Elastic wave propagation in anisotropic polycrystals
inferring physical properties of glacier ice
Rathmann, Nicholas M. M.; Grinsted, Aslak; Mosegaard, Klaus; Lilien, David A. A.; Westhoff, Julien; Hvidberg, Christine S. S.; Prior, David J. J.; Lutz, Franz; Thomas, Rilee E. E.; Dahl-Jensen, Dorthe

Published in:
Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences

DOI:
10.1098/rspa.2022.0574

Publication date:
2022

Document version
Publisher's PDF, also known as Version of record

Document license:
CC BY

Citation for published version (APA):
Elastic wave propagation in anisotropic polycrystals: inferring physical properties of glacier ice

Nicholas M. Rathmann¹, Aslak Grinsted¹, Klaus Mosegaard¹, David A. Lilien², Julien Westhoff¹, Christine S. Hvidberg¹, David J. Prior³, Franz Lutz³, Rilee E. Thomas³ and Dorthe Dahl-Jensen¹,²

¹Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark
²Centre for Earth Observation Science, University of Manitoba, Winnipeg, Canada
³Department of Geology, University of Otago, Dunedin, New Zealand

An optimization problem is proposed for inferring physical properties of polycrystals given ultrasonic (elastic) wave velocity measurements, made across multiple sample orientations. The feasibility of the method is demonstrated by inferring both the effective grain elastic parameters and the grain c-axis orientation distribution function (ODF) of ice-core samples from Priestley glacier, Antarctica. The method relies on expanding the ODF in terms of a spherical harmonic series, which allows for a non-parametric estimation of the sample ODF. Moreover, any linear combination of the Voigt (strain) and Reuss (stress) homogenization scheme is allowed, although for glacier ice, the exact choice is found to matter little for bulk elastic behaviour, and thus for inferred physical properties, too. Finally, the accuracy of the inferred grain elastic parameters is discussed, including the well-posedness and shortcomings of the inverse problem, relevant for future adoptions in glaciology, geology and elsewhere.

© 2022 The Authors. Published by the Royal Society under the terms of the Creative Commons Attribution License http://creativecommons.org/licenses/by/4.0/, which permits unrestricted use, provided the original author and source are credited.
1. Introduction

Polycrystalline materials consist of numerous individual grains of different size, shape and crystallographic orientation. Many naturally occurring inorganic materials, as well as manufactured materials, are polycrystalline, including glacial ice, minerals, metals and ceramics. Being able to non-destructively evaluate the internal structure of polycrystals is of great interest in disciplines such as glaciology, geology and seismology, where material samples are often not directly accessible (e.g. the mineral aggregate of Earth’s upper mantle) or sparse and valuable (e.g. glacier ice samples recovered from deep ice cores).

Of particular interest is the ability to infer the crystal orientation fabric (henceforth fabric), understood as the distribution of grain orientations, needed to determine the bulk viscous [1,2] and elastic [3,4] anisotropy of glacier ice and olivine (the most abundant upper-mantle mineral). Monocrystals (isolated grains) of ice are often approximated as viscously [5] and elastically [6] transversely isotropic with a symmetry axis that coincides with the crystal optical c-axis (figure 1a). Likewise, olivine monocrystals are viscously [7] and elastically [8] anisotropic, although with a different crystal symmetry. Thus, as the fabric evolves during flow in polycrystalline glacier ice, or in the mineral aggregate of the upper mantle, so should the bulk directional viscosity and elasticity structure, relevant for understanding glacier ice flows [9–12], seismic wave propagation ([13], and references therein) and the coupling between plate motions and the sublithospheric mantle (e.g. [3,14]). Furthermore, in the case where fabric evolution is dominated by the strain-induced rotation of grain orientations (that is, crystal recrystallization processes are slow), grain orientations can provide a unique record of past and present deformation in glaciers and ice sheets [12,15–19], and in the lithosphere and sublithospheric mantle [20].

In this work, we revisit the method of using elastic wave propagation as a way to infer physical properties of polycrystals; specifically, as a way to infer the c-axis orientation distribution function (henceforth ODF; figure 1b,c) and the effective grain elastic parameters of glacier ice. Over the last decade (but not limited thereto), this method has received a lot of attention in the glaciological literature, involving sonic logging of ice-core boreholes [21,22], and seismic surveys conducted over ice sheets using active [17,23–30] and passive (earth and ice quakes) [31–36] wave sources. These studies rely on the fact that P- and S-wave travel times are affected by fabric anisotropy, including the splitting of S-waves (acoustic birefringence) into fast and slow quasi-S waves (elaborated on below).

Also investigated extensively is the possibility of non-destructively inferring the c-axis ODF of ice-core samples by measuring ultrasonic P- and S-wave velocities (or phase velocities) through the samples at multiple orientations (figure 2) [37–43], a problem also of great interest in the broader material sciences community (see e.g. [44], and references therein). Recently, Hellmann et al. [38] found that for sufficiently small ice grains, measured P-wave velocities agree well with modelled velocities. Using a similar experimental setup, but additionally considering the propagation of S-waves, Lutz et al. [37] constructed an optimization problem and demonstrated that c-axis ODFs of ice-core samples, drilled in the shear margin of Priestley glacier, Antarctica, could indeed be inferred.

The approach by Lutz et al. [37] relies on minimizing the misfit between modelled and observed phase velocities by parametrizing the ODF as a horizontal single-maximum cluster of c-axes, similar to shear margin fabrics found elsewhere [45–48], and similar to other forward-model problems [4,17,49,50]. However, a priori constraining the fabric anisotropy to be of a predetermined type, while useful, does not provide a general method for inferring truly unknown ODFs. Even if the most common fabric types found in polar ice masses [51,52] were successfully parameterized, it is not immediately clear how to account for the broader class of fabrics where recrystallization has taken place (e.g. causing multiple preferred c-axis directions).

Here, we extend the methodology of Gusmeroli et al. [21] and Lutz et al. [37] by reformulating the optimization (inverse) problem such that no particular fabric anisotropy is presupposed, made possible by expanding the c-axis ODF in terms of a spherical harmonic series, inspired
Figure 1. (a) Monocrystal lattice composed of hexagonal cells with the crystal c-axis orthogonal to the basal plane (grey plane). Monocrystals are modelled as isotropic in the basal plane (transversely isotropic), characterized by the directional enhancements of the first Lamé coefficient ($\hat{\lambda}$), S-wave modulus ($\hat{\mu}$) and P-wave modulus ($\hat{\gamma}$). (b) Polycrystals are modelled as an ensemble of interactionless grains. (c) Example of a single-maximum c-axis orientation distribution function ($\psi / N$) and its principal directions ($m_i$). (Online version in colour.)

Figure 2. Schematic cross-section of the ultrasonic P- and S-wave experiments conducted on ice-core samples by Lutz et al. [37] and Hellmann et al. [38]. Grid lines show the displacement of material lines as P- or S-waves propagate through the sample (exaggerated). Vectors $\hat{k}$ and $\hat{p}$ denote the direction of wave propagation and wave polarization, respectively. The coordinate system defined here is identical to that used below. (Online version in colour.)

by the broader material sciences community (e.g. [44,50,53–55]). Using this representation, we demonstrate how either the ODF can be inferred if the effective elastic parameters of grains are known or vice-versa, followed by discussing the well-posedness of the inverse problem, relevant for future applications in glaciology, geology and elsewhere. We begin, however, by first introducing the general problem of elastic wave propagation in anisotropic polycrystals.

2. Background

(a) Bulk elastic constitutive equation

The Cauchy–Navier equation

$$\rho \frac{\partial^2 u}{\partial t^2} = \nabla \cdot \sigma$$  (2.1)
calculating the bulk, grain-ensemble-averaged stress tensor subject to simple stress or strain homogenizing stress field (Reuss's hypothesis) over the polycrystal scale (figure 1). Grains (monocrystals) subject to either a homogeneous strain field (Voigt's hypothesis) or Voigt's hypothesis assumes

\[ \sigma' = \lambda \text{tr}(\epsilon')I + 2\mu \epsilon' - \lambda(1 - \lambda)(\epsilon' : c^2)I + \text{tr}(\epsilon')c^2 \]

where \( \sigma' \) and \( \epsilon' \) are the microscopic stress and strain tensors, respectively. The anticommutator is defined as \( \{ A, B \} = A \cdot B + B \cdot A \) for arbitrary tensors \( A \) and \( B \), : is the double inner product, \( c' \) is the \( r \)th repeated outer product of \( c \) with itself, and \( I \) is the identity.

