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Calculation of Modulus in Different Directions for Single-Crystal Alloys

Single crystal turbine blade alloys have directional elastic properties, so that the orientation of the crystallographic structure relative to the geometrical axes of the engineered component assumes considerable importance in controlling performance, particularly in terms of creep, fatigue and vibration frequencies.

This Measurement Note describes methods of obtaining the directional elastic properties based on tensor notation, and correlates these with the angular dependence of the more-familiar Young's modulus and shear modulus.

The effects of temperature on measured modulus are also described.

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Introduction

The objective of this Note is to provide a simple means of calculating Young's modulus in a particular crystallographic direction appropriate for single crystal nickel-base turbine blade materials, to provide data for undertaking the calculations, and to provide information on the temperature dependence of moduli.

Nomenclature and equations

Crystallographically cubic single crystals have three independent crystallographic tensor stiffnesses (C_{ij}) or compliances (S_{ij}) (i, j = 1 to 6), specifically (i, j) = (1, 1), (1, 2) and (4, 4). The **effective Young's modulus *E*** in a given direction is a function of these elements and the angles of this direction to the principal crystallographic directions. The simplest notation is in terms of compliances and Euler angles (θ, φ) where θ is the azimuthal angle from the [001] direction and φ is the equatorial angle from the [010] direction in the (011) plane (Figure 1). The angle θ is equivalent in X-ray stereographic representations to 'theta' (UK notation) and 'alpha' or 'primary' (US notation). The angle φ is thought to be equivalent to 'rho' (UK notation) but does not correspond with one of the four US convention angles.

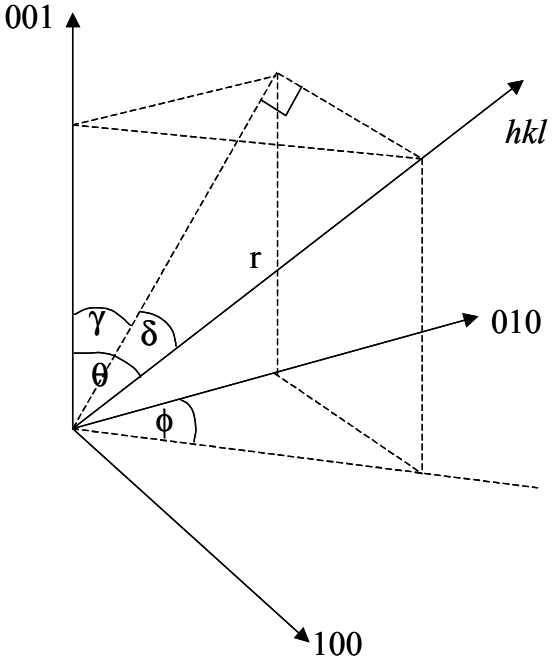

Figure 1: *Orientation nomenclature*

Following the notation of Hermann *et al.* [1]:

$$E\ (\theta,\varphi) = (S_{11} - 2SJ)^{-1} \qquad (1)$$

where: $S = S_{11} - S_{12} - S_{44}/2$

and $J = \sin^2\theta \cdot \cos^2\theta + \sin^4\theta \cdot (1 - \cos 4\varphi)/8$

Thus if S_{11}, S_{12} and S_{44} are known for a given composition, $E(\theta,\varphi)$ can be calculated from equation (1).

The situation regarding shear modulus *G* is much more complex. Except in the specific circumstances of a round rod test-piece, the apparent shear modulus depends on the cross sectional geometry and its rotational orientation relative to the crystallographic axes [2]. For the case of round rods, the shape dependence disappears and a relationship of the following form can be used:

$$G_{meas}(\theta,\varphi) = ((S_{44} + 4SJ)(1-\delta))^{-1} \qquad (2)$$

where δ is a coupling factor of the order 0.005. However, this may over or underestimate the true shear modulus of a non-round shape. It should also be well noted that a curious and complicating consequence of directional elasticity is that applying a pure twist to an off-axis rod or bar also leads to it curving [2].

