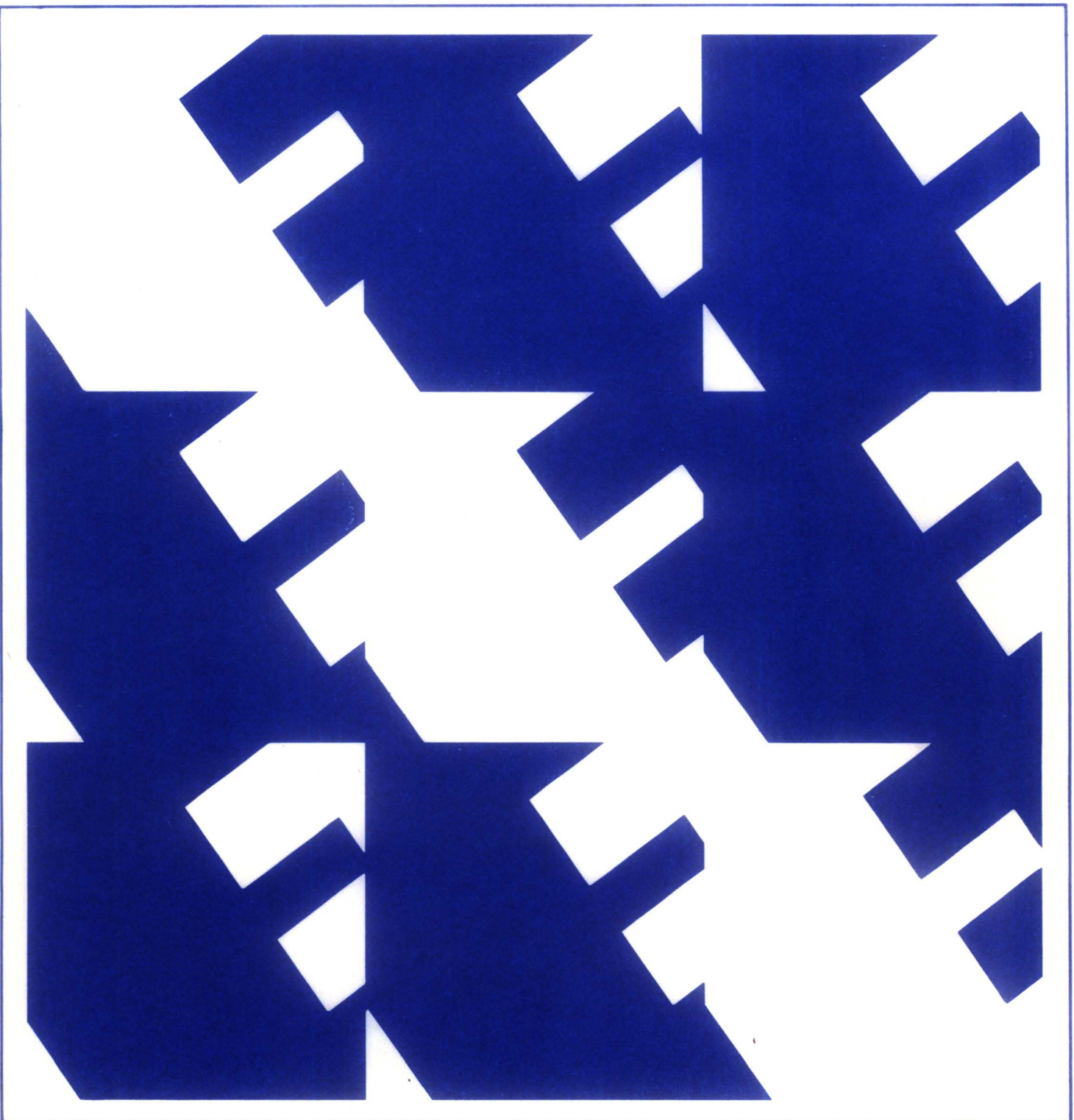


IEEE Standard on Piezoelectricity

ANSI/IEEE Std 176-1978



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IEEE Standard on
Piezoelectricity

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Foreword

(This Foreword is not a part of IEEE Std 176-1978, Standard on Piezoelectricity.)