The elastic parameters \( \lambda, \mu \) and \( \gamma = \lambda + 2\mu \) are the usual isotropic first Lamé coefficient, isotropic S-wave modulus and isotropic P-wave modulus. The remaining elastic parameters \( \hat{\lambda}, \hat{\mu} \) and \( \hat{\gamma} \), are the corresponding anisotropic enhancements along \( c \) and \( a \perp c \) (figure 1a) in the sense that the stiffness matrix is

\[
C = \begin{bmatrix}
\gamma & \lambda & \hat{\lambda} & 0 & 0 & 0 \\
\lambda & \gamma & \hat{\lambda} & 0 & 0 & 0 \\
\hat{\lambda} & \hat{\lambda} & \gamma & 0 & 0 & 0 \\
0 & 0 & 0 & \hat{\mu} \mu & 0 & 0 \\
0 & 0 & 0 & 0 & \hat{\mu} \mu & 0 \\
0 & 0 & 0 & 0 & 0 & \mu
\end{bmatrix}
\]

Note that equations (2.2) and (2.3) reduce to the constitutive equation of an isotropic elastic material for \( \hat{\lambda}, \hat{\mu}, \hat{\gamma} = 1 \).

Although the stiffness matrix (2.3) is the starting point for many glaciological applications (e.g., [4, 21, 28, 37, 38, 49, 58, 59]), the coordinate-independent form (2.2) is advantageous when calculating the bulk, grain-ensemble-averaged stress tensor subject to simple stress or strain homogenization assumptions. In this paper, we follow previous work by considering the simplest homogenization schemes [3] where polycrystals are regarded as an ensemble of interactionless grains (monocrystals) subject to either a homogeneous strain field (Voigt’s hypothesis) or homogeneous stress field (Reuss’s hypothesis) over the polycrystal scale (figure 1b). That is, Voigt’s hypothesis assumes \( \epsilon' = \epsilon \), and Reuss’s hypothesis assumes \( \sigma' = \sigma \).

The bulk stress tensor when subject to Voigt’s hypothesis, \( \sigma_{\text{Voigt}} \), is, therefore, given by the grain-averaged stress tensor, \( \sigma_{\text{Voigt}} = \langle \sigma' \rangle \), yielding

\[
\sigma_{\text{Voigt}} = \lambda \text{tr}(\epsilon)I + 2\mu \epsilon - \lambda(1 - \hat{\lambda})(\epsilon : (c^2))I + \text{tr}(\epsilon)(c^2)
+ [(1 + \hat{\gamma})\gamma - 2(\hat{\lambda} + 2\hat{\mu})]\epsilon : (c^4) - 2\mu(1 - \hat{\mu})\epsilon : (c^2),
\]

(2.4)

where \( \langle c' \rangle \) is the \( r \)th-order structure tensor (moment) of the c-axis distribution function \( \psi \):

\[
\langle c' \rangle = \frac{1}{N} \int_{\Omega} c' \psi \; d\Omega.
\]

(2.5)

Here, \( d\Omega = \sin(\theta) \; d\theta \; d\phi \) is the infinitesimal solid angle, and \( N = \int_{\Omega} \psi \; d\Omega \) is the total number of grains. Note that, in effect, the bulk stress tensor (2.4) depends only on the lowest \( (r = 2) \) and second-lowest \( (r = 4) \) even moments of \( \psi \), and that equal-sized grains are assumed by virtue of (2.5) (assumption revisited in the Discussion).

The bulk stress tensor when subject to Reuss’s hypothesis, \( \sigma_{\text{Reuss}} \), requires vectorizing the inverse relationship of (2.2) and is less straightforward to determine. For the sake of brevity, we refer the reader to appendix A for details.

The difference between bulk elastic moduli calculated using Voigt’s hypothesis compared to Reuss’s hypothesis has previously been estimated not to exceed 4.2% for glacier ice [60].
Although this suggests that either homogenization might be used for glacier ice, we shall consider both homogenization schemes in the following. We furthermore also consider the so-called Hill-average [61], defined as the linear combination

\[ \sigma = (1 - \alpha)\sigma_{\text{Reuss}} + \alpha\sigma_{\text{Voigt}}, \]  

(2.6)

for \( \alpha = 1/2 \), which often reproduces experimental estimates well [3,61].

(b) Fabric representation

Following previous work (e.g. [44,50,53–55,62,63]), we expand \( \psi \) in terms of a spherical harmonic series

\[ \psi(\theta, \phi) = \sum_{l=0}^{L} \sum_{m=-l}^{l} \psi_{lm} Y_{lm}(\theta, \phi), \]  

(2.7)

where \( \psi_{lm} \) are the complex expansion coefficients, and \( L \) is the wave-mode truncation above which finer-scale structure in \( \psi \) is unresolved. In this case, the total number of grains is simply \( N = \sqrt{4\pi \psi_{0}^0} \), and \( \psi \) being real implies that \( \psi_{lm}^* = (-1)^m \psi_{lm}^{*} \). The ODF is by definition the normalized distribution of \( c \)-axis orientations

\[ \text{ODF} = \frac{\psi}{N}, \]  

(2.8)

which depends on the normalized coefficients \( \hat{\psi}_{lm} = \psi_{lm}/\psi_{0}^0 \).

Given the harmonic expansion (2.7), \( \langle c^2 \rangle \) is exactly [64]

\[ \langle c^2 \rangle = \frac{1}{3} I + \sqrt{\frac{2}{15}} \begin{bmatrix} \text{Re}[\hat{\psi}_2^0] - \frac{1}{2\sqrt{3}} \hat{\psi}_2^0 & \text{Re}[\hat{\psi}_1^0] \\ \text{Im}[\hat{\psi}_2^0] & \text{Re}[\hat{\psi}_1^0] - \frac{1}{2\sqrt{3}} \hat{\psi}_2^0 \\ -\text{Re}[\hat{\psi}_2^0] & \text{Im}[\hat{\psi}_1^0] \end{bmatrix}_{\text{sym.}}. \]  

(2.9)

The entries of \( \langle c^4 \rangle \) are likewise given by linear combinations of \( \hat{\psi}_{2}^m \), but additionally depend on the higher-order expansion coefficients \( \hat{\psi}_{4}^m \) (see appendix B).

Although ODFs may in general include yet higher wavenumber components \( \hat{\psi}_{l}^m \neq 0 \) for \( l > 4 \) when small-scale structure is present (e.g. strong \( c \)-axis clustering), the homogenized elastic problem depends only on \( \langle c^2 \rangle \) and \( \langle c^4 \rangle \), and hence only on the lowest \( (l = 2) \) and second-lowest \( (l = 4) \) wavenumber components. That is, the homogenized elastic problem depends exclusively on the harmonic ODF components shown in figure 3, which may be arbitrarily scaled or rotated in the horizontal plane depending on the magnitude and phase of \( \hat{\psi}_{l}^m \).

(c) Plane wave propagation

We consider the usual monochromatic plane wave solutions to equation (2.1),

\[ \mathbf{u} = p \exp[i(kx - \omega t)], \]  

(2.10)

where \( k = k\hat{k} \) is the wavevector with magnitude \( k \), \( p \) is the polarization vector including the wave amplitude, \( \omega \) is the angular frequency of the wave and \( x \) is the position vector. It follows that equation (2.1), combined with (2.6), can be written as the eigenvalue problem

\[ \hat{Q} \cdot \mathbf{u} = \rho \left( \frac{\omega}{k} \right)^2 \mathbf{u}, \]  

(2.11)

where \( \hat{Q} \) is the normalized acoustic tensor

\[ \hat{Q} = (1 - \alpha)\hat{Q}_{\text{Reuss}} + \alpha\hat{Q}_{\text{Voigt}}, \]  

(2.12)
Figure 3. Harmonic components of the $c$-axis ODF that the structure tensors $\langle c^2 \rangle$ and $\langle c^4 \rangle$ depend on. The components may be arbitrarily scaled or rotated in the horizontal plane depending on the real and imaginary parts of the ODF expansion coefficients, $\hat{\psi}_m$, here shown for values of 1. (Online version in colour.)

and $V = \omega/k$ is the phase velocity of the wave. The Voigt contribution follows immediately from calculating $\nabla \cdot \sigma_{\text{Voigt}}$ using equation (2.4), giving

$$
\hat{Q}_{\text{Voigt}} = \mu I + (\mu + \nu) \hat{k}^2 - \lambda (1 - \hat{\lambda}) (\hat{k}^2, \langle c^2 \rangle) + [(1 + \gamma) - 2 (\hat{\lambda} + 2 \hat{\mu})] \langle c^4 \rangle : \hat{k}^2
$$

$$
- \mu (1 - \hat{\mu}) \left( \langle c^2 \rangle + (\langle c^2 \rangle : \hat{k}^2) I + [\hat{k}^2, \langle c^2 \rangle] \right).$$

The Reuss contribution, $\hat{Q}_{\text{Reuss}}$, is introduced in appendix A.