Angular dependency of modulus

Figure 2 shows the typical angular dependence of modulus for Rene N4 based on literature values of crystallographic compliances [3]. Shear modulus is computed for the simple case of round rods. Points to note are:

1. Young's modulus is a minimum along one of the crystallographic axes, θ = 0°, φ=0°, *i.e.* [001] direction;
2. As θ increases at φ = 0°, Young's modulus increases, nearly doubling for θ = 45°, φ = 0 °, *i.e.* [011] direction;
3. As θ increases at φ = 45°, Young's modulus increases by approximately 2.5 times for θ = 54°, φ = 45°, *i.e.* [111] direction;

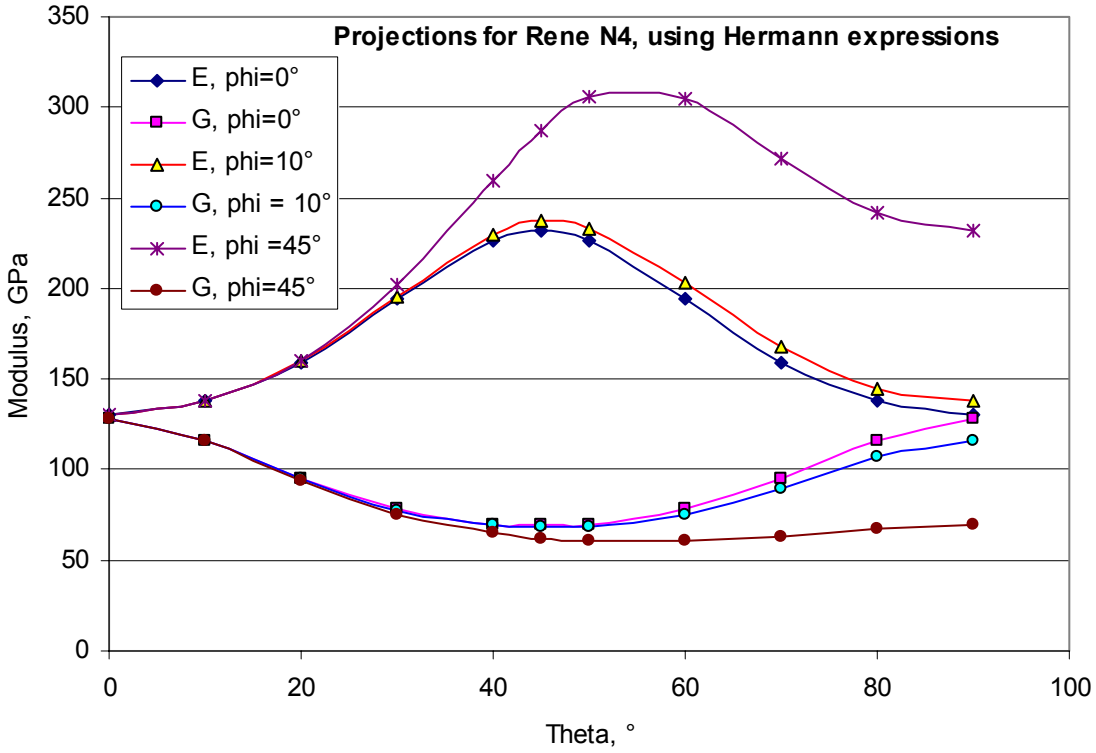

Figure 2: *Variation in Young's modulus and shear modulus with azimuthal and equatorial angle of direction relative to the crystallographic axes for alloy RENE N4 using compliance data from reference [3] and Hermann's formulation [1].*

4. For small angles of $\varphi < 25°$, the effect of φ on Young's modulus is negligible;
5. Shear modulus for twist about one of the crystallographic axes ($\theta = 0°$, $\varphi = 0°$) is a maximum;
6. Shear modulus drops with increasing angle θ to reach a minimum value at $\theta = 54°$, $\varphi = 45°$, *i.e.* [111] direction.

