

An American National Standard

IEEE Standard on Piezoelectricity

Sponsor
**Standards Committee
of the
IEEE Ultrasonics, Ferroelectrics, and Frequency Control Society**

Approved March 12, 1987

IEEE Standards Board

Approved September 7, 1987

American National Standards Institute

© Copyright 1988 by

The Institute of Electrical and Electronics Engineers, Inc

345 East 47th Street, New York, NY 10017, USA

No part of this publication may be reproduced in any form, in an electronic retrieval system or otherwise, without the prior written permission of the publisher.

IEEE Standards documents are developed within the Technical Committees of the IEEE Societies and the Standards Coordinating Committees of the IEEE Standards Board. Members of the committees serve voluntarily and without compensation. They are not necessarily members of the Institute. The standards developed within IEEE represent a consensus of the broad expertise on the subject within the Institute as well as those activities outside of IEEE which have expressed an interest in participating in the development of the standard.

Use of an IEEE Standard is wholly voluntary. The existence of an IEEE Standard does not imply that there are no other ways to produce, test, measure, purchase, market, or provide other goods and services related to the scope of the IEEE Standard. Furthermore, the viewpoint expressed at the time a standard is approved and issued is subject to change brought about through developments in the state of the art and comments received from users of the standard. Every IEEE Standard is subjected to review at least once every five years for revision or reaffirmation. When a document is more than five years old, and has not been reaffirmed, it is reasonable to conclude that its contents, although still of some value, do not wholly reflect the present state of the art. Users are cautioned to check to determine that they have the latest edition of any IEEE Standard.

Comments for revision of IEEE Standards are welcome from any interested party, regardless of membership affiliation with IEEE. Suggestions for changes in documents should be in the form of a proposed change of text, together with appropriate supporting comments.

Interpretations: Occasionally questions may arise regarding the meaning of portions of standards as they relate to specific applications. When the need for interpretations is brought to the attention of IEEE, the Institute will initiate action to prepare appropriate responses. Since IEEE Standards represent a consensus of all concerned interests, it is important to ensure that any interpretation has also received the concurrence of a balance of interests. For this reason IEEE and the members of its technical committees are not able to provide an instant response to interpretation requests except in those cases where the matter has previously received formal consideration.

Comments on standards and requests for interpretations should be addressed to:

Secretary, IEEE Standards Board
345 East 47th Street
New York, NY 10017
USA

Foreword

(This Foreword is not a part of ANSI/IEEE Std 176-1987, IEEE Standard on Piezoelectricity.)

The document presented herein is a revision of ANSI/IEEE Std 176-1978 which, in turn, had as its antecedents four earlier standards on piezoelectricity. These earlier standards were prepared within the Standards Committee framework of the IRE and later carried over and published as IEEE Standards: IEEE Std 176-1949 (R1971), Standards on Piezoelectric Crystals; IEEE Std 177-1978, Standard Definitions and Methods of Measurement for Piezoelectric Vibrators; IEEE Std 178-1958 (R1972), Standards on Piezoelectric Crystals: Determination of the Elastic, Piezoelectric, and Dielectric Constants—The Electromechanical Coupling Factor; and IEEE Std 179-1961 (R1971), Standards on Piezoelectric Crystals: Measurements of Piezoelectric Ceramics.

The relationship of ANSI/IEEE Std 176-1978 to the earlier standards cited above can be summarized as follows: ANSI/IEEE Std 176-1978 replaced IEEE Std 176-1959 and IEEE Std 178-1958. IEEE Std 177-1966 has continued in force up to the time this Foreword was written. IEEE Std 179-1961 has been allowed to lapse.

When ANSI/IEEE Std 176-1978 was written, the subcommittee that prepared it wanted to produce a standard that would be useful to persons doing analytical work as well as to those working with materials and designing devices. A large number of professionals within IEEE were then working in activities that involved extensive application of computer programs for computer-aided design and analysis. With this in mind, a heavy emphasis was placed on providing the analytical basis for piezoelectric formulations and for bringing definitions of angles and axes into agreement with those widely used in mathematical analysis. This thinking lay behind the sign changes associated with the angles for quartz. The same point of view is also the reason for the use of a right-handed coordinate system to describe both right-handed and left-handed quartz. Consequently, ANSI/IEEE Std 176-1978 attempted to introduce three major changes relative to the practices recommended in earlier standards:

(1) Use of a separate sign convention for the piezoelectric constants of quartz was abandoned. Over the years, in the course of its rise to prominence as the most important piezoelectric material, a number of different sign conventions have been associated with quartz. In order to bring the sign conventions for the constants of quartz into agreement with those used for other materials, the subcommittee decided in favor of changing the convention one more time.

(2) In part, some of the proliferation of sign conventions used with quartz was caused by the fact that quartz is an enantiomorphous material existing commonly in left-handed and right-handed forms. A second important change introduced by ANSI/IEEE Std 176-1978 was to abandon the practice of using a left-handed coordinate system with left-handed quartz and a right-handed coordinate system with right-handed quartz, using instead a right-handed coordinate system to specify the material constants for both forms of quartz and for any other enantiomorphous material. This decision was prompted by the desirability of preserving the sign conventions for vector and tensor quantities when doing analyses of device-related physical phenomena.

(3) Definitions of electromechanical coupling factors based on interaction energies were abandoned. In ANSI/IEEE Std 176-1978, when a piezoelectric solid having a simple shape was used dynamically as a singly resonant element, the material coupling factors were defined as they arose naturally in analytical solutions for electrically driven vibrations. On the other hand, when the piezoelectric solid was used essentially statically as part of a large resonant structure, the definitions of material coupling factors were based on ratios defined in terms of quantities arising in prescribed stress-strain cycles.

The three major changes in recommended practices, as described previously, have been continued in the present standard, even though the new sign conventions for quartz have not in the meantime gained much acceptance by the device industry using crystalline quartz.

This revision has left the basic content and structure of ANSI/IEEE Std 176-1978 unchanged. The following list of sections is given with the purpose of summarizing the contents of the sections and providing a brief indication of the changes that have been made.

Section 1. Introduction—1.1 contains a statement of the scope of the standard; 1.2 contains a discussion of units, and Table 1, which is a list of symbols and their units; and 1.3 lists references.

Section 2. Linear Theory of Piezoelectricity—This section provides a concise review of the physical quantities, theoretical concepts, and mathematical relationships basic to the linear theory of piezoelectricity. This section is essentially unchanged.