Nontrivial solutions to equation (2.11) require the determinant of $k^2 \hat{Q} - \rho \omega^2 I$ to vanish (Christoffel equation), yielding a polynomial equation of degree six in $k$. The six solutions generally consist of three forward propagating waves and three reversely propagating waves; specifically a quasi-P wave (qP) and two quasi-S waves (qS1 and qS2) in both the forward and reverse direction (quasi in the usual sense that $p \parallel k$ or $p \perp k$ cannot be assumed in anisotropic media for P and S waves, respectively). The waves qS1 and qS2 are henceforth assumed sorted such that they refer to the fast and slow quasi-S wave, respectively.

In the special case that $k$ is aligned with one of the coordinate axes, the problem reduces to that of finding the roots of a depressed cubic equation that can be solved analytically (not shown for brevity; see e.g. [59]). Without loss of generality, we take advantage of this by setting $\hat{k} = \hat{z}$ above and instead rotate the ODF accordingly. The rotation is that which sends $k$ to $\hat{z}$, made possible with Wigner’s $D$ matrix, in which case the rotated expansion coefficients are

$$
\hat{\psi}_m = \sum_{n=-l}^{l} (D_{mn}^l)^* \hat{\psi}_n. 
$$

While the ODF’s final azimuthal orientation will vary depending on the path taken when rotating $\hat{k}$ into $\hat{z}$ ($S^2$ is a curved space), this affects only the directions of the wave eigenpolarizations and not the phase velocities which are unambiguously defined.
3. Inferring physical properties

The physical properties of polycrystals may refer to different characteristics depending on the problem of interest. In the context of elastic wave propagation, we shall take it to mean (i) the effective grain elastic parameters
\[ \mathbf{g} = [\lambda, \mu, \hat{\lambda}, \hat{\mu}, \hat{\gamma}] \]
that reproduce observed phase velocities for a given homogenization scheme (\( \alpha \)) and ODF, and (ii) the expansion coefficients of the ODF
\[ \hat{\psi} = [\hat{\psi}_0^0, \hat{\psi}_1^0, \hat{\psi}_2^0, \hat{\psi}_3^0, \hat{\psi}_0^2, \hat{\psi}_1^2, \hat{\psi}_2^2, \hat{\psi}_3^2, \hat{\psi}_4^2] \]
that determine the fabric-induced acoustic anisotropy.

We are, therefore, interested in whether \( \mathbf{g} \) and \( \hat{\psi} \) can, for a given polycrystal, be inferred from elastic phase-velocity measurements made in the laboratory (figure 2). For this purpose, we propose solving an optimization problem that minimizes the modelled phase-velocity misfit with observations. Specifically, we consider minimizing the cost function
\[ J(\mathbf{g}, \hat{\psi}) = \sum_i \sum_{n=1}^N \beta_i (V_i(\theta_n, \phi_n; \mathbf{g}, \hat{\psi}) - V_{i,\text{obs}}(\theta_n, \phi_n))^2, \]
with respect to \( \mathbf{g} \) or \( \hat{\psi} \), given \( n = 1, \ldots, N \) measurements of the phase velocities \( V_i = \{V_{qP}, V_{qS1}, V_{qS2}\} \) at sample orientations prescribed in terms of the co-latitude and azimuth, \( \theta_n \) and \( \phi_n \). Here, the three phase-velocity misfits are taken to be equally weighted, \( \beta_{qP} = \beta_{qS1} = \beta_{qS2} \), but need not necessarily be so. Ideally, the three misfits should be weighted according to their noise/uncertainty. If the noise standard deviation is \( s \) for (say) measurements of \( V_{qP} \), the corresponding weight should be \( \beta_{qP} = 1/s^2 \). In this way, a correct weighting between certain and uncertain data are guaranteed. If, however, the uncertainties are of the same magnitude, weighting is unnecessary.

To test the methodology, we considered three ice-core samples, taken from shear margin of Priestley glacier, Antarctica, for which Thomas et al. [48] measured the c-axis distributions using electron back scatter diffraction, and Lutz et al. [37] measured the angular dependencies in ultrasonic phase velocities. Following Thomas et al. [48], the three samples are henceforth labelled as ‘003’, ‘007’ and ‘010’. All three samples consist of a strong c-axis cluster (single maximum) in the horizontal \( \hat{x}–\hat{y} \) plane that is sub-perpendicular to the direction of flow, \( \hat{y} \). Figure 4a–c shows the measured c-axes (green dots) and corresponding ODFs truncated at \( L = 4 \) (grey contours), the latter determined by solving the linear problem involving \( (c^4) \) and \( \hat{\psi}_m^4 \) (equation (B1)).

For all three samples, ultrasonic phase-velocity measurements were made at \( \theta = 90^\circ \) with azimuthal increments of \( \Delta\phi = 10^\circ \) (i.e. the horizontal \( \hat{x}–\hat{y} \) plane in figures 2 and 4a–c). We refer
demonstrates this, showing that taking temperature dependencies, inclusions and more (elaborated on in the Discussion). Figure 5 demonstrates this, showing that taking

\( a = 1/2 \) with the monocrystal parameters reported by

Bennett [39] (henceforth ‘B68’)

\[
\mathbf{g}_{\text{B68}} = [7.15 \text{ GPa}, 3.455 \text{ GPa}, 0.822, 0.886, 1.084],
\]

(3.4)

combined with the measured ODF of sample 007 (i.e. \( \hat{\psi} = \hat{\psi}_{\text{obs}} \)), does not result in predicted phase velocities (dashed blue lines) that match observed velocities (black dots; error bars denote measurement uncertainties).

Since the misfit is largely an offset in mean qP and qS velocities across the sample orientation, \( \phi \), one might suspect that adjusting the isotropic grain parameters \( \lambda \) and \( \mu \) (and hence \( \gamma \)) is sufficient to reduce the misfit. However, even for isotropic fabrics (\( \psi_i^m = 0 \) for \( l > 0 \)) without angular dependencies, the phase velocities depend on all five elastic parameters (not shown). It is, therefore, not exactly clear whether (or how) the anisotropic enhancements (\( \hat{\lambda}, \hat{\mu}, \hat{\gamma} \)) are to be adjusted to reduce the misfit.

Instead, we follow Gusmeroli et al. [21] by seeking to independently infer the optimal effective elastic parameters, \( \mathbf{g}_{\text{opt}} \), such that observed phase velocities (\( V_{i,\text{obs}} \)) are reproduced given the ODF of each sample observed by Thomas et al. [48]. Figure 6 shows the optimal elastic parameters inferred for each ice-core sample (triangles), and for each homogenization scheme (\( \alpha = 0, 1, 1/2 \)), determined by minimizing \( J \) following a Newton conjugate gradient descent using SciPy [72] with \( \nabla J \) evaluated numerically and a initial guess of \( \mathbf{g} = \mathbf{g}_{\text{B68}} \) but taking \( \hat{\lambda} = \hat{\mu} = \hat{\gamma} = 1 \) (elastically isotropic grains). The minimization of \( J \) was stopped once modelled qP velocities were approximately within the experimental uncertainty bounds, but we note that further descending \( J \) did not lead to much different results (i.e. over fitting was not an issue, at least for the fabrics considered here). While the isotropic parameters (\( \lambda, \mu, \gamma \)) are indeed found to take smaller values compared to the initial B68 guess (figure 6a–c), consistent with reducing the mean velocities across \( \phi \), the anisotropic enhancements (\( \hat{\lambda}, \hat{\mu}, \hat{\gamma} \)) are found to agree relatively well with B68 and other estimates (figure 6d–f). For reference, the solid blue line in figure 5a–c shows the resulting, predicted phase velocities for sample 007 given the inferred (best-fit) elastic parameters, \( \mathbf{g}_{\text{opt}} \), with \( \alpha = 1/2 \) (other \( \alpha \) lead to similar results).

