper levels are discussed in this subsection. Vertical profiles of the horizontally averaged temperature and supersaturation in the domain at the initial time are shown in Fig. 6. The concentration of ice crystals was horizontally averaged for each habit in the entire domain and also the average axis ratio was calculated by using concentration-weighted axis lengths. The average concentration and axis ratios, $\phi = c/a$ and $\psi = d/a$, for S-HCH and S-PCH at 20 min of simulation are shown in Fig. 7. The dominance of habits can be mainly understood from the habit frequency (Fig. 1) at 20 minutes of simulation. However, the effect of vertical advection and sedimentation is noticeable. The concentration for S-HCH, (Fig. 7a), shows that columnar crystals dominate at $z > 7$ km ($T < -30^\circ C$) and then plates at $4 < z < 6$ km ($-25 < T < -10^\circ C$). As shown in Fig. 6, the supersaturation over ice, $s_i$, stays around 0.2 at $z > 7$ km and temperature decreases with height at the initial time. The habit frequency (Fig. 1) shows that the habit of larger frequency between hexagonal monocrystals shifts from plates to columns across $T \sim -40^\circ C$ at $s_i \sim 0.2$. According to Fig. 7d, prediction of polycrystals (S-PCH) introduced the highest concentration of irregular polycrystals at $z > 4$ km ($T < -10^\circ C$), which can be expected from the frequency map, given the vertical profile of supersaturation at $T < -20^\circ C$ as well as vertical advection and sedimentation. Also, high concentrations of planar and columnar polycrystals were predicted at $6 < z < 8$ km ($-40^\circ C < T < -25^\circ C$) and $9 < z < 11$ km ($-56 < T < -46^\circ C$), respectively. The concentration of plates was reduced by up to two orders of magnitude from S-HCH, while concentration of columnar crystals is as high as the polycrystals at $z > 8$ km ($T < -40^\circ C$). According to Figs. 7a,d, the dendrites fell to $z = 2$ km ($T \sim 0^\circ C$) due to vertical advection and sedimentation. The average $\phi$ is similar between S-HCH and S-PCH (Figs. 7b,e). The irregular polycrystals already show growth of the average $\psi$ at this time.

The experiments S-HCH and S-PCH clearly show the potential importance of the habits in middle and upper levels due to habit-dependent sedimentation, and growth rate. Vertical displacement of ice crystals can be clearly seen by comparing 20 and 60 min of simulation (Figs. 7, 8). The plates in S-HCH fell into the low levels ($2 < z < 4$ km), while the irregular polycrystals in S-PCH fell into the levels ($2 < z < 4$ km) [see (a) and (d) of Figs. 7, 8]. At this time irregular polycrys-
FIG. 7. Vertical profiles of horizontally averaged concentration and axis lengths for each habit at 20 minutes of simulation: results from (top) S-HCH and (bottom) S-PCH. The solid lines indicate plates; dashed, dendrites; dashed-dotted, columns; gray solid, planar polycrystals; gray dashed-dotted, columnar polycrystals; and gray dashed, irregular poly-crystals.

FIG. 8. As in Fig. 7 but at 60 minutes of simulation.
tals in the low levels have significant growth of dendritic arms indicated by the $\psi$ in (f). It is because the polycrystals fell through the dendritic growth region ($-16^\circ < T < -12^\circ$C). Vertical profiles of the axis ratio $\phi$ in (b) and (c) of Figs. 7, 8] also indicate downward shifts, but the change at a level is combination of growth and vertical displacement.

The spatial distributions of number concentrations and mass contents of diagnosed habits at 90 min for S-HCH are shown in Fig. 9. The planar crystals are dominant in lower and middle levels ($2 < z < 6$ km), and the columnar crystals in middle and upper levels ($6 < z < 10$ km). The columns with relatively large mass that were originally formed in the upper levels ($z > 8$ km) are slowly falling, as indicated by the mass content. The extension of the inherent growth ratio and use of the frequency map for hexagonal crystals resulted in the spatial distribution of habits that is a mixture of two extreme cases, one with columnar growth and another with planar growth defined for $T < -20^\circ$C (EXP2 and EXP3), simulated in HT07 at this time (see Figs. 12 and 14 of HT07).

