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Investigating the influence of the grain size and distribution on the macroscopic dielectric properties of Antarctic firn

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Abstract:	<p>This study is based on the analysis of detailed measurements of firn dielectric properties performed in Antarctica through coring down to 106 meters. Dielectric measurements in the frequency band (0.4 - 2.5 GHz) have been carried out using an open-resonator probe. Density was also measured for the same samples. The experimental results confirmed the well-known dependence of the real part of permittivity ϵ' on depth and density, showing an increase of ϵ' with density. The imaginary part also increases with depth with a rather complex dependence on frequency, probably due to the presence of salts or impurities. The analysis of the experimental data was performed by implementing 3D and 2D full wave numerical models, to simulate a mixture of firn crystals at prescribed densities, corresponding to the measured densities on the ice cores. The numerical analysis of the ensemble of inclusions showed that the usual symmetric formulae used for modeling ice dielectric properties agree with the average results of the simulation but they are not able to explain the spreading of the measured data at given density. A dielectric model was developed allowing for quantification of the dependence of dielectric properties on density, by combining two models: one consisting in firn crystals into an air host, the other assuming the presence of air inclusions into an homogeneous firn host. The weighted equation is based on the volume fraction. A simple geometric shape (ellipsoidal) is assumed for both ice crystals and air inclusions. This kind of shape is reasonable for the purpose of the dielectric study. The result is a mixture, smoothly changing from firn particles in air (low density) to air bubbles in an ice matrix (high density). A statistical analysis has been accomplished to investigate the dependence of the dielectric properties on the geometrical arrangement of the inclusions. For that purpose, a large number of simulations with different arrangements (micro-states) giving rise to the same average density (macro-state) has been carried out. The permittivity change due to micro-state variability appears to be at least two-three times the model variation due to density alone, and comparable to the measured variability at a given depth, suggesting that firn structure has a significant effect on the dielectric properties.</p>
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Investigating the influence of the grain size and
distribution on the macroscopic dielectric
properties of Antarctic Firn

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1 Abstract

2 This study is based on the analysis of detailed measurements of firn dielectric
3 properties performed in Antarctica through coring down to 106 meters. Dielec-
4 tric measurements in the frequency band (0.4 – 2.5 GHz) have been carried out
5 using an open–resonator probe. Density was also measured for the same sam-
6 ples. The experimental results confirmed the well–known dependence of the
7 real part of permittivity ϵ' on depth and density, showing an increase of ϵ' with
8 density. The imaginary part also increases with depth with a rather complex
9 dependence on frequency, probably due to the presence of salts or impurities.

10 The analysis of the experimental data was performed by implementing 3D
11 and 2D full wave numerical models, to simulate a mixture of firn crystals at
12 prescribed densities, corresponding to the measured densities on the ice cores.
13 The numerical analysis of the ensemble of inclusions showed that the usual
14 symmetric formulae used for modeling ice dielectric properties agree with the
15 average results of the simulation but they are not able to explain the spreading
16 of the measured data at given density.

17 A dielectric model was developed allowing for quantification of the de-
18 pendence of dielectric properties on density, by combining two models: one
19 consisting in firn crystals into an air host, the other assuming the presence of
20 air inclusions into an homogeneous firn host. The weighted equation is based on
21 the volume fraction. A simple geometric shape (ellipsoidal) is assumed for both
22 ice crystals and air inclusions. This kind of shape is reasonable for the purpose
23 of the dielectric study. The result is a mixture, smoothly changing from firn

24 particles in air (low density) to air bubbles in an ice matrix (high density).

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26 of the dielectric properties on the geometrical arrangement of the inclusions.
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28 (micro–states) giving rise to the same average density (macro–state) has been
29 carried out. The permittivity change due to micro–state variability appears
30 to be at least two–three times the model variation due to density alone, and
31 comparable to the measured variability at a given depth, suggesting that firn
32 structure has a significant effect on the dielectric properties.

33 Keywords: Antarctica, dielectric measurements, ice cores, dielectric model,
34 full wave EM simulations, close-off, firn

35 **2 Introduction**

36 Remote sensing techniques employed to measure Antarctica ice thickness, such
37 as radars or radiometers, require an accurate estimation of ice dielectric prop-
38 erties. The real and imaginary part of ice permittivity is one of the most im-
39 portant variables determining the penetration depth or scattering of EM waves.

40 A variety of studies have been presented in the last decades to propose
41 models of electric permittivity of snow and firn. An early work by Polder and
42 van Santen (1946) computed the effective permittivity of a material consisting
43 of a host medium in which solid particles or empty holes, assumed of ellip-
44 soidal shape, are packed together. Tiuri et al. (1984) measured the complex

45 permittivity of firn at microwave frequencies, concluding that it is practically
46 independent of the microstructure for density up to 500 kg m^{-3} . Matzer (1996)
47 measured the permittivity of dry snow in 90 samples at different sites in the
48 Swiss and Austrian Alps and showed the strong dependence of the real part of
49 snow permittivity on density. The author also presented a formulation based on
50 the effective medium formula (Polder and van Santen, 1946), and he concluded
51 that the formulation for oblate spheroidal particles was the most appropriate
52 and that the structure of the firn crystals have an effect on permittivity.

53 The transition between snow, firn and ice is based on density. Firn be-
54 comes ice when the interconnecting air- or water-filled passageways between
55 the grains are sealed off, a process called pore close-off. This value depends
56 on density and it usually occurs around a density of 830 kg m^{-3} (Cuffey and
57 Paterson, 2010). In this study we will refer to firn, since the measured densities
58 are usually below this threshold.

59 A general overview of the different electromagnetic mixing models was
60 presented by Sihvola (1999), discussing a variety of approaches including clas-
61 sic mixing approaches, homogeneous and in-homogeneous inclusions, isotropic
62 and anisotropic media and others. Among the various models, the continu-
63 ous or bi-continuous random structure models showed promising results in the
64 interpretation and modeling of dielectric spectroscopy or remote sensing data.
65 Karkkainen et al. (2000) presented a numerical analysis of electromagnetic fields
66 in random dielectric materials. The calculated permittivity distribution were
67 compared with theoretical mixture models. They concluded that all the possible

68 permittivity values lie between the Wiener limits, and the values were almost
69 always between the Hashin–Shtrikman limits.

70 When studying the dielectric properties of firn the most relevant variables
71 are the density, at a macroscopic level, and orientation, size and shape of ice
72 crystals on a microscopic scale. The crystal size can be represented by the
73 average crystal area (Jun and Jacka, 1999), defined as the surface of an ellipse
74 whose long and short semi-axes correspond to the radii of the largest inscribed
75 circle and the smallest circumscribed circle, respectively, for a given crystal. The
76 average crystal area of Antarctic firn is a function of depth. Crystal orientation,
77 expressed for example by the crystallographic c-axis, has been shown to be
78 practically random in polar ice cores (Jun and Jacka, 1999). If the crystal
79 is roughly represented by an ellipsoid, which is acceptable for the purpose of
80 the dielectric model, another parameter possibly influencing permittivity is the
81 aspect ratio, which is descriptive of the crystal shape.