**Orientation fabric**

Given the B68 monocrystal parameters, Lutz et al. [37] showed that the ODF of samples 003, 007 and 010, can be inferred by minimizing the misfit between modelled and observed phase velocities, methodically similar to minimizing \( J \) above. Specifically, Lutz et al. [37] assumed a horizontal single-maximum fabric, parameterized in terms of its strength (cluster cone angle) and azimuthal orientation (two unknowns in total). This is different from our non-parametric representation of \( \psi \) which makes no a priori assumption about the fabric pattern. However, inferring all expansion coefficients, \( \hat{\psi}_l^m \) for \( l \leq 4 \), implies inferring a total of 14 unknowns (two real numbers and six complex numbers). Whether this constitutes a well-posed problem, in the usual sense that the best-fit ODF is unique and physically consistent, is not exactly clear.

At minimum, a physically consistent solution requires the eigenvalues of \( \langle c^2 \rangle \) and \( \langle c^4 \rangle \) to be strictly positive (the c-axis density function is strictly positive). Assuming the usual ordering \( a_1 \leq a_2 \leq a_3 \) and \( \hat{a}_1 \leq \hat{a}_2 \leq \hat{a}_3 \leq \hat{a}_4 \leq \hat{a}_5 \leq \hat{a}_6 \) for the eigenvalues of \( \langle c^2 \rangle \) and \( \langle c^4 \rangle \), respectively, it suffices
to require that $a_1 \geq 0$ and $\tilde{a}_1 \geq 0$. We include these constraints in the inverse problem by setting $J \rightarrow J + J_s$, where

$$J_s = -\eta(a_1 - s^2) - \tilde{\eta}(\tilde{a}_1 - \tilde{s}^2),$$

introduces two slack variables, $s$ and $\tilde{s}$ (two additional unknowns), that allow converting the inequality constraints into equality constraints. Here, $\eta$ and $\tilde{\eta}$ are Lagrange multipliers that must take values sufficiently large as to avoid $a_1 < 0$ and $\tilde{a}_1 < 0$ (evaluated a posteriori; see Discussion).

We find it surprisingly uncomplicated to infer all three sample ODFs by descending $J$ with an isotropic fabric as initial guess, resulting in ODFs in good agreement with the observed ODFs.
Figure 6. Monocrystal elastic parameters reported in the literature as a function of temperature (circles and lines), and optimal (best-fit) parameters inferred from the three ice-core samples (triangles). Uncertainties are denoted by error bars and shaded areas. (Online version in colour.)

We inferred all 14 degrees of freedom (i.e. both \( \langle c^2 \rangle \) and \( \langle c^4 \rangle \)) for each homogenization scheme (\( \alpha = 0, 1, 1/2 \)) given both B68 parameters (\( g_{\text{B68}} \)) and our optimal set (\( g_{\text{opt}} \)). Figure 5e,f shows the inferred ODFs of sample 007 for the Hill-average (\( \alpha = 1/2 \)) given \( g_{\text{B68}} \) and \( g_{\text{opt}} \), respectively. Because little difference is found among the three homogenization schemes, only results for the Hill-average are shown. For comparison, figure 5d shows the observed ODF (identical to figure 4b). The corresponding modelled phase velocities are shown in figure 5a–c as red lines.

Due to the above-mentioned discrepancy found between modelled and observed angular-mean velocities when using the B68 parameters, Lutz et al. [37] proposed replacing the absolute velocities \( V_i \) with the angular anomalies (i.e. subtracting the mean velocity)

\[
\delta V_i(\phi_n) = V_i(\phi_n) - \frac{1}{N} \sum_{n=1}^{N} V_i(\phi_n),
\]

when determining the best-fit ODF. For consistency with Lutz et al. [37], and for a robust gradient descent of \( J \) given \( g_{\text{B68}} \), we too, therefore, replaced \( V_i \) with \( \delta V_i \) in equation (3.3) when inferring \( \hat{\psi} \) given \( g_{\text{B68}} \).
4. Discussion

(a) Inferred elastic parameters

Our inferred optimal grain elastic parameters \( g_{\text{opt}} \) are found to generally fall within the range of previous experimental estimates for monocrystals (figure 6). Since the inferred parameters are to be understood as the best-fit parameters given possible shortcomings of the forward model, the fact that values agree with experimental estimates suggests relatively accurate model physics. Indeed, consistent with previous work, we find that the choice of homogenization scheme \( \alpha \) matters little for the bulk elastic behaviour; Nanthikesan & Shyam Sunder [60] found that choosing \( \alpha = 0 \) over \( \alpha = 1 \) makes a difference of 4.2% in bulk elastic parameters for glacier ice. Among the three relatively strong single-maximum fabrics considered here, the inferred parameters varied at most per sample for different \( \alpha \) by \( \delta \lambda = 1.6\%, \delta \mu = 0.2\%, \delta \delta = 4.7\%, \delta \hat{\mu} = 2.2\%, \delta \hat{\nu} = 2.0\% \).

Important factors known to affect bulk elastic behaviour, but not accounted for here, include temperature [6,66–68,73], porosity (e.g. air bubble inclusions) [38], static pressure (not relevant here; values in figure 6 are for an atmospheric reference pressure) [74], grain sizes [38,75,76] and the influence of grain boundary sliding/stiffness [77–79]. Accounting for these effects might, therefore, further (i) reduce the spread in inferred parameters between the three samples and (ii) reduce discrepancies with experimental estimates in the literature.

Neglecting grain sizes and shapes might have influenced our inferred elastic parameters in at least two ways: (i) Elvin [77] found that grain shapes are more important when grain boundary sliding is active, compared to the elastic anisotropy of grains (on the homogenized properties) when grain boundary sliding is prohibited and (ii) Hellmann et al. [38] showed how calculated phase velocities cannot be expected to match measured ultrasonic phase velocities unless samples contain a large ensemble of small grains relative to the pulse wavelength (i.e. phase-velocity dispersion due to grain scattering is negligible). The source signal pulse used to generate our velocity dataset [37] had a dominant frequency of 1 MHz, resulting in a dominant wavelength of approximately 3.8 mm in the three samples. With an average grain size among the samples of approximately 1 mm [48], the effect of grain scattering on measured phase velocities cannot be entirely neglected. Although modelling the effect of grain boundary sliding (e.g. [78]) is out of the scope of this work, we tested the influence of grain sizes by re-inferred \( g_{\text{opt}} \) upon replacing each sample ODF with its grain-size-weighted equivalent. While sophisticated methods exist for deriving the volume of a single grain from its cross-sectional area (e.g. [80]), we take a much simpler approach by approximating the grain volume fraction (the ideal grain weight) by the measured grain cross-sectional area fraction. Table 1 shows the resulting relative changes in \( g_{\text{opt}} \) compared to figure 6. We find, overall, rather small changes, suggesting that neglecting grain sizes is neither able to explain the parameter differences found between the three samples, nor to explain discrepancies with existing estimates in the literature (insofar as grains are, on average, small enough that grain scattering is negligible).

Since all three samples were subject to identical temperatures in the laboratory \( T = −23^\circ\text{C} \), we are left to speculate that differences in inferred parameters between the three samples might, in part, be due to uncertainties in measured phase velocities, and might, in part, be due to observed anisotropies in preferred bubble shapes or aligned cracks in the samples [37,48].

The discrepancies found between our inferred parameters (especially \( \lambda, \mu, \nu \) and existing experimental estimates could, on the other hand, be the result of temperature dependencies. The temperature dependency of \( g \) for a monocrystal (as reported in the literature; figure 6) is likely to be different from that of \( g_{\text{opt}} \) for a polycrystal: Vaughan et al. [73] and Sayers [78] argued that observed decreases in bulk stiffnesses \( C_{11} = \nu \) and \( C_{66} = \mu \) (and hence \( \lambda \)) with increasing temperature are caused by a decrease in grain boundary stiffness due to liquid phases developing on grain boundaries associated with pre-melting conditions. Indeed, Sayers [35] and Llorens et al. [79] have recently argued that the observed decrease in S-wave velocity found to occur near the base of ice sheets [31] might be explained [32] by a film of liquid water forming along
repeating experiments such as those conducted by Lutz making it an under-determined problem to extract the individual elastic parameters from such both fabric and all five elastic parameters (at least under Voigt and Reuss homogenizations),

Some estimates indicate liquid phases can exist on grain boundaries at temperatures as low as

\[ \eta \approx 2000; \]

(see Text S5) for pre-melting conditions (note that estimates by Bass et al. [68] and Green & Mackinnon [69] have relatively large uncertainties).