The spatial distributions of number concentrations and mass contents of diagnosed habits at 20 and 90 min for S-PCH are shown in Figs. 10 and 11, respectively. As shown in Figs. 7 and 10, plates and dendrites existed at 20 min at $2 < z < 6$ ($-25^\circ < T < 0^\circ$C) with dendrites formed in the area of water saturation. However, most of those in the domain fell to the melting zone, and only plates formed at the west boundary with low mass content exist at 90 min. The irregular polycrystals were formed at $z > 5.5$ km ($T < -20^\circ$C) and over the area with relatively low supersaturation over ice ($0.05 < s_i < 0.2$) before 20 min (see Fig. 7). The planar and columnar polycrystals were associated with higher supersaturation, as discussed in the next subsection. Sedimentation and vertical advection of the irregular polycrystals led to the dominance in low and middle levels at 90 min. Comparison of Figs. 9 and 11 indicates that maximums of mass content for S-PCH are larger than those of S-HCH. As shown in Fig. 8, the average $\phi$ of plates is larger than 0.25, which means plates have larger capacitance than irregular polycrystals for a given radius. However, since irregular polycrystals had larger maximum dimension than plates for a given mass, which is not generally true for the empirical relationships of these habits, terminal velocity (capacitance) of irregular polycrystals was calculated to be smaller (larger) than plates for the mass. Therefore, the longer time for depositional growth and larger mass growth of the irregular polycrystals than plates for a given mass resulted in the larger maximum mass content. Assumptions about the growth model of mass and geometry as well as habit growth regimes are critical components of SHIPS, particularly in the upper and middle levels where they ultimately can affect the spatial distribution of concentration and mass content in the lower levels significantly.

**Fig. 9.** Comparison of number concentrations and mass contents for diagnosed habits after 90 minutes of vapor deposition simulation (S-HCH). The gray shading indicates the logarithm of number concentration per liter: $\log_{10} (L^{-1})$. The thin black contours indicate 0.01 and 0.05 ($g \ m^{-1}$), and the thick black contours 0.1, 0.2, and 0.3 ($g \ m^{-1}$).
FIG. 10. Comparison of number concentrations and mass contents for diagnosed habits after 20 minutes of vapor deposition simulation (S-PCH). The gray shading indicates the logarithm of number concentration per liter: log10(L^-1). The thin black contours indicate 0.01 and 0.05 (g m^-3), and the thick black contours 0.1, 0.2, and 0.3 (g m^-3).

FIG. 11. As in Fig. 10 but at 90 minutes of simulation.
c. Habit distributions and nucleation processes

Different nucleation processes show distinct characteristics in creating spatial and size distributions of ice particles. The ice nucleation rates in concentration and average maximum dimension of nucleated ice crystals are shown for each process in Figs. 12 and 13, using 20-min simulation from PCH as an example. These show that the deposition–condensation freezing process nucleates small particles of diameter $D < 10 \mu m$, with a large concentration tendency of more than $1 L^{-1} s^{-1}$. The immersion (homogeneous) freezing processes nucleate relatively large ice crystals of up to $D = 41 \mu m$ ($D = 24 \mu m$) with a concentration tendency of $1 (10) L^{-1} s^{-1}$. The concentration tendency due to contact freezing is much smaller than the others by two or more orders of magnitude, although the nucleated mass can be as large as those from the immersion and homogeneous freezing processes. Regions of significant concentration tendency by immersion and homogeneous freezing processes are located over the windward slope of the two peaks of the Cascades ($y \sim 210$ and $310 km$ and $z > 6 km$). These are associated with strong vertical motion in the regions ($2-5 m s^{-1}$). The contact freezing nucleation process is active at $3 < z < 5 km$ ($-15^\circ < T < -5^\circ C$). The deposition–condensation freezing occupies a wider area of stratiform clouds where the vapor is saturated over ice. Note that the temperature range of the active immersion freezing process ($-35^\circ < T \leq -20^\circ C$) in these model simulations corresponds to the high frequency of planar polycrystals in Bailey and Hallett’s frequency map (Fig. 1), whereas that of the homogeneous freezing process ($T \leq -55^\circ C$) corresponds to the high frequency of irregular and columnar polycrystals.