Section 3. Crystallography Applied to Piezoelectric Crystals—A large part of the material in this section was first presented in IEEE Std 176-1949 and 178-1958 and substantially revised when included in ANSI/IEEE Std 176-1978. A number of changes have been made in this section. Several errors in Table 3, “Summary of Crystal Systems,” all having to do with the point group symbols for the cubic system, have been corrected. The subsection 3.2.5.1, Application to Quartz, has been rewritten to clarify the relationship of the sign conventions of the present standard to those used in IEEE Std 176-1949. A major omission of the subcommittee that prepared ANSI/IEEE Std 176-1978 was a table showing all the piezoelectric, dielectric, and elastic constants for both right-handed and left-handed quartz in a right-handed coordinate system. This should have been done because quartz has been and continues to be the most important piezoelectric material for technological and commercial applications, and because quartz exists commonly in both forms. This oversight has been corrected by the inclusion of Table 6, “Elasto-Piezo-Dielectric Matrices for Right- and Left-Handed Quartz.” To further supplement the information on quartz and the conventions associated with rotated cuts, Table 7, entitled “Elasto-Piezo-Dielectric Matrix for Right-Handed Quartz,” has been added and Fig 6, entitled “Illustration of a Doubly Rotated Quartz Plate, the SC Cut, Having the Notation $(YXw/l) 22.4^\circ/-33.88^\circ$,” has been included. Fig 5 in the 1978 version of this standard showed a GT cut of quartz as an example of a doubly rotated cut and had an error in the drawing. This error has been corrected.

Section 4. Wave and Vibration Theory—This section presents the results of analyses for plane wave motions and vibrations in piezoelectric solids. The reader primarily interested in doing laboratory measurements need not be concerned with the mathematical details of this section; however, this section does contain several cautionary remarks of importance when resonator theory is used to interpret experimental results. An important reason for including this section in the standard is that the analyses shown lead naturally to the definitions of electromechanical coupling factors for a number of cases of practical interest. In addition, this section provides the equations used in deriving numerical results from the experimental techniques discussed in Section 5. Several of the equations in this section have been changed to correct sign errors that appeared in the 1978 version.

Section 5. Simple Homogeneous Static Solutions—This section presents the equations applicable for quasi-static mechanical behavior and provides definitions of quasi-static material coupling factors. No changes have been made in this section.

Section 6. Measurement of Elastic, Piezoelectric, and Dielectric Constants—This section presents a brief review of the measuring techniques and the important equations used to determine the electroelastic constants characterizing piezoelectric materials. It includes a presentation of methods employing pulse-echo techniques and high overtone modes as well as the more conventional fundamental-mode resonator techniques. It replaces the earlier treatment of measurement techniques contained in IEEE Std 178-1958. The range of applicability of the measuring techniques and the advantages and disadvantages associated with the different methods are discussed. The definition of f_p , originally defined in IEEE Std 177-1966 for the simple equivalent circuit as the parallel resonance frequency, is generalized to cover the case of materials with high coupling factors. No changes have been made in this section.

Section 7. Bibliography—Except for a few minor changes, the Bibliography remains essentially the same as in IEEE Std 176-1978.

ANSI/IEEE Std 176-1978 was prepared during the period from 1967 to 1978. The members of the Subcommittee on Piezoelectric Crystals who participated in this work over this period were the following:

A. H. Meitzler, *Chair*

D. Berlincourt
G. A. Coquin

F. S. Welsh, III

H. F. Tiersten
A. W. Warner

The credits for the primary authorship of the various sections are as follows:

Section 1.: A. H. Meitzler

Section 2.: H. F. Tiersten

Section 3.: A. W. Warner, D. Berlincourt, A. H. Meitzler, and H. F. Tiersten

Section 4.: H. F. Tiersten

Section 5.: D. Berlincourt

Section 6.: G. A. Coquin and F. S. Welsh, III

In addition to the names mentioned above, there were others who were associated with the subcommittee at various times during the period in which this standard was prepared and who made valuable contributions to the work of the subcommittee. Those whose names should be mentioned here include R. Bechmann, J.L. Bleustein, E.M. Frymoyer, and R.T. Smith. The preparation of the final draft of ANSI/IEEE Std 176-1978 benefited greatly from the coordination of activities and the moderation of differences of opinion accomplished by J. E. May, who in 1977 served as the Chairman of the IEEE Technical Committee on Transducers and Resonators.

The present version of this document was begun in 1985 and completed review during 1986. The draft of the revised standard was prepared by A. H. Meitzler with the help of contributions from A. Ballato and H. F. Tiersten and with the additional help of a list of suggested changes and comments compiled by T. R. Meeker. The members of the IEEE Subcommittee on Piezoelectric Crystals who participated in the review process at the time were as follows:

T. R. Meeker, *Chair*

A. Ballato (ex officio)
D. T. Bell
E. Hafner

W. H. Horton
J. A. Kusters
A. H. Meitzler
R. C. Smythe

H. F. Tiersten
W. L. Smith
A. W. Warner

The following persons were on the balloting committee that approved this document for submission to the IEEE Standards Board:

A. Ballato
D. C. Bradley
L. N. Dworsky
W. H. Horton

J. A. Kusters
T. R. Meeker
A. H. Meitzler
B. K. Sinha

R. C. Smythe
W. L. Smith
H. F. Tiersten
A. W. Warner

When the IEEE Standards Board approved this standard on March 12, 1987, it had the following membership:

Donald C. Fleckenstein, *Chair*
Marco W. Migliaro, *Vice Chair*
Sava I. Sherr, *Secretary*

James H. Beall
Dennis Bodson
Marshall L. Cain
James M. Daly
Stephen R. Dillon
Eugene P. Fogarty
Jay Forster
Kenneth D. Hendrix
Irvin N. Howell

Leslie R. Kerr
Jack Kinn
Irving Kolodny
Joseph L. Koepfinger*
Edward Lohse
John May
Lawrence V. McCall
L. Bruce McClung

Donald T. Michael*
L. John Rankine
John P. Riganati
Gary S. Robinson
Frank L. Rose
Robert E. Rountree
William R. Tackaberry
William B. Wilkens
Helen M. Wood

*Member emeritus

CLAUSE	PAGE
1. Introduction	1
1.1 Scope	1
1.2 Symbols and Units	1
1.3 References	2
2. Linear Theory of Piezoelectricity.....	4
2.1 General	4
2.2 Mechanical Considerations	4
2.3 Electrical Considerations	5
2.4 Linear Piezoelectricity	6
2.5 Boundary Conditions	9
2.6 Alternate Forms of Constitutive Equations.....	10
3. Crystallography Applied to Piezoelectric Crystals	11
3.1 General	11
3.2 Basic Terminology and the Seven Crystal Systems.....	11
3.3 Conventions for Axes.....	17
3.4 Elasto-Piezo-Dielectric Matrices for All Crystal Classes	21
3.5 Use of Static Piezoelectric Measurements to Establish Crystal Axis Sense.....	22
3.6 System of Notation for Designating the Orientation of Crystalline Bars and Plates	25
4. Wave and Vibration Theory	29
4.1 General	29
4.2 Piezoelectric Plane Waves	29
4.3 Thickness Excitation of Thickness Vibrations.....	30
4.4 Lateral Excitation of Thickness Vibrations.....	34
4.5 Low-Frequency Extensional Vibrations of Rods.....	35
4.6 Radial Modes in Thin Plates	39
5. Simple Homogeneous Static Solutions	41
5.1 General	41
5.2 Applicable Equations	42
5.3 Applicability of Static Solutions in the Low-Frequency Range (Quasistatic).....	44
5.4 Definition of Quasistatic Material Coupling Factors	44
5.5 Nonlinear Low-Frequency Characteristics of Ferroelectric Materials (Domain Effects).....	45
6. Determination of Elastic, Piezoelectric, and Dielectric Constants	46
6.1 General	46
6.2 Dielectric Constants	47
6.3 Static and Quasistatic Measurements	47
6.4 Resonator Measurements	49
6.5 Measurement of Plane-Wave Velocities	59
6.6 Temperature Coefficients of Material Constants	63
7. Bibliography.....	64

An American National Standard

IEEE Standard on Piezoelectricity

1. Introduction

1.1 Scope

This standard on piezoelectricity contains many equations based upon the analysis of vibrations in piezoelectric materials having simple geometrical shapes. Mechanical and electrical dissipation are never introduced into the theoretical treatment, and except for a brief discussion of nonlinear effects in Section 5., all the results are based on linear piezoelectricity in which the elastic, piezoelectric, and dielectric coefficients are treated as constants independent of the magnitude and frequency of applied mechanical stresses and electric fields.