Modulus measurement

There are several ways of measuring the elastic moduli of anisotropic materials. Perhaps the simplest is to take a bar test-piece and determine its flexural and torsional mode resonances or natural frequencies, and to use the standard formulae to compute the effective axial modulus and effective shear modulus for twist about that axis. Standards have been prepared for these methods in ASTM, CEN and ISO, *e.g.* ASTM C1198, C1259, EN 843-2, ISO 17561. Alternatively, the ultrasonic pulse velocity can be measured and related to the moduli.

Provided that a sufficient number of test-pieces with different orientation angles are measured, it is possible then to use equations (1) and (2) to determine the tensor compliance values with a high level of accuracy. Note that round rods are preferred to avoid problems with the interpretation of torsional measurements. The use of rectangular section bars strictly requires knowledge of a third orientation angle.

Effect of alloy composition

As shown in Table 1, the effect of alloy composition on the tensor compliance values is a minor one, and most single-crystal nickel base superalloys seem to have similar behaviour.

Table 1: *Tensor compliance values from various sources*

Alloy	Tensor compliance values, GPa^{-1}			Source
	S_{11}	S_{12}	S_{44}	
CMSX486	0.007709	-0.002950	0.007773	NPL [5]
CM186LC	0.0077	-0.0037	0.0074	NPL [4]
Rene N4	0.007645	-0.002921	0.007828	Dandekar [3]
CMSX4	0.00795	-0.00290	0.00760	Hermann* [1] (* Note: these data have been read from plots)
CMSX6	0.00795	-0.00295	0.00770	
SRR99	0.00795	-0.00300	0.00780	

Table 2: *Example calculation of moduli from compliance tensor parameters*

Modulus calculation			CMSX486		s11	0.007986	c11	198.2578
Rods	Angles, °				s12	-0.00277	c12	105.2865
US convention	Alpha	-			s44	0.007619	c44	131.2508
UK convention	Theta	Rho	Angle function		s	0.006947		
Euler convention	Theta	Phi	J	2*J	4*J	E theory	Gtheory	
	0	0	0.0000	0.0000	0.0000	125.22	125.85	
	10	0	0.0292	0.0585	0.1170	131.93	114.23	
	20	0	0.1032	0.2066	0.4131	152.65	92.58	
	30	0	0.1875	0.3750	0.7500	185.84	76.16	
	40	0	0.2425	0.4849	0.9698	216.57	68.26	
	45	0	0.2500	0.5000	1.0000	221.59	67.30	
	50	0	0.2425	0.4849	0.9698	216.57	68.26	
	54	0	0.2261	0.4523	0.9045	206.42	70.43	
	60	0	0.1875	0.3750	0.7500	185.84	76.16	
	70	0	0.1033	0.2066	0.4132	152.65	92.58	
	80	0	0.0292	0.0585	0.1170	131.93	114.23	
	90	0	0.0000	0.0000	0.0000	125.22	125.85	

Example calculation of angle dependence of moduli

Table 2 is from an Excel spreadsheet designed to compute the angular dependence of moduli for given input crystallographic compliances. The strong orientation dependence is clear.

Effects of temperature

With rising temperature there is a monotonic drop in modulus. The effect is broadly similar for all nickel-based superalloys, as shown by some examples in Figure 3.

The temperature dependences of the tensor elastic compliances and elastic stiffness are shown in Table 3 for alloy CMSX486 in the form of polynomial fits. Also included in this table are the polynomial fits for the normalised change from room temperature of Young's modulus (E/E_{25}) and shear modulus (G/G_{25})for the near [001] direction. These data can be considered representative of many nickel-based alloys with an uncertainty of typically ±2%. Caution should be exercised in extrapolating these relationships beyond 900 °C, the limit of the modulus measurements.