82 From the dielectric point of view, firn is modeled as a binary mixture,
83 made of “pure” firn/ice and air. Different approaches (Sihvola, 1999) bring to
84 symmetric formulae, where inclusions and host can be interchanged with no
85 consequence on the effective permittivity, or to non–symmetric formulae based
86 on the Maxwell Garnett theory, where the host material is that having the
87 dominant volume fraction.

88 An analytic formula is only able to represent the average measured di-
89 electric constant as a function of density or volume fraction. The choice of a
90 non–symmetric model involving firn inclusions in air appears reasonable for

91 low-density material, while it does not appear meaningful for high-density
92 material where a suspension of air bubbles into an ice host is physically more
93 based. No analytic formula is able to handle inclusions having different shapes,
94 size and orientation. Therefore a numerical method of analysis is needed.

95 Direct measurements of the dielectric properties of Antarctic ice, such as
96 “dielectric profiling” (DEP) measurements on sampled firn cores, are scarcely
97 common in the literature. The first comprehensive measurement was performed
98 by Moore (1988), with a profiled firn core of 130 m depth in Antarctica, to mea-
99 sure the reflection coefficient and electrical conductivity to derive the dielectric
100 properties. However, the measurement was limited to the range of 20 Hz to
101 300 kHz. Wolff et al. (1997) and Wolff (2000) focused on conductivity measure-
102 ments, but the early attempts to measure firn’s permittivity by DEP (Moore,
103 1988) were not pursued with more extensive campaigns and at higher frequen-
104 cies of interest for space-borne radar and radiometers. Suguyama et al. (2010)
105 measured the permittivity of the upper 1 meter snow layer at 35 locations, along
106 a transect of approximately 50 km, using a transmission-line resonator. The
107 measurements provided information in the horizontal direction, but to a shallow
108 depth of 1 meter. Grimm et al. (2015) analyzed dielectric spectra (0.1 Hz – 1
109 MHz) of 49 firn samples in Antarctica. However, they did not explore higher
110 frequencies and did not collect detailed and extensive measurement on a single
111 core down to over 100 meters depth. Overall, there is need to obtain detailed
112 DEP in depth (at least at up to the close-off) in the frequency bands where
113 space-borne radar and radiometers operate.

114 This study reports the results of direct measurement of dielectric prop-
115 erties, density and specific surface area, performed at Dome-C in Antarctica
116 (Concordia Experimental Station) down to 106 meters, through the collection of
117 firn cores. The dielectric measurements were performed by an open-resonator
118 probe (Olm et al., 2019), providing high accuracy measurements of both the
119 real and the imaginary parts, in four narrow frequency bands around 400, 880,
120 1100 and 2500 MHz, as a function of depth z and density ρ . Measurements of
121 the complex permittivity of firn were performed in situ and later repeated on the
122 same samples transported in a cold laboratory. For the aim of interpreting the
123 variability of experimental permittivity at given density, two- and three- di-
124 mensional numerical models has been implemented, based on the Finite Element
125 (FE) method. Computed dielectric permittivities are compared to experimental
126 data and to existing mixture models to obtain a formulation for firn permittivity
127 allowing to take in account the variability due to the microscopic arrangement
128 of firn crystals.

129 **3 Materials and Methods**

130 The dielectric measurements described here have been conducted at the Concor-
131 dia Station in Antarctica (73°30'S 123°00'E), on a core of firn drilled down to 106
132 meters depth. Measurements were performed on core slices of 10 cm thickness,
133 whose density was also measured and recorded. A total of 930 samples have
134 been measured *in situ*, i.e. one every 10 cm, with two different open-coaxial

135 resonant probes, the first operating at about 900 MHz in air (2700 MHz in
136 second harmonic), the second at 400 MHz in air (1200 in second harmonic).
137 Measurements concerned depths from about 3 to 106 m, because the first 3 me-
138 ters of core were damaged. Sample temperature was -20 °C. The samples were
139 later moved into a cold laboratory in Firenze (Italy), where measurements were
140 repeated at -19 °C, on 92 samples spaced about 1 m between them. In both
141 cases only one point per sample was measured, with the exception of a limited
142 number of them for testing purposes.

143 The electromagnetic technique used for dielectric measurement, based on
144 a open-resonator probe, is thoroughly described in Olmi et al. (2019). The
145 frequency band of interest for the study is 400–2500 MHz, because of the remote
146 sensing applications relevant for the study itself.

147 The density of the samples used for dielectric measurements was directly
148 deduced from mass and volume measurements. The diameter and height of each
149 sample, assumed to be cylindrical in shape, were measured with a caliper, and
150 mass was measured with a precision balance. Largest uncertainty came from the
151 volume measurement, and accuracy of such density measurements on cohesive
152 firn core samples is estimated to be better than 10 %.

153 In this work we will not be concerned with the variation of dielectric
154 properties with frequency, the attention being focused on the dependence of
155 permittivity on firn structure at a fixed frequency. Therefore, we will refer all
156 future considerations to a nominal frequency of 1 GHz, although the data are
157 shown for the measured frequencies.

158 **4 Theory**

159 **4.1 Numerical Simulation**

160 The dielectric model consists in a host medium containing a random distribution
161 of inclusions (spheres, ellipsoids), of different size and orientation, possibly over-
162 lapping. The host medium can be air and the inclusions ice crystals, or the op-
163 posite. Borrowing the notion from statistical physics, we define “micro–state”
164 a specific geometrical arrangement of inclusions. The average physical proper-
165 ties (the “macro–state”) are obtained in principle by averaging on all possible
166 micro–states. Therefore, generating geometrical arrangements corresponding
167 to the same material density, we can compute the macro–state permittivity by
168 averaging on the micro–states. At the same time, by looking at the statisti-
169 cal distribution of the micro–state permittivity we obtain information on the
170 influence of the geometrical arrangement on the complex permittivity variation.

171 Both three–dimensional (3D) and two–dimensional (2D) models have
172 been implemented. The composite material fills a section of a parallel–plate
173 wave–guide supporting a transverse electromagnetic (TEM) propagation mode.
174 In the 3D case, the parallel–plate guide is realized by imposing a “perfect–magnetic
175 wall” condition on two surfaces normal to the magnetic field vector, as shown
176 in Figure 1. The EM wave, propagating along the y direction, has the electric
177 field polarized in the z –direction and the magnetic field in the x –direction.
178 The input port is the $y=0$ plane, while a perfect electric reflector is placed at a
179 distance d from it.

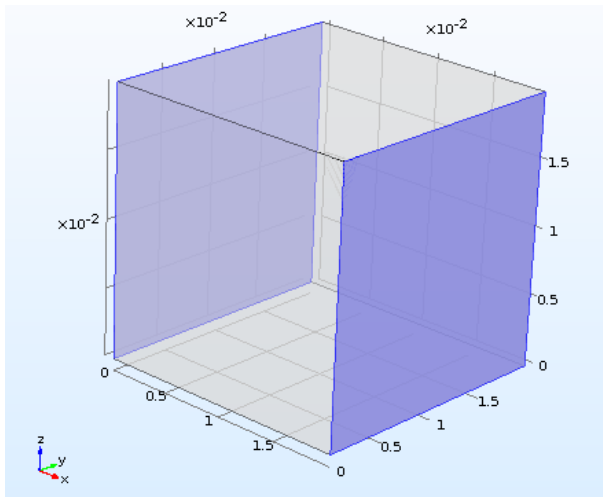


Figure 1: Geometry of the TEM waveguide. Electric field is z -directed, magnetic field is x -directed, wave propagation is along y . The “grayed” surfaces are the perfect magnetic walls.

