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DP-927

AEC RESEARCH AND DEVELOPMENT REPORT

TENSOR PROPERTIES OF ORIENTED METALS

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Printed in USA. Price $1.00
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664533

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Metals, Ceramics, and Materials
(TID-4500, 34th Ed.)

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October 1964

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CONTRACT AT(07-2)-1 WITH THE
UNITED STATES ATOMIC ENERGY COMMISSION

ABSTRACT

The theory for predicting anisotropic physical properties that result from preferred grain orientation was generalized, in analogy to the theory of linear homogeneous strain, to permit prediction of physical properties in all directions of the material from preferred orientation measurements in six or more directions. The theory is applicable to those properties that can be described to a first approximation by a second-order tensor, such as electrical resistivity, thermal coefficient of linear expansion, heat conductivity, thermal e.m.f., magnetic susceptibility, and irradiation growth.

CONTENTS

LIST OF TABLES AND FIGURES

Table

Figure

TENSOR PROPERTIES OF ORIENTED METALS

INTRODUCTION

In previous communications[1-5], a theory was developed for predicting anisotropic physical properties that result from preferred grain orientation in metals. The physical properties that were studied were thermal expansion coefficients[4] and irradiation growth[1,5].

The equations that were developed for predicting the physical properties were based on two assumptions:

(a) The properties of the polycrystalline aggregate were average values of the properties of the individual grains over all orientations. This assumption ignored interactions between grains, lattice distortions at the grain boundary, and any phenomena that occurred at the grain boundaries. The assumption must have been reasonably good, however, since the growth index, G_N,[5] and the thermal expansion coefficient, α_N,[4] which were derived by this simple averaging process indicated good agreement between theory and experiment, as shown by the data reproduced in Table I and Figure 1.

(b) The deformation was linear and homogeneous.

The grain orientation distribution, used in the equations for predicting physical properties, was expressed mathematically as a function, $P(u,\phi)$, where $P(u,\phi)$ is the number of grains whose crystallographic axes make angles (u,ϕ) with the direction in which the physical property is being predicted. The function $P(u,\phi)$ was synthesized from a set of measured relative diffraction intensities.[4]

The present report shows that the analogy to linear homogeneous strain tensor theory can be carried a step further; that is, one can develop a theory which will predict physical properties <u>in all directions</u> of a sample rather than <u>in a single direction</u> as has been the case to date.

This information was presented in abbreviated form at the 21st Pittsburgh Diffraction Conference (November 6, 7, 8, 1963) and in detailed form at the X-Ray Preferred Orientation Meeting held at the National Lead Company of Ohio (December 5, 6, 1963).

TABLE I

Calculated[a] Versus Measured Thermal Expansion Coefficient, α_N, for Alpha-Rolled Uranium Plate[4]

Direction	Measured α_N[7] (25 to 100°C)	Calculated α_N (25 to 100°C)
Longitudinal	9.2	9.07
Transverse	19.9	19.12
Normal	21.0	20.63

(a) Calculations were made using equation 4, i.e.,

$$\alpha_N = \alpha_a \int_0^1 \int_0^{\pi/2} P(u,\phi)(1-u^2)\sin^2\phi\,du\,d\phi + \alpha_b \int_0^1 \int_0^{\pi/2} P(u,\phi)(1-u^2)\cos^2\phi\,du\,d\phi + \alpha_c \int_0^1 \int_0^{\pi/2} P(u,\phi)u^2\,du\,d\phi$$

which assumes linear homogeneous deformation.

