### LECTURE 4: REPRESENTATION QUADRICS:

### Review Questions:

- 1. What is the difference between an anisotropic property and an isotropic property? Name some of each class. Which properties are likely to be tensors?
- 2. What is the definition of a second rank tensor property? There are two alternative definitions, can you specify both? What are a few second rank tensor properties?
- We talked a lot about transformations, why? Write the transformation law for a second rank tensor in at least two different notations.
- 4. What are principal values and principal directions? What is a necessary and sufficient condition that principal axes and principal values exist?
- 5. Suppose that one knows the principal directions for a second rank tensor property. What is the value that would be measured for a direction with direction cosines I<sub>1</sub> I<sub>2</sub> I<sub>3</sub>.?

### Quadrics:

We seek a convenient geometrical representation of the tensor property.

A surface in 3-d is a good possibility. Why? (Consider the representation of the tensor when the coordinate axes are the principal directions.)

# Equation for a quadric surface:

$$A_{11}x_{1}^{2} + A_{22}x_{2}^{2} + A_{33}x_{3} + A_{12}x_{1}x_{2} + A_{13}x_{1}x_{3} + A_{23}x_{2}x_{3} + A_{1}x_{1} + A_{2}x_{2} + A_{3}x_{3} + C = 0$$

- 1. Can show that the components of the equation for a quadric in 3-d transform like a tensor.
- 2. Infer that each symmetric 2<sup>nd</sup> rank tensor represented by a quadric
- 3. Direction and magnitude of the effect can be given by a geometric construction using the representation quadric.

Quadric Surfaces:

Ellip. Paraboloid

Hyper. Paraboloid

Ellipsoid 
$$\frac{x^2}{\Delta^2} + \frac{y^2}{R^2} + \frac{z^2}{C^2} = 1$$

 $\frac{x^2}{A^2} + \frac{y^2}{B^2} + \frac{z^2}{C^2} = 1$  Vertices at (±a, 0,0) if a2>b2,a2>c2

Real or imaginary ellipse; point if tangent plane

Ellip. Hyp. 1 Sheet 
$$\frac{x^2}{A^2} + \frac{y^2}{B^2} - \frac{z^2}{C^2} = 1$$

Doubly ruled surface; contains two families of generators

Tensor property would have no value in one direction

Ellip. Hyp. 2 Sheet 
$$\frac{x^2}{A^2} - \frac{y^2}{B^2} - \frac{z^2}{C^2} = 1$$

Tensor property would have no

value in one direction

$$A^2 B^2 C^2$$

Not symmetric

Ellip. Paraboloid 
$$\frac{x^2}{A^2} + \frac{y^2}{B^2} = z$$

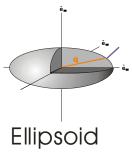
 $\frac{x^2}{A^2} - \frac{y^2}{B^2} = z$ 

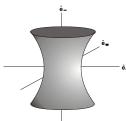
Not symmetric

Elliptic Cone

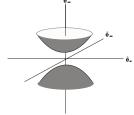
 $\frac{x^2}{A^2} + \frac{y^2}{B^2} = \frac{z^2}{C^2}$ 

Not symmetric





Hyperboloid of 1 Sheet



Hyperboloid of 2 Sheets

Because symmetric second rank tensors have values that are defined for all directions, focus on the set of quadrics expressible as ellipsoids.

The other quadrics are not defined in some directions or are not symmetric.

If lines, flat planes, cylinders, points and etc are eliminated, the general equation for a quadric surface that corresponds to the indicial form above is

$$A_{11}X_1^2 + A_{22}X_2^2 + A_{33}X_3^2 + A_{12}X_1X_2 + A_{13}X_1X_3 + A_{23}X_2X_3 + A_{21}X_1X_2 + A_{31}X_1X_3 + A_{32}X_2X_3C = 0$$

If 
$$A_{ij}=A_{ji}$$
, then 
$$A_{11}X_1^2 + A_{22}X_2^2 + A_{33}X_3^2 + \\ 2A_{12}X_1X_2 + 2A_{13}X_1X_3 + 2A_{23}X_2X_3 + C = 0$$

This equation represents an ellipsoid of revolution, and can be written in indicial form as  $A_{ii}x_{i}x_{i} + C = 0$  (1).

Now for a given vector with components,  $x_i$ , a transformation of axes gives new components  $\mathbf{X'}_k = \mathbf{a}_{kl} \mathbf{X}_l$  and the inverse  $\mathbf{X}_l = \mathbf{a}_{kl} \mathbf{X'}_k$ .

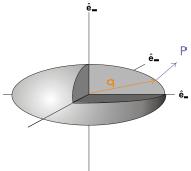
Plug the forward transformation into (1) to get  $A_{ij}a_{ki}x'_k a_{ij}x'_l + C = 0$  and  $A_{ij}a_{ki}a_{ij} x'_k x'_l + C = 0$ 

Because the equation in the transformed space is  $A'_{kl} x'_k x'_l + C = 0$ , then by inspection

$$A'_{kl} = a_{ki}a_{lj}A_{ij}$$

The components of the equation for an ellipsoid transform like those of a symmetric tensor.

# Size of the representation quadric:



Suppose a property is given by  $q_i = S_{ij}p_j$ .

Recall that for any direction relative to the principal axes space, the magnitude of the property in that direction is  $S = S_{ij}I_iI_j$ .

Now consider a representation quadric with unit dimension,  $S_{ij}x_ix_j = 1$ .

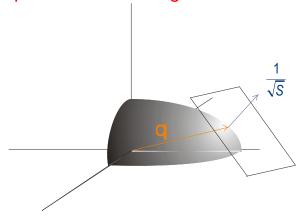
For a vector  $q_i = |q|I_i$ , then plugging into the quadric equation  $S_{ij}|q|I_j|q|I_j = 1$ 

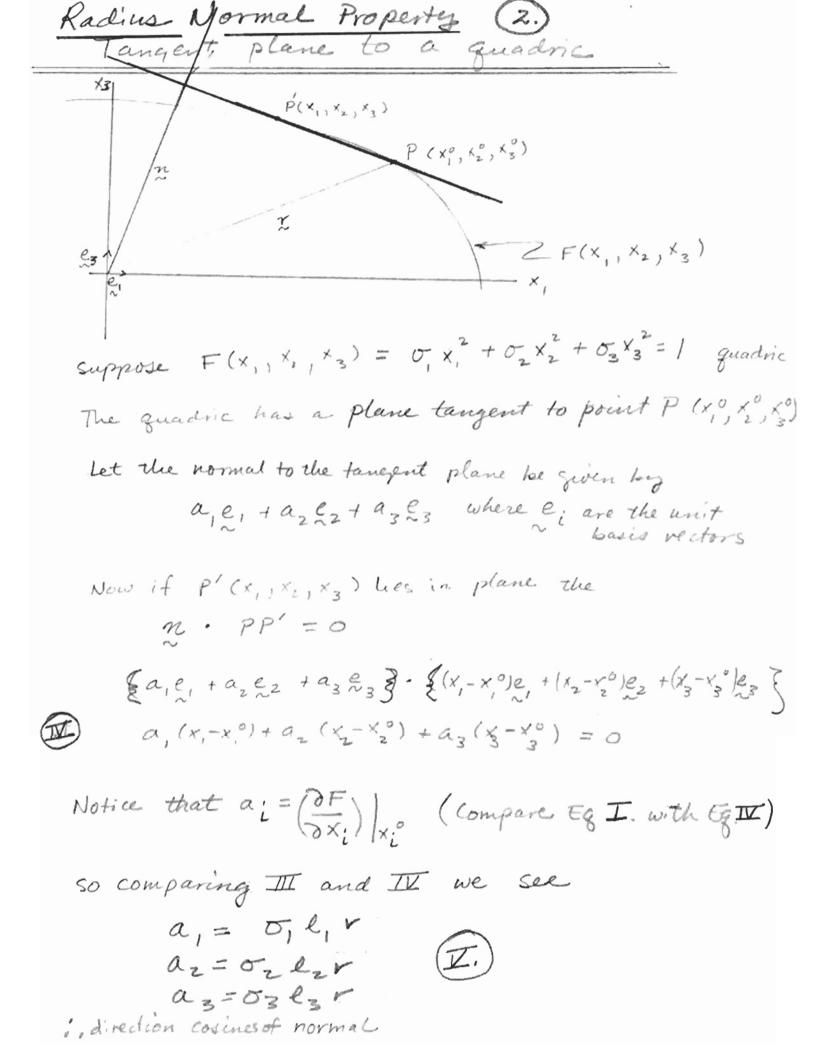
And therefore, 
$$S_{ij}I_{i}I_{j} = \frac{1}{|q|^{2}}$$
 and  $\overline{|q| = \frac{1}{\sqrt{S}}}$ 

The magnitude of the property in a given direction is the inverse of the square root of the radius vector of the quadric in that direction.

# Radius Normal Property:

The effect vector is normal to the plane tangent to the quadric at the intersection of the driving force direction (i.e. the radius of the quadric in the driving force direction).





# Radius Normal Property



At the point (x1, x2, x3) is

$$(x_1-x_1^\circ) (\frac{\partial F}{\partial x_1})_0 + (x_2-x_2^\circ) (\frac{\partial F}{\partial x_2})_0 + (x_3-x_3^\circ) (\frac{\partial F}{\partial x_3})_0 = 0$$

The representation quadric is given by  $1 = \sigma_{ij} x_i x_j$  which in principal coordinates becomes  $1 = \sigma_{11} x_1 x_1 x_2 x_1$ , i.e.

$$1 = \sigma_1 x_1^2 + \sigma_2 x_2^2 + \sigma_3 x_3^2$$

Looking at the sketch below we see that x1 = rl1, x2 = rl2, x3 = rl3

By taking the partial derivatives of Eqn. II and substituting them into I we obtain

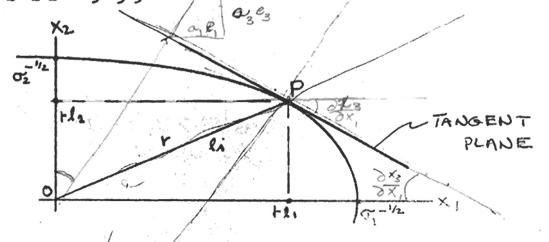
$$(x_1-rl_1) \sigma_1 rl_1 + (x_2-rl_2) \sigma_2 rl_2 + (x_3-rl_3) \sigma_3 rl_3 = 0$$

or 
$$\sigma_1 r l_1 x_1 + \sigma_2 r l_2 x_2 + \sigma_3 r l_3 x_3 = \sigma_1 r^2 l_1^2 + \sigma_2 r^2 l_2^2 + \sigma_3 r^2 l_3^2$$

but 
$$\sigma_1 r^2 l_1^2 + \sigma_2 r^2 l_2^2 + \sigma_3 r^2 l_3^2 = 1$$

 $\sigma_1 r l_1 x_1 + \sigma_2 r l_2 x_2 + \sigma_3 r l_3 x_3 = 1$  is the Eqn. of the tangent plane

to the quadric



II

 $\pi$ 

I

	Radius Normac Propertie Nyc p23. 3.
=	First find direction cosines of letted, Pi Suppose Po = 0; 3;
	In Principle Avis Representation
	$\sigma_{ij} = \begin{bmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_2 & 0 \\ 0 & 0 & \sigma_3 \end{bmatrix}$
	50 P = [ 5,81 , 5282) 5303] = 5:8i
	If 8: = 18/li where li are direct covenes
	then direction cosines of D are proportioned
	notice that direction cosine of P (Eg III)
	are proportional to direction covenes of
	normal (E2 V.)

in parallel with the direction of the effect radius normal property.

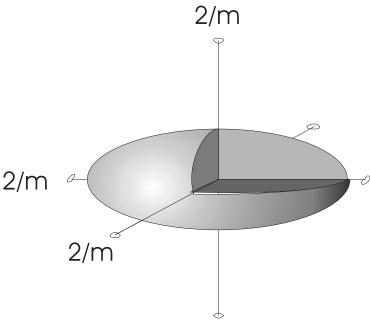
# Effect of symmetry:

Any second rank symmetric tensor has inherent symmetry m m m. That is, the tensor

- 1. Is centrosymmetric: Tensor relation is satisfied when  $-\mathbf{r}$  is substitute for  $\mathbf{r}$ .
- 2. Has three mirror planes perpendicular to the principal directions
- 3. Has two-fold rotation axes parallel to the principal directions.

The exact shape of the property and its quadric and the orientation of the quadric with respect to the crystal are restricted by the point group symmetry.

Neumann's Principle: The symmetry elements of any physical property must include the symmetry elements of the point group of the crystal. The physical property may be more symmetric, but not less.



### Relationship between quadric and crystal axes:

**Triclinic**: Point group classes  $1, \boxed{1}$ : Quadric has more symmetry that both classes. No restriction on relative orientation of quadric. No restriction on the principal values. Need to measure six components to the tensor. (Three directions and three values).

**Monoclinic**: 2, m, 2/m: One principal direction of the ellipsoid must be aligned along the 2-fold axes. Other axes may be in any orientation. No restriction on the principal values. Need to measure four components (three principal values and one angle).

**Orthorhombic**: 222, *mm*2, *mmm*: Inherent symmetry of the quadric just matches the symmetry of the most symmetric point group. Axes of crystal and the principal directions of the quadric must be aligned. No restriction on the principal values. Need to measure three principal values.

**Tetragonal:** 4,  $\overline{4}$ ,  $\overline{4/m}$ , 422, 4mm,  $\overline{4}$ 2m, 4/mmm: Two principal values of the quadric must be equal. Principal directions must be parallel to the crystal axes. Need to measure two principal values.

**Trigonal:** 3,  $\boxed{3}$ , 32, 3m,  $\boxed{3m}$ : Two principal values must be equal. One principal direction must be aligned with 3 fold. Two principal values must be measured.

**Hexagonal:** 6,  $\overline{6}$ , 3m,  $\overline{6/m}$ , 622, 6mm,  $\overline{6}m2$ , 6/mmm: Two principal values must be equal. One principal direction must be aligned with 3 fold. Two principal values must be measured.

**Cubic:** 23, m3, 432,  $\overline{43}m$ ,  $\overline{m3}m$ : All three principal values must be equal. The property is isotropic. Only one measurement must be made.

Table 3. (After Nye).

Opt Class Isotropic	System Cubic	Charac. Symmetry 4 3-folds	Shape and Orientation Sphere	# ind. Coeff. 1	Tensor in conv. orient.  (a 0 0 0 0 a 0 0 0 a 0 0 a 0 0 a 0 0 a 0 0 a 0 0 a 0 0 a 0 0 a 0 0 0 a 0 0 0 a 0 0 0 0 a 0 0 0 0 a 0 0 0 0 a 0 0 0 0 0 a 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Uniaxial	Tetragonal Hexagonal Trigonal	<ol> <li>4-fold</li> <li>6-fold</li> <li>3-fold</li> </ol>	Quadric of revolution about the principal symmetry axis	2	$ \begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & c \end{pmatrix} $
Biaxial	Orthorhombic	$3 \perp \text{2-folds}$	General quadiric aligned to crystal axes	3	$ \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix} $
	Monoclinic		General quadric with one principal axis aligned to diad	4	$ \begin{pmatrix} a & 0 & d \\ 0 & b & 0 \\ d & 0 & c \end{pmatrix} $
	Triclinic	Center or no	General quadric with no relation to crystal axes	6	$\begin{pmatrix} a & e & d \\ e & b & f \\ d & f & c \end{pmatrix}$

### SUMMARY:

## Tensor properties:

Many properties are represented by tensors.
 Situation always arises if rank of cause is not equal to rank of effect or if properties are anisotropic (i.e. property varies with direction in crystal)

2. If Property relates Prop has Rank

Scalar $\Rightarrow$ Vector 1 Vector $\Rightarrow$ Vector 2  $2^{\text{nd}}$  Rank $\Rightarrow$ 2<sup>nd</sup> Rank 4

For examples, see the accompanying table.

3. Number of components (values necessary to specify the property) goes up with rank.

3<sup>n</sup> where n is the rank of the tensor property.

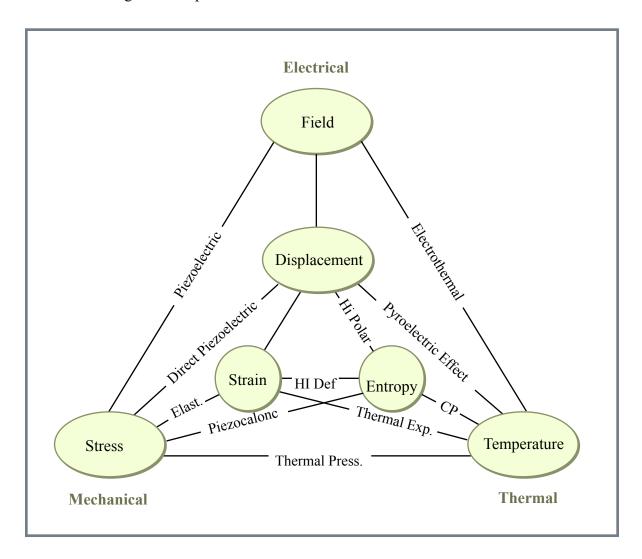
The actual values depend on the choice of the coordinate system, but the tensor properties has invariants which do not depend on that choice.

- 4. If a property relates one vector to another the property is a second rank tensor. All second rank tensors transform according a particular tensor transformation law.
- 5. The symmetry elements of any physical property must include the symmetry elements of the point group of the crystal.
- 6. For any second rank symmetric tensor there are three mutually perpendicular directions for which cause and effect are in the same direction. The directions are the principal directions and the values are the principal values.
- 7. The magnitude of a  $2^{nd}$  rank tensor property in a direction  $[l_1, l_1, l_3]$  is given by  $S = S_{ij} l_i l_j$

# Quadric Surfaces: Summary

- 1. Representation quadrics are a method to visualize a 2<sup>nd</sup> rank symmetric tensor property.
- 2. Correspondence between the visualization and the tensor property occurs because the coefficients of the quadric equation transform in the same way as the tensor.
- 3. The direction and magnitude of the effect is given by a geometric construction on the representation quadric. For a given direction, the magnitude of the property is given by  $1/r^2$  where r is the radius of the quadric at the point of

intersection. The direction of the effect is given by the normal to the plane tangent at the point of intersection.



Adapted from Nye, 1957.

### **BIBLIOGRAPHY**

- Dove, M.T., *Structure and Dynamics: An Atomic View of Materials*, 334 pp., Oxford University Press, Oxford, 2003.
- Malvern, L.E., *Introduction to the Mechanics of a Continuous Medium*, Prentice Hall, Englewood Cliffs, NJ, 1969.
- Nye, J.F., *Physical Properties of Crystals*, 322 pp., Oxford University Press, Oxford, UK, 1957.
- Zwikker, C., *Physical Properties of Solid Materials*, 300 pp., Pergamon Press, London, 1954.