180 Computing permittivity by means of the 3D model is very time-consuming,
 181 in particular for densities that require a large partial volume fraction of the “in-
 182 clusion” phase. The statistical analysis to be performed on the ensembles of
 183 micro-states, requires the electromagnetic computation to be repeated hun-
 184 dreds of times for a given density value. It was observed that, for a given
 185 density, the distribution of the real and imaginary parts are practically identi-
 186 cal for a 3D model of prolate spheroids and for a 2D model of ellipses, having
 187 semi-axes and orientation in the same range of values. As an example, figure 2
 188 respectively refer to 3D and 2D distributions giving rise to a firm density of 800
 189 kg m^{-3} .

190 The difference among 3D and 2D simulation is not only in the additional
 191 dimension of the former, which dramatically increases the number of degrees

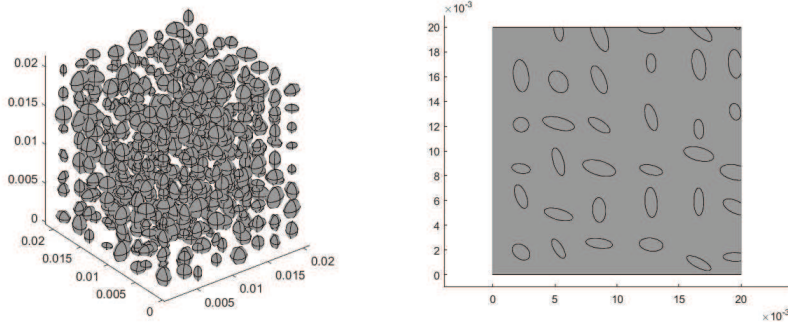


Figure 2: 3D distribution of spheroids and 2D distribution of ellipses (air inclusions in firn) corresponding to an firn density of 800 kg m^{-3} .

192 of freedom of the FEM problem (or, in other terms, the order of the system of
 193 equations to be solved). Both in the 3D and 2D case, the inclusions are modeled
 194 as geometric parts and, as such, they require to be meshed (with tetrahedra in
 195 the 3D case or triangles in 2D). As a consequence, a geometry having a large
 196 number of inclusions, possibly overlapping, requires a huge number of mesh
 197 elements. Our approach, in the 2D case, is to generate the proper geometry
 198 (i.e. the distribution of inclusion giving the required average density of firn) and
 199 to include the information about the inclusion topology in a space-dependent
 200 permittivity $\epsilon(x, y)$, which is a continuous analytical function. Although that
 201 function has sharp edges at the interface between two materials (host/inclusion),
 202 the geometry and the mesh topology of the problem remain unchanged.

203 Table 1 shows the differences between 2D and 3D for 400 micro-states,
 204 for a material having a density $\rho = 800 \pm 0.36\% \text{ kg m}^{-3}$.

205 The almost perfect equivalence among 3D and 2D models suggests re-

Table 1: Comparison between the 3D and 2D mode

3D		2D	
ϵ'	ϵ''	ϵ'	ϵ''
$2.8 \pm 2.5\%$	$1.25 \times 10^{-3} \pm 4.7\%$	$2.8 \pm 2.3\%$	$1.32 \times 10^{-3} \pm 4.5\%$

206 sorting to a 2D model for the statistical purpose. The electromagnetic model
 207 used to compute the complex permittivity of firm is reduced to a section of
 208 parallel-plate waveguide, excited at one end (input port) by a TEM mode and
 209 short-circuited at the other end (Figure 3).

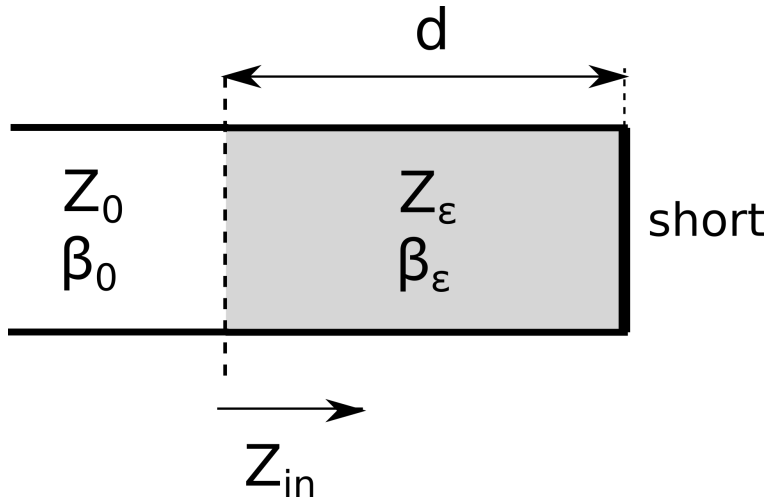


Figure 3: Transmission line equivalent circuit of the plane-wave propagation problem

210 The complex reflection coefficient computed at the input port contains the
 211 information about the permittivity of the material filling the waveguide. The
 212 choice of a full-wave solution, analogous to what proposed in Karkkainen et al.
 213 (2000), has been preferred to the quasi-static approach proposed by Tuncer

214 et al. (2001) and frequently used in the modeling of random media, e.g. in Zhao
 215 et al. (2004). The reason is that while the scale of the inclusions is such to fulfill
 216 the requirements for a quasi–static approximation at about 1 GHz, the necessity
 217 of having a sufficient volume (surface in 2D) to include a suitable number of firn
 218 particles of different size brings to a macroscopic dielectric sample whose size is
 219 not sufficiently smaller than the wavelength in firn. If the mean surface of the
 220 inclusions is in the order of 1 mm^2 , simulating firn with porosity 0.5, a sample
 221 surface of 1000 mm^2 contains 500 inclusions. Assuming a rectangular sample
 222 surface, the characteristic length (CL) is in the order of the square root of 1000,
 223 which is about $1/10$ of the wavelength in air, and $1/6$ of the wavelength (λ) in
 224 firn. These values are too large for a quasi–static approximation, requiring at
 225 least $\text{CL} < \lambda/20$.

226 The reflection coefficient at the input of the firn–filled space is computed
 227 in terms of the impedance $Z_{in} = jZ_\epsilon \tan(\beta d)$ at the same interface:

$$\Gamma_{in} = \frac{Z_{in} - Z_0}{Z_{in} + Z_0} = \frac{j \tan(\beta d) - \sqrt{\epsilon}}{j \tan(\beta d) + \sqrt{\epsilon}} \quad (1)$$

228 where:

$$\beta = k_0 \sqrt{\epsilon} \quad (2)$$

$$Z_\epsilon = Z_0 / \sqrt{\epsilon} \quad (3)$$

229 are the complex wave number and characteristic impedance in firn, respectively,

230 while k_0 and Z_0 are the same quantities in air. The reason for including a “vir-
 231 tual” section in air (actually, it is zero length) is that the FEM code normalizes
 232 the computed scattering parameters to the free space impedance. The algo-
 233 rithm for computing the complex permittivity ϵ uses a FEM engine, based on
 234 COMSOL Multiphysics[®], integrated in MATLAB[®] code by LiveLink[®].