The document presented here has as its antecedents four earlier standards on piezoelectricity, originally prepared within the Standards Committee framework of the IRE and later carried over and published as IEEE Standards: IEEE Std 176-1949 (Reaff 1971), Piezoelectric Crystals (ANSI C83.3-1951 (R1972)); IEEE Std 177-1966, Definitions and Methods of Measurement for Piezoelectric Vibrators (ANSI C83.17-1970); IEEE Std 178-1958 (Reaff 1972), Determination of the Elastic, Piezoelectric, and Dielectric Constants of Piezoelectric Crystals and also the Electromechanical Coupling Factor (ANSI C83.23-1960 (R1972)); and IEEE Std 179-1961 (R1971), Measurements of Piezoelectric Ceramics (ANSI C83.24-1962 (R1972)).

In the years that have elapsed since the publication of these four standards, the need has become clear for the preparation of a new, more comprehensive treatment that eliminates errors, includes more material on piezoelectric materials of recent interest, and provides a clearer statement of the theoretical basis for many of the concepts and equations of fundamental importance in the field. The present work, representing the culmination of these objectives, replaces IEEE Stds 176 and 178. There is only a slight overlap in the coverage of IEEE Std 177 and this standard, and a somewhat greater overlap of information contained in this standard with IEEE Std 179. In places where differences in treatment of technical details exist, the recommendations of this standard shall apply.

This new standard introduces several important changes in and additions to practices recommended in the four cited standards. The two important changes are the following:

- (1) Use of a separate sign convention for the piezoelectric constants of quartz has been abandoned.
- (2) Definitions of electromechanical coupling factors based on interaction energies have been abandoned. In this standard, when a piezoelectric solid having a simple shape is used dynamically as a singly resonant element, the material coupling factors are defined as they arise naturally in analytical solutions for electrically driven vibrations. On the other hand, when the piezoelectric solid is used essentially statically as part of a larger resonant structure, the definitions of material coupling factors are based on ratios defined in terms of quantities arising in prescribed stress-strain cycles.

Besides these changes, a number of important additions have been made to the standard on piezoelectricity.

Section 2. This section provides a concise review of the physical quantities, theoretical concepts, and mathematical relationships basic to the linear theory of piezoelectricity.

Section 3. This section is a revision of the material originally covered in IEEE Stds 176 and 178. All the illustrations used in IEEE Std 176 to show examples from different crystal systems have been dropped, tables of crystalline properties have been revised, and a number of errors have been corrected. The subject of enantiomorphic forms is treated in greater detail than before. The material related to the piezoelectric determination of the sense of the crystal axes and to systems of notation for designating oriented bars and cuts has been clarified. This section contains tables frequently referenced by individuals doing either theoretical or experimental work with piezoelectric materials.

Section 4. This section presents the results of analyses for plane wave motions and vibrations in piezoelectric solids. Some material in this section overlaps material contained in IEEE Std 179. Definitions of electromechanical coupling factors for a number of cases of practical interest are given. This section provides the equations used in deriving numerical results from the experimental techniques discussed in Section 5. The reader primarily interested in doing laboratory measurements need not concern himself 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.

Section 5. This section presents the equations applicable for quasi-static mechanical behavior and provides definitions of quasi-static material coupling factors.

Section 6. 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. The range of applicability of the measuring techniques and the advantages and disadvantages associated with different methods are discussed. The definition of f_p , originally defined in IEEE Std 177 for the simple equivalent circuit as the parallel resonance frequency, is generalized to cover the case of materials with high coupling factors.

This standard has benefited from the contributions of many people, including members of the IEEE Subcommittee on Piezoelectric Crystals (primarily responsible for the preparation of this standard) and members of the jointly sponsoring parent IEEE technical committees, the IEEE Technical Committee on Transducers and Resonators and the IEEE Technical Committee on Frequency Control and Time. The credit for the primary authorship of the various sections is 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 here, there are others who were associated at various times with the committee over the ten-year period in which this standard was prepared and who made valuable contributions to the work of the committee. Among those whose names should be mentioned here are R. Bechmann, J. L. Bleustein, E. M. Frymoyer, and R. T. Smith.