Real materials involve mechanical and electrical dissipation. In addition, they may show strong nonlinear behavior, hysteresis effects, temporal instability (aging), and a variety of magneto-mechano-electric interactions. For example, poled ferroelectric ceramics, commonly called piezoelectric ceramics, are a class of materials of major importance in commercial applications; yet because of the presence of ferroelectric domains, they exhibit a variety of nonlinearities and aging effects which are not within the scope of this standard. Although this standard does not treat nonlinear or aging effects in ceramics, it does present the equations commonly used to determine the piezoelectric properties of poled ceramic materials and uses the elastoelectric matrices of the equivalent crystal class ($6mm$) in a number of examples.

It is not possible to state concisely a specific set of conditions under which the definitions and equations contained in this standard apply. In many cases of practical interest mechanical dissipation is the most important limitation on the validity of an analysis carried out for an ideal piezoelectric material. ANSI/IEEE Std 177-1966 [5]¹ discusses in detail the electrical characteristics of resonators made of materials with mechanical losses and the simple equivalent circuit that can be used to represent these resonators in a frequency range near fundamental resonance. Section 6. of this standard also provides discussion of the bounds imposed on the application of this standard to real materials. In brief, measurements based on this standard will be most meaningful when they are carried out on piezoelectric materials with small dissipations and negligible nonlinearities, like single-crystal dielectric solids or high-coupling-factor ceramics.

1.2 Symbols and Units

All equations and physical constants appearing in this standard are written in the International System of Units (SI units), according to ANSI/IEEE Std 268-1982 [2]. Table 1 lists many of the symbols used and, where appropriate, shows the units associated with the physical quantities designated by the symbols.

¹The numbers in brackets correspond to those of the references listed in 1.3; when preceded by B, they correspond to the bibliography in Section 7.

1.3 References

This standard is written to be a self-contained document useful to the reader without requiring other standards to be at hand. However, the reader may find that standards covering other related specialized topics, such as dielectric materials, piezoelectricity, and piezomagnetism may aid implementation of this standard. A list of these related references is given here.

[1] ANSI/EIA 512-1985, Standard Methods for Measurement of the Equivalent Electrical Parameters of Quartz Crystal Units, 1 kHz to 1 GHz.²

[2] ANSI/IEEE Std 268-1982, American National Standard Metric Practice.³

[3] ASTM D150-87, Tests for AC-Loss characteristics and Dielectric Constant (Permittivity) of Solid Electrical Insulating Materials.⁴

[4] IEC 444 (1973), Basic Method for the Measurement of Resonance Frequency and Equivalent Series Resistance of Quartz Crystal Units by Zero-Phase Technique in a π -Network.⁵

[5] IEEE Std 177-1978, Standard Definitions and Methods of Measurement for Piezoelectric Vibrators.

[6] IEEE Std 178-1958 (R1972), Standards on Piezoelectric Crystals: Determination of the Elastic, Piezoelectric, and Dielectric Constants of Piezoelectric Crystals—The Electromechanical Coupling Factor.

[7] IEEE Std 179-1961 (R1971), Standards on Piezoelectric Crystals: Measurements of Piezoelectric Ceramics.

[8] IEEE Std 319-1971, IEEE Standard on Magnetostrictive Materials: Piezomagnetic Nomenclature.

²ANSI/EIA publications can be obtained from the Sales Department, American National Standards Institute, 1430 Broadway, New York, NY 10018, or from the Standards Sales Department, Electronic Industries Association, 2001 I Street, NW, Washington, DC 20006.

³IEEE publications can be obtained from the Service Center, The Institute of Electrical and Electronics Engineers, 445 Hoes Lane, PO Box 1331, Piscataway, NJ 08855-1331.

⁴ASTM documents are available from American Society for Testing and Materials, 1916 Race Street, Philadelphia, PA 19103.

⁵IEC documents are available in the US from the Sales Department, American National Standards Institute, 1430 Broadway, New York, NY 10018.

Table 1—List of Symbols and Their Units

Symbol	Meaning	SI Unit
a, b, c	Natural axes of crystal	meter
a	Radius of a disk	meter
c_{ijkl}, c_{pq}	Elastic stiffness constant	newton per square meter
C	Capacitance	farad
C_0	Shunt capacitance in resonator equivalent circuit	farad
C_1	Series capacitor in resonator equivalent circuit	farad
d_{ijk}, d_{ip}	Piezoelectric constant	meter per volt = coulomb per newton
D (superscript)	At constant electric displacement	
D_i	Electric displacement component	coulomb per square meter
e_{ijk}, e_{ip}	Piezoelectric constant	coulomb per square meter
E (superscript)	At constant electric field	volt per meter
E_i	Electric field component	volt per meter
f	Frequency	hertz
f_1	Lower critical frequency, maximum admittance (lossless)	hertz
f_2	Upper critical frequency, maximum impedance (lossless)	hertz
f_a	Antiresonance frequency (zero reactance)	hertz
f_r	Resonance frequency (zero susceptance)	hertz
f_m	Frequency of maximum impedance	hertz
f_n	Frequency of minimum impedance	hertz
f_p	Frequency of maximum resistance	hertz
f_s	Frequency of maximum conductance	hertz
Δf	$f_p - f_s$	hertz
g_{ijk}, g_{ip}	Piezoelectric constant	volt meter per newton = square meter per coulomb
H	Electromechanical enthalpy density	joule per cubic meter
h_{ijk}, h_{ip}	Piezoelectric constant	volt per meter = newton per coulomb
$J_1(z)$	Modified quotient of cylinder functions (Eq 112)	
k_{31}^l	Rod extensional coupling factor with transverse excitation	
k_{33}^l	Rod extensional coupling factor with longitudinal excitation	
k_{15}^t	Thickness-shear coupling factor	
k_{33}^t	Thickness-extensional coupling factor	
k_p	Planar coupling factor	
l	Length	meter
L_1	Series inductance in resonator equivalent circuit	henry
M	Resonator figure of merit	
m	Mirror or reflection plane in a crystal	
n_i	Outwardly directed unit normal	
R_1	Series resistance in resonator equivalent circuit	ohm
s_{ijkl}, s_{pq}	Elastic compliance constant	square meter per newton
S	An arbitrary surface	square meter