The formation of polycrystals through immersion and homogeneous freezing has a large impact on the spatial distribution of polycrystalline habits. Concentrations of diagnosed habits for PCL and PCLH are shown in Figs. 14 and 15. It can be seen that the concentration of ice crystals is close to the $N_{p, x}$ in these simulations owing to the lower threshold in the dynamic model. Comparison of PCL and PCLH indicates that the area with different dominant habits clearly corresponds to the area of active immersion and homogeneous freezing nucleation processes ($200 < y < 250 km$ and $300 < y < 350 km$ at $z > 6 km$). PCLH assumes that all the ice crystals form hexagonal monocrystals after the freezing nucleation processes, while PCL generates polycrystals by using habit frequency tables. Therefore, PCLH shows more hexagonal monocrystals and less polycrystals in the areas of active immersion and homogeneous freezing processes than PCL does. The habit distributions of PCL and PCLH in the stratiform clouds at $y < 200 km$ are almost identical due to no active immersion and homogeneous freezing processes. PCH and PCHH show similar differences to those between PCL and PCLH but with higher concentration $O(100 L^{-1})$ in the regions where the deposition nucleation process is active.

The frequency of diagnosed habits was calculated for five temperature ranges in the entire domain and over the first 3 hours of simulation (Table 2). The temperature ranges are $T \leq -40^\circ C (z > 8.1 km), -40^\circ < T \leq -30^\circ C (6.8 < z < 8.1 km), -30^\circ < T \leq -20^\circ C (5.5 < z < 6.8 km), -20^\circ < T \leq -10^\circ C (4 < z < 5.5 km), and -10^\circ < T \leq 0^\circ C (2.2 < z < 4 km)$. Note that this analysis includes the sedimentation effects of ice crystals. Therefore, the habit frequency is not only a function of the temperature and moisture at the local grid cell. With the formation of polycrystals by the freezing processes (PCH and PCL), irregular polycrystals are the most dominant habit at $T \leq -20^\circ C$. At $T \leq -40^\circ C$, if the freezing is not the mechanism to produce polycrystals (PCHH and PCLH), columnar crystals prevail with a frequency of more than 40%. At $T \leq -20^\circ C$ the fraction of irregular polycrystals increases with temperature for PCH and PCHH. Furthermore, the formation of polycrystals by freezing processes has a large impact on planar monocrystals for $-30^\circ < T \leq -20^\circ C$. When the polycrystals are formed with freezing, planar monocrystals take on less than 1% of the concentration. However, when the monocrystals are formed with the freezing, they show a frequency of 25% for PCHH and 71% for PCLH. At $T > -20^\circ C$ the plates and dendrites prevail, except for PCL where the irregular polycrystals have the largest frequency due to sedimentation. The frequency of columnar crystals increases in the layer $-10^\circ < T \leq 0^\circ C$ from the above layer due to the columnar growth region ($T \sim -6^\circ C$).

It is important to mention that the simulations without immersion and homogeneous freezing processes (PCHN and PCLN) still produce the highest frequency of irregular polycrystals in temperature ranges $-40^\circ < T \leq -10^\circ C$, which are comparable to cases including the freezing processes. However, frequencies of the planar and columnar polycrystals turned out to be less than PCH and PCL. This is simply because the concentration nucleated by immersion and homogeneous freezing processes was removed, so the relative contribution of crystals that form in high saturation was reduced. PCHN and PCLN maintained higher supersaturation over the mountainous area ($y > 210 km$) than PCH and PCL. The supercooled liquid hydrometeors act as the source of moisture through a vapor deposition process in PCHN and PCLN rather than the source.
FIG. 12. Concentration tendency of ice nucleation processes for PCH at 20 min: (a) deposition–condensation nucleation, (b) contact freezing nucleation, (c) immersion freezing nucleation, (d) homogeneous freezing nucleation, and (e) total.

FIG. 13. Initial maximum dimension of ice crystals produced by ice nucleation processes for PCH at 20 min: (a) deposition–condensation freezing nucleation, (b) contact freezing nucleation, (c) immersion freezing nucleation, (d) homogeneous freezing nucleation, and (e) total.
FIG. 14. Concentration for diagnosed habits for PCL at 20 min. The contours indicate 10^3 L^{-1}.

FIG. 15. As in Fig. 14 but for PCLH.
of concentration and mass of ice crystals through the freezing nucleation processes. The effect of nucleating hexagonal monocrystals instead of polycrystals also appears in the mean maximum dimension and standard deviation of particle size distributions (PSDs) for $T \leq -20^\circ C$ (Table 2). Since polycrystals tend to be more compact than columnar monocrystals given a mass, the mean and standard deviation of PCH (PCL) is smaller than for PCHH (PCLH).