Although several studies have also investigated how P- and S-wave velocities depend on temperature for polycrystalline ice [74,81,82], measured P- and S-wave velocities depend on both fabric and all five elastic parameters (at least under Voigt and Reuss homogenizations), making it an under-determined problem to extract the individual elastic parameters from such measurements.

To further explore how temperature influences the effective elastic parameters, we propose repeating experiments such as those conducted by Lutz et al. [37] but for a larger range of laboratory temperatures, combined with our inversion scheme for inferring \( g_{\text{opt}} \). To that end, adopting the methodology by Sayers [35] might be useful, whereby the effect of water at grain boundaries is represented by an additional (superimposed) grain boundary shear compliance, the strength of which (as a function of temperature) would also constitute an unknown.

(b) Inferred orientation fabrics

The accuracy of our inferred ODFs (goodness of fit) can be quantified in more detail by calculating the eigenvalues of \( \langle c^2 \rangle \) and \( \langle c^4 \rangle \). Table 2 shows the \( \langle c^2 \rangle \) eigenvalues \((a_1,a_2,a_3)\) and smallest \( \langle c^4 \rangle \) eigenvalue \((\tilde{a}_1)\) for both observed and inferred ODFs, suggesting, overall, that our method can reasonably infer the strength of the principal fabric direction, \( a_3 \).

The inequality constraints were fulfilled across all inversions by selecting \( \eta = 0 \) and \( \tilde{\eta} \approx 2000; \) that is, we found no need to impose \( a_1 \geq 0 \) if \( \tilde{a}_1 \geq 0 \) was constrained. While this suggests that it suffices to constrain \( \tilde{a}_1 \geq 0 \) in future adoptions, we emphasize that the constraints must always

Table 1. Change in inferred elastic parameters (compared to figure 6) if ODFs are constructed by weighing each grain c-axis by its grain-area fraction.

<table>
<thead>
<tr>
<th>source</th>
<th>( \delta \lambda ) (%)</th>
<th>( \delta \mu ) (%)</th>
<th>( \delta \lambda' ) (%)</th>
<th>( \delta \lambda'' ) (%)</th>
<th>( \delta \lambda''' ) (%)</th>
<th>( \delta \lambda'''' ) (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>sample 003</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \alpha = 0 )</td>
<td>-0.2</td>
<td>-0.2</td>
<td>-0.2</td>
<td>-0.2</td>
<td>-0.2</td>
<td>-0.2</td>
</tr>
<tr>
<td>( \alpha = 1 )</td>
<td>-0.0</td>
<td>-0.0</td>
<td>-0.2</td>
<td>-0.0</td>
<td>-0.0</td>
<td>-0.0</td>
</tr>
<tr>
<td>( \alpha = 1/2 )</td>
<td>-0.1</td>
<td>-0.1</td>
<td>-0.2</td>
<td>-0.1</td>
<td>-0.1</td>
<td>-0.1</td>
</tr>
<tr>
<td>sample 007</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \alpha = 0 )</td>
<td>-0.3</td>
<td>-0.3</td>
<td>-0.5</td>
<td>-0.3</td>
<td>-0.3</td>
<td>-0.3</td>
</tr>
<tr>
<td>( \alpha = 1 )</td>
<td>0.1</td>
<td>0.1</td>
<td>-0.3</td>
<td>0.1</td>
<td>0.1</td>
<td>0.1</td>
</tr>
<tr>
<td>( \alpha = 1/2 )</td>
<td>-0.1</td>
<td>-0.1</td>
<td>-0.4</td>
<td>-0.1</td>
<td>-0.1</td>
<td>-0.1</td>
</tr>
<tr>
<td>sample 010</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \alpha = 0 )</td>
<td>-0.3</td>
<td>-0.3</td>
<td>-1.0</td>
<td>-0.3</td>
<td>-0.3</td>
<td>-0.3</td>
</tr>
<tr>
<td>( \alpha = 1 )</td>
<td>0.7</td>
<td>0.7</td>
<td>-0.5</td>
<td>0.7</td>
<td>0.7</td>
<td>0.7</td>
</tr>
<tr>
<td>( \alpha = 1/2 )</td>
<td>0.3</td>
<td>0.3</td>
<td>-0.7</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
</tr>
</tbody>
</table>
be evaluated \textit{a posteriori}, and both $\eta$ and $\tilde{\eta}$ adjusted if needed. We mention in passing that only slightly negative eigenvalues ($a_1 \simeq -0.08$) were found if no constraints were applied.

The relative errors in the strength of the two smallest-eigenvalue directions are found to be somewhat larger compared to $a_3$. To further improve the misfit \textit{in general}, we believe that it is necessary to carefully consider the ODF definition: similar to above, the ODF should, ideally, be understood as a grain-volume-fraction-weighted distribution. While our inferred ODFs can indeed be interpreted as such, the measured sample ODFs (and hence eigenvalues in table 2) assume equal-sized grains by virtue of equation (2.5). We find, however, very similar eigenvalues when using the grain cross-sectional area fraction as $c$-axis weights (not shown). We leave further attempts for understanding the mismatch between inferred and observed fabric eigenvalues for future work, but note that our optimal parameters give, regardless, the best reproduction of the strength of the principal fabric direction ($a_3$), which is also clear from comparing figure 5d–f.

\textbf{(c) Well-posedness of inverse problem}

\textbf{(i) Elastic parameters and measurement scheme}

In the case where the sought-after ODF is truly unknown, having accurate effective grain elastic parameters as a function of temperature, and other relevant parameters, is crucial. Only then can the absolute velocities be reproduced (full versus dashed lines in figure 5a–c), allowing $V_i$—and not the angular anomalies, $\delta V_i$—to enter the misfit $J$ when inferring the ODF (i.e. $\hat{\psi}$). Since a rotationally symmetric fabric around the measurement plane is indistinguishable from an isotropic fabric if $\delta V_i$ is used, using $\delta V_i$ is not an attractive \textit{general} approach. Of course, if multiple non-overlapping measurement planes are considered, this might help constrain the problem. However, for cylindrical-shaped ice-core samples (figure 2), this may require further cutting of samples, possibly causing loss of valuable ice for other purposes (e.g. climatic records), and therefore at odds with being a non-destructive method. Indeed, Lutz \textit{et al.} \cite{37} estimated that approximately 12 equi-spaced measurement directions ($\Delta \phi = 30^\circ$ increments) are needed to infer a single-maximum ODF, which seems difficult to accomplish for e.g. two orthogonal measurement planes without further cutting ice-core samples. To that end, we speculate that if it is possible to further cut samples (maybe requiring a different instrument design than shown in figure 2), measuring phase velocities along the unique eigenvectors of $(c^2)$ and $(e^4)$-eigentensors for each harmonic mode shown in figure 3 might contain the most information per total number of measurements.

\textbf{(ii) Additional synthetic experiments}

In addition to the experimental data considered above, we constructed a set of synthetic experiments to search for pitfalls when attempting to infer other fabrics commonly found (or expected to exist) in glacier ice. Specifically, we generated synthetic phase-velocity datasets with $g_{68}$ parameters given a girdle fabric ($c$-axes distributed along a great circle on $S^2$) and multi-maxima fabrics (fabrics dominated by modes $l = 4, m > 0$). We considered two sampling planes, $\hat{x}$–$\hat{y}$ and $\hat{x}$–$\hat{z}$, and found that, in either case, ODFs could be inferred reasonably well (not shown).
Figure 7. Seismic survey schemes. (a) Excited waves are reflected of the ice–bed interface and recorded at surface-based receivers. (b) Excited waves are recorded at receivers inside an ice core borehole. $P_{ij}$ denote the set of survey locations on the surface. (Online version in colour.)

While more work is needed to understand the well-posedness as a function of fabric type and choice of sampling plane, we, therefore, believe that our method might also be useful for glacier ice subject to extensional (flank) flow, or even recrystallization-affected fabrics such as those thought to exist in warm or highly stressed areas of ice sheets (e.g. near bumpy basal topography, in warm basal ice or in ice-stream shear margins) [83–85].