Symbol	Meaning	SI Unit
S (superscript)	At constant strain	
S_{ij}, S_p	Strain component	
T (superscript)	At constant stress	
T_i	Traction vector component	newton per square meter
t	Thickness	meter
T_{ij}, T_p	Stress component	newton per square meter
v	Velocity	meter per second
w	Width	meter
X, Y, Z	Rectangular axes of a crystal	meter
x_i	Rectangular coordinate axis	meter
X	Electric circuit reactance	ohm
Y	Electric circuit admittance	siemens
Z	Electric circuit impedance	ohm
α, β, γ	Angles between crystallographic axes	second
β_{ij}	Impermittivity components	meter per farad
ϵ_0	Permittivity of free space	farad per meter
ϵ_{ij}	Permittivity component	farad per meter
Γ	Motional capacitance constant	farad per meter
θ	Temperature	kelvin
ρ	Mass density	kilogram per cubic meter
σ	Entropy	joule per kelvin
σ	Planar Poisson's ratio	
τ	Time	second
ϕ	Scalar electric potential	volt
ϕ, Θ, Ψ	Angles used in rotational symbol	
ω	Angular frequency ($2\pi f$)	hertz

2. Linear Theory of Piezoelectricity

2.1 General

In linear piezoelectricity the equations of linear elasticity are coupled to the charge equation of electrostatics by means of the piezoelectric constants. However, the electric variables are not purely static, but only quasistatic, because of the coupling to the dynamic mechanical equations. Thus, in order to provide an appropriate theoretical basis for the material covered in this standard, the relevant mechanical and electrical field variables will be briefly defined and the pertinent mechanical and electrical equations presented in this section.

2.2 Mechanical Considerations

The Cartesian components of the infinitesimal mechanical displacement of a material point are denoted by u_i .

NOTE — Cartesian tensor notation is used throughout this standard. See Jeffreys [B1]. For a more complete discussion of mechanical displacement, see Tiersten ([B2], Chapter 3, Section 1.).

The symmetric portion of the spatial gradient of the mechanical displacement determines the strain tensor S_{ij} .

NOTE — A comma followed by an index denotes partial differentiation with respect to a space coordinate.

Thus,

$$S_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}) \quad (1)$$

where

$$u_{i,j} = \partial u_i / \partial x_j$$

The antisymmetric portion of the mechanical displacement gradient determines the infinitesimal local rigid rotation ([B2], Chapter 3, Section 2.), which is allowed to take place without constraint in the continuum, and is of no consequence in this standard. The velocity of a point of the continuum is given by

$$v_i = \dot{u}_i = \partial u_i / \partial \tau \quad (2)$$

where τ denotes the time. The mass per unit volume is denoted by ρ , which will be a constant for any material throughout this standard.

The mechanical interaction between two portions of the continuum, separated by an arbitrary surface S , is assumed to be given by the traction vector, which is defined as the force per unit area T_i acting across a surface at a point and dependent on the orientation of the surface at the point.

NOTE — For a more complete discussion of traction, see ([B2], Chapter 2, Section 1.).

In fact the existence of the traction vector and the integral form of the equations of the balance of linear momentum determine ([B2], Chapter 2, Section 2.) the existence of the stress tensor T_{ij} , which is related to the traction vector T_j by the relation

$$T_j = n_i T_{ij} \quad (3)$$

where n_i denotes the components of the outwardly directed unit normal to the surface across which the traction vector acts. Clearly, T_{ij} is a second-rank tensor.

NOTE — The summation convention for repeated tensor indices is employed throughout. See [B1], Chapter 1.

From Eq 3 and the integral forms of the equations of the balance of linear momentum result the stress equations of motion:

$$T_{ij,i} = \rho \ddot{u}_j \quad (4)$$

where, from the conservation of angular momentum, the stress tensor T_{ij} is symmetric.

In linear theory the components of the vectorial flux of mechanical energy across a surface are given by $(-T_{ij})$.

2.3 Electrical Considerations

In piezoelectric theory the full electromagnetic equations are not usually needed. The quasielectrostatic approximation is adequate because the phase velocities of acoustic waves are approximately five orders of magnitude less than the velocities of electromagnetic waves.

NOTE — For more detail concerning the nature and limitations of the approximation, see ([B2], Chapter 4, Section 4.).

Under these circumstances magnetic effects can be shown to be negligible compared to electrical effects. In electrical theory the Cartesian components of the electric field intensity and electric displacement are denoted, respectively, by E_i and D_i . In MKS units these two vectors are related to each other by

$$D_i = \epsilon_0 E_i + P_i \quad (5)$$

where P_i denotes the components of the polarization vector, and the permittivity of free space ϵ_0 is given by

$$\epsilon_0 = 8.854 \cdot 10^{-12} \text{ F/m} \quad (6)$$

The electric field vector E_i is derivable from a scalar electric potential φ :

$$E_i = -\varphi, i \quad (7)$$

The electric displacement vector D_i satisfies the electrostatic equation for an insulator,

$$D_{i,i} = 0 \quad (8)$$

It should be noted that although the electric field equations appear to be static, they are time dependent because they are coupled to the dynamic mechanical equations presented in 2.2. The time-dependent vector flux of electrical energy across a surface is given by $(+ \varphi_i)$, which is the degenerate form taken by the Poynting vector in the quasistatic electric approximation.

NOTE — For details concerning the derivation of the degenerate form of the Poynting vector for the quasistatic electric field, see ([B2], Chapter 4, Sections 3. and 4.).

2.4 Linear Piezoelectricity

The conservation of energy ([B2], Chapter 5, Sections 1.–3.) for the linear piezoelectric continuum results in the first law of thermodynamics:

$$\dot{U} = T_{ij}\dot{S}_{ij} + E_i\dot{D}_i \quad (9)$$

where U is the stored energy density for the piezoelectric continuum. The electric enthalpy [B3] density H is defined by

$$H = U - E_i D_i \quad (10)$$

and from Eqs 9 and 10 there results

$$\dot{H} = T_{ij}\dot{S}_{ij} - D_i\dot{E}_i \quad (11)$$

Eq 11 implies

$$H = H(S_{kp}, E_k) \quad (12)$$

and from Eqs 11 and 12 there result

$$T_{ij} = \partial H / \partial S_{ij} \quad (13)$$

$$D_i = -\partial H / \partial E_i \quad (14)$$

where it should be noted that

$$\partial S_{ij} / \partial S_{ji} = 0, \quad i \neq j \quad (15)$$

in taking the derivatives called for in Eq 13.