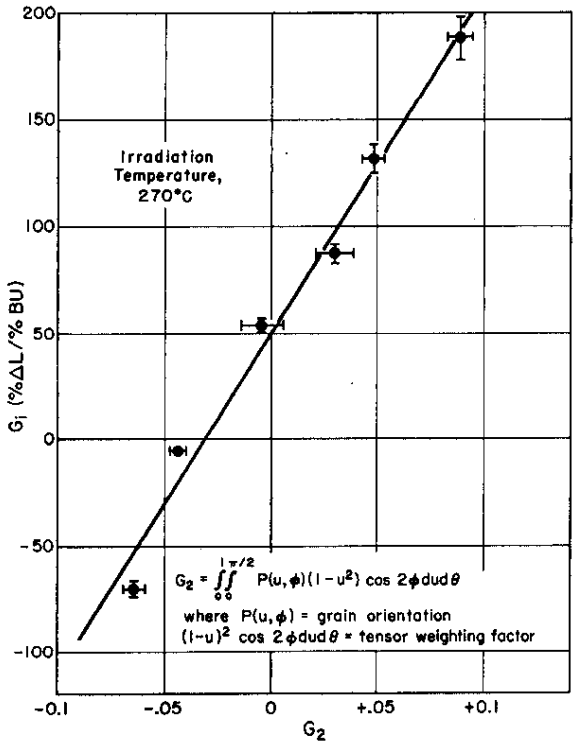

FIG. 1 GROWTH RATE, G_i, VERSUS G_2 FOR UNRESTRAINED URANIUM ROD[5]
(Irradiated in NaK Capsules)

SUMMARY

The theory for predicting anisotropy in physical properties due to grain orientation is generalized, in analogy to the theory of homogeneous strain, to permit the prediction of physical properties in all directions of the sample from preferred orientation measurements in six or more directions. Assuming no prior knowledge of the preferred orientation, the optimum six directions are those lying along the edges of an equilateral tetrahedron.

It is shown that if α_N represents the thermal expansion coefficient, for any direction N, then α_N is given by the symmetric tensor

$$\alpha_N = (a\ b\ c) \begin{pmatrix} \alpha_{11} & \alpha_{12} & \alpha_{13} \\ \alpha_{21} & \alpha_{22} & \alpha_{23} \\ \alpha_{31} & \alpha_{32} & \alpha_{33} \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix}$$

where a, b, and c are the direction cosines which the direction N makes with a set of orthogonal axes.

If $P(u,\phi)$ is measured for six or more directions, then α_N can be calculated for the six directions and the α_{ij} determined by matrix inversion from the above equation. A parallel treatment is valid for the growth index G_N.

The theory was tested on a section of hot-rolled uranium sheet on which preferred orientation measurements were made to determine α_N in 15 directions of the sheet. The α_N for six directions were used to determine the α_{ij}. The α_N calculated for all 15 directions from these α_{ij} were in good agreement with the measured values of α_N for the 15 directions. The α_{ij} are also determined from a least-squares fit of the data for all 15 directions. These α_{ij} give α_N which are in better agreement with the measured α_N than the α_{ij} determined from six directions.

An IBM-704 computer program was written which, beginning with the α_N and their corresponding direction cosines a, b, and c, computes the α_{ij}, the principal roots, the direction cosines of the principal axes, compares measured α_N with calculated α_N, and calculates the determinant of the matrix used to compute the α_{ij}, the correlation coefficient, and the standard deviation of the least-squares fit used to compute the α_{ij}.

DISCUSSION

DEVELOPMENT OF A GENERAL TENSOR FOR CALCULATING IRRADIATION GROWTH AND THERMAL EXPANSION COEFFICIENTS IN URANIUM

For the case of linear homogeneous elastic strain, the strain in any direction, N, can be represented by an equation for a surface of second degree,[6] i.e.,

$$\epsilon_N = \epsilon_{11}a^2 + \epsilon_{22}b^2 + \epsilon_{33}c^2 + 2\epsilon_{12}ab + 2\epsilon_{13}ac + 2\epsilon_{23}bc \quad (1)$$

where a, b, and c are the direction cosines of direction N; ϵ_{11}, ϵ_{22}, and ϵ_{33} are the normal strains; and ϵ_{12}, ϵ_{13}, and ϵ_{23} are the shear strains. Since there are only six strain coefficients, a knowledge of ϵ_N in six directions will permit solution of equation 1 for the ϵ_{ij} and thereby permit calculation of ϵ_N in any direction. A convenient form for expressing equation 1 is the symmetric tensor (i.e., $\epsilon_{ij} = \epsilon_{ji}$).