235 The procedure for computing ϵ is the following. Given the desired density
 236 value ρ_D , distributions of ellipses with random orientation (between 0 and $\pi/2$)
 237 are generated to fulfil a requirement about the “computed” density $\rho_C = \rho_D \pm$
 238 Δ . An algorithm was written in MATLAB[®] to generate a certain number of
 239 particles of variable size and shape at spatial intervals (fixed on physical basis,
 240 as described later), to achieve a target density corresponding to the measured
 241 density as function of depth. During the iterations the algorithm adjusts the
 242 lengths of the semi-axes, the aspect ratio (AR) and the angle of the generated
 243 ellipses.

244 The complex permittivity ϵ computed inverting (1) for density values ρ_C
 245 belonging to the interval $(\rho_D - \Delta, \rho_D + \Delta)$ automatically takes into account the
 246 dependence on density. The operation of inverting (1) maps the Γ interval onto
 247 an ϵ interval, depending on the density variation:

$$(\Gamma(\rho_D - \Delta), \Gamma(\rho_D + \Delta)) \rightarrow (\epsilon(\rho_D - \Delta), \epsilon(\rho_D + \Delta))$$

248 In relatively shallow firn the average crystal area (ACA) of Antarctic
 249 firn/ice increases about linearly with depth. From Lipenkov et al. (1989) and
 250 Jun and Jacka (1999) the ACA changes from about 0.4–0.9 mm² at a depth of

251 10 m to $1.4\text{--}1.6\text{ mm}^2$ at 100 m. Arnaud et al. (1998) presented experimental
252 data and a physical model (Arnaud et al., 2000) on the transformation of dry
253 snow to firn and the of snow/firn and ice in the upper part of the polar sheets.
254 Few data are available concerning the dependence of crystal orientation on depth
255 for shallow firn, but it is reasonable (see, for example Jun and Jacka (1999))
256 to assume a random orientation for the c -axis. Moreover, the orientation of
257 elliptical inclusions does not have a marked effect on the average permittivity
258 in a medium with randomly oriented inclusions (Sihvola, 1999), as an expected
259 effect of the random dipole polarization moment. That characteristic has been
260 confirmed by the numerical simulations described later in this paper.

261 In Azuma et al. (1999) the aspect ratio at the lowest reported depth (about
262 100 m) is about 1.7. We can reasonably assume a linear dependence of the
263 average aspect ratio between 1 and about 2 from the surface to 100 m depth,
264 as an effect of firn compression.

265 For each density, a number (*e.g.* 100) of simulations are conducted to
266 investigate the dependence of the dielectric properties on the micro-state con-
267 figurations. From experiments, the dependence of density with depth is known.
268 For each couple (depth, density) set in the numerical model, the average aspect
269 ratio and the average particle diameter is fixed, and two sets of simulations are
270 performed: one involving firn inclusions in air host medium, the other involving
271 air inclusions in an ice host medium.

272 4.2 Dielectric mixing formulae

273 The effective permittivity of a random mixture (Sihvola, 2000) cannot be sum-
274 marized by a closed-form analytic expression, although some work on the ana-
275 lytical treatment of a dielectric containing random metallic inclusions has been
276 done in the recent past (Koledintseva et al., 2006).

277 The results from numerical simulations of random inclusions in a host
278 material do not agree with homogenisation formulas like that of Bruggeman
279 (Sihvola, 1999) or, which is the same, the frequently used formula derived from
280 the theory developed by Polder and van Santen (1946). The reason is that such
281 formulae are symmetric in the permittivity of the inclusion material (ϵ_i) and of
282 the host environment (ϵ_e):

$$(1 - v) \frac{\epsilon_e - \epsilon_m}{\epsilon_e + 2\epsilon_m} + v \frac{\epsilon_i - \epsilon_m}{\epsilon_i + 2\epsilon_m} = 0 \quad (4)$$

283 where ϵ_m is the (effective medium) mixture permittivity and v is the volume
284 fraction of the inclusion material. Numerically simulated dielectrics do not
285 exhibit such a symmetry: the effective permittivity of an arrangement of ice
286 inclusions in air, computed as a function of the density, is different from the
287 permittivity of an arrangement of air inclusions in ice. As a consequence, if the
288 inclusions were supposed to all have the same shape, the generalized Maxwell
289 Garnett (MG) approach for ellipsoidal inclusions would be the correct choice
290 (Sihvola, 1999). Actually, the MG formula is inherently non symmetrical so,
291 given the density ρ of the material, and computing the air volume fraction v (ρ_I

292 is the density of pure ice):

$$v = \frac{\rho_I - \rho}{\rho_I - 1} \quad (5)$$

293 leading to two different dielectrics: (1) an ice bulk medium containing a volume
294 fraction v of air, or (2) an arrangement of firm inclusions having a total volume
295 fraction $1 - v$, in air. Dielectrics (1) and (2) are described by two different MG
296 formulas.

297 Just to show the connection between the MG approach and the Bruggeman
298 formula, suppose the inclusions are oblate spheroids with semi-axis a and b in
299 the ratio $\theta = b/a = 2$. The dielectric constant ϵ_i , assumed real, of the inclusions
300 can be that of ice (3.15) or air (1). Correspondingly, the dielectric constant of
301 the external medium ϵ_e will be 1 and 3.15, respectively.

302 Given the spheroid eccentricity $e = \sqrt{\theta^2 - 1}$, the MG formula for random
303 inclusions involves the depolarization factors along axes parallel to the main
304 directions (denoted by the numerals 1 to 3), given by (Sihvola, 1999):

$$A_1 = \frac{1 + e^2}{e^3} (e - \tan^{-1}(e)) \quad (6)$$

$$A_2 = \frac{1 - A_1}{2} \quad (7)$$

$$A_3 = A_2 \quad (8)$$

305 The effective MG dielectric constant ϵ_M is:

$$\epsilon_M = \epsilon_e + \epsilon_e \frac{\frac{v}{3} \sum_{k=1}^3 f(\epsilon_i, \epsilon_e, A_k)}{1 - \frac{v}{3} \sum_{k=1}^3 A_k f(\epsilon_i, \epsilon_e, A_k)} \quad (9)$$

306 where:

$$f(\epsilon_i, \epsilon_e, A_k) = \frac{\epsilon_i - \epsilon_e}{\epsilon_e + A_k(\epsilon_i - \epsilon_e)} \quad (10)$$

307 By exchanging the role of inclusion and host, two non-intersecting curves
 308 are obtained as function of the air volume fraction v . With reference to figure 4,
 309 the dashed line is the dielectric constant of an ice host with air inclusions, while
 310 the dotted curve is the dielectric constant of an air host with ice inclusions,
 311 both as a function of the air volume fraction. The curves do not assume the
 312 same value in $v = 0.5$, because of the formula asymmetry and, furthermore,
 313 they have slightly different maximum and minimum values for pure ice (clearly
 314 they coincide for $v = 1$, i.e. in pure air). But, if it is reasonable that quasi-pure
 315 ice (e.g. at firn/ice transition where density is about 830 kg m^{-3}) is “solid ice
 316 with air bubbles”, and it is equally meaningful to consider snow as “ice crystals
 317 suspended in air”, a transition between the upper and the lower model of Figure
 318 4 must be defined.