In linear piezoelectric theory the form taken by H is

$$H = \frac{1}{2} c_{ijkl}^E S_{ij} S_{kl} - e_{kij} E_k S_{ij} - \frac{1}{2} \epsilon_{ij}^S E_i E_j \quad (16)$$

where c_{ijkl}^E , e_{kij} , and ϵ_{ij}^S are the elastic, piezoelectric, and dielectric constants, respectively. In general there are 21 independent elastic constants, 18 independent piezoelectric constants, and 6 independent dielectric constants. From Eqs 13, 14, and 16 with Eq 15 there result the piezoelectric constitutive equations:

$$T_{ij} = c_{ijkl}^E S_{kl} - e_{kij} E_k \quad (17)$$

$$D_i = e_{ikl} S_{kl} + \epsilon_{ij}^S E_j \quad (18)$$

Note that the substitution of Eqs 10 and 18 into Eq 16 yields

$$U = \frac{1}{2} c_{ijkl}^E S_{ij} S_{kl} + \frac{1}{2} \epsilon_{ij}^S E_i E_j \quad (19)$$

and there is no piezoelectric interaction term in the positive definite stored energy function U . Since the e_{kij} do not appear in Eq 19, the positive definiteness of U places restrictions on the c_{ijkl}^E and the ϵ_{ij}^S , but not on the e_{kij} . Note further that the substitution of Eqs 1 and 7 into Eqs 17 and 18, and then Eqs 17 and 18 into Eqs 4 and 8 yields the four differential equations

$$c_{ijkl}^E u_{k,li} + e_{kij} \varphi_{,ki} = \rho \ddot{u}_j \quad (20)$$

$$e_{kij} u_{i,jk} - \epsilon_{ij}^S \varphi_{,ij} = 0 \quad (21)$$

in the four dependent variables u_j and φ . Eqs 20 and 21 are the three-dimensional differential equations for the linear piezoelectric continuum.

No notational distinction between the isothermal and adiabatic material constants is made in this standard. The scalar symbols θ and σ are recommended for temperature and entropy to avoid confusion with the tensor symbols S_{ij} and T_{ij} employed in this standard. Of course, under rapidly varying conditions, the adiabatic values of the constants are understood, and under slowly varying or static conditions, the isothermal values are understood. The form of the constitutive equations given in Eqs 17 and 18 is the only one that is useful for the three-dimensional continuum when

no boundaries are present, because it is the only form that yields Eqs 20 and 21 from Eqs 4 and 8. There are, however, other forms of the constitutive equations, and these become useful in certain specific instances when boundaries are present. The alternate forms that appear most frequently in the literature are presented and discussed in 2.6.

In order to write the elastic and piezoelectric tensors in the form of a matrix array, a compressed matrix notation is introduced in place of the tensor notation, which has been used exclusively heretofore. This matrix notation consists of replacing ij or kl by p or q , where i,j,k,l take the values 1, 2, 3 and p,q take the values 1, 2, 3, 4, 5, 6 according to Table 2.

The identifications

$$c_{ijkl}^E \equiv c_{pq}^E, \quad e_{ikl} \equiv e_{ip}, \quad T_{ij} \equiv T_p \quad (22)$$

are made. Then the constitutive Eqs 17 and 18 can be written:

$$T_p = c_{pq}^E S_q - e_k^E E_k \quad (23)$$

$$D_i = e_{iq} S_q + \epsilon_{ik}^S E_k \quad (24)$$

where

$$\begin{aligned} S_{ij} &= S_p \quad \text{when } i = j, p = 1, 2, 3 \\ 2S_{ij} &= S_p \quad \text{when } i \neq j, p = 4, 5, 6 \end{aligned} \quad (25)$$

NOTE — The summation convention for all repeated indices is understood.

Table 2—Matrix Notation	
<i>ij or kl</i>	<i>p or q</i>
11	1
22	2
33	3
23 or 32	4
31 or 13	5
12 or 21	6

It should be noted that when the compressed matrix notation is used, the transformation properties of the tensors become unclear. Hence, the tensor indices must be employed when coordinate transformations are to be made. It should also be noted that the time-dependent vector flux of piezoelectric energy is the sum of the mechanical and electrical terms mentioned in 2.2 and 2.3, respectively, and is given by

$$- (T_{ij} \dot{u}_j - \phi \dot{D}_i) \quad (26)$$

2.5 Boundary Conditions

In the presence of boundaries the appropriate boundary conditions must be adjoined to the differential Eqs 20 and 21 of the linear piezoelectric continuum. If there is a material surface of discontinuity, then across the surface there are the continuity conditions ([B2], Chapter 5, Section 4.; Chapter 6, Section 4.)

$$n_i T_{ij}^I = n_i T_{ij}^{II} \quad (27)$$

$$u_j^I = u_j^{II} \quad (28)$$

$$n_i D_i^I = n_i D_i^{II} \quad (29)$$

$$\varphi^I = \varphi^{II} \quad (30)$$

where I indicates the values of the variables on one side and II the values of the variables on the other side of the surface of discontinuity, and n_i denotes the components of the unit normal to the surface. At a traction-free surface, the boundary conditions, Eq 27, become

$$n_i T_{ij} = 0 \quad (31)$$

At a displacement-free surface, the boundary conditions, Eq 28, become

$$u_j = 0 \quad (32)$$

In more general cases different combinations of Eqs 31 and 32 apply. If the appropriate dielectric constant of the material is large compared to the dielectric constant of air (vacuum), the boundary condition, Eq 29, at an air-dielectric interface becomes, approximately,

$$n_i D_i = 0 \quad (33)$$

where D_i is the electric displacement in the material. On a surface with an electrode φ must be either specified or some relation between φ and $n_i D_i$ given. If the electrodes are short-circuited and the reference potential is zero,

$$\varphi = 0 \quad (34)$$

at each electrode. If a pair of electrodes operates into a circuit of admittance Y , the condition is

$$I = \int_A n_i \dot{D}_i ds = \pm YV \quad (35)$$

where the $\pm$ depends on the orientation of the coordinate axes, A represents the area of the electrode, and the voltage V is related to the potential difference according to

$$V = \varphi(1) - \varphi(2) \quad (36)$$

NOTE — For a discussion of circuit admittance, see ([B2], Chapter 15).

2.6 Alternate Forms of Constitutive Equations

For the unbounded piezoelectric medium, the only form of the constitutive equations which is of any value is given in Eqs 17 and 18. Some other forms of the constitutive equations are

$$S_{ij} = s_{ijkl}^E T_{kl} + d_{kij} E_k \quad (37)$$

$$D_i = d_{ikl} T_{kl} + \epsilon_{ik}^T E_k \quad (38)$$

and

$$S_{ij} = s_{ijkl}^D T_{kl} + g_{kij} D_k \quad (39)$$

$$E_i = -g_{ikl} T_{kl} + \beta_{ik}^T D_k \quad (40)$$

and

$$T_{ij} = c_{ijkl}^D S_{kl} - h_{kij} D_k \quad (41)$$

$$E_i = -h_{ikl} S_{kl} + \beta_{ik}^S D_k \quad (42)$$

These latter forms of the constitutive equations, although exact, are employed in approximations which are valid under certain limiting circumstances. The utility of any one of these three pairs of constitutive equations depends on the fact that certain variables on the right-hand sides are approximately zero under appropriate circumstances. Consequently, the set to use in a given instance depends crucially on the specific geometrical, mechanical, and electrical circumstances. As an example, for low-frequency vibrations of a rod one would use either Eqs 37 and 38 or Eqs 39 and 40, because under these circumstances all stress components vanish, either exactly or approximately, except for the extensional stress along the length of the rod. However, it is not at all clear whether to use the first or the second set unless more specific information concerning the shape of the cross section and placement of electrodes is given. In fact, in a given instance it is quite possible that a different set of constitutive equations somewhere between the two would be useful.

