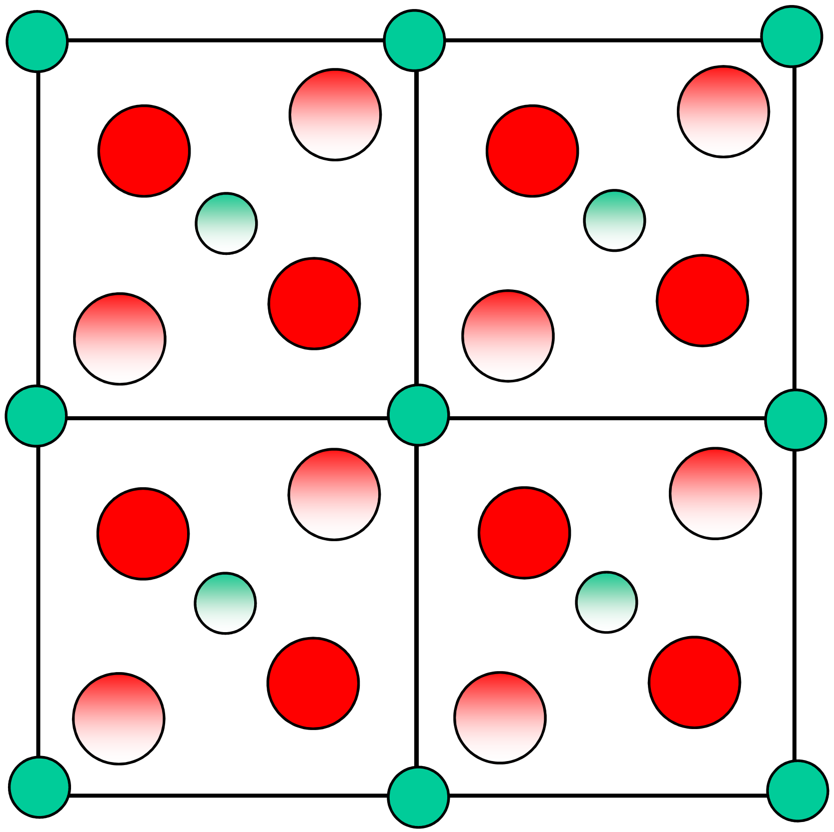
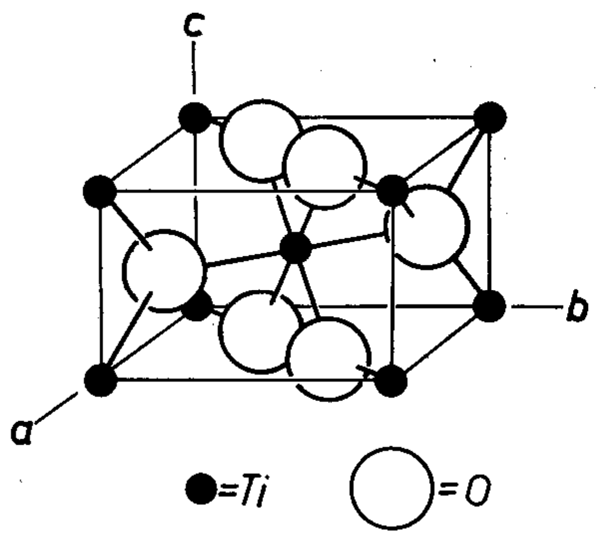
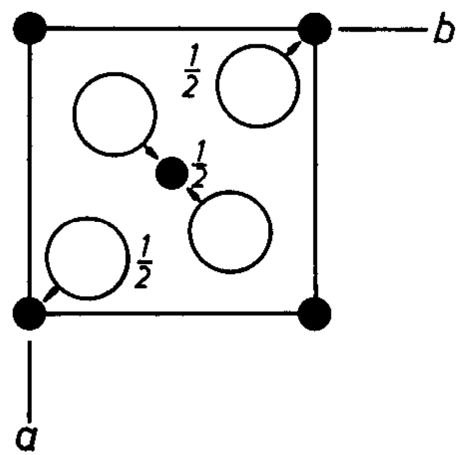
Rutile, TiO_2



