

Orientation Dependence of Elastic Constants for Ice

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ABSTRACT

Orientation dependence of Young's and shear moduli of ice single crystals has been calculated at various temperatures using the most up-to-date values of elastic constants and classical equations derived for hexagonal materials. Young's modulus is a maximum whereas shear modulus has a minimum value along the c-axis. Along a direction 50° to the c-axis, the shear modulus has a maximum value and the Young's modulus, a minimum. Average values of polycrystal moduli calculated from single crystal values showed only mild temperature dependence.

1. INTRODUCTION

Knowledge of the mechanical properties of ice is indispensable for the design of structures off the Arctic coast or on large ice sheets such as those on Antarctica and Greenland, and for icebreakers and other vessels operating in ice infested waters. Ice is a crystalline material having a hexagonal structure with tetrahedral coordination for the O-ions. During the formation of ice sheets over lakes and oceans columnar grains are usually formed with some definite crystallographic orientations, depending upon the conditions of freezing. In many instances very large columnar grains up to several centimeters in diameter are formed during the growth of an ice sheet. The mechanical properties of ice, hence the strength of an ice sheet, depend on the orientation of the grains in it. The strength of ice in the field is often related to the values of elastic moduli, in particular, Young's modulus E and the rigidity (or shear) modulus G . Hence it is worthwhile studying the orientation dependence of elastic constants of ice, for developing suitable rheological models of its mechanical behaviour, especially in the early part of the stress-strain curve and under high rates of deformation as under impact of an ice sheet with a structure.

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2. CALCULATION OF SINGLE CRYSTAL ELASTIC CONSTANTS

In general, stresses and strains are functions of elastic moduli C and compliances S . The standard equations relating stresses and strains for a hexagonal crystal are well known.^{1,2} Values of E and G are usually determined in the laboratory by measuring the velocity of propagation of longitudinal and transverse sound waves in the material.

Equations for the moduli (Young's E , and shear or rigidity G) measured in a direction at an angle ϕ with the hexagonal axis are²

$$E^{-1} = S_{11}(1-\cos^2\phi)^2 + S_{33}\cos^4\phi + (2S_{13}+S_{44})\cos^2\phi(1-\cos^2\phi) \quad (1)$$

$$G^{-1} = S_{44} + [S_{11}-S_{12}-(S_{44}/2)](1-\cos^2\phi) + 2(S_{11}+S_{33}-2S_{33}-S_{44})\cos^2\phi(1-\cos^2\phi) \quad (2)$$

where S_{ij} are the elastic compliances.

Values of compliances S_{ij} are obtained from the values of elastic constants C_{ij} using relationships that can be derived from the fundamental equations given by Love¹ (see also Ref. 2.)

$$\begin{aligned} S_{44} &= C_{44}^{-1} \\ S_{11}-S_{12} &= (C_{11}-C_{12})^{-1} \\ S_{11}+S_{12} &= C_{33}/X \\ S_{13} &= -C_{13}/X \\ S_{33} &= (C_{11}+C_{12})/X \end{aligned} \quad (3)$$

$$\text{where } X = \frac{C_{33}(C_{11}+C_{12})-2C_{13}^2}{[S_{33}(S_{11}+S_{12})-2C_{13}^2]^{-1}}$$

When $\phi=0$, Eqns (1) and (2) reduce to,

$$E_c = C_{33}^{-1} \text{ and } G_c = C_{44}^{-1} \quad (4)$$

which are the values of moduli parallel to the hexagonal axis. When $\phi = 90^\circ$, the values of the moduli along the basal planes are obtained from Eqns (1) and (2),

$$E_a = S_{11}^{-1} \text{ and } G_a = [S_{11}-S_{12}+(S_{44}/2)]^{-1} \quad (5)$$

The elastic constants C_{ij} and hence the compliances S_{ij} are dependent on the temperature of a material, and for ice the most accepted temperature dependence of elastic constants are those given by Dantl.^{3,4} Dantl's equations are of the form :

$$C_{ij}(T) = C_{ij}(0)[1-aT-bT^2] \quad (6)$$

where $C_{ij}(T)$ is the value at temperature $T^\circ\text{C}$ and $C_{ij}(0)$ is the value at 0°C . The values of the constants a and b were determined by ultrasonic pulse-echo method and fitting proper curves to the measured data in the temperature range of 0°C to -140°C .