The relations between the coefficients appearing in the four sets of constitutive equations, Eqs 17, 18 and Eqs 37–42, may be written

$$\begin{aligned} c_{pr}^E s_{qr}^E &= \delta_{pg}, & c_{pr}^D s_{qr}^D &= \delta_{pq} \\ \beta_{ik}^S \epsilon_{jk}^S &= \delta_{ij}, & \beta_{ik}^T \epsilon_{jk}^T &= \delta_{ij} \\ c_{pq}^D &= c_{pq}^E + e_{kp} h_{kq}, & s_{pq}^D &= s_{pq}^E - d_{kp} g_{kq} \\ \epsilon_{ij}^T &= \epsilon_{ij}^S + D_{iq} e_{jq}, & \beta_{ij}^T &= \beta_{ij}^S - g_{iq} h_{jq} \\ e_{ip} &= d_{iq} c_{qp}^E, & d_{ip} &= \epsilon_{ik}^T g_{kp} \\ g_{ip} &= \beta_{ik}^T d_{kp}, & h_{ip} &= g_{iq} c_{qp}^D \end{aligned} \quad (43)$$

using the compressed notation introduced in 2.4 and where $i, j, k = 1, 2, 3$ and $p, q, r = 1, 2, 3, 4, 5, 6$ and δ_{ij} is the $3 \cdot 3$ unit matrix and δ_{pq} is the $6 \cdot 6$ unit matrix. As a consequence of Eqs 22 and 25 the following relations hold:

$$\begin{aligned}
 s_{pq}^E &= s_{ijkl}^E, \quad i = j \text{ and } k = l, \quad p, q = 1, 2, 3 \\
 s_{pq}^E &= 2s_{ijkl}^E, \quad i = j \text{ and } k \neq l, \quad p = 1, 2, 3, \quad q = 4, 5, 6 \\
 s_{pq}^E &= 4s_{ijkl}^E, \quad i \neq j \text{ and } k \neq l, \quad p, q = 4, 5, 6
 \end{aligned} \tag{44}$$

and similar relationships hold for s_{pq}^D :

$$\begin{aligned}
 d_{iq} &= d_{ikl}, \quad k = l, \quad q = 1, 2, 3 \\
 d_{iq} &= 2d_{ikl}, \quad k \neq l, \quad q = 4, 5, 6
 \end{aligned} \tag{45}$$

and similar relationships hold for g_{iq} . The piezoelectric constants h_{iq} are related to the h_{ijl} in the same way that e_{iq} are related to the e_{ikl} , and the elastic constants c_{pq}^D are related to the c_{ijkl}^D in the same way that the c_{pq}^E are related to the c_{ijkl}^E .

3. Crystallography Applied to Piezoelectric Crystals

3.1 General

The gap between the treatment of piezoelectric solids using the theoretical concepts of continuum mechanics, as presented in Section 2., and the application of the equations of that section to particular piezoelectric materials is spanned by the branch of science called crystallography. Most piezoelectric materials of interest for technological applications are crystalline solids. These can be single crystals, either formed in nature or formed by synthetic processes, or polycrystalline materials like ferroelectric ceramics which can be rendered piezoelectric and given, on a macroscopic scale, a single-crystal symmetry by the process of poling. Since the theoretical principles developed in Section 2. are presented with the generality of tensor formulations, connection of the theory of Section 2. with real piezoelectric materials requires as a first step the definition of crystal axes within the different crystallographic point groups and the association of the crystal axes with the Cartesian coordinate axes used in mathematical analysis. In addition to axis identification and association, the science of crystallography provides a highly developed nomenclature and a wealth of data useful to engineers and scientists working with piezoelectric crystals. Such data are, for example, atomic cell dimensions and angles, interfacial angles, optical properties, and X-ray properties.

3.2 Basic Terminology and the Seven Crystal Systems

The term *crystal* is applied to a solid in which the atoms are arranged in a single pattern repeated throughout the body. In a crystal the atoms may be thought of as occurring in small groups, all groups being exactly alike, similarly oriented, and regularly aligned in all three dimensions. Each group can be regarded as bounded by a parallelepiped, and each parallelepiped regarded as one of the ultimate building blocks of the crystal. The crystal is formed by stacking together in all three dimensions replicas of the basic parallelepiped without any spaces between them. Such a building block is called a *unit cell*. Since the choice of a particular set of atoms to form a unit cell is arbitrary, it is evident that there is a wide range of choices in the shapes and dimensions of the unit cell. In practice, that unit cell is selected which is most simply related to the actual crystal faces and X-ray reflections, and which has the symmetry of the crystal itself. Except in a few special cases, the unit cell has the smallest possible size.

In crystallography the properties of a crystal are described in terms of the natural coordinate system provided by the crystal itself. The axes of this natural system, indicated by the letters a , b , and c , are the edges of the unit cell. In a cubic crystal, these axes are of equal length and are mutually perpendicular; in a triclinic crystal they are of unequal lengths and no two are mutually perpendicular. The faces of any crystal are all parallel to planes whose intercepts on the a , b , c axes are small multiples of unit distances or else infinity, in order that their reciprocals, when multiplied by a small common factor, are all small integers or zero. These are the indices of the planes. In this nomenclature we have, for example, faces (100), (010), (001), also called the a , b , c faces, respectively. In the orthorhombic, tetragonal, and cubic

systems, these faces are normal to the a , b , c axes. Even in the monoclinic and triclinic systems, these faces contain, respectively, the b and c , a and c , and a and b axes. As referred to the set of rectangular axes X , Y , Z , these indices are in general irrational except for cubic crystals.

Depending on their degrees of symmetry, crystals are commonly classified into seven systems: triclinic (the least symmetrical), monoclinic, orthorhombic, tetragonal, trigonal, hexagonal, and cubic. The seven systems, in turn, are divided into point groups (classes) according to their symmetry with respect to a point. There are 32 such classes, eleven of which contain enantiomorphous forms (see 3.3.2). Twelve classes are of too high a degree of symmetry to show piezoelectric properties. Thus twenty classes can be piezoelectric. Every system contains at least one piezoelectric class. A convenient summary of the 32 classes with examples is given in Table 3.

The international crystallographic system [B4] (Hermann-Mauguin notation) plays a key role in the interpretation of Table 4. In this system, an axis of rotation is indicated by one of the numbers 1, 2, 3, 4, 6. The number indicates through its reciprocal the part of a full rotation about the axis which is required to bring the crystal into an equivalent position in regard to its internal structural properties. The number 1 indicates no symmetry at all, since any structure must come back into coincidence after a complete rotation, while 2 indicates a twofold axis of rotation. The Symbols $\bar{1}$, $\bar{2}$, $\bar{3}$, $\bar{4}$, $\bar{6}$ indicate axes of rotatory inversion. The symbol i implies a simple center of inversion. The symbol σ is equivalent to a reflection plane, and since reflection planes are so important a feature of the structure, the symbol for such a plane, m , is written instead of σ . If an axis has a reflection plane perpendicular to it, this fact is written as part of the symbol for that axis by following the number which describes the symmetry of the axis with the notation $/m$.