319 The simplest transition is a linear transformation from the former (a/i: air
 320 in ice) to the latter (i/a: ice in air), or in other words to compute the mixture
 321 dielectric constant ϵ_m as follows, where the inclusion volume fraction has been
 322 substituted by the material density ρ which is the parameter of interest:

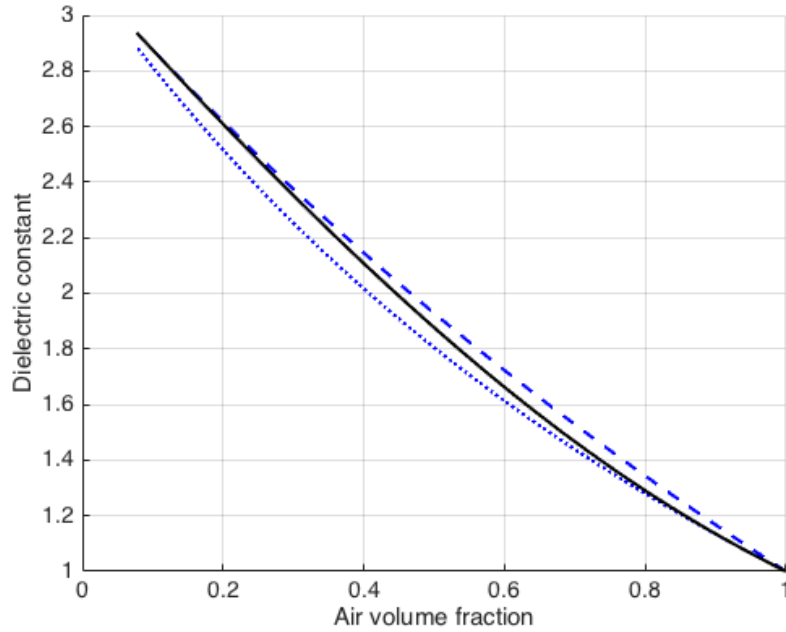


Figure 4: Dielectric constant of an ice/air mixture computed by the MG formula, as a function of the volume fraction (see text)

$$\epsilon_m(\rho) = [1 - \eta(\rho)] \epsilon_{i/a}(\rho) + \eta(\rho) \epsilon_{a/i}(\rho) \quad (11)$$

323 with:

$$\eta(\rho) = \frac{\rho - 1}{\rho_I - 1} \quad (12)$$

324 Such a linear relation is such that the dielectric constant for $v = 0.5$ is
 325 exactly the mean value between those of the upper and lower curves at the same
 326 volume fraction. The solid line in figure 4, representing the linear transformation

327 from the a/i to the i/a model, almost perfectly corresponds with the dielectric
328 constant computed by the Bruggeman formula (4), confirming the validity of
329 the linear transformation. Figure 5 shows such a correspondence: the maximum
330 percentage deviation from the Bruggeman formula is less than 0.7 %.

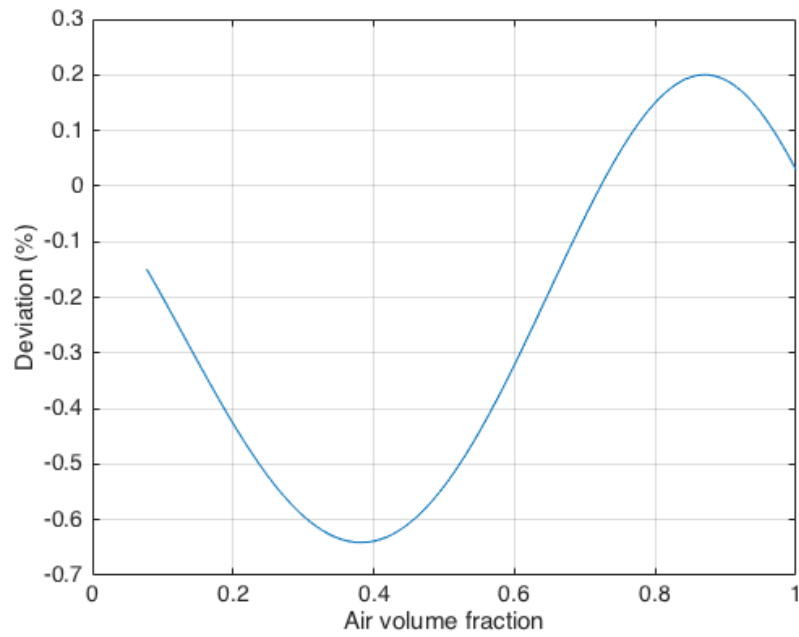


Figure 5: Relative percentage deviation of the linear formula (11) from the Bruggeman effective dielectric constant

331 5 Results

332 5.1 Experimental Results

333 The measurement procedure and, in particular, the electromagnetic model of
334 the open-resonator probe, is described elsewhere (Olmí et al., 2019). Two
335 cavity resonators are used, operating in first and second harmonics.

336 Briefly summarizing, for each cavity two calibration measurements are
337 conducted – one in air, one with the probe placed on a reference dielectric –
338 at the beginning and at the end of a session (usually half a day), after a full
339 calibration of the vector network analyzer used to measure the transmission
340 through the microwave cavity.

341 Figure 6 depicts the dielectric constant as function of depth at four fre-
342 quencies (first and second resonant mode of the two cavity resonators employed),
343 while figure 7 shows the measured loss tangent at the same frequency values.
344 The smooth lines of both dielectric constant and loss tangent are a result of a
345 “smoothed” calibration procedure, not of a direct smoothing or interpolation
346 of the measured data. The transmission coefficient in every session is inverted
347 to give the complex permittivity using the “local” calibration, i.e. that relative
348 to the session (red dots). As an alternative, the calibration parameters at each
349 frequency can be used to build a smoothed calibration curve, which brings to
350 the solid-line values in figures 6 and 7.