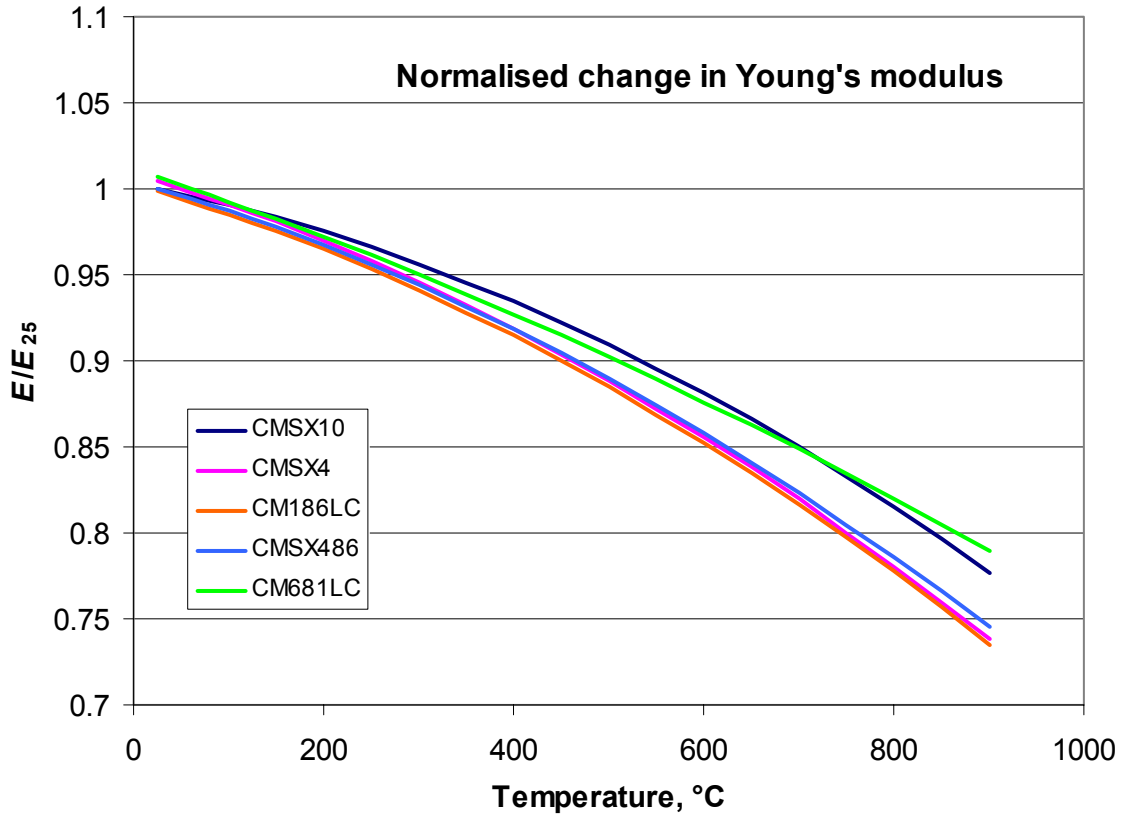

Figure 3: *Fractional change in Young's modulus close to the [001] direction as a function of temperature for several nickel-based alloys. Also included is the alloy CM681LC cast equiaxially.*

Table 3: *Polynomial fits of the compliance parameters, stiffness parameters, and near (001) axis modulus changes from 25 °C values as functions of temperature for alloy CMSX486*

Parameter	Polynomial function (T = temperature in °C)
S_{11}	+2.28042E-09 T^2 + 7.90394E-07 T + 7.62713E-03
S_{12}	-8.85389E-10 T^2 - 4.39668E-07 T - 2.76680E-03
S_{44}	+1.28059E-09 T^2 + 1.21277E-06 T + 7.37661E-03
C_{11}	-3.78195E-05 T^2 - 9.91763E-03 T + 2.24063E+02
C_{12}	-2.56446E-05 T^2 + 7.76370E-03 T + 1.27405E+02
C_{44}	-8.60735E-06 T^2 - 2.64720E-02 T + 1.35852E+02
E/E_{25}	-1.50578298E-07 T^2 - 1.565686E-04 T + 1.01640
G/G_{25}	-7.835196E-08 T^2 - 1.904995E-04 T + 1.00400

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