The assumed habits for the freezing nucleation processes can significantly affect the conditional frequency of habits given a maximum dimension. The PSDs of ice particles were calculated by grouping the simulated samples in the domain into the five temperature ranges as defined for the analysis of habit frequency. Along with it, the conditional frequency of diagnosed habits given a maximum dimension was calculated. The results for PCL and PCLH at 90 minutes of simulation are shown in Fig. 16. The average PSDs for PCH and PCHH or PCL and PCLH are very similar, and the difference in conditional frequency of habits shows the effect of polycrystal formation by the freezing processes. Comparison of conditional frequencies for PCL and PCLH clearly shows that hexagonal monocrystals of PCLH reached much higher concentration in 10–100 $\mu m$ at $T \leq -20^\circ C$ than those of PCL, and it corresponds to the size produced by the freezing nucleation. Note that the immersion and homogeneous freezing process are potentially quite important because the potential concentration of liquid hydrometeors nucleated from CCN is much higher than that of solid hydrome-

Table 2. Moments of average particle size distribution and concentration frequency of habits for five temperature ranges. Concentration (Conc), mean maximum dimension (MD), and standard deviation of maximum dimension (Std dev) are given in L$^{-1}$, mm, and mm, respectively; P denotes plates; D, dendrites; C, columnar crystals; CP, columnar polycrystals; PP, planar polycrystals; and IP, irregular polycrystals. The frequency is in percent (%). Approximate heights (km) for the temperature ranges ($^\circ C$) are also indicated in parentheses.

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</tbody>
</table>
teors nucleated from IN by two to three orders of magnitude and also because the process nucleates particles with large initial size and mass. Figure 17a shows the concentration of supercooled liquid hydrometeors by using ambient temperature and diameter of liquid hydrometeors at 20 min for PCL. The concentration decreases with a decrease of temperature and an increase of size. At $T = -20^\circ$C the size of the supercooled liquid hydrometeor ranges between 10 to 100 $\mu$m. The nucleation rates by the immersion and homogeneous freezing processes are shown in Figs. 17b,c, respectively. Even though Bigg’s formula (see appendix B of HT07) for $-40^\circ < T < -20^\circ$C and $5 < D < 100$ $\mu$m indicates low probability of freezing (about 0.0001 to 0.1), the concentration of supercooled liquid hydrometeors is high enough to produce a rate of more than 1.0 L$^{-1}$s$^{-1}$. The rate is significant compared to the $N_{IN}$ available for PCL and PCLH.

Fig. 16. Average particle size distribution and conditional frequency of habits in the five temperature ranges for (left) PCL and (right) PCLH at 90 min. Open circles connected with lines indicate the size distribution. In the legend for the frequency, P denotes plates; D, dendrites; C, columns; CP, columnar polycrystals; PP, planar polycrystals; and IP, irregular polycrystals.
d. Effect of ice nuclei concentration

The IN concentration, $N_{\text{IN}}$, affects habit frequency observed at a given level through change in ice supersaturation, $s_i$, during the nucleation period of ice crystals and change in freezing processes. PCH experienced a larger decrease in $s_i$ ($<15\%$) in stratiform clouds ($y < 200$ km) at $6 < z < 8$ km, at least after 20 min, than PCL ($s_i \approx 25\%$ to $30\%$). It is a result of a high concentration of ice crystals that consumed available humidity. This resulted in the growth of planar polycrystals for PCL during the nucleation period ($D < 20 \mu m$) in stratiform clouds with deposition-condensation freezing nucleation. Similarly, $s_i$ at $200 < y < 220$ km and $6 < z < 8$ km for PCH was lower ($\sim 20\%$) from 60 to 120 min than PCL ($20\% < s_i < 45\%$). At the same time, the tendency of the immersion freezing process in PCH was significantly reduced in the area from 20 min, while PCL sustained a similar magnitude. It is because the decrease in $s_i$ due to the high concentration of ice crystals led to a decrease in CCN activation tendency and, therefore, few supercooled droplets available for the freezing process. As a result, PCL predicted a much higher concentration of planar polycrystals especially over the high topography ($200 < y < 275$ km) than PCH, which is reflected for $-40^\circ < T \leq -20^\circ$C of Table 2. In the same manner, columnar polycrystals in PCL were found to have higher concentration at $T \leq -40^\circ$C and $200 < y < 275$ km than those in PCH.