351 It clearly appears that the real part of permittivity weakly depends on
352 frequency and exhibit the same dependence with depth. The same is not true

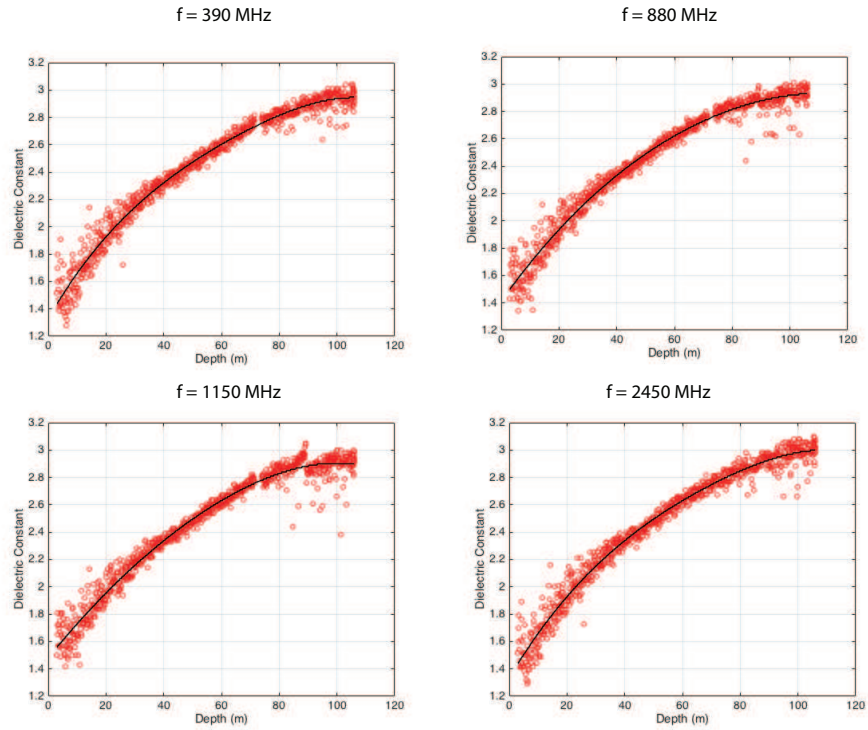


Figure 6: Real part of complex permittivity versus depth

353 for the imaginary part, whose dependence on frequency appears rather complex,
 354 probably due to the presence of salts or impurities, although generally increas-
 355 ing with depth. This could hopefully be confirmed by a cross-check with the
 356 findings of physical-chemical analyses currently in progress.

357 Figure 8 shows the measured density of the core slices as a function of the
 358 slice depth. The dependence of density ρ on depth z appears to be described
 359 by a power-law relation:

$$\rho(z) = az^b + c \quad (13)$$

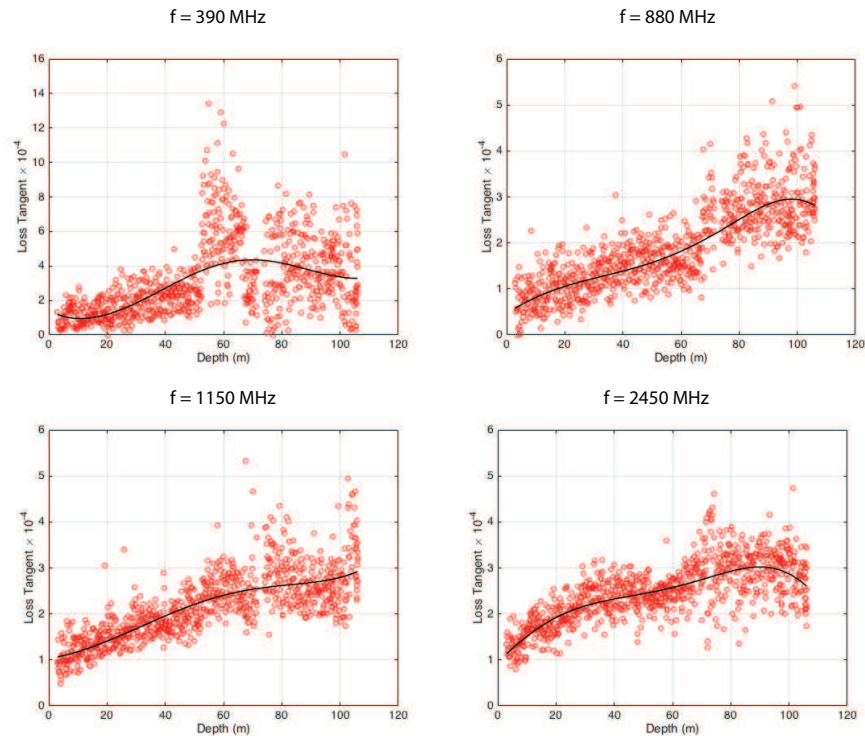


Figure 7: Loss tangent versus depth

360 which corresponds to the solid line in the figure. The dashed line refers to
 361 the bi-exponential fitting model introduced by Arthern et al. (2013), whose
 362 rationale is based on the existence of a critical density where a discontinuity
 363 appears in the derivative of $\rho(z)$. That kind of relationship does not appear to
 364 describe well our experimental data.

365 5.2 Numerical Results

366 Two sets of simulations are conducted, to follow the procedure summarized by
 367 equation (11). The first set allows to compute $\epsilon_{i/a}(\rho, z)$, the second $\epsilon_{a/i}(\rho, z)$,

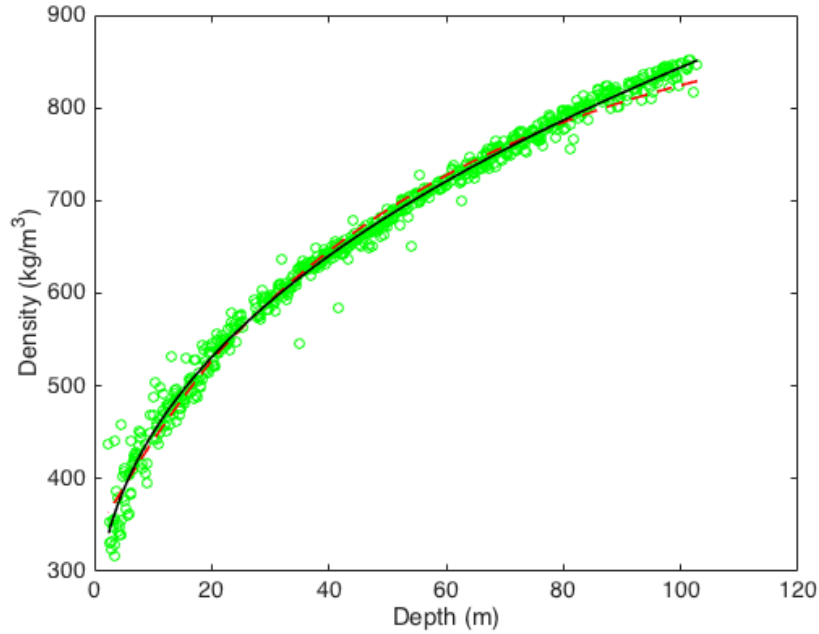


Figure 8: Density $\rho(z)$ versus depth: comparison between the power-law fitting (solid black line) and the bi-exponential fitting (dashed red line)

368 where “i/a” and “a/i” mean “ice in air” and “air in ice” respectively, as in
 369 Section 4.2.

370 5.2.1 Statistical Analysis

371 For each density value (macro-state) we obtain a set of micro-states by the
 372 procedure outlined in the previous section. As an example, figure 9 (left) shows
 373 a configuration of firn inclusions (black) in air (white) corresponding to a density
 374 of 400 kg m^{-3} , and (right) a configuration of air inclusions (white) in a ice host
 375 material (black). It is clear from figure 9 how the depth, hence the density,

376 plays a role in the variation of shape and size of the inclusions.