(iii) Seismic surveys over ice sheets

Recent seismic surveys [17,25–29,34], conducted at the surface of ice sheets, indicate an increasing interest in applying seismic methods to infer the in situ physical properties of ice sheets (typically fabric). Much like our approach and in radio-glaciological methods (e.g. [86–88]), many seismic methods also rely on shear-wave splitting (travel-time anomalies) to characterize the fabric anisotropy. However, unlike laboratory experiments where the sample-of-interest can easily be rotated relative to the ultrasonic transducer (figure 2), seismic surveys are in practice constrained to walk-away seismic profiling (figure 7), limiting the range of incident angles that waves can be excited to propagate along (in analogy to limiting the range of $\phi$ in this study). If a similar optimization problem is, therefore, sought for seismic velocity data (where the fabric would, in a sense, be the depth-averaged fabric), the well-posedness of the problem must be treated carefully: the number of surface measurements needed is not clear and will depend on the number of redundant propagation directions considered, which, in turn, depends on the fabric symmetries that are, in principle, unknown. To elaborate, consider a vertical single-maximum fabric that is horizontally isotropic, common to many places in ice sheets [51,52]. If a survey is conducted over an ice column with such a fabric, rotating the surface wave source around the common midpoint in the surface plane ($P_0$ in figure 7a) at multiple radial distances (rings in figure 7a) would not provide additional information unless absolute velocities $V_i$ and not $\delta V_i$ are considered in cost function $J$, and hence requires good estimates of the effective grain elastic parameters as discussed above.

If, on the other hand, seismic receivers can be moved vertically along a borehole (e.g. [37])—an experimental setup where receivers do not rely on reflections of the ice–bed interface—a greater range of incident angles could in theory be achieved (figure 7b). In that case, care must, however, be exercised to ensure the depth-averaged fabric is a good approximation throughout the ice
column, as such a method would sample only part of the ice column depending on the receiver depth.

(iv) State of the art in material sciences

Determining the ODF from bulk wave velocity measurements is also of great interest in the broader material sciences community and especially the metals community (see e.g. [44], for an overview). Recently, an intrinsically well-posed inverse problem for determining the ODF was developed by Lan et al. [44,89] and later validated against neutron diffraction experiments [90,91]. The method relies on averaging the monocrystal phase-velocity function, \( V'_{i}(\hat{k}) \), over the ODF to construct the polycrystalline phase-velocity function, \( V_{i}(\hat{k}) \). By expanding both \( V'_{i}(\hat{k}) \) and the ODF in terms of a spherical harmonic series, the corresponding harmonic expansion coefficients for \( V_{i}(\hat{k}) \) follow from a convolution problem and are given by

\[
(V_{i})^{m}_{l} = K^{0}_{l} \hat{\psi}^{m}_{l},
\] (4.1)

where the harmonic expansion coefficients of the kernel function, \( K^{0}_{l} \), depend on the expansion coefficients of \( V'_{i}(\hat{k}) \) (see [44], for details).

Compared to our method, this approach is attractive for several reasons: (i) no assumptions are made about the monocrystal constitutive equation since \( V'_{i}(\hat{k}) \) can simply be fitted to observations (although (4.1) is a special case that assumes transversely isotropic grains), (ii) higher-order ODF coefficients can in principle be inferred whereas our method is limited to \( l \leq 4 \) coefficients and (iii) the problem is mathematically well posed in the sense that the ODF expansion coefficients, \( \hat{\psi}^{m}_{l} \), are uniquely defined by (4.1) for a given harmonic expansion of \( V'_{i}(\hat{k}) \) and \( V_{i}(\hat{k}) \).

Of course, this method can in practice be ill-posed in the same way as discussed above: if bulk phase velocities are measured along too few propagation directions (which depends on the fabric symmetries), multiple sets of expansion coefficients \( (V_{i})^{m}_{l} \) might reproduce observed bulk velocities, and determining \( \hat{\psi}^{m}_{l} \) from (4.1) could be ambiguous even though (4.1) is well posed. This is not to say that both methods result in similar inferred ODFs; descending the cost function \( J \) does not guarantee reaching the global minimum, and the minimum found will in general depend on the initial guess. However, our method benefits from the ability to seamlessly include multiple lines of observations (e.g. qP, qS1 and qS2 phase velocities simultaneously) and additional constraints through the Lagrange multiplier method. For glaciological purposes, the latter ability is particularly relevant since ensuring the inferred ODF is strictly positive (positive eigenvalues) is important when calculating fabric-induced anisotropic viscosities. Using the above de-convolution method, Lan et al. [44] found that inferred ODFs were not always strictly positive.

(d) Relevance for geological materials

Ultrasonic measurements are also made during deformation experiments on rocks to help understand processes and evolving mechanics. For example, during uniaxial compression tests, ultrasound monitoring can be applied to monitor the evolution of cracks and thus damage in breaking rocks [92], a valuable technique when applied in parallel with acoustic emission [93,94]. Such data have implications for understanding active faults [95], and have a role in constraining real time monitoring, for faults, CO2 sequestration [96] and geothermal energy systems. Application during non-brittle laboratory deformation tests is, however, difficult because of technical challenges in conducting ultrasonic work at high temperatures, and so far has been limited to salt [97] and ice [98].

Other work in the geosciences considers lower frequency (seismic) data that can characterize the structure of the crust [99–101], the upper mantle [13,102,103] and the deeper Earth [104,105]. Virtually all work that relates measurements of seismic anisotropy to the fabrics of rocks does so through forward modelling of the elastic properties of fabrics (e.g. [106–108], and references therein). Our inverse methodology might, therefore, be useful as an additional way to constrain
fabrics in situations where multiple receiver stations record the same seismic event (usually earthquake). In this case, we believe that caveats regarding the well-posedness of the inverse problem are similar to those discussed above in a glaciological context.

5. Conclusion

We revisited the method of using ultrasonic (elastic) P- and S-wave velocity measurements to non-destructively infer physical properties of polycrystals. Specifically, we proposed an optimization problem for inferring the grain c-axis orientation distribution function (ODF) and effective grain elastic parameters of glacier ice in a mixed stress–strain homogenization scheme, which relies on minimizing the modelled wave-velocity misfits with observations across multiple sample orientations.

Our method is inspired by, and builds on, the methodology of Gusmeroli et al. [21] and Lutz et al. [37], but is free of constraints that the ODF must be of a predetermined type, made possible by expanding the c-axis distribution function in terms of a spherical harmonic series (non-parametric approach) similar to developments made in the broader material sciences community (e.g. [44,50,53–55]). Using the same ice-core data as Lutz et al. [37] from the shear margin of Priestley glacier, Antarctica, we demonstrated that our method is a feasible approach for inferring both the ODF of ice-core samples and the effective grain elastic parameters of the homogenization scheme.

In line with past work [60], we found that the forward problem (calculated wave velocities) is relatively insensitive to the exact choice of stress–strain homogenization scheme for glacier ice, and therefore inferred properties are, too.

We showed how physical constraints can be imposed on the inversion, such as requiring strictly positive eigenvalues of the inferred ODF. The degree to which such constraints are enforced (Lagrange multiplier magnitude) should be adjusted a posteriori and possibly (but not necessarily) on a per-sample basis.

We found that using accurate, effective values for the grain elastic parameters is important when inferring truly unknown ODFs, and that using existing monocrystal (single crystal) estimates from the literature might, therefore, not suffice for all inverse problems. Only when using accurate values (that may depend on temperature, porosity, static pressure, etc.) can absolute velocities enter the cost function of the optimization problem—providing more information to the optimization problem—central for future adoptions of our method in e.g. large-scale seismic surveys, or for determining the strength of the principal c-axis direction most accurately in ultrasound experiments.

There is, however, room for further improving the misfit between inferred and observed ODFs, such as measured by the smallest fabric eigenvalues. We suggest future work should treat the inferred ODF as a grain-volume-fraction-averaged distribution, and comparisons with observed ODFs should ideally reflect this; that way, uncertainties associated with assuming equal-sized grains are at least reduced. Nonetheless, we believe that our work demonstrates that constructing a classical optimization problem, combined with a spectral-space representation of the c-axis distribution, provides a viable, general approach for inferring c-axis distributions and effective grain elastic parameters of anisotropic polycrystals such as glacier ice.

Data accessibility. The data and model code for reproducing the plots of this paper are available at https://github.com/nicholasmr/specfab.

Authors’ contributions. N.M.R.: conceptualization, formal analysis, investigation, methodology, project administration, resources, software, supervision, validation, visualization, writing—original draft, writing—review and editing; A.G.: conceptualization, methodology, writing—original draft, writing—review and editing; K.M.: methodology, writing—review and editing; D.A.L.: methodology, writing—review and editing; J.W.: methodology, writing—review and editing; C.S.H.: methodology, writing—review and editing; D.J.P.: data curation, funding acquisition, investigation, methodology, writing—review and editing; F.L.: data curation, investigation, writing—review and editing; R.E.T.: data curation, investigation, writing—review and editing; D.D.-J.: funding acquisition, writing—review and editing.
Conflict of interest declaration. We declare we have no competing interests.