Another effect of $N_{\text{IN}}$ to habit frequency at a level is through the sedimentation of ice crystals. The difference in $N_{\text{IN}}$ can lead to the difference in maximum dimension of ice crystals. Comparison of the mean maximum dimensions for PCH and PCL shown in Table 2 indicates that PCL has a larger dimension of ice crystals at $T > -20^\circ$C ($z < 6$ km) as well as standard deviation. However, the mean maximum dimension over the domain decreases by decreasing $N_{\text{IN}}$ at $T < -20^\circ$C because the concentration of small crystals nucleated by the freezing processes in orographic wave clouds ($y > 300$ km and $z > 5.5$ km) is larger than that at $y < 300$ km by three orders of magnitude for PCL. Spatial distributions of the mean maximum dimension at 90 min are shown for PCH and PCL in Figs. 18 and 19. PCL simulates columnar crystals with $100 < D < 300 \mu m$ at $y < 250$ km and $z > 8$ km ($T < -40^\circ$C), whereas PCH with $30 < D < 100 \mu m$. The maximum dimension of irregular polycrystals in PCL is larger than those in PCH in the stratiform clouds ($y < 200$ km), but it decreases in the active freezing nucleation area at $y > 200$ km owing to the high concentration. As a result of the faster growth rate, one can see the clearer sedimentation of large irregular polycrystals into the dendritic growth regime $-20^\circ < T \leq 0^\circ$C in PCL than in PCH. Thus, $N_{\text{IN}}$ can change habit frequency through vapor deposition growth rate and subsequent sedimentation.

e. Comparison of simulated habit distributions with observations

This subsection compares simulated habit distributions in PCH and PCL with observations from the winter orographic storm on 13–14 December 2001 during
Fig. 18. Comparison of maximum dimension averaged for each diagnosed habit at 90 min for PCH. The black contour indicates a maximum dimension of 0.1 cm.

Fig. 19. As in Fig. 18 but for PCL.
the IMPROVE-2 campaign. As discussed in HT07, aircraft observation by Woods et al. (2005) indicates the existence of assemblages of sectors, sideplanes, and plates at $4 < z < 6$ km as well as unrime plates. Rimed cold-type crystals, dendrites, aggregates of dendrites, graupel-like snow, and graupels were observed at $2.5 < z < 4$ km. Figure 20 shows the concentration and mass content for diagnosed habits for PCH at 90 minutes of simulation. The magnitude of mass content simulated with PCH at 90 min was larger than PCL, and closer to observation-based estimates by Woods et al. Both simulations predicted plates at $4 < z < 6$ km and dendrites at $z < 4$ km (see Figs. 18 and 19). PCH produced a high concentration and mass content of irregular polycrystals falling to $z = 4$ km at 90 min, whereas irregular polycrystals in PCL have faster sedimentation than PCH due to greater depositional growth than PCH. PCH predicted negligible concentration of planar polycrystals, which include the sideplanes, radiating assemblage of plates, and others in SHIPS, over the windward slope of the Cascades, while PCL predicted a higher concentration at $z > 6$ km (see Table 2 and Figs. 18–20). These results suggest that the actual $N_{IN}$ could have been smaller above 4 km than PCH, or that upward vertical motion should have been stronger than simulated to produce higher supersaturation necessary for planar polycrystals. As reported by Woods et al., the cold-type crystals were associated with altostratus clouds formed by an upper-level front. Since this study does not simulate the upper-level front as well as collision processes, further comparison with the observation is not appropriate. Nevertheless, the framework of polycrystal prediction made it possible to predict qualitatively similar crystal habits for the case.

Next, the simulations are compared with frequency analyses reported for other cases. Although a more direct comparison for a specific case has to be done to validate the framework for predicting polycrystals with SHIPS, the following preliminary comparison supports the approach taken with SHIPS.

Korolev et al. (2000) observed ice particles with $D > 125$ μm in stratiform clouds and classified them into four categories: spheres, irregulars, needles/columns, and dendrites. Since Table 2 includes ice particles of all sizes, habit frequency was recalculated for the simulated crystals with $D > 125$ μm and frequency of plates,
and all the polycrystals were categorized as irregulars (Fig. 21). The observed frequency of irregular particles ranged from 70% to 90% for $D > 125 \mu m$ (see their Fig. 6). It increases with a decrease of temperature and the peak shifts from $T \sim -37^\circ C$ to $-30^\circ C$ with size possibly due to sedimentation. On the other hand, the simulated frequencies of irregular crystals show more variability over $T$, and the peak frequencies, except for PCLH, appear to be shifted to warmer temperature than in Korolev et al. (2000). The observed peak frequencies for columnar crystals at $T > -10^\circ C$ and $T < -40^\circ C$ can be found in all simulations, but the simulated frequencies at $T < -40^\circ C$ are higher than observed by about 40%-90%. The high frequency is evident in the PSD from PCL (Fig. 16) for $D > 200 \mu m$. The dominance of columns can be linked to the average $s_1 \sim 15\%$ in the stratiform clouds ($y < 200 \text{ km}$), which is favorable for formation of columnar crystals (Fig. 1). This study did not simulate radiative cooling at the cloud top, which would have increased the $s_1$ to produce column polycrystals in the region. All simulated frequencies of dendrites increase from $-20^\circ C < T < -10^\circ C$ toward $0^\circ C$ and reach more than 30%. The observation shows the peak at $-20^\circ C < T < -10^\circ C$ and then decreasing with $T$. The reduction with $T$ may be related to the riming process in real clouds. Note that Korolev et al. included heavily rimed particles, graupels, and others with characteristics that do not fall into the categories of needles, dendrites, or spheres into irregulars, whereas this study only simulates nucleation, vapor deposition, and melting. The habit frequency of all but PCLH is qualitatively similar to the observation. However, simulations with aggregation and riming processes as well as radiative cooling must be carried out in order to compare with the observations more rigorously.