These values, for the five fundamental elastic constants needed to calculate the elastic moduli using Eqns (1) to (3) are :

C_{ij}	$a(10^{-3})$	$b(10^{-6})$
C_{11}	1.489	1.85
C_{12}	2.072	3.62
C_{13}	1.874	0
C_{33}	1.629	2.93
C_{44}	1.601	3.62

To obtain $C_{ij}(0)$, the values of elastic constants determined by Gammon *et al*⁵⁻⁷ and claimed to be the most accurate to date for ice, were used. Using the method of Brillouin spectroscopy to determine the acoustic wave propagation velocity in ice, Gammon *et al* determined the adiabatic values of elastic constants in four different kinds of ice: artificial ice frozen from distilled water, clear monocrystalline glacier ice, bubbly lake ice, and sea ice. The weighted average of these measurements corrected to -16°C were :

$C_{11} = 13.929 \pm 0.041$, $C_{12} = 7.082 \pm 0.039$, $C_{13} = 5.765 \pm 0.023$, $C_{33} = 15.010 \pm 0.046$ and $C_{44} = 3.014 \pm 0.011$, all values in GPa. Using these values in Eqn (6) for $T = -16^{\circ}\text{C}$, the calculated values of $C_{ij}(0)$ are : $C_{11}(0) = 13.6112$, $C_{12}(0) = 6.8610$, $C_{13}(0) = 5.5972$, $C_{33}(0) = 14.6394$ and $C_{44}(0) = 2.9414$ GPa. These values were used in conjunction with Eqns (1) to (6) to calculate values of Young's modulus E and shear or rigidity modulus G , as a function of angle of orientation ϕ between the c -axis and the direction of interest, for various temperatures between 0°C and -196°C (77°K).

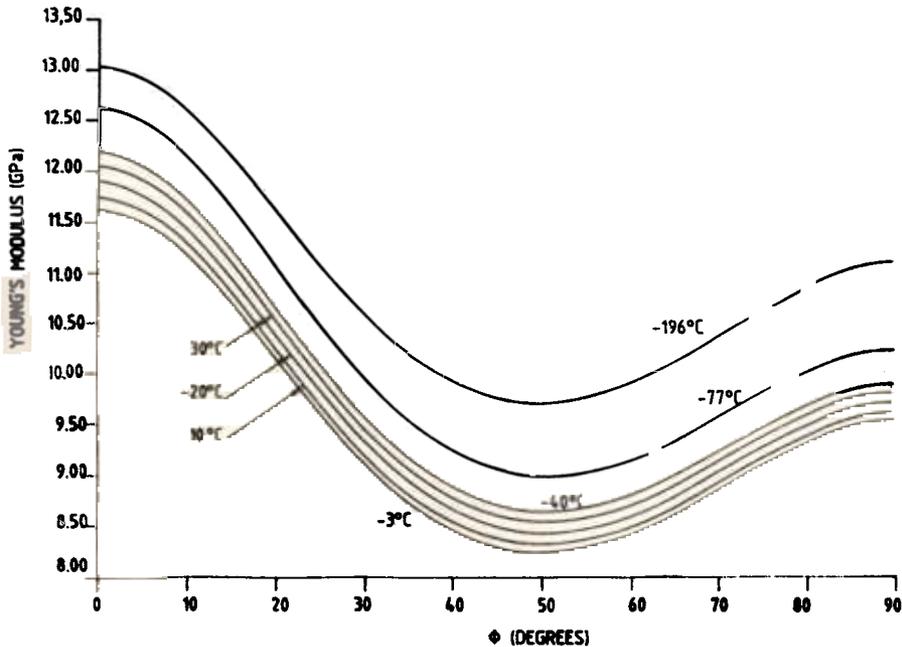


Figure 1. Variation of Young's modulus of ice with angle of orientation between c -axis and direction of measurement.

The variations of E and G with ϕ and T ($^{\circ}\text{C}$) are shown in Figs.1&2 respectively. Figure 3 shows the variations of the Young's and shear moduli parallel to the c -axis (E_c, G_c), and those parallel to the basal plane (E_a, G_a).