$$\epsilon_N = (a\ b\ c)\begin{pmatrix}\epsilon_{11} & \epsilon_{12} & \epsilon_{13}\\ \epsilon_{21} & \epsilon_{22} & \epsilon_{23}\\ \epsilon_{31} & \epsilon_{32} & \epsilon_{33}\end{pmatrix}\begin{pmatrix}a\\ b\\ c\end{pmatrix} \quad (2)$$

If the assumption is made that the nature of α_N and G_N is such that they can be described by an equation of the type employed to describe linear homogeneous deformation, i.e., equation 2, then

$$\alpha_N = (a\ b\ c)\begin{pmatrix}\alpha_{11} & \alpha_{12} & \alpha_{13}\\ \alpha_{21} & \alpha_{22} & \alpha_{23}\\ \alpha_{31} & \alpha_{32} & \alpha_{33}\end{pmatrix}\begin{pmatrix}a\\ b\\ c\end{pmatrix} \quad (3)$$

or $$\alpha_N = \alpha_{11}a^2 + \alpha_{22}b^2 + \alpha_{33}c^2 + 2\alpha_{12}ab + 2\alpha_{13}ac + 2\alpha_{23}bc \quad (4)$$

and

$$G_N = (a\ b\ c)\begin{pmatrix}G_{11} & G_{12} & G_{13}\\ G_{21} & G_{22} & G_{23}\\ G_{31} & G_{32} & G_{33}\end{pmatrix}\begin{pmatrix}a\\ b\\ c\end{pmatrix} \quad (5)$$

or $$G_N = G_{11}a^2 + G_{22}b^2 + G_{33}c^2 + 2G_{12}ab + 2G_{13}ac + 2G_{23}ac \quad (6)$$

As in the case of the strain tensor, the values of α_{ij} and G_{ij} may be determined in a straightforward fashion if six (or more) values of α_N and G_N are known. A given value of α_N or G_N is calculated from the equations[4,2]

$$\alpha_N = \left[\alpha_a \int_0^1 \int_0^{\pi/2} P(u,\phi)(1-u^2)\sin^2\phi \, du d\phi \right.$$

$$+ \alpha_b \int_0^1 \int_0^{\pi/2} P(u,\phi)(1-u^2)\cos^2\phi \, du d\phi \qquad (7)$$

$$\left. + \alpha_c \int_0^1 \int_0^{\pi/2} P(u,\phi) u^2 \, du d\phi \right] \div \int_0^1 \int_0^{\pi/2} P(u,\phi) \, du d\phi$$

and $$G_N = \left[\int_0^1 \int_0^{\pi/2} P(u,\phi)(1-u^2)\cos 2\phi \, du d\phi \right] \div \int_0^1 \int_0^{\pi/2} P(u,\phi) \, du d\phi \qquad (8)$$

where for each sample direction, N, a set of relative diffraction intensities are measured and these are used to synthesize a grain orientation distribution function $P(u,\phi)$.

Once the α_{ij} or G_{ij} are determined from six of the measured directions then α_N and G_N can be calculated directly from equations 3 and 5 for <u>any</u> desired direction. Regarding the selection of the six directions for measurement, they must be so chosen that the determinant of the coefficients of the α_{ij} is not equal to zero (for instance, no more than three directions may be coplanar). If no prior knowledge of the preferred orientation is assumed, the optimum six directions are those lying along the edges of an equilateral tetrahedron (Figure 2).