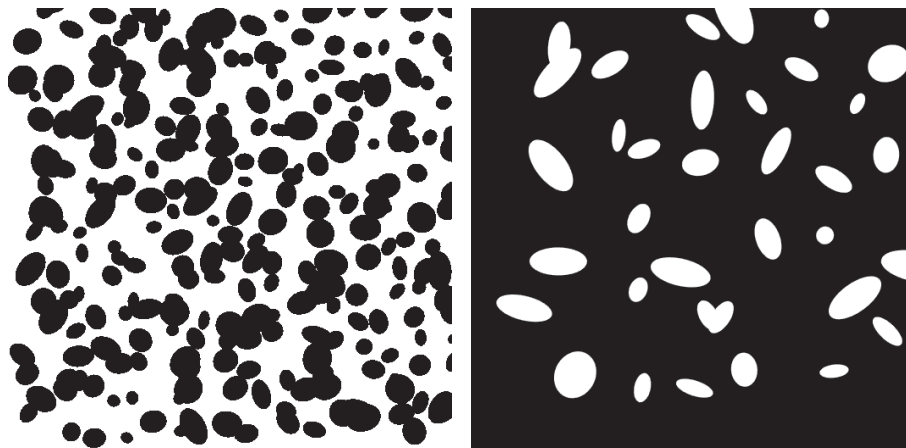


Figure 9: Micro-states. $\rho = 400 \text{ kg m}^{-3}$ (left) and $\rho = 800 \text{ kg m}^{-3}$ (right)

377 The density corresponding to a macro-state in a simulation is allowed
378 to have a small interval of variation around the set value, to be able to apply
379 a sort of de-trending to the computed complex permittivity values. In fact,
380 although several formulas exist, see for example Kovacs et al. (1995), relating
381 the real part of permittivity to density and, of course, a fitting of ϵ versus ρ can
382 be performed over the entire density range, we found that greater accuracy in
383 de-trending is achieved by “zooming” into a small region of densities.

384 Denoting by $\Delta\epsilon'$ and $\Delta\epsilon''$ the de-trended values of ϵ' and ϵ'' , we obtain
385 from simulations the results presented in Figure 10 for a density of 400 kg m^{-3} .

386 Very similar results are obtained for a density of 840 kg m^{-3} , as depicted
387 in Figure 11. To summarize, we observe that the dielectric constant (real part)
388 has a 3σ variation of 0.08 for each value in the whole density range. The 3σ

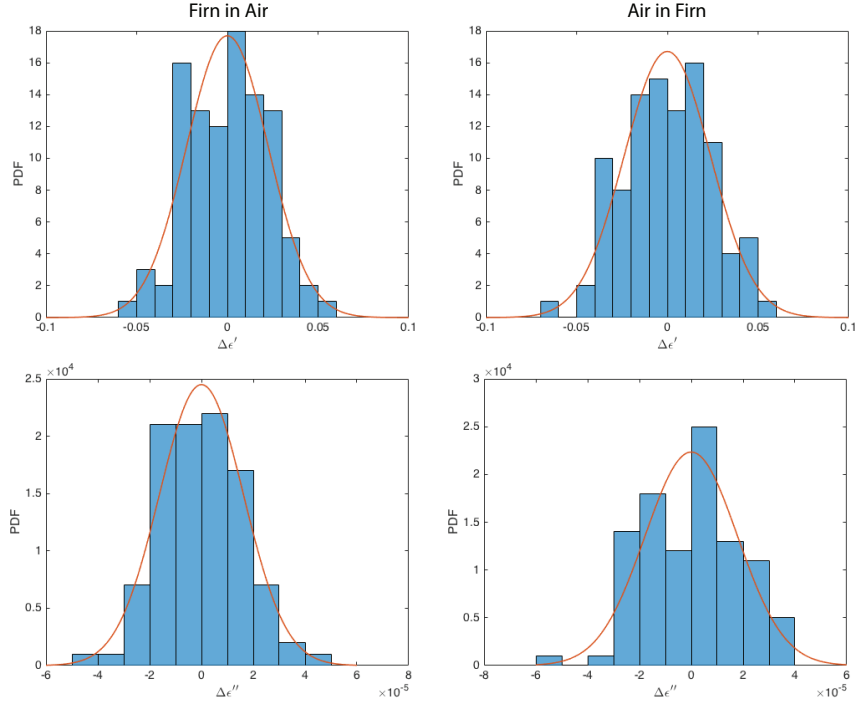


Figure 10: $\Delta\epsilon'$ (top plates) and $\Delta\epsilon''$ (bottom plates) for $\rho = 400 \text{ kg m}^{-3}$

389 variation is 6×10^{-5} and 9×10^{-5} for dielectric losses at 400 kg m^{-3} and 840 kg
 390 m^{-3} respectively. The micro-state variability is entirely responsible of such a
 391 variation, as the change with density has been dropped out by the de-trending
 392 procedure.

393 5.2.2 Discussion

394 Figure 12 compares the experimental results of ϵ as a function of depth with
 395 the results of the numerical model. The dashed lines are the $\pm 3\sigma$ values around
 396 the mean, i.e. the values between the dashed curves include about 99% of
 397 the possible dielectric constants computed by the models as a function of the

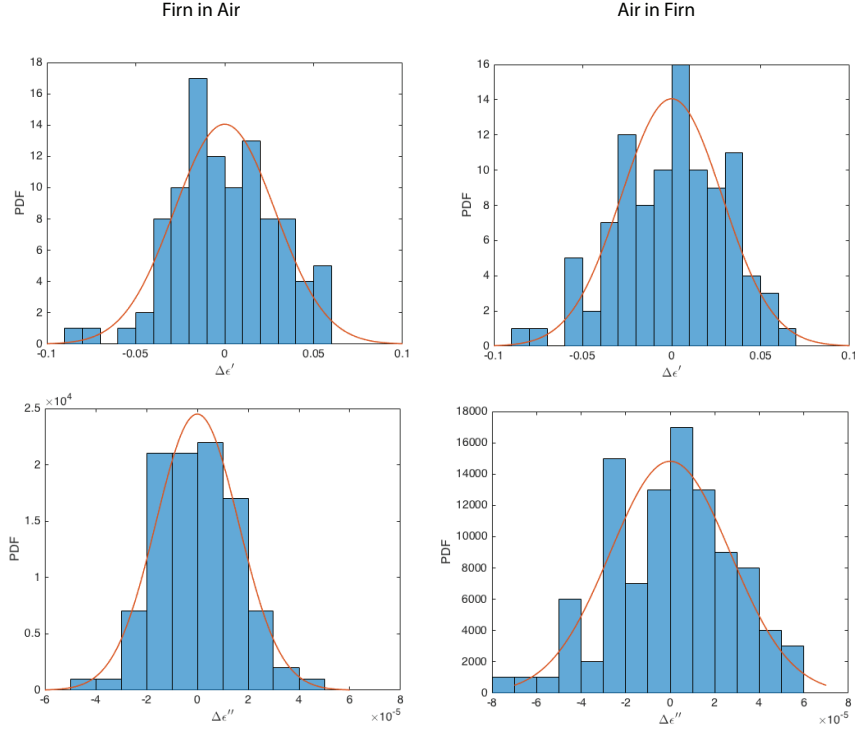


Figure 11: $\Delta\epsilon'$ (top plates) and $\Delta\epsilon''$ (bottom plates) for $\rho = 840 \text{ kg m}^{-3}$

398 micro-state configurations. The solid line is computed applying the linear
 399 relation (11), while the dash-dot line is computed by the Bruggeman formula.