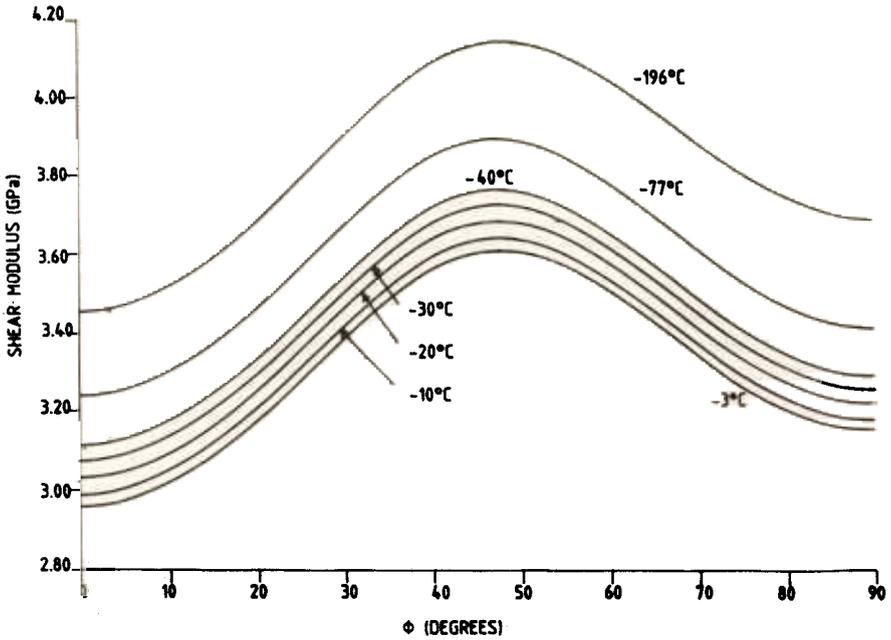


Figure 2. Variation of shear or rigidity modulus with angle of orientation.

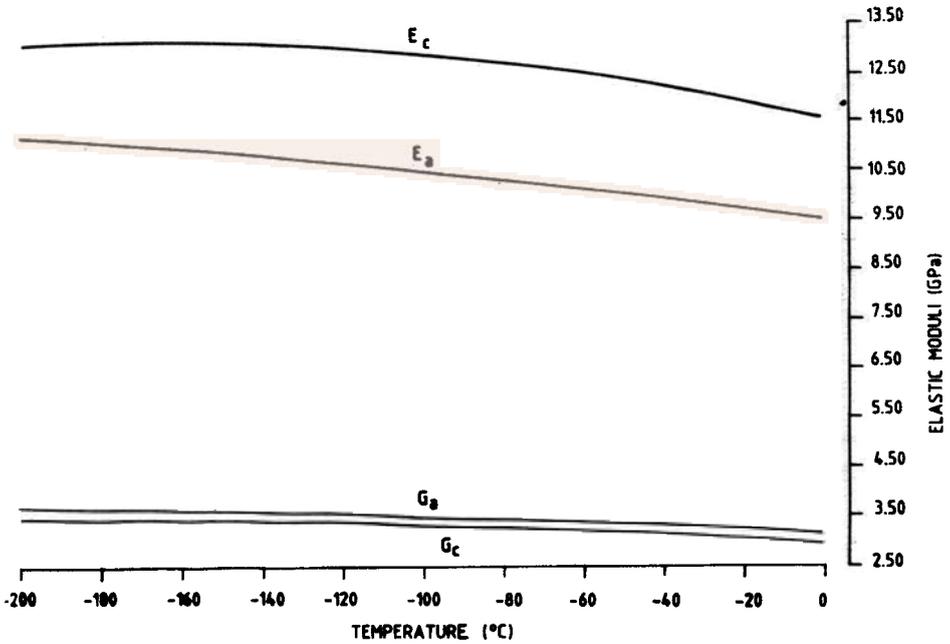


Figure 3. Variation of Young's and shear moduli parallel to (E_c, G_c), and normal to (E_a, G_a) the c -axis, with temperature.