Baker and Lawson (2006) and Lawson et al. (2006a) show that for wave and cirrus clouds with $-60^\circ C < T < -27^\circ C$, polycrystals of rosette shapes dominate the mass size distribution for $D > 100 \mu m$, while spheroids occupy the range $10 < D < 20 \mu m$ (see Figs. 13 and 5 of their papers, respectively). The mass size distribution and mass conditional frequency of habits of PCH and PCL were calculated for $-60^\circ C < T < -27^\circ C$ in the orographic wave cloud region ($y > 280 \text{ km}$) at 90 min (Fig. 22). PCL shows the dominance of columnar polycrystals for $60 < D < 300 \mu m$, which agrees with the observations except that SHIPS does not have spheroids. Interestingly, columns and plates in PCH have significant fractions for $D > 200 \mu m$. These hexagonal monocrystals were formed in the edge of high supersaturation for PCH and PCL, but the high frequency over the large size simulated for PCH can be simply attributed to the high $N_{IN}$. This would suggest that it may be possible for hexagonal monocrystals to be observed in wave and cirrus clouds with high $N_{IN}$.

5. Discussion

The SHIPS framework for predicting polycrystals appears to provide a robust explanation of the behavior of the observed crystal habit. The fact that the mass and length growth rates for polycrystals as well as for hexagonal crystals in cold temperatures ($T < 20^\circ C$) are first-order approximations, and that the growth rates of the coordinates of the center of gravity (especially for irregular polycrystals) were parameterized subjectively rather than physically are examples of weaknesses in the SHIPS formulation that should be considered. The following discussion addresses major concerns and points necessary to improve the prediction of polycrystals as well as hexagonal crystals at low temperature.
a. Formation of polycrystals

The quantitative conditions for forming polycrystals from nucleation processes and from a riming process are still not fully understood. In the literature, rapid freezing of a large liquid hydrometeor is considered to be one of the key formation processes of polycrystals (Pruppacher and Klett 1997). This study assumed one frequency map constructed by BH04a for all the nucleation processes. As BH04a described, the most likely ice nucleation process that occurred on filaments drawn from soda-lime glass was deposition–condensation freezing for $T > -40^\circ C$ and deposition freezing for $T < -40^\circ C$. Bacon et al. (2003) studied the initial growth of small ice crystals ($100 - 200 \mu m$) at $T = 38^\circ C$ and $0 < s_i < 10\%$ with the electrodynamic levitation technique. They reported that crystals grown from frozen droplets exhibited isometric compact habits at vapor excesses of less than about 0.05 g m$^{-3}$ and polycrystal habits at higher excess for $T > -22^\circ C$. At lower temperature, frozen droplets tended to be polycrystalline and florid. On the other hand, frost “seeds” ($D < 10 \mu m$) developed into a pristine hexagonal prism with final axis ratios different from those of frozen droplets at all temperatures. They concluded that the concentration of crystalline defects in the initial particle is an important factor to determine the particle shape in addition to environment temperature and humidity. The reason why BH04a has multiple habits formed at a given $T$ and $s_i$ may be the difference in the concentration of defects. Thus, it is important to clarify the connection of habits to the nucleation process, freezing or deposition nucleation, for cloud modeling applications.