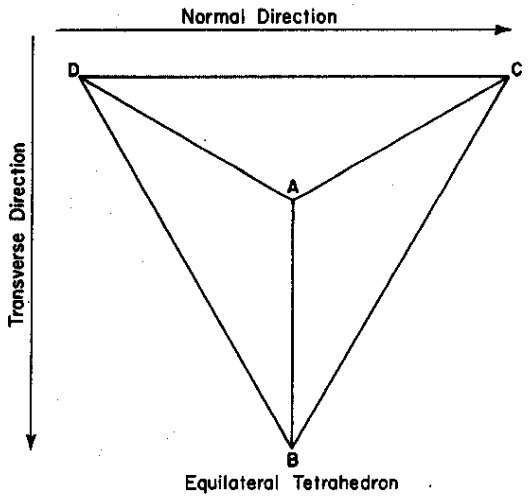

FIG. 2 DIRECTIONS FOR PREFERRED ORIENTATION MEASUREMENTS IN ROLLED URANIUM SHEET

It is well known that a set of coordinate axes can always be found in which the cross terms in a, b, and c of equation 1 will vanish, i.e.,

$$\epsilon_N = \epsilon_{11}a^2 + \epsilon_{22}b^2 + \epsilon_{33}c^2 \qquad (9)$$

We call these strains the principal strains (or principal roots) and the axes the principal axes. Similarly, for α_N and G_N

$$\alpha_N = \alpha_{11}a^2 + \alpha_{22}b^2 + \alpha_{33}c^2 \qquad (10)$$

and

$$G_N = G_{11}a^2 + G_{22}b^2 + G_{33}c^2 \qquad (11)$$

If the principal directions are known a priori, then α_N or G_N need be measured only along these principal directions to determine α_N or G_N in all directions.

COMPUTER PROGRAM FOR DETERMINING α_{ij} OR G_{ij}, AND FOR DETERMINING THE PRINCIPAL AXES

An IBM-704 computer program was already available[2] for computing α_N or G_N and these values along with the direction cosines provide the input data for the new IBM-704 computer program. The computer program employs matrix inversion to determine α_{ij}. If more than six α_N are fed in as data then a least-squares method is used to determine α_{ij}. Having determined α_{ij}, the computer then determines the principal axes and the principal roots. The format consists of input data, α_{ij}, calculated versus measured α_N, the correlation coefficient of the least-squares fit, the standard deviation, the value of the determinant of the matrix used in the computation of α_{ij}, the principal roots and the direction cosines of the principal roots. A typical format is shown as Table IV. The computer program is available at the Savannah River Laboratory.

EXPERIMENTAL PROCEDURE

The material selected for the experimental verification of the above treatment was a section of alpha-rolled uranium sheet. Samples were prepared as described in Reference 1 for 15 directions of the plate. To get the most uniform distribution for the first six directions, they were machined

along directions corresponding to the edges of an equilateral tetrahedron as illustrated in Figure 3. The other nine directions were chosen so as to require a minimum amount of additional machining. The techniques used to machine the samples are illustrated in Figure 3.