3. CALCULATION OF POLYCRYSTAL ELASTIC CONSTANTS FROM SINGLE CRYSTAL VALUES

In the case of polycrystalline ice with equiaxed grains, as one observes at the bottom of the growing ice sheets below the columnar grains, the elastic constants can be calculated by considering it as an isotropic body composed of a large number of small single crystals oriented at random. Since no exact solution is available, several approximate methods have been suggested. In all these methods, the macroscopic elastic moduli and compliances \bar{C}_{ij} and \bar{S}_{ij} are related to the crystal moduli and compliances C_{ij} and S_{ij} by the general equations,

$$\bar{C}_{ij} = \sum_{kl} a_{ijkl} C_{kl} \quad (7)$$

$$\bar{S}_{ij} = \sum_{kl} b_{ijkl} S_{kl} \quad (8)$$

where the coefficients a_{ijkl} and b_{ijkl} are obtained from a combination of elastic constants and compliances,

The best averages for materials having hexagonal crystallographic symmetry are those given by Voigt⁸ for the uniform strain assumption, and by Reuss⁹ for the uniform stress assumption. For an isotropic nonporous body there are only three independent constants on the left hand side of Eqn (7) and (8). These are given by Markham,¹⁰

$$\begin{aligned} \bar{C}_{11} &= (8C_{11} + 3C_{33} + 4C_{13} + 8C_{44})/15 \\ \bar{C}_{12} &= (C_{11} + C_{33} + 5C_{12} + 8C_{13} - 4C_{44})/15 \\ \bar{C}^{44} &= (\bar{C}^{11} - \bar{C}^{12})/2 = (7C_{11} + 2C_{33} - 5C_{12} - 4C_{13} + 12C_{44})/30 \end{aligned} \quad (9)$$

and

$$\begin{aligned} \bar{S}_{11} &= (8S_{11} + 3S_{33} + 4S_{13} + 2S_{44})/15 \\ \bar{S}_{12} &= (S_{11} + S_{33} + 5S_{12} + 8S_{13} - S_{44})/15 \\ \bar{S}_{44} &= 2(\bar{S}_{11} - \bar{S}_{12}) = (14S_{11} + 4S_{33} - 10S_{12} - 8S_{13} + 6S_{44})/15 \end{aligned} \quad (10)$$

From these the values of shear moduli calculated for the uniform strain (Voigt) case and uniform stress (Reuss) case are, respectively,

$$G_V = \bar{C}_{44} \text{ and } G_R = (\bar{S}_{44})^{-1} \quad (11)$$

Figure 4 shows the variation of these with temperature.

As the materials of hexagonal crystallographic symmetry, with $C_{11} \neq C_{33}$ undergo shear deformation when subjected to uniform hydrostatic pressure, the bulk modulus K , depends on whether the condition of uniform stress or uniform strain is specified. The bulk modulus, defined by the uniform pressure required to produce a bulk strain dV/V (where V is the volume of material), is given by Reuss⁹

$$K_R = (2S_{11} + S_{33} + 2S_{12} + 4S_{13})^{-1} \quad (12)$$

Under uniform strain (Voigt⁸), the bulk modulus given in terms of the stiffnesses are,

$$K_V = (2C_{11} + C_{33} + 2C_{12} + 4C_{13})/9 \quad (13)$$

The variation of K_R and K_V with temperature is also shown in Fig. 4. Figure 4 shows