It may be possible to predict the amount of mass produced by the freezing processes in SHIPS and diagnose if the shape of ice crystal is a spheroid, faceted hexagonal monocrystal, or faceted polycrystalline crystal. Bacon et al. (2003) states that nonisometric habits develop only after the crystal masses reach nearly 1000 times the masses of the original drops based on previously published reports. Better quantitative understanding of the growth of supercooled droplets to polycrystals is necessary over a wide temperature range.

b. Modeling growth of hexagonal monocrystals in cold temperature

This study used columnar and planar inherent growth ratios for $T \leq -20^\circ C$ to take into account the comparable frequency of plates and columns. According to CL94, the ratio of growth of each axis length is modeled as $dc/da = \Gamma(T)/c/a$. The inherent growth ratio $\Gamma(T)$ is a ratio of the deposition coefficients for the basal and prism faces, which is a function of only ambient temperature. The ambient moisture is reflected in the parameterization of deposition (apparent) density, which is used to calculate the growth of axis lengths. Nelson and Baker (1996) presented a physically consistent vapor growth model based on the assumption that the flux of vapor to the crystal surface is uniform over each flat crystal face. As discussed by Nelson and Baker in their model, $dc/da$ is just the ratio of the deposition coefficients for the two faces, which are modeled to be a function of the size and ambient conditions as temperature and humidity. Formulated either way, the growth model has to be able to take into account the growth of plates and columns at one temperature with different humidity.

Aircraft observations and laboratory experiments showed that pristine bullet rosettes can grow into more complex shape with sideplane and irregular shapes as they experience warmer temperature (Bailey and Hall 2004b; Baker and Lawson 2006). It may be possible to model such transitions with SHIPS by referring to
axis lengths of hexagonal crystals in polycrystals if the transition is reflected in the inherent growth ratio.

Diagnosing $a$ and $c$ axis lengths of polycrystals may not be possible if only one mass component for an ice crystal is used. For a given mass, the maximum dimension of polycrystals and monocrystals is similar, which means that $a$ and $c$ axis lengths of a monocrystal and those of the monocrystal in a polycrystal can be quite different. Thus, mixing of those lengths between monocrystals and polycrystals may produce unrealistic mass–length relationships.

c. Prognostic variables for polycrystals

Even in a Lagrangian simulation of an ice particle, the prediction of geometry of polycrystals is challenging due to the fact that the growth data along the crystalline axis for polycrystals is limited and that the geometry itself is difficult to describe by only a few parameters. This study used the coordinates of gravity and number of extra crystalline structures to “categorize” the types of polycrystals (Fig. 2). The frequency of crystals diagnosed to be polycrystals in the model actually depends on the assigned volume in the parameter space to habits, as well as the frequency of formation observed by BH04a. If one knows the 3D geometry of a polycrystal, it is possible to vigorously calculate the coordinates and number of crystalline structures from it. The integral of mass moment of a polycrystal over a coordinate system can be advected in Eulerian models, and the division of the integral by mass predicted would give the coordinate of the center of gravity. However, at this moment it is not clear that the habit can be identified from the space defined with coordinates of gravity and number of extra crystalline structures. BH04a shows a variety of polycrystals such as crossed plates, gohei twins, scrolls, spearheads, and overlapping parallel plates in $-40 ^\circ C < T \leq -20 ^\circ C$. They describe a family of sideplanes in terms of a twin boundary structure (TBS). Therefore, the length and number of TBSs may be used as PPVs. A similar challenging problem of the geometry can be found in the automatic diagnosis of habits from CPI images of ice particles. Baker and Lawson (2006) and Lawson et al. (2006a,b) developed the software using “focus,” “cutoff,” “Crystal,” “Length,” “Width,” “Perimeter,” and “h1–h6 from radial harmonics.” The parameters, “$h1$–$h6$,” are the first six harmonic frequencies. Similar methodology could be applied to the prognostic variables of polycrystals in SHIPS. Construction of a database with minimum characteristic physical parameters that clearly define spaces for each habit would be useful to improving diagnoses of polycrystals in the numerical model and the automatic habit diagnosis for instruments as well as the database of growth rates along crystallographic directions for polycrystals.