The designation for any class of symmetry is made up in the international system of one, two, or three symbols, each indicating the symmetry with respect to *one* type of direction in the crystal. Crystallographically identical directions are grouped together under one symbol. Thus a cubic NaClO_3 crystal has *three* twofold rotation axes and *four* threefold rotation axes, but the symbol is 23, because each twofold axis is identical, and each threefold axis is identical. Only where the crystallographic directions are not identical are different symbols used. The first symbol refers to the principal axis of the crystal if there is one, indicating the type of symmetry of the axis and the existence of a mirror plane perpendicular to that axis, if any. The second symbol refers to the symmetry of the second most important crystal direction, giving the symmetry along that axis and a mirror plane perpendicular to it, if any. The third symbol states the symmetry along the third most important direction. Table 3 lists the international point group symbols for all 32 point groups, and Table 4 provides clarification by identifying the symmetry directions for each crystal system. In all but the cubic system, both the second and third directions need not be symmetry directions; in the cubic system, the third direction need not be a symmetry direction; and in the absence of symmetry, no symbol is given.

To characterize a piezoelectric crystal, a set of piezoelectric constants is needed; and in order to make them unambiguous, a sign convention is necessary for both the constants and the axis sense. A specific relation between the a , b , c axes of crystallography and the X , Y , Z axes is given in 3.2.1–3.2.6, and summarized in Table 3. The reader is cautioned at this point that, without general agreement on sign conventions, there can be much confusion. Data expressed in terms of one abc – XYZ relation look very different from the same data in terms of another abc – XYZ relation. In this standard, the positive senses of the XYZ axes are defined such that certain piezoelectric constants are positive. Details for determining senses of the XYZ axes are described in 3.5. The choice of the positive sense is arbitrary in some cases. A discussion of static measurements related to sign determination will be found in 6.3.

3.2.1 The Triclinic System

A triclinic crystal has neither symmetry axes nor symmetry planes. The lengths of the three axes are in general unequal; and the angles α , β , and γ between axes b and c , c and a , and a and b , respectively, are also unequal. The a axis has the direction of the intersection of the faces b and c (extend the faces to intersection if necessary), the b axis has the direction of the intersection of faces c and a , the c axis has the direction of the intersection of faces a and b (see Table 3).

The X , Y , Z axes are associated as closely as possible with the a , b , c axes, respectively. The Z axis is parallel to c , Y is normal to the ac plane, and X is thus in the ac plane. The $+Z$ and $+X$ axes are chosen so that d_{33} and d_{11} are positive. The $+Y$ axis is chosen so that it forms a right-handed system with $+Z$ and $+X$.

Table 3—Summary of Crystal Systems

Crystal System	International Point Groups		Axis Identification, Crystallographic				Axis Identification, Rectangular			Schoenflies Symbol	Example	Formula
	Short	Full	<i>c</i>	<i>a</i>	<i>b</i>		<i>X</i>	<i>Y</i>	<i>Z</i>			
Triclinic $c_0 < a_0 < b_0$; $\alpha, \beta > 90^\circ$	p	1	1					1(010)		C_1	Aminoethyl ethanolamine hydrogen <i>d</i> -tartrate (AET)	$C_8H_{17}O_7N_2$
								1(010)			Copper sulfate pentahydrate	$CuSO_4 \cdot 5H_2O$
Monoclinic $c_0 < a_0, \beta > 90^\circ$; $\alpha = \gamma = 90^\circ$	p	2	2	2				$1(100)$	<i>c</i>	C_2	Ethylene diamine tartrate (EDT)	$C_6H_{14}N_2O_6$
	p	<i>m</i>	<i>m</i>		<i>/m</i>			$1(100)$	<i>c</i>	$C_8(C_{1h})$	Lithium trihydrogen selenite	$LiH_3(SeO_3)_2$
		$2/m$	$2/m$					$1(100)$	<i>c</i>	C_{2h}	Gypsum	$CaSO_4 \cdot 2H_2O$
Orthorhombic $c_0 < a_0 < b_0$; $\alpha = \beta = \gamma = 90^\circ$	p	222	222	2	2	2		<i>a</i>	<i>b</i>	$D_2(V)$	Rochelle salt, except between Curie points	$NaKC_4H_4O_6 \cdot 4H_2O$
	p	<i>mm</i> 2	$2 \frac{2}{m} \frac{2}{m}$	(See Note 1)			(See Note 1)			C_{2h}	Barium sodium niobate	$Ba_2NaNb_5O_{15}$
		<i>mmm</i>	mmm	2	2	2		<i>a</i>	<i>b</i>	$D_{2h}(V_h)$	Barite	$BaSO_4$
Tetragonal $a_0 = b_0$; $\alpha = \beta = \gamma = 90^\circ$	p	4	4	<i>c</i>	<i>a</i> ₁	<i>a</i> ₂		(a_1)	<i>c</i>	C_4	Potassium strontium niobate	$KSrNb_5O_{15}$
	p	$4/m$	$4/m$	4	†	†		(a_1)	<i>c</i>	S_4	Anorthite	$Ca_2Al_2SiO_7$
		422	422	4	†	†		(a_1)	<i>c</i>	C_{4h}	Scheelite	$CaWO_4$
	p	$4mm$	$4mm$	4	2	2		(a_1)	<i>c</i>	D_4	Nickel sulfate hexahydrate, Paratellurite	$NiSO_4 \cdot 6H_2O$, TeO_2
	p	$2m$	$2m$	4	<i>/m</i>	<i>/m</i>		(a_1)	<i>c</i>	C_{4v}	Barium titanate	$BaTiO_3$
		$4/m \frac{2}{m} \frac{2}{m}$	$4/m \frac{2}{m} \frac{2}{m}$	4	2	2	(See Note 2)	(a_1)	<i>c</i>	$D_{2d}(V_d)$	Ammonium dihydrogen phosphate (ADP)	$NH_4H_2PO_4$
				4	2	2		(a_1)	<i>c</i>	D_{4h}	Zircon	$ZrSiO_4$
Trigonal $(a_0)_1 = (a_0)_2 = (a_0)_3$	p	3	3	<i>c</i>	<i>a</i> ₁	<i>a</i> ₂	<i>a</i> ₃			Any two	Sodium periodate trihydrate	$NaIO_4 \cdot 3H_2O$
				3	†	†		(a_1)	<i>c</i>	C_3	Dolomite	$CaCo_3MgCO_3$
	p	32	32	3	2	2	2	(a_1)	<i>c</i>	$C_3(S_6)$	α -quartz	SiO_2
	p	3m	3m	3	<i>/m</i>	<i>/m</i>	<i>/m</i>	(a_1)	<i>c</i>	D_3	Lithium niobate	$LiNbO_3$