Funding. The research leading to these results has received funding from the Villum Foundation, investigator grant nos. 16572 and 23261, and the Independent Research Fund Denmark (DFF), grant no. 2032-00364B.

Acknowledgements. We wish to thank two anonymous reviewers for providing comments that helped improve the scope and relevance of our paper. Notably, this includes addressing the relevance of our method for other fabric types found in glacier ice, and for the broader material science community.

Appendix A. Stress homogenization

The starting point for deriving the Reuss-averaged stress tensor, \( \sigma_{\text{Reuss}} \), and acoustic tensor, \( \tilde{Q}_{\text{Reuss}} \), is the inverse of the constitutive equation (2.2):

\[
\epsilon' = \frac{\hat{\lambda}^2 \lambda^2 - \hat{\gamma} \gamma \lambda}{2\mu \chi} \text{tr}(\sigma') I + \frac{1}{2\mu} \sigma' + \frac{\hat{\lambda} \lambda + 2\mu - \hat{\gamma} \gamma \lambda}{2\mu \chi} \left[ (\sigma': c^2) I + \text{tr}(\sigma') c^2 \right] 
+ \left( \frac{4\mu \lambda (1 + \hat{\lambda}) + 4\mu^2 + \hat{\gamma} \gamma^2 - \hat{\lambda}^2 \lambda^2}{2\mu \chi} \right) \sigma' : c^4 + \frac{1 - \hat{\mu}}{2\mu \mu} \{ \sigma', c^2 \},
\]

(A1)

where \( \chi = 2\hat{\gamma} \gamma (\lambda + \mu) - \hat{\lambda}^2 \lambda^2 \).

(a) Stress tensor

Calculating the Reuss grain-average of equation (A1) and subsequently vectorizing the equation according to

\[
V(X_{ij}) = [X_{11}, X_{21}, X_{31}, X_{12}, \ldots, X_{33}]^T, \quad (A2)
\]

can be shown to give

\[
V(\langle \epsilon' \rangle) = P \cdot V(\sigma_{\text{Reuss}}), \quad (A3)
\]

where \( P \) is the \( 9 \times 9 \) matrix

\[
P = \frac{\hat{\lambda}^2 \lambda^2 - \hat{\gamma} \gamma \lambda}{2\mu \chi} V(I_3) V(I_3) + \frac{1}{2\mu} I_9 + \frac{\hat{\lambda} \lambda + 2\mu - \hat{\gamma} \gamma \lambda}{2\mu \chi} \left( V((c^2) V(I_3) + V(I_3) V((c^2)) \right) 
+ \left( \frac{4\mu \lambda (1 + \hat{\lambda}) + 4\mu^2 + \hat{\gamma} \gamma^2 - \hat{\lambda}^2 \lambda^2}{2\mu \chi} \right) F((c^4)) + \frac{1 - \hat{\mu}}{2\mu \mu} \left( (c^2) \otimes I_3 + I_3 \otimes (c^2) \right), \quad (A4)
\]

and \( F(X_{ijlm}) \) is the \( 9 \times 9 \) matrix

\[
F(X_{ijlm}) = \begin{bmatrix}
X_{1111} & X_{1121} & X_{1131} & X_{1112} & \cdots & X_{1133} \\
X_{2111} & X_{2121} & X_{2131} & X_{2112} & \cdots & X_{2133} \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
X_{3311} & X_{3321} & X_{3331} & X_{3312} & \cdots & X_{3333}
\end{bmatrix}. \quad (A5)
\]
Here, $\otimes$ is the generalized Kronecker (outer) product, and $I_m$ is the $m \times m$ identity matrix. It follows that

$$\sigma_{\text{Reuss}} = \mathcal{V}^{-1} \left( \mathbf{P}^{-1} \cdot \mathcal{V}(\langle \epsilon \rangle) \right), \quad (A\ 6)$$

where $\mathcal{V}^{-1}$ reverts the vectorization.

(b) Acoustic tensor

The acoustic tensor under the Reuss hypothesis follows from writing $\nabla \cdot \sigma_{\text{Reuss}}$ in its vectorized form, combined with equation (A 6), giving

$$\nabla \cdot \sigma_{\text{Reuss}} = (I \otimes [\partial_x, \partial_y, \partial_z]) \cdot \mathcal{V}(\sigma_{\text{Reuss}}) = (I \otimes [\partial_x, \partial_y, \partial_z]) \cdot \mathbf{P}^{-1} \cdot \mathcal{V}(\langle \epsilon \rangle), \quad (A\ 7)$$

which allows $\hat{Q}_{\text{Reuss}}$ to be identified for $\hat{k} = \hat{z}$ by writing out the components (not shown):

$$\hat{Q}_{\text{Reuss}} = \frac{1}{2} \begin{bmatrix} (P^{-1})_{33} + (P^{-1})_{37} & (P^{-1})_{36} + (P^{-1})_{38} & 2(P^{-1})_{39} \\ (P^{-1})_{63} + (P^{-1})_{67} & (P^{-1})_{66} + (P^{-1})_{68} & 2(P^{-1})_{69} \\ (P^{-1})_{93} + (P^{-1})_{97} & (P^{-1})_{96} + (P^{-1})_{98} & 2(P^{-1})_{99} \end{bmatrix}. \quad (A\ 8)$$

Appendix B. Fourth-order structure tensor

The fourth-order structure tensor, $\langle \epsilon^4 \rangle$, can conveniently be written in Mandel’s $6 \times 6$ notation, $\mathcal{M}(\langle \epsilon^4 \rangle)$:

$$\mathcal{M}(\langle \epsilon^4 \rangle) = \begin{bmatrix} \langle \epsilon^4 \rangle_{1111} & \langle \epsilon^4 \rangle_{1122} & \langle \epsilon^4 \rangle_{1133} & \sqrt{2} \langle \epsilon^4 \rangle_{1123} & \sqrt{2} \langle \epsilon^4 \rangle_{1131} & \sqrt{2} \langle \epsilon^4 \rangle_{1112} \\ \langle \epsilon^4 \rangle_{2211} & \langle \epsilon^4 \rangle_{2222} & \langle \epsilon^4 \rangle_{2233} & \sqrt{2} \langle \epsilon^4 \rangle_{2223} & \sqrt{2} \langle \epsilon^4 \rangle_{2231} & \sqrt{2} \langle \epsilon^4 \rangle_{2212} \\ \langle \epsilon^4 \rangle_{3311} & \langle \epsilon^4 \rangle_{3322} & \langle \epsilon^4 \rangle_{3333} & \sqrt{2} \langle \epsilon^4 \rangle_{3323} & \sqrt{2} \langle \epsilon^4 \rangle_{3331} & \sqrt{2} \langle \epsilon^4 \rangle_{3312} \\ \sqrt{2} \langle \epsilon^4 \rangle_{2311} & \sqrt{2} \langle \epsilon^4 \rangle_{2322} & \sqrt{2} \langle \epsilon^4 \rangle_{2333} & 2 \langle \epsilon^4 \rangle_{2323} & 2 \langle \epsilon^4 \rangle_{2331} & 2 \langle \epsilon^4 \rangle_{2312} \\ \sqrt{2} \langle \epsilon^4 \rangle_{3111} & \sqrt{2} \langle \epsilon^4 \rangle_{3122} & \sqrt{2} \langle \epsilon^4 \rangle_{3133} & 2 \langle \epsilon^4 \rangle_{3123} & 2 \langle \epsilon^4 \rangle_{3131} & 2 \langle \epsilon^4 \rangle_{3112} \\ \sqrt{2} \langle \epsilon^4 \rangle_{1211} & \sqrt{2} \langle \epsilon^4 \rangle_{1222} & \sqrt{2} \langle \epsilon^4 \rangle_{1233} & 2 \langle \epsilon^4 \rangle_{1223} & 2 \langle \epsilon^4 \rangle_{1231} & 2 \langle \epsilon^4 \rangle_{1212} \end{bmatrix}. \quad (B\ 1)$$

In this notation, the double contraction with (say) $\epsilon$ is given by $\langle \epsilon^4 \rangle : \epsilon = \mathcal{M}^{-1}[\mathcal{M}(\langle \epsilon^4 \rangle) : \mathcal{M}(\epsilon)]$, where $\mathcal{M}(\epsilon) = [\epsilon_{xx}, \epsilon_{yy}, \epsilon_{zz}, \sqrt{2} \epsilon_{xy}, \sqrt{2} \epsilon_{xz}, \sqrt{2} \epsilon_{yz}]$ and $\mathcal{M}^{-1}$ re-establishes the tensorial form.