400 The results on the statistical variation of the imaginary part, and hence
 401 of the loss tangent, are similar. Of course, the computation of the imaginary
 402 part of the ice/air mixture depends on the true value of the imaginary part of
 403 pure ice at the frequency of interest, which is not so well defined as the real part
 404 (Figure 13). As for the real part, the dashed lines correspond to 3σ variation
 405 around the mean value.

406 The average dielectric constant computed by (11), with the variance based

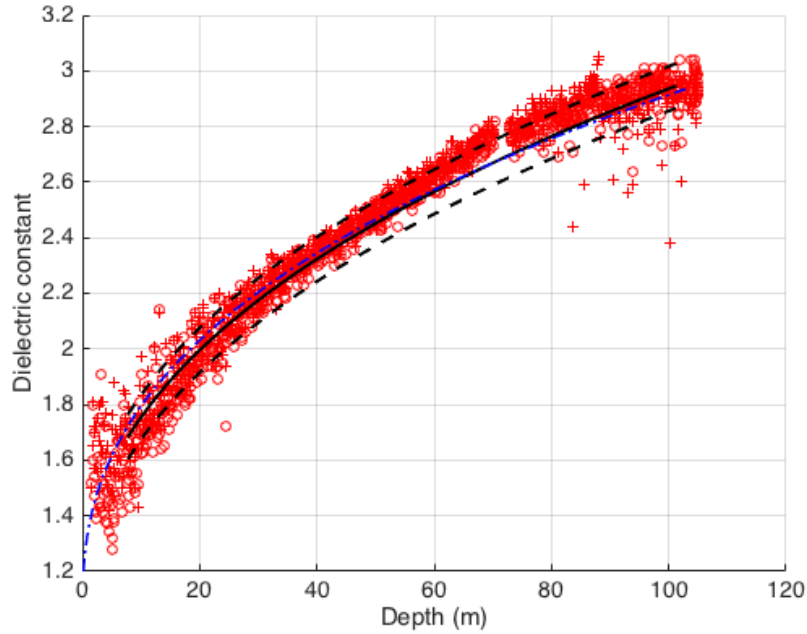


Figure 12: Dielectric constant versus depth: comparison between the experimental data at 880 MHz (red circles) and at 1.15GHz (red crosses) and the results of the full-wave numerical model at 1 GHz

407 on the statistical analysis, represents quite well the experimental behaviour, like
 408 the Bruggeman formula does, only slightly over-estimating the dielectric con-
 409 stant at low depth (lower than 20 meters), i.e. in the lower range of densities.
 410 The statistical analysis allows to visualize the expected variability of the average
 411 dielectric constant due to the micro-state variability. The variance of the ex-
 412 perimental data at a given depth is very similar, although some outliers appear
 413 as a consequence of the local variation of density at the close-off depths.

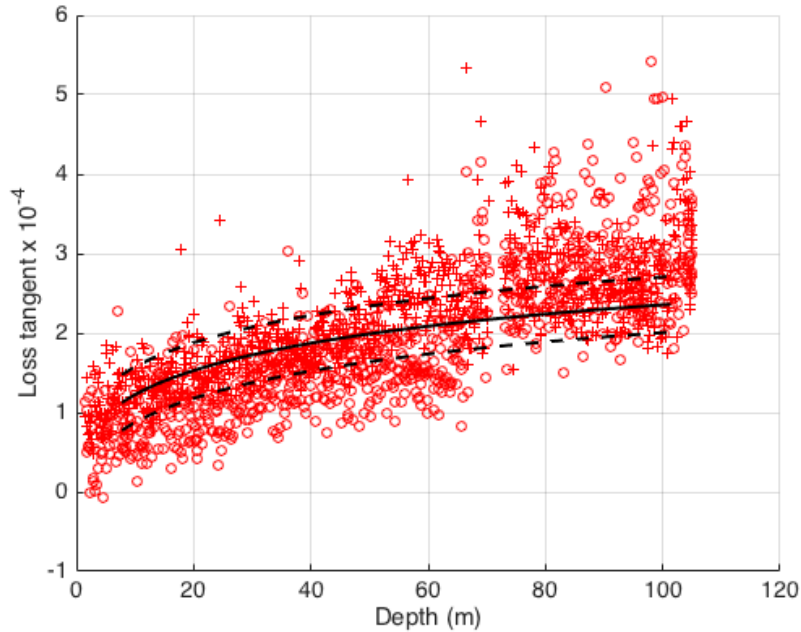


Figure 13: Loss tangent versus depth: comparison between the experimental data at 880 MHz (red circles) and at 1.15GHz (red crosses) and the results of the full-wave numerical model at 1 GHz

414 6 Conclusions

415 In this study detailed measurements of firm dielectric properties were performed
 416 through the collection of firm cores down to 106 meters, by using a resonator.
 417 Detailed measurements of the real and imaginary dielectric permittivity were
 418 performed on the ice cores providing an extended dataset of dielectric properties
 419 with depth. Density was also measured for the same samples. The experimental
 420 results confirmed the dependence of the real part with depth and density. In-
 421 creasing depth and density corresponds to an increase in the real permittivity.

422 A power–law equation was derived to fit the data. The imaginary part also
423 increases with depth but it does not follow the same clear trend, its dependence
424 on frequency appears rather complex, probably due to the presence of salts or
425 impurities.

426 The analysis of the experimental data was performed by first implement-
427 ing 3D and 2D full wave numerical models, by generating random ensembles of
428 inclusions , to simulate a mixture of firn crystals at prescribed densities, corre-
429 sponding to the measured densities on the ice cores. The numerical analysis of
430 the ensemble of inclusions showed that the common symmetric functions used for
431 ice dielectric properties do not agree with the results of the simulation and with
432 the measured data. These results show that a host of ice crystals into air signif-
433 icantly differs from a host of air bubbles into ice, and therefore non–symmetric
434 formulations should be used. A single non–symmetric formulation is not suf-
435 ficient to continuously represent the whole density range. Moreover, analytical
436 formulae are unable to account for the effect of randomness, size/shape hetero-
437 geneity, particle packing on the average firn permittivity.

438 To solve this problems a dielectric model was developed, allowing for quan-
439 tification of the dependence of the dielectric properties on density. The model
440 was developed by combining two models: one of firn crystals into an air host,
441 and air inclusions into an ice host. The weighted equation is based on the vol-
442 ume fraction (density). The result is a mixture smoothly changing from firn
443 particles in air (low density) to air bubbles in an ice matrix (high density).
444 The implementation of such a mixture model by means of a numerical model

445 allowed to investigate the dependence of complex permittivity at all densities
446 in the range 350–840 kg m⁻³, on the average firn characteristics, e.g. crystal
447 area, shape and orientation, and on the average crystal arrangement. For this
448 purpose, a statistical analysis has been conducted showing how the variability
449 of the micro–states affects the average permittivity. The permittivity change
450 due to micro–state variability appears to be at least two–three times that due
451 to the measured variability of density at a given depth, therefore concluding
452 that firn structure has a significant effect on the dielectric properties.

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Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: