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Subject	ANSYS Tip of the Week: Conversion of Piezoelectric Material Data		

1. Introduction:

Conversion of material properties of piezoelectric ceramics (such as PZT) has caused many users confusion because of the difference between manufacturer-supplied data and the format required by ANSYS. This memo hopes to clarify this point and to provide users with information on conversion routines.

Section 2 outlines the general constitutive equations and provides a framework for the following discussion. Sections 3-6 cover converting manufacturer's data to ANSYS data for the stiffness matrix, dielectric constants, and piezoelectric constants.

2. Background Information:

Before proceeding to conversion routines, the basic constitutive relationship of piezoelectric materials will be outlined. Some notation may be non-standard, although the author has tried to keep consistent with notation in published data as well as Ch. 11 of the ANSYS Theory Manual.

T = mechanical stress

S = mechanical strain

D = electric displacement (also referred to in ANSYS as electric flux density)

E = electric field

The above notation (all capital letters) is used for both variables (vectors) and superscript notation indicating evaluation of properties.

The constitutive relationship usually given by manufacturers or published data/reports is in the following form:

$$\{S\} = [s^E]\{T\} + [d]\{E\}$$
$$\{D\} = [d]^t\{T\} + [\varepsilon^T]\{E\} \qquad \text{Eqns. 1 \& 2}$$

where

$\{T\}$ = stress vector (six components x, y, z, yz, xz, xy)

$\{S\}$ = strain vector (six components x, y, z, yz, xz, xy)

$\{D\}$ = electric displacement vector (three components x, y, z)

$\{E\}$ = electric field vector (three components x, y, z)

$[s^E]$ = compliance matrix evaluated at constant electric field, i.e. short circuit

$[d]$ = piezoelectric matrix relating strain/electric field

$[d]^t$ = piezoelectric matrix relating strain/electric field (transposed)

$[\varepsilon^T]$ = dielectric matrix evaluated at constant stress, i.e. mechanically free

On the other hand, ANSYS requires data in the following form (taken from Equation 11.1-1 in the ANSYS Theory Manual):

$$\{T\} = [c^E]\{S\} - [e]\{E\}$$
$$\{D\} = [e]^t\{S\} + [\varepsilon^S]\{E\}$$
Eqns. 3 & 4

where

$\{T\}$ = stress vector (six components x, y, z, xy, yz, xz)
$\{S\}$ = strain vector (six components x, y, z, xy, yz, xz)
$\{D\}$ = electric displacement vector (three components x, y, z)
$\{E\}$ = electric field vector (three components x, y, z)
$[c^E]$ = stiffness matrix evaluated at constant electric field, i.e. short circuit
$[e]$ = piezoelectric matrix relating stress/electric field
$[e]^t$ = piezoelectric matrix relating stress/electric field (transposed)
$[\varepsilon^S]$ = dielectric matrix evaluated at constant strain, i.e. mechanically clamped

In order to convert the manufacturer's data presented in the form of Equations 1 & 2 to ANSYS notation (Equations 3 & 4), Equation 1 needs to be based on stress rather than strain. The following manipulations can be performed:

$$\{S\} = [s^E]\{T\} + [d]\{E\}$$
$$[s^E]\{T\} = \{S\} - [d]\{E\}$$
$$\{T\} = [s^E]^{-1}\{S\} - [s^E]^{-1}[d]\{E\}$$
Eqns. 5-7

Since Equation 2 relates electric displacement to strain rather than stress, Equation 7 can then be plugged back into Equation 2:

$$\{D\} = [d]^t\{T\} + [\varepsilon^T]\{E\}$$
$$\{D\} = [d]^t\left([s^E]^{-1}\{S\} - [s^E]^{-1}[d]\{E\}\right) + [\varepsilon^T]\{E\}$$
$$\{D\} = [d]^t[s^E]^{-1}\{S\} + \left([\varepsilon^T] - [d]^t[s^E]^{-1}[d]\right)\{E\}$$
Eqns. 8-10

Upon comparison of Equation 7 & 10 with Equations 3 & 4, one can obtain the relationship between manufacturer-supplied data and ANSYS-required values:

$$[c^E] = [s^E]^{-1}$$
$$[\varepsilon^S] = [\varepsilon^T] - [d]^t[s^E]^{-1}[d]$$
$$[e] = [s^E]^{-1}[d] = [d]^t[s^E]^{-1}$$
Eqns. 11-13

These equations will form the basis of the conversion routines discussed shortly. Note that the manufacturer's data has mechanical vector in the form {x, y, z, yz, xz, xy} whereas ANSYS's mechanical vector is in the form {x, y, z, xy, yz, xz}.

3. Stiffness/Compliance Matrix:

There are three ways in which a user can input stress-strain data. One can use MP commands to specify orthotropic material properties (EX, NUXY, GXY). Otherwise, a user can input an anisotropic elastic matrix with TB,ANEL. At 5.6, the *TBOPT* field of the TB command controls whether this is read as a stiffness or compliance matrix.[1]

Assuming polarization in the 3-axis (z-axis), one can "map" manufacturer data to ANSYS data to generate a compliance matrix:

$$\left[s^E\right] = \left[c^E\right]^{-1} = \begin{bmatrix} s_{11}^E & s_{12}^E & s_{13}^E & 0 & 0 & 0 \\ & s_{11}^E & s_{13}^E & 0 & 0 & 0 \\ & & s_{33}^E & 0 & 0 & 0 \\ & & & s_{66}^E & 0 & 0 \\ & & & & s_{44}^E & 0 \\ & & & & & s_{44}^E \end{bmatrix}$$

If s_{66}^E is not available, it can be determined from $s_{66}^E = 2\left(s_{11}^E - s_{12}^E\right)$.[2] Note that if the user wants to input stiffness matrix, he/she must calculate $\left[c^E\right] = \left[s^E\right]^{-1}$. The user will need to do this to calculate the other constants as noted in subsequent sections. The user can invert the compliance matrix in Microsoft Excel using the MINVERSE function. For the TB,ANEL command, either matrix (stiffness matrix or compliance matrix) can be input.

To input this data as compliance, the user can issue the following commands:

```
TB,ANEL,1,1,,1            ! Material #1, 1 TEMP, TBOPT=1 for compliance input
TBDATA, 1,se11,se12,se13  ! Input first row
TBDATA, 7,se11,se13       ! Input second row
TBDATA,12,se33            ! Input third row
TBDATA,16,se66            ! Input fourth row
TBDATA,19,se44            ! Input fifth row
TBDATA,21,se44            ! Input sixth row
```

One needs to replace all values of `se12` above with appropriate numerical values of compliance.

On the other hand, to input this data as stiffness, the user can issue the following commands:

```
TB,ANEL,1,1,,0            ! Material #1, 1 TEMP, TBOPT=0 for stiffness input
TBDATA, 1,ce11,ce12,ce13  ! Input first row
TBDATA, 7,ce11,ce13       ! Input second row
TBDATA,12,ce33            ! Input third row
TBDATA,16,ce66            ! Input fourth row
TBDATA,19,ce44            ! Input fifth row
TBDATA,21,ce44            ! Input sixth row
```

One needs to replace all values of `ce12` above with appropriate numerical values of stiffness, as calculated by the inverse of the compliance matrix (using either mathematics/matrix programs such as MATLAB or Mathcad or spreadsheet programs such as Excel, as mentioned above).

[1] At 5.5 and prior, the compliance/stiffness matrix with TB,ANEL was controlled with a KEYOPT(2) setting for SOLID5/98 and KEYOPT(6) for PLANE13

[2] $s_{66}^E = \dfrac{1}{G_{xy}} = \dfrac{2\left(1+\nu_{xy}\right)}{E_x} = 2\left(s_{11}^E - s_{12}^E\right)$

An alternative method instead of using TB,ANEL is to use MP commands. Assuming polarization in the 3-axis (z-axis), the user can also convert manufacturer data to ANSYS data. Recall from Equation 2.1-4 in the ANSYS Theory Manual:

$$[D]^{-1} = \left[s^E\right] = \left[c^E\right]^{-1} = \begin{bmatrix} 1/E_x & -\nu_{xy}/E_y & -\nu_{xz}/E_z & 0 & 0 & 0 \\ & 1/E_y & -\nu_{yz}/E_z & 0 & 0 & 0 \\ & & 1/E_z & 0 & 0 & 0 \\ & & & 1/G_{xy} & 0 & 0 \\ & & & & 1/G_{yz} & 0 \\ & & & & & 1/G_{xz} \end{bmatrix}$$

Using the above relationship, one can input the stiffness via orthotropic MP commands as follows:

$$EX = \frac{1}{s_{11}^E} = EY$$

$$EZ = \frac{1}{s_{33}^E}$$

$$GXY = \frac{1}{s_{66}^E} = \frac{1}{2\left(s_{11}^E - s_{12}^E\right)}$$

$$GYZ = \frac{1}{s_{44}^E} = GXZ$$

$$NUXY = -\frac{s_{12}^E}{s_{11}^E}$$

$$NUYZ = -\frac{s_{13}^E}{s_{33}^E} = NUXZ$$

To input this data, one can issue the following commands:

```
MP,EX  ,1,1/se11          ! Material #1, Elastic modulus
MP,EY  ,1,1/se11
MP,EZ  ,1,1/se33
MP,NUXY,1,-se12/se11      ! minor Poisson's ratio
MP,NUYZ,1,-se13/se33
MP,NUXZ,1,-se13/se33
MP,GXY ,1,1/se66          ! Shear modulus
MP,GYZ ,1,1/se44
MP,GXZ ,1,1/se44
```

One needs to replace all values of `se12` above with appropriate numerical values of compliance.

4. Permittivity Matrix:

The permittivity matrix evaluated at constant strain is input into ANSYS. Oftentimes, manufacturers' data has permittivity evaluated at constant stress, so conversion is necessary.

As noted in Equation 12, one can calculate the dielectric constants based on constant strain from the following relationship:

$$\left[\varepsilon^S\right] = \left[\varepsilon^T\right] - [d]^t \left[s^E\right]^{-1} [d]$$

After evaluating Equation 12 above, the user can input permittivity. The permittivity matrix has only diagonal terms:

$$\left[\varepsilon^S\right] = \begin{bmatrix} \varepsilon_{11}^S & 0 & 0 \\ & \varepsilon_{11}^S & 0 \\ & & \varepsilon_{33}^S \end{bmatrix} = \varepsilon_o \begin{bmatrix} K_{11}^S & 0 & 0 \\ & K_{11}^S & 0 \\ & & K_{33}^S \end{bmatrix}$$

where $K_{11}^S = \dfrac{\varepsilon_{11}^S}{\varepsilon_o}$ is relative permittivity.

In ANSYS, although the user has the choice of inputting permittivity as an absolute value ε_{33}^T or relative value K_{33}^T, starting from 5.4, the relative value is the recommended choice. Assuming polarization in the 3-axis (z-direction), this can be input with the MP commands as follows:

```
EMUNIT,EPZRO,8.85e-12      ! Define free-space permittivity
MP,PERX,1,reps11           ! Material #1
MP,PERY,1,reps11
MP,PERZ,1,reps33
```

One should replace all values of `reps33` above with appropriate numerical values of *relative* permittivity.[3]

5. Density Input:

Density needs no conversion. It is input with the MP command as follows:

```
MP,DENS,1,dens             ! Material #1
```

One needs to replace the value of `dens` above with the appropriate numerical value of density.

[3] As noted above, the user has the option of inputting relative or absolute permittivity. Any small value (<1) will be automatically recognized as absolute permittivity by ANSYS, so the user does not need to take any special action.

6. Piezoelectric Constant Matrix:

Usually, manufacturers' data has $[d]$, which relates mechanical strain to electric field. However, ANSYS requires $[e]$, relating mechanical stress to electric field, so conversion is necessary.

Note from Equation 13 above, a relationship between $[e]$ and $[d]$ is established as follows:

$$[e] = \left[s^E\right]^{-1}[d] = [d]^t\left[s^E\right]^{-1}$$

where, assuming polarization in the 3-axis (z-direction) and symmetry in the unpolarized directions ($d_{32} = d_{31}$ and $d_{24} = d_{15}$):

$$[d]^t = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & d_{15} \\ 0 & 0 & 0 & 0 & d_{15} & 0 \\ d_{31} & d_{31} & d_{33} & 0 & 0 & 0 \end{bmatrix}$$

Recall from the above discussions that manufacturers' data assumes the mechanical vector as {x, y, z, yz, xz, xy} corresponding to {1, 2, 3, 4, 5, 6} indexes. Row 4 needs to be shifted to Row 5, and, similarly, Row 5 → Row 6, Row 6 → Row 4. Hence, d_{15} and d_{24} are shifted one across.

The user can use this matrix with $\left[s^E\right]^{-1} = \left[c^E\right]$ to evaluate $[e]$ (with 4, 5, 6 rows properly modified), which will become:

$$[e] = \begin{bmatrix} 0 & 0 & e_{31} \\ 0 & 0 & e_{31} \\ 0 & 0 & e_{33} \\ 0 & 0 & 0 \\ 0 & e_{15} & 0 \\ e_{15} & 0 & 0 \end{bmatrix}$$

To input this data, one can issue the following commands:

```
TB,PIEZ,1                   ! Material #1, piezo matrix
TBDATA, 3,e31               ! Input first row
TBDATA, 6,e31               ! Input second row
TBDATA, 9,e33               ! Input third row
TBDATA,14,e15               ! Input fifth row
TBDATA,16,e15               ! Input sixth row
```

One needs to replace all values of `e33` above with appropriate numerical values of piezo constants.

7. Conclusion & Future Work:

This memo provided background information on the constitutive laws of piezoelectric ceramics, both in manufacturer-supplied form as well as ANSYS notation. Sections 3-6 develop the equations needed to convert material data to a form acceptable for use with ANSYS.

The attached Excel worksheet contains conversion routines to provide the user with a simple way to produce material library data with the poling direction in either the z- or y-directions. Export the sheet as CSV (comma-separated text), and this can be directly input into ANSYS. Sample material properties are provided as well. Note that the author makes no guarantee or assumes no liability for any data in the Excel worksheet.

John Thompson at ANSYS Technical Support has also issued a similar memo and a very useful PIEZMAT macro to facilitate conversion of data. CSI or the author of this document can be contacted to obtain this macro and document.

In the future, the author may add a separate document for conversion of piezoelectric material properties if the data is assuming the constitutive equations written in terms of strain and electric field (i.e., if one has the analogous $[g]$ coefficients instead of $[d]$ matrix). 2D material definition will also be added (i.e., change poling direction to y-axis).

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