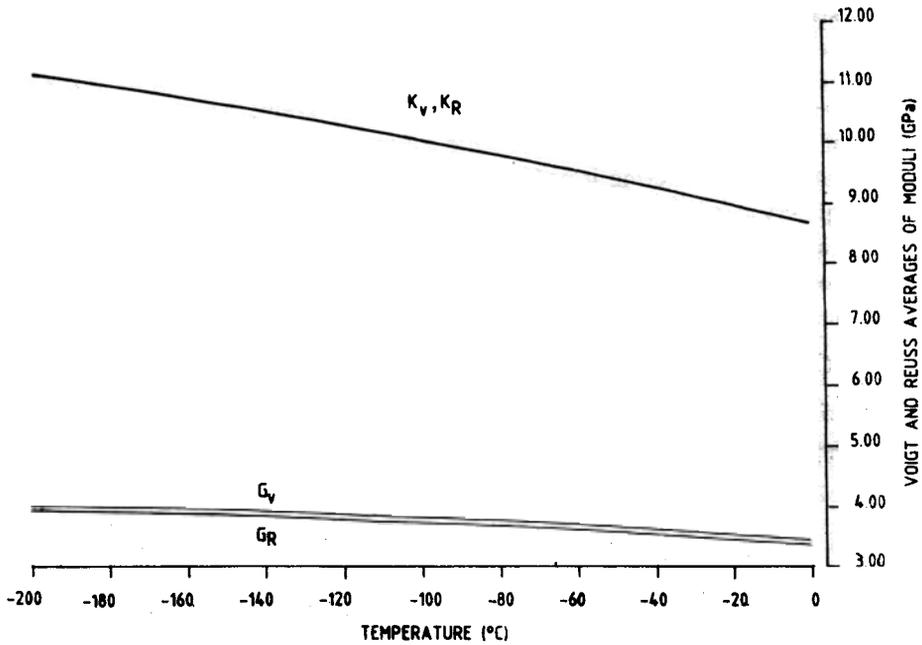


Figure 4. Variation of the Voigt and Reuss averages of shear (G_V , G_R) and bulk (K_V , K_R) moduli with temperature.

that, at a particular temperature, while the Voigt average of shear modulus for ice is slightly larger than the Reuss average, the Voigt and Reuss averages of bulk moduli have identical values.

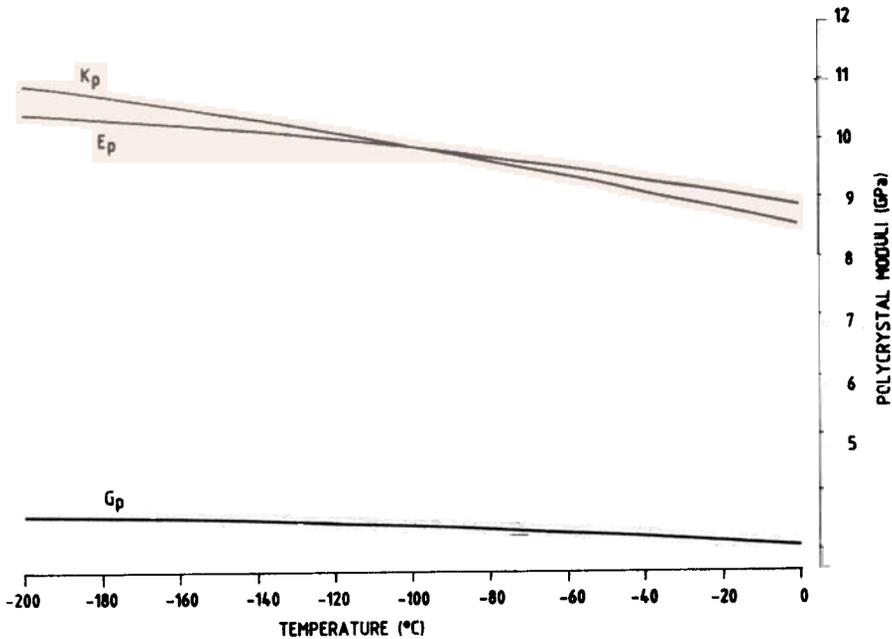


Figure 5. Variation of the shear (G_p), bulk (K_p) and Young's (E_p) moduli for polycrystalline ice, with temperature.

As a very rough approximation, the moduli of a polycrystalline material can be taken to be the average of the values obtained from the Voigt and Reuss extremes,

$$\begin{aligned} \text{Shear or rigidity modulus} \quad G_p &= (G_V + G_R)/2 \\ \text{Bulk modulus} \quad K_p &= (K_V + K_R)/2 \end{aligned} \quad (14)$$

and

$$\text{Young's modulus} \quad E_p = 9K_p G_p / (3K_p + G_p)$$

where the subscript p indicates values for polycrystalline material. Using the values of C_{ij} for ice at various temperatures, the calculated values of G , K and E for a few selected temperatures are shown in Table 1. The variation of G , K and E for polycrystalline ice with temperature is shown in Fig. 5.