Crystal System	International Point Groups		Axis Identification, Crystallographic			Axis Identification, Rectangular			Schoenflies Symbol	Example	Formula
	Short	Full	<i>c</i>	<i>a</i>	<i>b</i>	<i>X</i>	<i>Y</i>	<i>Z</i>			
(See 2.2.5)	<i>m</i>	$\frac{2}{3} \frac{2}{m}$	2	2	2	(<i>a</i> ₁)		<i>c</i>	<i>D</i> _{3d}	Calcite	CaCO ₃
Hexagonal $(a_0)_1 = (a_0)_2 = (a_0)_3$ (See 2.2.5)	p	6	6	†		(<i>a</i> ₁)		<i>c</i>	<i>C</i> ₆	Lithium iodate	LiIO ₃
	p	$\frac{6}{m}$	6	†		(<i>a</i> ₁)		<i>c</i>	<i>C</i> _{3h}	Lithium peroxide	Li ₂ O ₃
		622	6	2	2	(<i>a</i> ₁)		<i>c</i>	<i>C</i> _{6h}	Apatite	CaF ₂ ·3Ca ₃ P ₂ O ₈
	p	6mm	6	/m	/m	(<i>a</i> ₁)		<i>c</i>	<i>D</i> ₆	β-quartz	SiO ₂
	p	$\frac{6}{m}$	6	2	2	(<i>a</i> ₁)		<i>c</i>	<i>C</i> _{6v}	Cadmium sulfide	CdS
	p	$\frac{6}{m} \frac{2}{m} \frac{2}{m}$	6	2	2	(<i>a</i> ₁)		<i>c</i>	<i>D</i> _{3h}	Benitoite	BaTiSi ₃ O ₉
Cubic $a_0 = b_0 = c_0; \alpha = \beta = \gamma = 90^\circ$			<i>a</i> ₁	<i>a</i> ₂	<i>a</i> ₃	(<i>a</i> ₁)	(<i>a</i> ₂)	(<i>a</i> ₃)			
	23	23	2	2	2	(<i>a</i> ₁)	(<i>a</i> ₂)	(<i>a</i> ₃)	<i>T</i>	Bismuth germanium oxide	Bi ₁₂ GeO ₂₀
	$\frac{2}{m} \frac{3}{m}$	$\frac{2}{m} \frac{3}{m}$	2	2	2	(<i>a</i> ₁)	(<i>a</i> ₂)	<i>a</i> ₃	<i>T</i> _h	Pyrite	FeS ₂
	432	432	4	4	4	(<i>a</i> ₁)	(<i>a</i> ₂)	<i>a</i> ₃	<i>O</i>	Cadmium fluoride	CdF ₂
	3m	3m	4	4	4	(<i>a</i> ₁)	(<i>a</i> ₂)	(<i>a</i> ₃)	<i>T</i> _d	Gallium arsenide	GaAs
	$\frac{4}{m} \frac{3}{m} \frac{2}{m}$	$\frac{4}{m} \frac{3}{m} \frac{2}{m}$	4	4	4	(<i>a</i> ₁)	(<i>a</i> ₂)	(<i>a</i> ₃)	<i>O</i> _h	Sodium chloride	NaCl

NOTES:

1 — *Z* is the polar axis, which may be *a*, *b*, or *c*. Depending on whether *a*, *b*, or *c* is polar, the full international point group symbol is *2mm*, *m2m*, or *mm2*, respectively. *X* is parallel to the smaller of the nonpolar axes. Thus in classes *2mm*, *m2m*, and *mm2*, *X* is chosen parallel to *c*, *a*, and *a*, respectively.

2 — In class *2m* the axial choice is as listed here for six of the space groups. For the other six the *a* axis is chosen at 45 degrees to the twofold axes in order to have the smallest unit cell. In all cases *X* and *Y* are chosen parallel to the twofold axes. See 2.2.4.

3 — Axes whose sense is determined by the sign of a piezoelectric constant. It does not necessarily have a polar axis. For † and * see text.

3.2.2 The Monoclinic System

A monoclinic crystal has either a single axis of twofold symmetry or a single plane of reflection symmetry, or both. Either the twofold axis or the normal to the plane of symmetry (they are the same if both exist, and this direction is called the unique axis in any case) is taken as the b or Y axis. Of the two remaining axes, the smaller is the c axis. In class 2, $+Y$ is chosen so that d_{22} is positive; $+Z$ is chosen parallel to c (sense trivial), and $+X$ such that it forms a right-handed system with $+Z$ and $+Y$. In class m , $+Z$ is chosen so that d_{33} is positive, and $+X$ so that d_{11} is positive, and $+Y$ to form a right-handed system.

**Table 4—
Significant Symmetry Directions for the International (Hermann-Mauguin) Symbol***

Crystal System	First Symbol	Second Symbol	Third Symbol
Triclinic	None		
Monoclinic	b (1)		
Orthorhombic	a (1)	b (1)	c (1)
Tetragonal	c (1)	a (2)	[110] (2)
Trigonal	c (1)	a (3)	
Hexagonal	c (1)	a (3)	Digonal (3) [1010 axis]
Cubic	a (3)	[111] (4)	[110] (6)

*The number after each direction indicates the multiplicity of that direction in the crystal.

NOTE — Positive and negative may be checked using a carbon-zinc flashlight battery. The carbon anode connection will have the same effect on meter deflection as the $+$ end of the crystal axis upon *release* of compression. For more detail see 3.5 and 6.3.

3.2.3 The Orthorhombic System

An orthorhombic crystal has three mutually perpendicular twofold axes or two mutually perpendicular planes of reflection symmetry, or both. The a , b , c axes are of unequal length. For classes 222 and $2/m\ 2/m\ 2/m$ unit distances are chosen such that $c_0 < a_0 < b_0$. For the remaining class, which is polar, Z will always be the polar axis regardless of whether it is a , b , c in the crystallographer's notation. Axes X and Y will then be chosen so that X is parallel to the remaining axis that is smallest. This class therefore may be properly designated $mm2$, $2mm$, or $m2m$, depending on whether c , a , or b is the polar axis. Axis sense is trivial except for the polar class for which $+Z$ is chosen such that d_{33} is positive.

NOTE — See note in 3.2.2.

3.2.4 The Tetragonal System

A tetragonal crystal has a single fourfold axis or a fourfold inversion axis. The c axis is taken along this fourfold axis, and the Z axis lies along c . The a and b axes are equivalent and are usually called a_1 and a_2 . There are seven classes of tetragonal crystals, five of which can be piezoelectric; these are classes 4 , $2m$, 422 , and $4mm$. Three of these have no twofold axes to guide in a choice of an a axis; however, for all of them except $2m$ there is no alternative to the choice of an a axis in such a way as to make the unit cell of smallest volume. In class $2m$, which has a twofold axis, the smallest cell may not have its a axis parallel to this axis. There are twelve possible arrangements of matter (space groups) that have symmetry $2m$. Of these twelve, six have the smallest cell when the a axis is an axis of twofold symmetry, and six have the smallest cell when a is chosen at 45 degrees to twofold axes (while still perpendicular to the c axis). The international tables for X-ray crystallography [B5] now use the smallest cell in all twelve cases. In