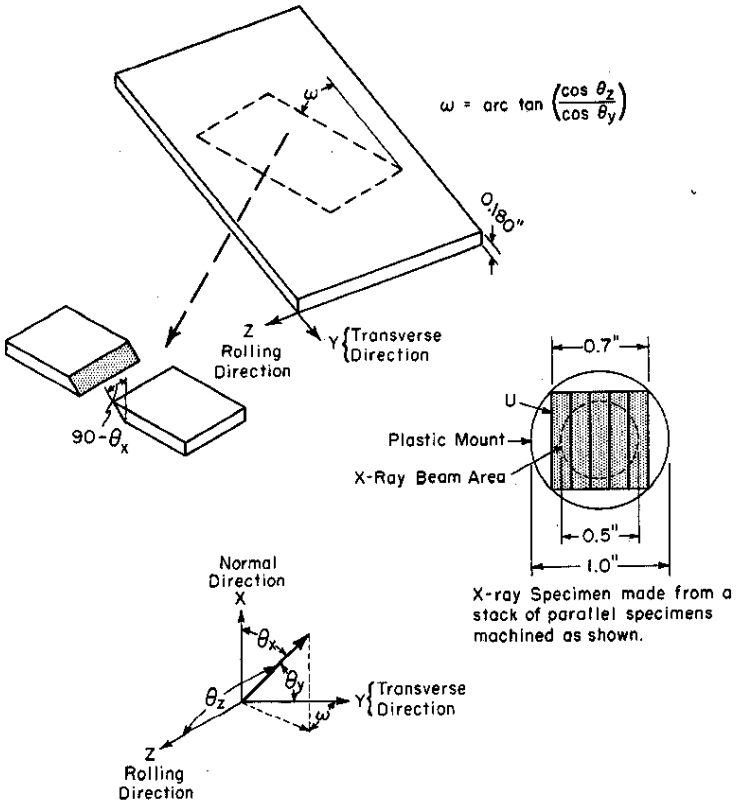

FIG. 3 METHOD OF MACHINING SPECIMENS

Prior to preparing the samples, 50 runs were made at different depths in the normal direction of the plate. The data showed a 0.005-inch texture gradient on the outer surfaces of the plate; these surfaces were ground off to remove the texture gradient before the samples were prepared for the final measurements.

The integrated diffraction intensities for 20 planes (hkl) of uranium were measured for each direction with an automated Norelco diffractometer and a scintillation detector. The planes used are given in Reference 2. Fifteen runs were made on each sample, at 15 different depths with mechanical and electropolishing at each depth. The 15 runs assured a sufficient statistical population of grains and care was taken to remove all cold work by electropolishing before each run. The 95% confidence interval of the mean of the measured values for each sample is given in Table III.

EXPERIMENTAL PROOF FOR THE GENERAL TENSOR

The validity of the assumption that α_N and G_N can be represented by a tensor of the same form as that used for linear homogeneous deformation was demonstrated by comparing the values of α_N and G_N obtained from the preferred orientation measurements using equations 7 and 8 with those calculated from equations 3 and 5. First, α_N and G_N were calculated from the $P(u,\phi)$ for each of the 15 directions. These are called measured α_N and G_N since each $P(u,\phi)$ is determined from a set of measured diffraction intensities from a particular direction in the sample. Six of the measured α_N and G_N were used to determine α_{ij} and G_{ij} (by matrix inversion). These values of G_{ij} and α_{ij} were then used to calculate α_N and G_N for the other nine directions using equations 3 and 5. The calculated and measured G_N and α_N are compared in Table II.

TABLE II

Calculated Versus Measured G_N and α_N for Alpha-Rolled Uranium Plate

(Six directions chosen along edges of equilateral tetrahedron)

Direction Cosines			G_N		α_N	
a	b	c	Measured	Calculated	Measured	Calculated
1.00000	0	0	-0.260	-0.260	18.50	18.50
-0.50000	-0.86603	0	-0.114	-0.114	19.07	19.07
0.50000	-0.86603	0	-0.118	-0.118	19.37	19.37
0	0.57738	-0.81649	0.145	0.145	13.46	13.47
0.50000	-0.28866	-0.81649	0.157	0.157	12.14	12.14
-0.50000	-0.28866	-0.81649	0.150	0.150	12.21	12.21
0	0	1.00000	0.331	0.308	8.91	9.42
0	1.00000	0	-0.064	-0.068	19.40	19.46
0	-0.81649	-0.57738	0.065	0.095	16.32	15.41
0	0.94284	-0.33326	-0.034	-0.051	18.71	18.81
0	0.3326	0.94284	0.271	0.291	10.48	10.07
-0.50000	0	-0.86603	0.176	0.162	11.54	11.78
-0.50000	0	0.86603	0.182	0.235	11.34	11.60
-0.50000	-0.86603	0	-0.116	-0.049	19.35	19.07
-0.50000	0	-0.86603	0.195	0.227	11.16	11.78
Range of deviation			0.004 to 0.067		0.06 to 0.91	
Average deviation			0.017		0.23	

NOTE: The "boxed" data were used to calculate the α_{ij} and G_{ij}. The G_N and α_N data listed under "Calculated" were calculated from these α_{ij} and G_{ij} using equations 3 and 5. The term "Measured α_N and G_N" means α_N and G_N calculated from equations 7 and 8 using the measured $P(u,\phi)$ distribution function.