Like $\langle \epsilon^2 \rangle$, the entries of $\langle \epsilon^4 \rangle$ are linear combinations of $\hat{\psi}_j^m$. Following Rathmann et al. [64] by repeatedly expanding products in (2.5) between two spherical harmonics in terms of a new spherical harmonic series (contraction rule), it can be shown that

$$B \equiv \mathcal{M}(\langle \epsilon^4 \rangle) = B^{(0)} + B^{(2)} + B^{(4)}, \quad (B\ 2)$$
where \( \mathbf{B}^{(0)} \) is an isotropic contribution, \( \mathbf{B}^{(2)} \) depends on the \( l = 2 \) modes, and \( \mathbf{B}^{(4)} \) depends on the \( l = 4 \) modes. The three terms in (B.2) are given by

\[
\mathbf{B}^{(0)} = \frac{1}{15} \begin{bmatrix}
3 & 1 & 1 & 0 & 0 & 0 \\
1 & 3 & 1 & 0 & 0 & 0 \\
1 & 1 & 3 & 0 & 0 & 0 \\
0 & 0 & 0 & 2 & 0 & 0 \\
0 & 0 & 0 & 0 & 2 & 0 \\
0 & 0 & 0 & 0 & 0 & 2
\end{bmatrix},
\]

\[
\mathbf{B}^{(2)} = \frac{2}{7\sqrt{5}} \begin{bmatrix}
\mathbf{B}_{11}^{(2)} & \mathbf{B}_{12}^{(2)} \\
\mathbf{B}_{12}^{(2)} & \mathbf{B}_{22}^{(2)}
\end{bmatrix}, \quad \mathbf{B}^{(4)} = \frac{1}{21\sqrt{5}} \begin{bmatrix}
\mathbf{B}_{11}^{(4)} & \mathbf{B}_{12}^{(4)} \\
\mathbf{B}_{12}^{(4)} & \mathbf{B}_{22}^{(4)}
\end{bmatrix},
\]

where

\[
\mathbf{B}_{11}^{(2)} = \begin{bmatrix}
-\dot{\psi}_2^0 + \sqrt{6}\text{Re}[\dot{\psi}_2^2] & -\frac{1}{3}\dot{\psi}_2^0 & \frac{1}{6}\dot{\psi}_2^0 + \frac{1}{\sqrt{6}}\text{Re}[\dot{\psi}_2^2] \\
\text{sym.} & -\dot{\psi}_2^0 - \sqrt{6}\text{Re}[\dot{\psi}_2^2] & \frac{1}{6}\dot{\psi}_2^0 - \frac{1}{\sqrt{6}}\text{Re}[\dot{\psi}_2^2] \\
\frac{1}{3}\dot{\psi}_2^0 - \sqrt{\frac{2}{3}}\text{Re}[\dot{\psi}_2^2] & -\sqrt{\frac{2}{3}}\text{Im}[\dot{\psi}_2^2] & -\sqrt{\frac{2}{3}}\text{Re}[\dot{\psi}_2^2]
\end{bmatrix},
\]

\[
\mathbf{B}_{22}^{(2)} = \begin{bmatrix}
\frac{1}{3}\dot{\psi}_2^0 + \sqrt{\frac{2}{3}}\text{Re}[\dot{\psi}_2^2] & -\sqrt{\frac{2}{3}}\text{Im}[\dot{\psi}_2^2] & \sqrt{\frac{2}{3}}\text{Im}[\dot{\psi}_2^2] \\
\text{sym.} & -\frac{2}{3}\dot{\psi}_2^0 \\
\frac{1}{\sqrt{3}}\text{Im}[\dot{\psi}_2^2] & -\sqrt{3}\text{Re}[\dot{\psi}_2^2] & -\sqrt{3}\text{Im}[\dot{\psi}_2^2]
\end{bmatrix},
\]

\[
\mathbf{B}_{12}^{(2)} = \begin{bmatrix}
\sqrt{3}\text{Im}[\dot{\psi}_2^2] & -\frac{1}{\sqrt{3}}\text{Re}[\dot{\psi}_2^2] & -\sqrt{3}\text{Im}[\dot{\psi}_2^2] \\
\sqrt{3}\text{Im}[\dot{\psi}_2^2] & -\sqrt{3}\text{Re}[\dot{\psi}_2^2] & -\sqrt{3}\text{Im}[\dot{\psi}_2^2]
\end{bmatrix},
\]

and

\[
\mathbf{B}_{11}^{(4)} = \begin{bmatrix}
\frac{3}{2\sqrt{5}}\dot{\psi}_4^0 - 2\text{Re}[\dot{\psi}_4^2] + \sqrt{7}\text{Re}[\dot{\psi}_4^2] & \frac{1}{\sqrt{10}}\dot{\psi}_4^0 - \sqrt{7}\text{Re}[\dot{\psi}_4^2] & -2\sqrt{\frac{7}{5}}\dot{\psi}_4^0 + 2\text{Re}[\dot{\psi}_4^2] \\
\text{sym.} & \frac{3}{2\sqrt{5}}\dot{\psi}_4^0 + 2\text{Re}[\dot{\psi}_4^2] + \sqrt{7}\text{Re}[\dot{\psi}_4^2] & -2\sqrt{\frac{7}{5}}\dot{\psi}_4^0 - 2\text{Re}[\dot{\psi}_4^2]
\end{bmatrix},
\]

\[
\mathbf{B}_{11}^{(4)} = \begin{bmatrix}
\frac{1}{\sqrt{10}}\dot{\psi}_4^0 & -2\sqrt{\frac{7}{5}}\dot{\psi}_4^0 + 2\text{Re}[\dot{\psi}_4^2] \\
\text{sym.} & \frac{3}{2\sqrt{5}}\dot{\psi}_4^0 + 2\text{Re}[\dot{\psi}_4^2] + \sqrt{7}\text{Re}[\dot{\psi}_4^2]
\end{bmatrix}.
\]
\[
B_{22}^{(4)} = \\
\begin{bmatrix}
-4\sqrt{5} \psi_4^0 - 4\text{Re}[\psi_4^2] & -4\text{Im}[\psi_4^2] & \sqrt{2}\text{Re}[\psi_4^1] + \sqrt{14}\text{Re}[\psi_4^4] \\
4\sqrt{5} \psi_4^0 + 4\text{Re}[\psi_4^2] & -\sqrt{2}\text{Im}[\psi_4^2] + \sqrt{14}\text{Im}[\psi_4^4] \\
\text{sym.} & \sqrt{\frac{2}{5}} \psi_4^0 - 2\sqrt{7}\text{Re}[\psi_4^4] \\
\end{bmatrix}.
\]

\[
B_{12}^{(4)} = \\
\begin{bmatrix}
-\text{Im}[\psi_4^1] + \sqrt{7}\text{Im}[\psi_4^3] & 3\text{Re}[\psi_4^1] - \sqrt{7}\text{Re}[\psi_4^3] & \sqrt{2}\text{Im}[\psi_4^2] - \sqrt{14}\text{Im}[\psi_4^4] \\
-3\text{Im}[\psi_4^1] - \sqrt{7}\text{Im}[\psi_4^3] & \text{Re}[\psi_4^1] + \sqrt{7}\text{Re}[\psi_4^3] & \sqrt{2}\text{Im}[\psi_4^2] + \sqrt{14}\text{Im}[\psi_4^4] \\
4\text{Im}[\psi_4^1] & -4\text{Re}[\psi_4^1] & -2\sqrt{2}\text{Im}[\psi_4^4] \\
\end{bmatrix}.
\]

References


39. Bennett HF. 1968 *An investigation into velocity anisotropy through measurements of ultrasonic wave velocities in snow and ice cores from Greenland and Antarctica.* Madison, WI: The University of Wisconsin-Madison.


78. Sayers CM. 2018 Increasing contribution of grain boundary compliance to polycrystalline ice elasticity as temperature increases. J. Glaciol. 64, 669–674. (doi:10.1017/jog.2018.56)