Table 1. Values of Young's shear, and bulk moduli for polycrystalline ice, at different temperatures

Polycrystal moduli (GPa)			
T(C)	E_p	G_p	K_p
-1.0	9.021	3.400	8.678
-3.0	9.045	3.408	8.708
-5.0	9.069	3.417	8.738
-10.0	9.128	3.438	8.812
-16.0	9.197	3.463	8.899
-20.0	9.242	3.480	8.957
-30.0	9.352	3.519	9.098
-40.0	9.458	3.557	9.237
-77.0	9.811	3.683	9.722
-196.0	10.538	3.932	10.989

4. DISCUSSIONS

At all temperatures the Young's modulus has the highest value along the c -axis, i.e., $\phi = 0$; and it decreases as ϕ increases as shown in Fig. 1. It reaches a minimum value for $\phi \approx 50^\circ$ beyond which it increases again. Also, for any particular value of ϕ the value of E is higher, the lower the temperature.

The shear modulus G , on the other hand (Fig 2), has the lowest value for $\phi = 0$, i.e., along the c -axis, and it increases with increasing ϕ , reaching a peak at about 50° and then decreases for further increase in ϕ .

Figure 3 shows the specific cases of temperature dependence of moduli parallel to the c -axis and basal plane. Although the temperature dependence is small for these moduli, it can be seen that the values increase monotonically with decreasing

temperature, except for E_c parallel to the c -axis. Also noteworthy is the fact that at any temperature, the value of shear modulus parallel to the basal plane is slightly larger than that parallel to c -axis, whereas in the case of Young's modulus, the value parallel to c -axis is larger than that normal to it.

For ice, data on experimentally measured values of E and G as a function of orientation ϕ do not exist in the literature, for a comparison with the calculated values. Some indirect evidence of this orientation effect can however be quoted. Carter and Michel¹¹ measured the variation of the tensile and compressive strengths of $S1$ type of ice (columnar grained ice with preferred vertical orientation of c -axis) with orientation ϕ , and their results did indeed show a decrease in strength as ϕ increased from 0° to 45° , beyond which strength increased again. The variation of strength (compressive and tensile) with ϕ observed by them (see also Figs 2.4 and 2.5 of Michel,¹² pp. 93, 95) is very similar to the variation of E with ϕ presented in Fig 1 from the present calculations. Hence, it could be surmised that the observed orientation dependence of uniaxial strength of columnar grained ice could at least be partly attributed to the orientation dependence of Young's modulus.

Field measurements¹³ of strength of ice cores taken parallel to and normal to the ice surface in the Beaufort Sea showed that, for a particular loading rate, the horizontal cores had a much smaller yield strength than the vertical ones. For unaligned columnar grained ice, the uniaxial compressive strength of vertical specimens is slightly more than three times the uniaxial strength of horizontal ones. For granular ice, the vertical strength is only 10 per cent greater than the horizontal strength. Although several factors such as grain boundaries, air bubbles, segregation of impurities, etc. could cause such differences in directional strengths, the effect of orientation dependence of moduli cannot entirely be ruled out.

There are no experimental data available on the orientation dependence of the strength of ice tested under pure shear to compare with the orientation dependence of shear modulus shown in Fig 2. It may be worthwhile carrying out tests under pure shear on ice samples with various orientations, to verify the orientation dependence of shear strength and shear modulus.

Finally, the values of the polycrystalline moduli [Young's (E_p), shear (G_p) and bulk (K_p)], and their temperature dependence (Fig 5) obtained from the present calculations are of the same magnitude as reported in literature.¹⁴ As seen in Fig 5, E and G vary only slightly with temperature, but K increases more steeply with decreasing temperature than the other two moduli.

5. CONCLUSIONS

Orientation dependence of single crystal elastic constants for ice were calculated and the values of Young's modulus and shear modulus were found to have considerable dependence on the direction of measurement with respect to c -axis. At any temperature, Young's modulus was maximum along the c -axis where shear modulus had a minimum value. The Young's modulus had the minimum value, and shear modulus had the maximum value along a direction at an angle of about 50° to the

c-axis. The difference between the maximum and minimum values was about 35 per cent for the Young's modulus and 21.5 per cent for shear modulus.

The average values of moduli for polycrystalline ice and their temperature dependence were also calculated. For polycrystalline ice, the Young's and shear moduli were only mildly temperature dependent, whereas the bulk modulus showed a stronger temperature dependence and increased with decreasing temperature.

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