The agreement between theory and experiment is good. As a further refinement all 15 directions were used to determine, by least-squares fitting, the best set of α_{ij} and G_{ij}. The measured and calculated α_N and G_N for these α_{ij} and G_{ij} are shown in Table III. The agreement is excellent.

TABLE III

Calculated Versus Measured G_N and α_N for Alpha-Rolled Uranium Plate

(Fifteen directions, includes the six directions employed in Table II)

Direction Cosines			G_N		α_N	
a	b	c	Measured	Calculated	Measured	Calculated
1.00000	0	0	-0.260	-0.252	18.50	18.32
-0.50000	-0.86603	0	-0.114	-0.117	19.07	19.27
0.50000	-0.86603	0	-0.118	-0.118	19.37	19.44
0	0.57738	-0.81649	0.145	0.170	13.47	12.97
0.50000	-0.28866	-0.81649	0.157	0.151	12.14	12.26
-0.50000	-0.28866	-0.81649	0.150	0.154	12.21	12.20
0	0	1.00000	0.331	0.318	8.91	9.21
0	1.00000	0	-0.064	-0.072	19.40	19.70
0	-0.81649	-0.57738	0.065	0.076	16.32	15.94
0	0.94284	-0.33326	-0.034	-0.041	18.71	18.71
0	0.33326	0.94284	0.271	0.287	10.48	10.21
-0.50000	0	-0.86603	0.176	0.177	11.54	11.49
-0.50000	0	0.86603	0.182	0.174	11.34	11.49
-0.50000	-0.86603	0	-0.116	-0.117	19.35	19.27
-0.50000	0	-0.86603	0.195	0.177	11.16	11.49
Average deviation			0.009		0.20	
Range of deviation			0 to 0.025		0 to 0.50	
Average 95% confidence limit of measured values			0.009		0.13	

NOTE: The "Measured α_N and G_N" were computed from equations 7 and 8 using the measured $P(u,\phi)$. The "Calculated α_N and G_N" were computed from equations 3 and 5. The α_{ij} and G_{ij} used in equations 3 and 5 were determined by least squares from all 15 measured α_N and G_N.

Hence, α_N and G_N have been shown to have a tensor form which can be described by an equation of the second degree. Although measurements in only an arbitrary six directions are needed to determine the coefficients, α_{ij} and G_{ij}, of the equations, comparison of Tables II and III shows that the more directions one measured the greater the precision of α_{ij} and G_{ij}.

GEOMETRICAL DESCRIPTION OF THE THERMAL EXPANSION COEFFICIENT TENSOR FOR ALPHA-ROLLED PLATE

If the coordinate axes are taken in the direction of the principal axes, then equation 4 reduces to equation 10 and

$$x = \alpha_{11}a, \quad y = \alpha_{22}b, \quad \text{and } z = \alpha_{33}c$$

where x, y, and z are the principal axes and α_{11}, α_{22}, and α_{33} are the principal roots.

Putting these values for a, b, and c into the identity relation for the direction cosines, $a^2 + b^2 + c^2 = 1$, we obtain

$$\frac{x^2}{\alpha_{11}^2} + \frac{y^2}{\alpha_{22}^2} + \frac{z^2}{\alpha_{33}^2} = 1 \qquad (12)$$

which is the equation of an ellipsoid when α_{11}, α_{22}, and α_{33} are all positive. The principal roots α_{11}, α_{22}, and α_{33} for alpha-rolled plate, given in Table IV, are all positive. For this condition, the surface is an ellipsoid as shown in Figure 4. The principal directions are nearly coincident with the fabrication directions. The thermal expansion coefficient for any direction in the plate may be obtained from Figure 4 by constructing a vector from the origin, in the given direction, to the surface of the ellipsoid. The length of the vector is the thermal expansion coefficient α_N. For the plate studied, the α_N is minimum in the rolling direction and about equal in the transverse and normal directions.

TABLE IV

Computer Format Used for Calculating the General Tensor

Input Data				
	Direction Cosines			
G_N	a	b	c	α_{ij}
18.50000	1.00000	0.	0.	α_{11} 0.18317377E 02
19.07000	-0.50000	-0.86603	0.	α_{22} 0.19699620E 02
19.37000	0.50000	-0.86603	0.	α_{33} 0.92141126E 01
13.47000	0.	0.57738	-0.81649	α_{12} -0.10021067E-00
12.14000	0.50000	-0.28866	-0.81649	α_{13} -0.22868335E-02
12.21000	-0.50000	-0.28866	-0.81649	α_{23} -0.27611174E-00
8.91000	0.	0.	1.00000	
19.40000	0.	1.00000	0.	
16.32000	0.	-0.81649	-0.57738	
18.71000	0.	0.94284	-0.33326	
10.48000	0.	0.33326	0.94284	
11.54000	-0.50000	0.	-0.86603	
11.34000	-0.50000	0.	0.86603	
19.35000	-0.50000	-0.86603	0.	
11.16000	-0.50000	0.	-0.86603	

Statistics	
Observations	15
Cor. Coeff.	0.99987408
Stand. Dev.	0.33200252E-11
Determinant	0.55349638E 03

Respectively Actual and Fitted Values					
18.50000	18.31738	19.07000	19.26743	19.37000	19.44100
13.47000	12.97019	12.14000	12.26409	12.21000	12.20250
8.91000	9.21411	19.40000	19.69962	16.32000	15.94422
18.71000	18.70878	10.48000	10.20523	11.54000	11.48802
11.34000	11.49198	19.35000	19.26743	11.16000	11.48802

Principal Roots		Direction Cosines for Principal Axes			
1	0.18310224E 02	Root (1)	-0.99744	-0.07146	0.00242
2	0.92068437E 01	Root (2)	0.00064	0.02631	0.99965
3	0.19714042E 02	Root (3)	0.07129	-0.99711	0.02621

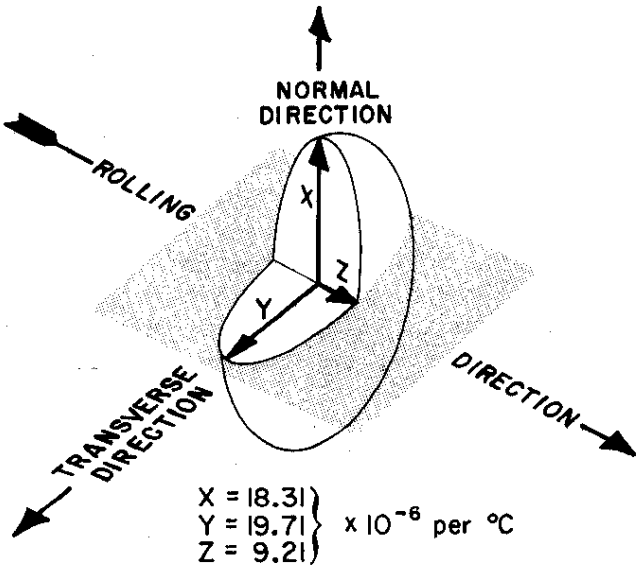

FIG. 4 STRAIN TENSOR FOR THERMAL EXPANSION COEFFICIENT OF ALPHA-ROLLED URANIUM PLATE

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