The preparation of the final draft of this standard has benefited greatly from the coordination of activities and moderation of differences of opinion accomplished by J. E. May, Chairman of the IEEE Technical Committee on Transducers and Resonators.

This standard was prepared by the IEEE Subcommittee on Piezoelectric Crystals which consisted of the following members:

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An American National Standard

IEEE Standard on Piezoelectricity

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, Definitions and Methods of Measurement for Piezoelectric Vibrators, 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

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_{ijk}, 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	

(Continued on page 10)

Table 1 (Continued)

Symbol	Meaning	SI Unit
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
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^P	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

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.

1.1 Units. All equations and physical constants appearing in this standard are written in the International System of Units (SI units), according to IEEE Std 268-1976, ASTM/IEEE Standard Metric Practice (ANSI Z210.1-1976,

ASTM E380-76). Table 1 lists many of the symbols used and, where appropriate, shows the units associated with the physical quantities designated by the symbols.

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 elec-

tric 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 [1]. For a more complete discussion of mechanical displacement, see Tiersten [2, ch 3, sec 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,

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

where

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

The antisymmetric portion of the mechanical displacement gradient determines the infinitesimal local rigid rotation [2, ch 3, sec 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

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

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 $\mathbf{T}_i$ 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 [2, ch 2, sec 1]. Also, see [3].

In fact the existence of the traction vector and the integral form of the equations of the balance of linear momentum determine [2, ch 2, sec 2] the existence of the stress tensor T_{ij} , which is related to the traction vector $\mathbf{T}_j$ by the relation

$$\mathbf{T}_j = n_i \mathbf{T}_{ij} \quad (\text{Eq 3})$$

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 [1, ch 1].

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

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

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 $(-T_{ij}\dot{u}_j)$.

2.3 Electrical Considerations. In piezoelectric theory the full electromagnetic equations are not 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 [2, ch 4, sec 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

$$D_i = \epsilon_0 E_i + P_i \quad (\text{Eq 5})$$

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

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

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

$$E_i = -\varphi_{,i} \quad (\text{Eq 7})$$

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

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

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 $(+\varphi \dot{D}_i)$, 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 [2, ch 4, sec 3 and 4].

2.4 Linear Piezoelectricity. The conservation of energy [2, ch 5, secs 1–3] for the linear piezoelectric continuum results in the first law of thermodynamics:

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

where U is the stored energy density for the piezoelectric continuum. The electric enthalpy [4] density H is defined by

$$H = U - E_i D_i \quad (\text{Eq 10})$$

and from Eqs 9 and 10 there results

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

Eq 11 implies

$$H = H(S_{kl}, E_k) \quad (\text{Eq 12})$$

and from Eqs 11 and 12 there result

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

$$D_i = -\partial H / \partial E_i \quad (\text{Eq 14})$$

where it should be noted that

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

in taking the derivatives called for in Eq 13.

In linear piezoelectric theory the form taken by H is

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

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:

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

$$D_i = e_{ikl} S_{kl} + \epsilon_{ik}^S E_k \quad (\text{Eq 18})$$

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

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

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

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

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

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.

Table 2
Matrix Notation

ij or kl	p or q
11	1
22	2
33	3
23 or 32	4
31 or 13	5
12 or 21	6

The identifications

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

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

$$T_p = c_{pq}^E S_q - e_{kp} E_k \quad (\text{Eq 23})$$

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

where

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

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

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

$$-(T_{ij} \dot{u}_j - \varphi \dot{D}_i). \quad (\text{Eq 26})$$

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 [2, ch 5, sec 4; ch 6, sec 4]

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

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

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

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

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

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

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

$$u_j = 0. \quad (\text{Eq 32})$$

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,

$$n_i D_i = 0 \quad (\text{Eq 33})$$

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,

$$\varphi = 0 \quad (\text{Eq 34})$$

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

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

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

$$V = \varphi(1) - \varphi(2). \quad (\text{Eq 36})$$

NOTE: For a discussion of circuit admittance, see [2, ch 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

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

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

and

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

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

and

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

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

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

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

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 3×3 unit matrix and δ_{pq} is the 6×6 unit matrix. As a consequence of Eqs 22 and 25 the following relations hold:

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

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

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

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. Because 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, 100, etc. 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 [5] (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 $\bar{1}$ implies a simple center of inversion. The symbol $\bar{2}$ 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 $\bar{2}$. 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

Table 3
Summary of Crystal Systems

Crystal System		Inter-national Point Groups		Axis Identification, Crystallographic <i>c a b</i>	Axis Identification, Rectangular <i>X Y Z</i>			+/- Axes (Note 3)	Schoen-flies Symbol	Example	Formula
		Short	Full								
Triclinic $c_o < a_o < b_o; \alpha, \beta > 90^\circ$	p	1	1		1(010)			Z X	C_1	Aminoethyl ethanolamine hydrogen <i>d</i> -tartrate (AET)	$C_8H_{17}O_7N_2$
		$\bar{1}$	$\bar{1}$		1(010)				$C_1(S_2)$	Copper sulfate pentahydrate	$CuSO_4 \cdot 5H_2O$
Monoclinic $c_o < a_o, \beta > 90^\circ; \alpha = \gamma = 90^\circ$	p	2	2	2	1(100)	<i>b</i>	<i>c</i>	Y	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>b</i>	<i>c</i>	Z X	$C_2(C_{1h})$	Lithium trihydrogen selenite	$LiH_3(SeO_3)_2$
		2/ <i>m</i>	$\frac{2}{m}$		1(100)	<i>b</i>	<i>c</i>		C_{2h}	Gypsum	$CaSO_4 \cdot 2H_2O$
Orthorhombic $c_o < a_o < b_o; \alpha = \beta = \gamma = 90^\circ$	p	222	222	2 2 2	<i>a</i>	<i>b</i>	<i>c</i>		$D_2(V)$	Rochelle salt, except between Curie points	$NaKC_4H_4O_6 \cdot 4H_2O$
	p	<i>mm</i> 2	(See Note 1)		(See Note 1)			Z	C_{2v}	Barium sodium niobate	$Ba_2NaNb_5O_{15}$
		<i>mmm</i>	$\frac{2}{m} \frac{2}{m} \frac{2}{m}$	2 2 2	<i>a</i>	<i>b</i>	<i>c</i>		$D_{2h}(V_h)$	Barite	$BaSO_4$
Tetragonal $a_o = b_o; \alpha = \beta = \gamma = 90^\circ$				<i>c a_1 a_2</i>							
	p	4	4	4 $\uparrow$	(<i>a</i> ₁)	(<i>a</i> ₂)	<i>c</i>	Z	C_4	Potassium strontium niobate	$KSr_2Nb_5O_{15}$
	p	$\bar{4}$	$\bar{4}$	$\bar{4} \uparrow$	(<i>a</i> ₁)	(<i>a</i> ₂)	<i>c</i>	Z	S_4	Anorthite	$Ca_2Al_2SiO_7$
		4/ <i>m</i>	$\frac{4}{m}$	4 $\uparrow$	(<i>a</i> ₁)	(<i>a</i> ₂)	<i>c</i>		C_{4h}	Scheelite	$CaWO_4$
	p	422	422	4 2 2	(<i>a</i> ₁)	(<i>a</i> ₂)	<i>c</i>	*	D_4	Nickel sulfate hexahydrate, Paratellurite	$NiSO_4 \cdot 6H_2O, TeO_2$