6. Conclusions

This paper proposed a framework to predict growth of polycrystals by vapor deposition in a way consistent with the simulation of monocrystals based on the history of ice crystals and current atmospheric conditions. At cold temperatures ($T < -20 ^\circ C$) and during the nucleation period ($D < 20 \mu m$), crystal habits were determined based on the ambient temperature and moisture, using a simple stochastic approach based on the habit frequency map constructed by BH04a. Two-dimensional idealized simulations of an orographic snowstorm during the IMPROVE-2 campaign showed the usefulness of the framework. The major findings are the following:

- During the early stage of growth, prediction of only hexagonal monocrystals with extended inherent ratio led to domination of columns in the upper level ($T < -30 ^\circ C$) and plates in the middle level ($-25 ^\circ C < T < -10 ^\circ C$). Prediction of polycrystals introduced the highest concentration of irregular polycrystals at $T < -10 ^\circ C$, which can be expected from the frequency map given the vertical profile of supersaturation. Also, high concentrations of planar and columnar polycrystals were predicted at $-6 < z < 8 \text{ km} (-40 ^\circ C < T < -25 ^\circ C)$ and $9 < z < 11 \text{ km} (-56 ^\circ C < T < -46 ^\circ C)$, respectively. Concentration of the plates was reduced by two orders of magnitude at these altitudes compared to the cases with only hexagonal monocrystals. Concentration of the columnar crystals remained as high as the polycrystals at $z > 8 \text{ km}$ ($T < -40 ^\circ C$). The difference in the spatial distribution of habits was found even more significant at the mature stage due to the sedimentation and mass growth of ice crystals. It was clearly shown that the growth rate and terminal velocity as well as the habit growth regimes in middle and upper levels are critical factors to model spatial distribution of ice crystals in lower levels.

- The immersion freezing process appears to be a key process for creating planar polycrystals because temperature and moisture of the active freezing process in the simulations corresponds to high frequency of planar polycrystals in the habit frequency map. For the same reason, the homogeneous freezing process was found to create columnar and irregular polycrystals. The assumed habits for the freezing processes were shown to change the conditional frequency of habits for $10 < D < 100 \mu m$ significantly. Since con-

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The spatial distributions predicted with polycrystals showed that IN concentration can modulate supersaturation by changing concentration of ice crystals, and in turn may change preferable habits for growth and tendency of freezing processes. The freezing tendency in orographic wave regions was significantly reduced due to a less active CCN activation process for the high IN case. Because of the two effects, planar and columnar polycrystals for the low IN case were more abundant in concentration than for the high IN case. Also, IN concentration was able to change the habit frequency analyzed at a given altitude through vapor deposition growth rate and subsequent sedimentation.

The spatial distributions predicted with polycrystals were qualitatively similar to those observed for the case study. Preliminary quantitative comparisons of the simulated habits were made with stratiform clouds observed by Korolev et al. (2000), a wave cloud by Baker and Lawson (2006), and a cirrus cloud by Lawson et al. (2006a), which showed modest agreement. The one discrepancy is in the simulated high frequency of columnar crystals at $T < -40^\circ$C compared with the observed frequency. The lack of a radiative cooling process at the cloud top and high concentration of IN in the simulations were thought to be the reason.

In order to improve the simulation and diagnosis of polycrystals, it is necessary to identify a limited set of characteristic physical parameters of polycrystals to predict in cloud-resolving models (CRMs). The next step would be to construct a database in laboratory experiments that provides relationships between the characteristic physical parameters and habits as well as the growth rate along the characteristic parameters. This research assumed that the habit frequency map by BH04a is valid for all of the nucleation processes simulated in our model. However, it is still not clear if the polycrystal formation actually depends on nucleation processes, namely, deposition nucleation and freezing nucleation processes. More research should be done on the quantitative growth conditions to form polycrystals and on the transition of small ice spheroids to polycrystals.

Overall, the comparisons between SHIPS and observations give cause for optimism. Certain details are not perfect, as we might expect from a new frontier in modeling. However, this is a first step to model the cause and effect relationships between the dynamics and growth processes of ice particles based on continuous growth history and physical principles. Unlike other frameworks for microphysics that attempt to classify crystals into rigid categories (conventional spectral bin models or bulk microphysics schemes), the SHIPS allows the cloud dynamics and the particle growth history to evolve crystals into their unique forms. For the first time, we have achieved a microphysics model that is probably teaching us how microphysical processes occur in real clouds rather than simply rediscovering the assumptions made to a parameterization. Although this approach is computationally expensive, the insight into the process that it provides justifies its cost, particularly for the development of radiative transfer theory through clouds formed of complex crystals. Such calculations are strongly dependent on these details of structure and their variation in space and SHIPS provides the details that are needed to develop these models.

Future studies are planned that include simulation of cirrus and orographic wave clouds with more direct comparison of nucleation processes and polycrystals. The next paper of this series will discuss simulations of aggregation and riming processes with SHIPS.

Acknowledgments. This research was sponsored by NASA (NNG04GA36G and NNX07AD43G). The authors are grateful to the anonymous reviewers for their suggestions.

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