	p	4 <i>mm</i>	4 <i>mm</i>	4 / <i>m</i> / <i>m</i>	(<i>a</i> ₁)	(<i>a</i> ₂)	<i>c</i>	Z	C_{4v}	Barium titanate	$BaTiO_3$
	p	$\bar{4}2m$	$\bar{4}2m$	4 2 2	(See Note 2)			Z	$D_{2d}(V_d)$	Ammonium dihydrogen phosphate (ADP)	$NH_4H_2PO_4$
		4/ <i>mmm</i>	$\frac{4}{m} \frac{2}{m} \frac{2}{m}$	4 2 2	(<i>a</i> ₁)	(<i>a</i> ₂)	<i>c</i>	*	D_{4h}	Zircon	$ZrSiO_4$
Trigonal $(a_o)_1 = (a_o)_2 = (a_o)_3$ (See 2.2.5)				<i>c a_1 a_2 a_3</i>				Any two			
	p	$\frac{3}{3}$	$\frac{3}{3}$	$\frac{3}{3} \uparrow$	(<i>a</i> ₁)		<i>c</i>		C_3	Sodium periodate trihydrate	$NaIO_4 \cdot 3H_2O$
				$\frac{3}{3} \uparrow$	(<i>a</i> ₁)		<i>c</i>		$C_{3i}(S_6)$	Dolomite	$CaCO_3MgCO_3$
	p	32	32	3 2 2 2	(<i>a</i> ₁)		<i>c</i>	X	D_3	α -quartz	SiO_2
	p	3 <i>m</i>	3 <i>m</i>	3 / <i>m</i> / <i>m</i> / <i>m</i>	(<i>a</i> ₁)		<i>c</i>	Z Y	C_{3v}	Lithium niobate	$LiNbO_3$
		$\bar{3}m$	$\bar{3} \frac{2}{m}$	$\bar{3} 2 2 2$	(<i>a</i> ₁)		<i>c</i>		D_{3d}	Calcite	$CaCO_3$
Hexagonal $(a_o)_1 = (a_o)_2 = (a_o)_3$ (See 2.2.5)	p	6	6	6 $\uparrow$	(<i>a</i> ₁)		<i>c</i>	Z	C_6	Lithium iodate	$LiIO_3$
	p	$\bar{6}$	$\bar{6}$	$\bar{6} \uparrow$	(<i>a</i> ₁)		<i>c</i>	X Y	C_{3h}	Lithium peroxide	Li_2O_3
		6/ <i>m</i>	$\frac{6}{m}$	6	(<i>a</i> ₁)		<i>c</i>		C_{6h}	Apatite	$CaF_2 \cdot 3Ca_3P_2O_8$
	p	622	622	6 2 2 2	(<i>a</i> ₁)		<i>c</i>		D_6	β -quartz	SiO_2
	p	6 <i>mm</i>	6 <i>mm</i>	6 / <i>m</i> / <i>m</i> / <i>m</i>	(<i>a</i> ₁)		<i>c</i>	Z	C_{6v}	Cadmium sulfide	CdS
	p	$\bar{6}m2$	$\bar{6}m2$	$\bar{6} 2 2 2$	(<i>a</i> ₁)		<i>c</i>	X	D_{3h}	Benitoite	$BaTiSi_3O_9$
		6/ <i>mmm</i>	$\frac{6}{m} \frac{2}{m} \frac{2}{m}$	6 2 2 2	(<i>a</i> ₁)		<i>c</i>		D_{6h}	Beryl	$3BeO \cdot Al_2O_3 \cdot 6SiO_2$
Cubic $a_o = b_o = c_o; \alpha = \beta = \gamma = 90^\circ$				<i>a_1 a_2 a_3</i>							
	p	23	23	2 2 2	(<i>a</i> ₁)	(<i>a</i> ₂)	<i>a</i> ₃	Z	T	Bismuth germanium oxide	$Bi_{12}GeO_{20}$
		<i>m</i> 3	$\frac{2}{m} 3$	2 2 2	(<i>a</i> ₁)	(<i>a</i> ₂)	<i>a</i> ₃	*	T_h	Pyrite	FeS_2
		432	432	4 4 4	(<i>a</i> ₁)	(<i>a</i> ₂)	<i>a</i> ₃	*	O	Cadmium fluoride	CdF_2
	p	$\bar{4}3m$	$\bar{4}3m$	$\bar{4} \bar{4} \bar{4}$	(<i>a</i> ₁)	(<i>a</i> ₂)	<i>a</i> ₃	Z	T_d	Gallium arsenide	$GaAs$
		<i>m</i> 3 <i>m</i>	$\frac{4}{m} \bar{3} \frac{2}{m}$	4 4 4	(<i>a</i> ₁)	(<i>a</i> ₂)	<i>a</i> ₃	*	O_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*, *c*, and *a*, respectively.

(2) In class *42m* 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 $\uparrow$ and $*$, see text.