Rutile, TiO_2

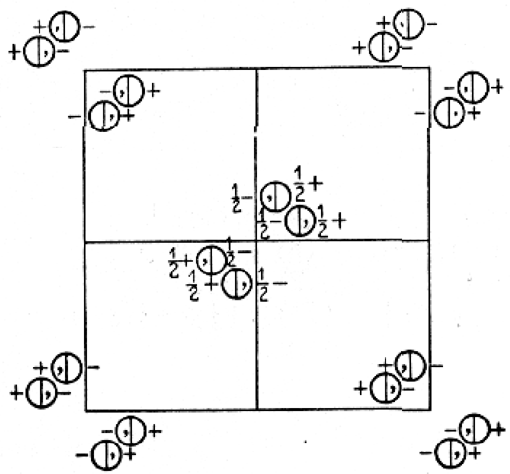
A		B		
Lattice	Basis	Space group	Positions of the atoms	
tetragonal P	Ti: 0,0,0 $\frac{1}{2},\frac{1}{2},\frac{1}{2}$	P 4_2/mnm	a	Ti: 0,0,0 $\frac{1}{2},\frac{1}{2},\frac{1}{2}$
$a_0 = 4.59$ Å $c_0 = 2.96$ Å	O: 0.3, 0.3, 0 0.8, 0.2, $\frac{1}{2}$ 0.2, 0.8, $\frac{1}{2}$ 0.7, 0.7, 0	$a_0 = 4.59$ Å $c_0 = 2.96$ Å	f	O: x,x,0 $\frac{1}{2}+x, \frac{1}{2}-x, \frac{1}{2}$ $\frac{1}{2}-x, \frac{1}{2}+x, \frac{1}{2}$ $\bar{x}, \bar{x}, 0$ $x = 0.3$

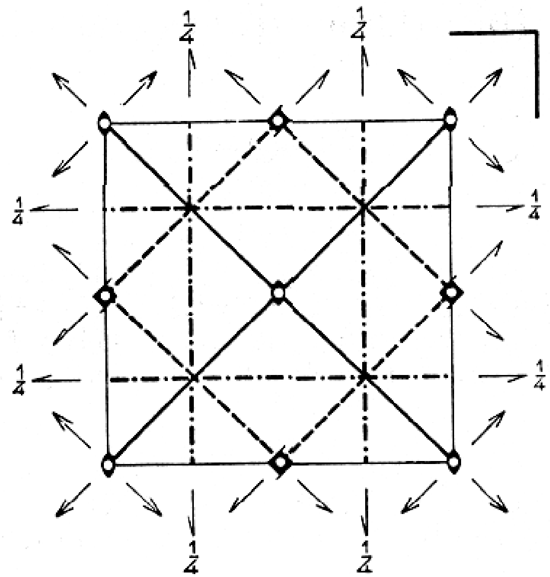




$P\,4_2/m\,n\,m$ D_{4h}^{14} $4/m\,m\,m$ Tetragonal

No. 136 $P\,4_2/m\;2_1/n\;2/m$ Patterson symmetry $P\,4/m\,m\,m$





Origin at centre $(m\,m\,m)$ at $2/m\;1\;2/m$

Asymmetric unit $0\leq x\leq \tfrac{1}{2};\quad 0\leq y\leq \tfrac{1}{2};\quad 0\leq z\leq \tfrac{1}{2};\quad x\leq y$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $4^{+}(0,0,\tfrac{1}{2})\quad 0,\tfrac{1}{2},z$	(4) $4^{-}(0,0,\tfrac{1}{2})\quad \tfrac{1}{2},0,z$
(5) $2(0,\tfrac{1}{2},0)\quad \tfrac{1}{4},y,\tfrac{1}{4}$	(6) $2(\tfrac{1}{2},0,0)\quad x,\tfrac{1}{4},\tfrac{1}{4}$	(7) $2\quad x,x,0$	(8) $2\quad x,\bar{x},0$
(9) $\bar{1}\quad 0,0,0$	(10) $m\quad x,y,0$	(11) $\bar{4}^{+}\quad \tfrac{1}{2},0,z;\ \tfrac{1}{2},0,\tfrac{1}{4}$	(12) $\bar{4}^{-}\quad 0,\tfrac{1}{2},z;\ 0,\tfrac{1}{2},\tfrac{1}{4}$
(13) $n(\tfrac{1}{2},0,\tfrac{1}{2})\quad x,\tfrac{1}{4},z$	(14) $n(0,\tfrac{1}{2},\tfrac{1}{2})\quad \tfrac{1}{4},y,z$	(15) $m\quad x,\bar{x},z$	(16) $m\quad x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

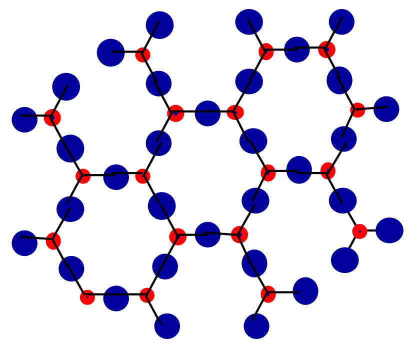
Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates	Reflection conditions
				General:
16	k	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{y}+\frac12,x+\frac12,z+\frac12$ (4) $y+\frac12,\bar{x}+\frac12,z+\frac12$ (5) $\bar{x}+\frac12,y+\frac12,\bar{z}+\frac12$ (6) $x+\frac12,\bar{y}+\frac12,\bar{z}+\frac12$ (7) $y,x,\bar{z}$ (8) $\bar{y},\bar{x},\bar{z}$ (9) $\bar{x},\bar{y},\bar{z}$ (10) $x,y,\bar{z}$ (11) $y+\frac12,\bar{x}+\frac12,\bar{z}+\frac12$ (12) $\bar{y}+\frac12,x+\frac12,\bar{z}+\frac12$ (13) $x+\frac12,\bar{y}+\frac12,z+\frac12$ (14) $\bar{x}+\frac12,y+\frac12,z+\frac12$ (15) $\bar{y},\bar{x},z$ (16) y,x,z	$0kl$: $k+l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
				Special: as above, plus
8	j	$..m$	x,x,z $\bar{x},\bar{x},z$ $\bar{x}+\frac12,x+\frac12,z+\frac12$ $x+\frac12,\bar{x}+\frac12,z+\frac12$ $\bar{x}+\frac12,x+\frac12,\bar{z}+\frac12$ $x+\frac12,\bar{x}+\frac12,\bar{z}+\frac12$ $x,x,\bar{z}$ $\bar{x},\bar{x},\bar{z}$	no extra conditions
8	i	$m..$	$x,y,0$ $\bar{x},\bar{y},0$ $\bar{y}+\frac12,x+\frac12,\frac12$ $y+\frac12,\bar{x}+\frac12,\frac12$ $\bar{x}+\frac12,y+\frac12,\frac12$ $x+\frac12,\bar{y}+\frac12,\frac12$ $y,x,0$ $\bar{y},\bar{x},0$	no extra conditions
8	h	$2..$	$0,\frac12,z$ $0,\frac12,z+\frac12$ $\frac12,0,\bar{z}+\frac12$ $\frac12,0,\bar{z}$ $0,\frac12,\bar{z}$ $0,\frac12,\bar{z}+\frac12$ $\frac12,0,z+\frac12$ $\frac12,0,z$	hkl : $h+k,l=2n$
4	g	$m.2m$	$x,\bar{x},0$ $\bar{x},x,0$ $x+\frac12,x+\frac12,\frac12$ $\bar{x}+\frac12,\bar{x}+\frac12,\frac12$	no extra conditions
4	f	$m.2m$	$x,x,0$ $\bar{x},\bar{x},0$ $\bar{x}+\frac12,x+\frac12,\frac12$ $x+\frac12,\bar{x}+\frac12,\frac12$	no extra conditions
4	e	$2.mm$	$0,0,z$ $\frac12,\frac12,z+\frac12$ $\frac12,\frac12,\bar{z}+\frac12$ $0,0,\bar{z}$	hkl : $h+k+l=2n$
4	d	$\bar{4}..$	$0,\frac12,\frac14$ $0,\frac12,\frac34$ $\frac12,0,\frac14$ $\frac12,0,\frac34$	hkl : $h+k,l=2n$
4	c	$2/m..$	$0,\frac12,0$ $0,\frac12,\frac12$ $\frac12,0,\frac12$ $\frac12,0,0$	hkl : $h+k,l=2n$
2	b	$m.mm$	$0,0,\frac12$ $\frac12,\frac12,0$	hkl : $h+k+l=2n$
2	a	$m.mm$	$0,0,0$ $\frac12,\frac12,\frac12$	hkl : $h+k+l=2n$

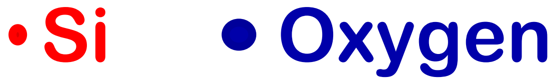
Crystalline vs. Non-crystalline

Crystalline materials...

- atoms pack in periodic, 3D arrays
- typical of: -metals
  -many ceramics
  -some polymers



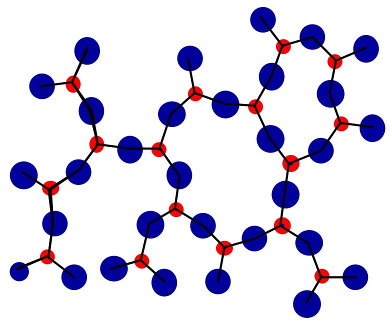
crystalline SiO_2



Non-crystalline materials...

- atoms have no periodic packing
- occurs for: -complex structures
  -rapid cooling

"amorphous" = non-crystalline

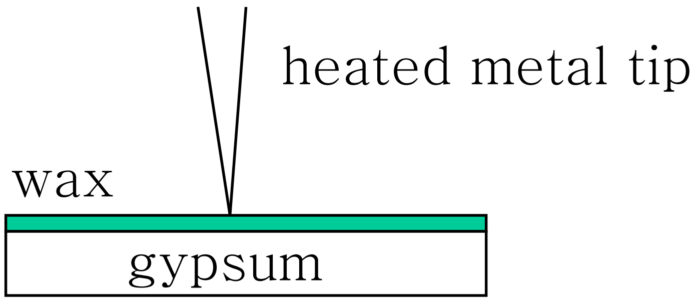


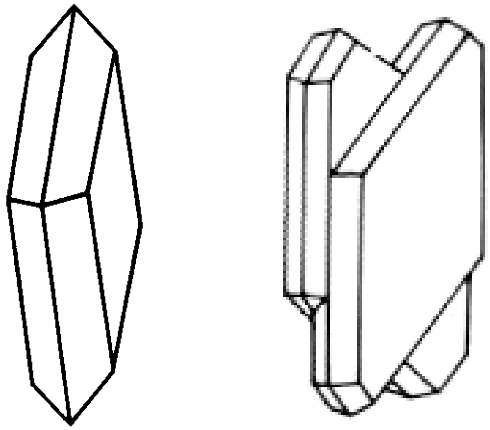
noncrystalline SiO_2

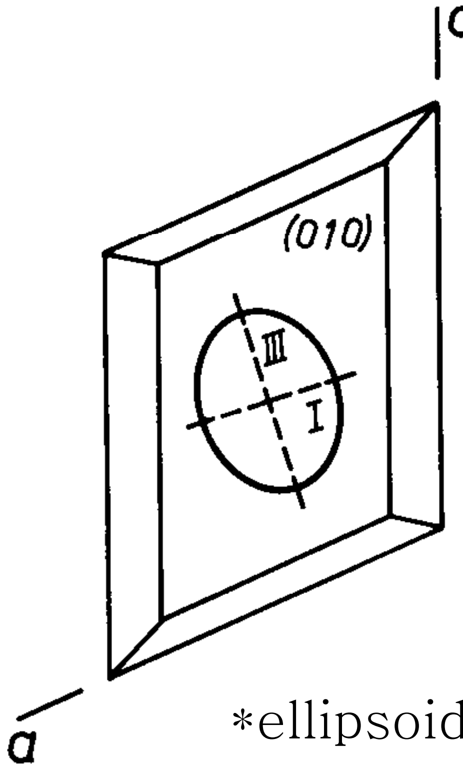
Thermal conductivity

ex) gypsum ($CaSO_4 2H_2O$)

Monoclinic

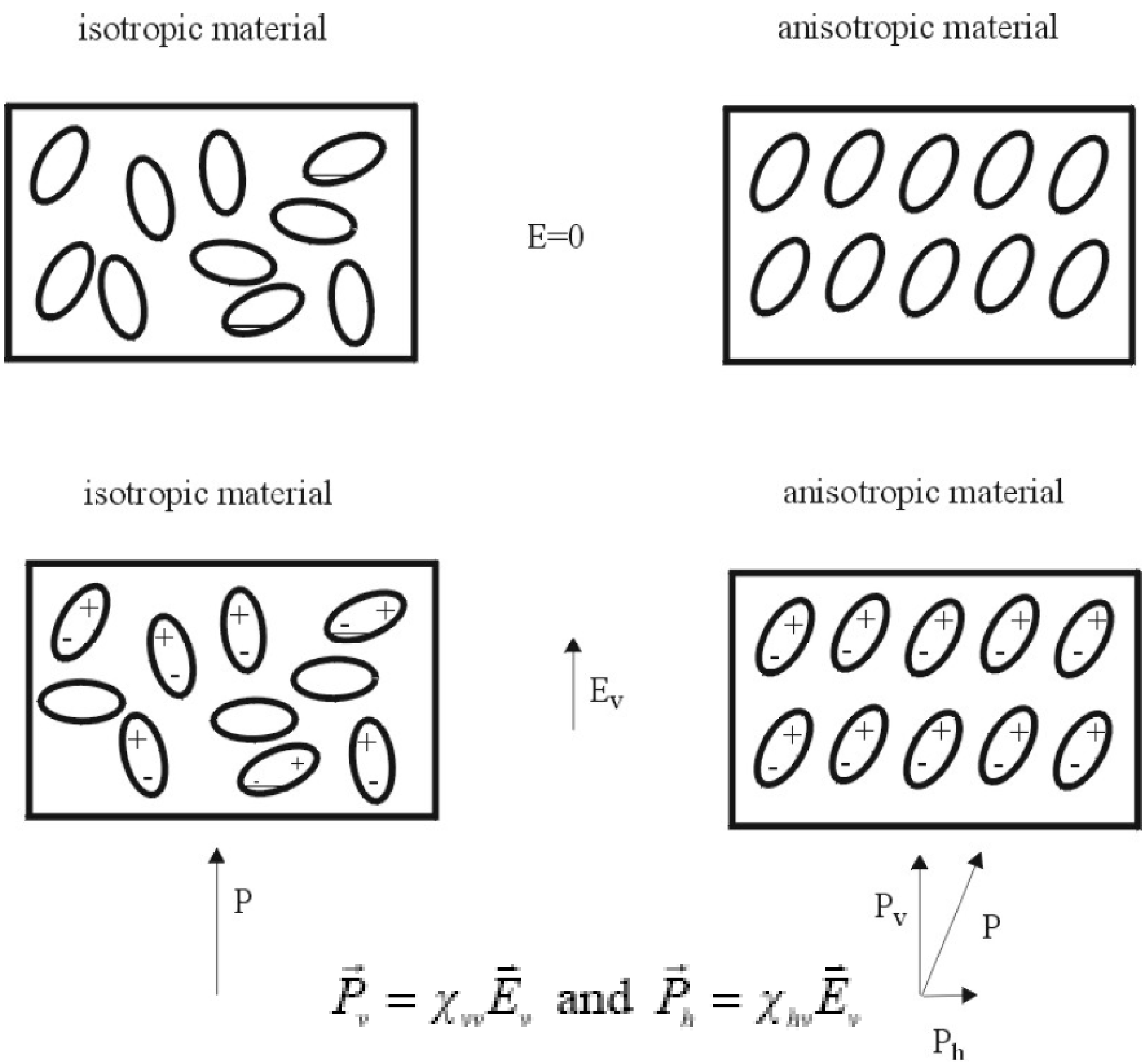






*ellipsoidal rather than circular

Electric susceptibility χ



$$\vec{P}_v = \chi_{vv}\vec{E}_v \text{ and } \vec{P}_h = \chi_{hv}\vec{E}_v$$

Physical Properties

- scalar (zero rank tensor)- non-directional physical

  quantities, a single number

  ex) density, temperature

- vector (first rank tensor)- magnitude and direction

  an arrow of definite length and direction

  ex) mechanical force, electric field, temperature gradient

  three mutually perpendicular axes Ox_1,Ox_2,Ox_3

  components $\vec{E} = [E_1, E_2, E_3]$

SUMMARY OF VECTOR NOTATION AND FORMULAE

In this book vectors are printed in bold-face type, thus, $\mathbf{p}$. The components of $\mathbf{p}$ referred to axes Ox_1, Ox_2, Ox_3 are p_1, p_2, p_3. We write

$$\mathbf{p} = [p_1, p_2, p_3],$$

and often denote $\mathbf{p}$ by p_i or $[p_i]$.

The *magnitude*, or *length*, of $\mathbf{p}$ is denoted by p:

$$p^2 = p_1^2+p_2^2+p_3^2 = p_i p_i.$$

A *unit vector* is one of unit length.

The *scalar product* of $\mathbf{p}$ and $\mathbf{q}$ is denoted by $\mathbf{p}\,.\,\mathbf{q}$:

$$\mathbf{p}\,.\,\mathbf{q} = p_i q_i = pq\cos\theta,$$

where θ is the angle between $\mathbf{p}$ and $\mathbf{q}$.

The *vector product* of $\mathbf{p}$ and $\mathbf{q}$ is denoted by $\mathbf{p}\wedge\mathbf{q}$:

$$\mathbf{p}\wedge\mathbf{q} = (pq\sin\theta)\mathbf{l},$$

where $\mathbf{l}$ is a unit vector perpendicular to $\mathbf{p}$ and $\mathbf{q}$ such that $\mathbf{p}$, $\mathbf{q}$, $\mathbf{l}$ form a right-handed set. The components of $\mathbf{p}\wedge\mathbf{q}$ referred to right-handed axes are

$$[p_2 q_3 - p_3 q_2,\ p_3 q_1 - p_1 q_3,\ p_1 q_2 - p_2 q_1].$$

The *gradient* of a scalar ϕ which varies with position is a vector denoted by $\operatorname{grad}\phi$:

$$\operatorname{grad}\phi = \left[\frac{\partial\phi}{\partial x_1}, \frac{\partial\phi}{\partial x_2}, \frac{\partial\phi}{\partial x_3}\right].$$

The *divergence* of a vector $\mathbf{p}$ which varies with position is a scalar denoted by $\operatorname{div}\mathbf{p}$:

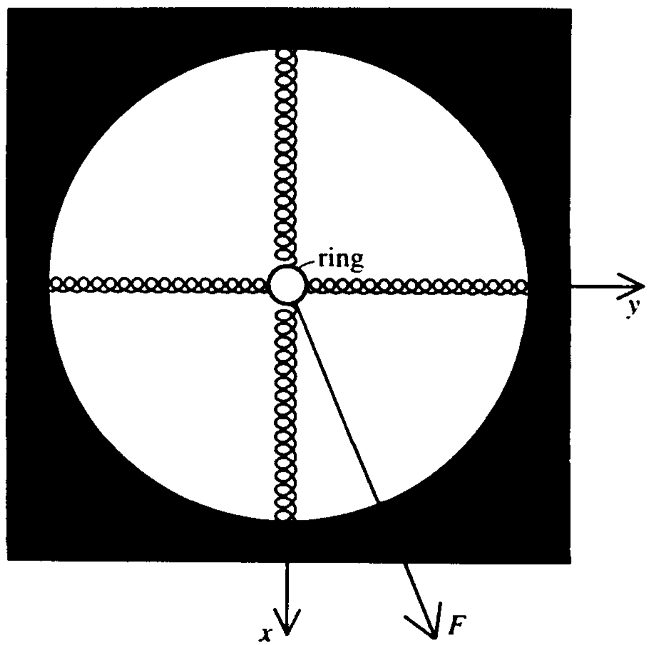
$$\operatorname{div}\mathbf{p} = \frac{\partial p_1}{\partial x_1}+\frac{\partial p_2}{\partial x_2}+\frac{\partial p_3}{\partial x_3} = \frac{\partial p_i}{\partial x_i}.$$

The *curl* of a vector $\mathbf{p}$ which varies with position is a vector denoted by $\operatorname{curl}\mathbf{p}$, whose components referred to right-handed axes are

$$\left[\frac{\partial p_3}{\partial x_2}-\frac{\partial p_2}{\partial x_3}, \frac{\partial p_1}{\partial x_3}-\frac{\partial p_3}{\partial x_1}, \frac{\partial p_2}{\partial x_1}-\frac{\partial p_1}{\partial x_2}\right].$$

Physical Properties

- second rank tensor
- mechanical analogy



central ring–2 pairs of springs

at right angle

springs on opposite sides are identical but have a different spring constant to perpendicular pair

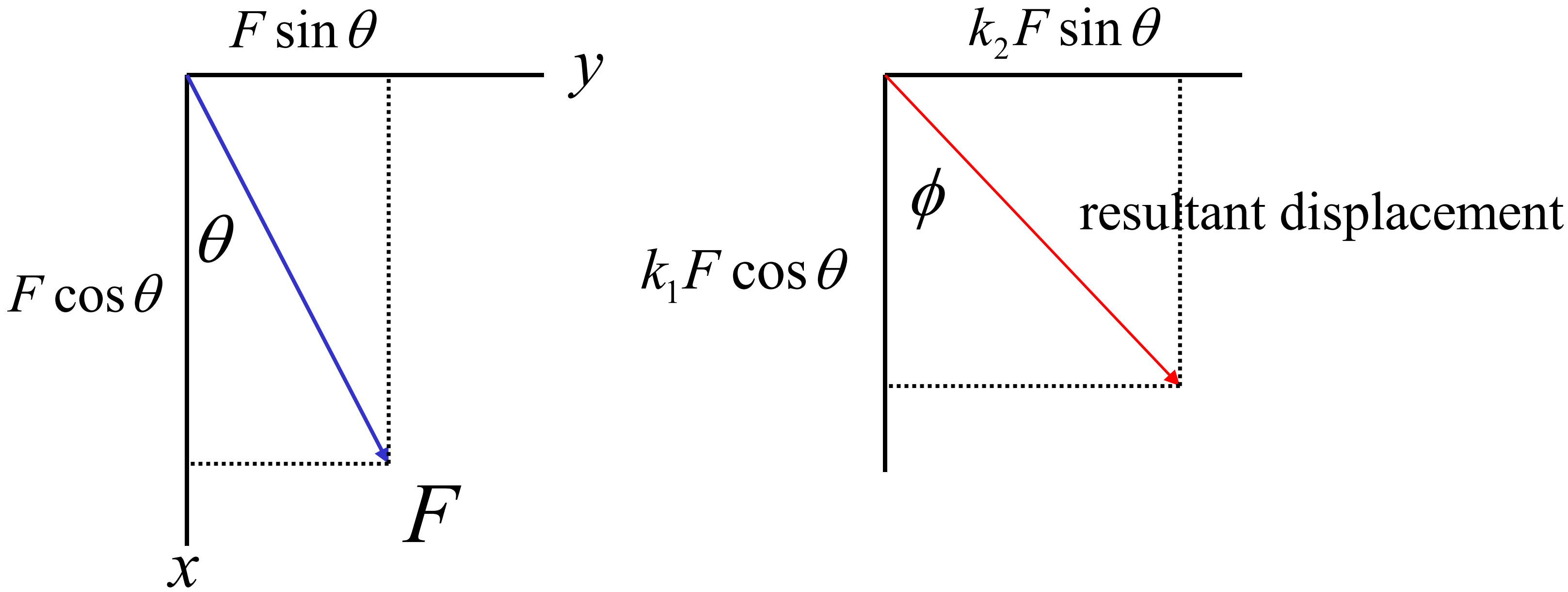
force (cause vector) → displacement (effect vector)

If a force is applied in a general direction, the displacement will not be in the same direction as the applied force (depends on relative stiffness)

Second Rank Tensor

- problem solving
  1. find components of the force F in the direction of each of the two springs
  2. work out the displacement which each force component would produce parallel to each spring
  3. combine two orthogonal displacement to find the resultant displacement

Second Rank Tensor



1. force $\vec{F} = [F\cos\theta, F\sin\theta]$
2. spring constant along x and y are k_1 and k_2, respectively
3. displacement $[k_1 F\cos\theta, k_2 F\sin\theta]$

resultant displacement $\tan\phi = \dfrac{k_2}{k_1}\tan\theta$

Second Rank Tensor

- consequences

1. In an anisotropic system, the effect vector is not, in general, parallel to the applied cause vector.
2. In two-dimensional example, there are two orthogonal directions along which the effect is parallel to the cause.
3. An anisotropic system can be analyzed in terms of components along these orthogonal principal directions, termed principal axes.

   Along these principal axes, the values of the physical property are termed the principal values.

Second Rank Tensor

- in 3-D, general direction- direction cosines, *l,m,n*
- a force $\vec{F}$ is applied in a general direction resulting in a displacement $\vec{D}$ at some angle φ to $\vec{F}$
- component of $\vec{D}$ in the direction of $\vec{F}$

$$D_F = D\cos\varphi$$

$$K = \frac{D\cos\varphi}{F} = \frac{D_F}{F}$$

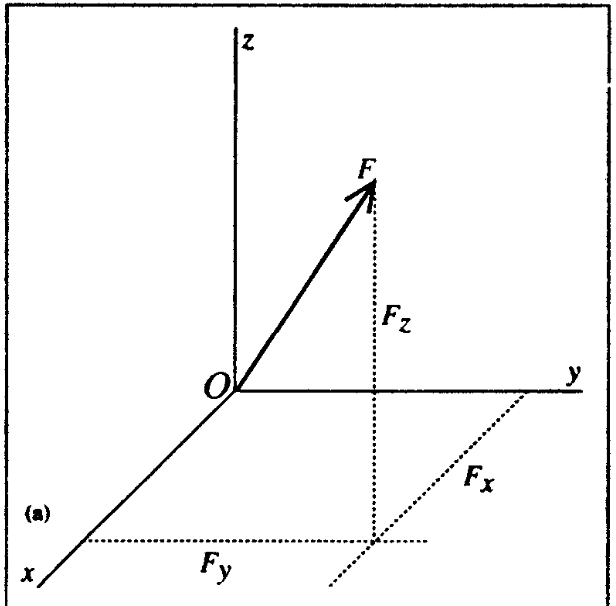
$$K = K(k_1, k_2, k_3)$$

- component of $\vec{F}$ along principal axes

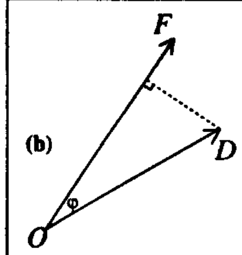
$$F_x = lF,\ F_y = mF,\ F_z = nF$$

- component of $\vec{D}$ along principal axes

$$D_x = k_1 lF,\ D_y = k_2 mF,\ D_z = k_3 nF$$

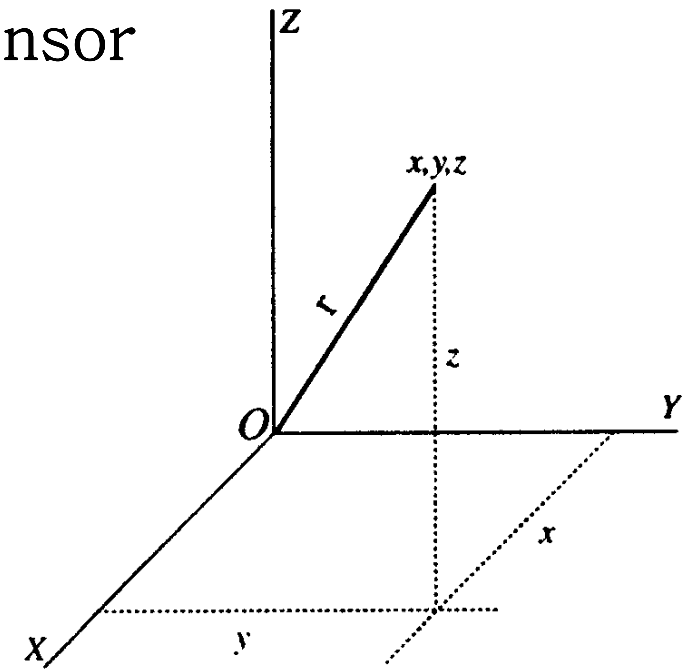


The direction cosines *l,m,n* of the direction of the Force *F* are given by the cosines of the angles between *F* and the *x,y,z* axes respectively.



The component of *D* in the direction of *F* is defined as $D_F = D\cos\varphi$

Second Rank Tensor



– $D_F = D_x l + D_y m + D_z n$

$$= k_1 F l^2 + k_2 F m^2 + k_3 F n^2$$

$$= (k_1 l^2 + k_2 m^2 + k_3 n^2) F$$

– $K = \dfrac{D_F}{F} = k_1 l^2 + k_2 m^2 + k_3 n^2$

– variation of a property K with direction

  – representation surface

direction cosine l, m, n

$$l = \frac{x}{r},\ m = \frac{y}{r},\ n = \frac{z}{r}$$

$$K = k_1 l^2 + k_2 m^2 + k_3 n^2 = k_1 (\frac{x}{r})^2 + k_2 (\frac{y}{r})^2 + k_3 (\frac{z}{r})^2$$

Second Rank Tensor

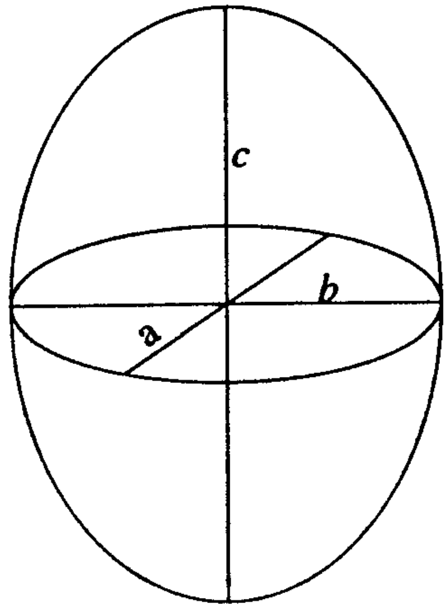
let $r^2 K = 1, \quad r = 1/\sqrt{K}$

$k_1 x^2 + k_2 y^2 + k_3 z^2 = 1$

if k_1, k_2, k_3 are positive, $k_1 x^2 + k_2 y^2 + k_3 z^2 = 1$ (ellipsoid)

normal form of the equation of an ellipsoid

$\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = 1$ ($a, b.c$: semiaxes)



representation surface

semiaxes: $\frac{1}{\sqrt{k_1}}, \frac{1}{\sqrt{k_2}}, \frac{1}{\sqrt{k_3}}$

In any general direction, the radius is equal to the value of $1/\sqrt{K}$ in that direction.

Second Rank Tensor

- electric field $\vec{E} \rightarrow$ current density $\vec{j}$

  i) if conductor is isotropic and obeys Ohm's law

$$\vec{j} = \sigma \vec{E}$$

$$\vec{E} = [E_1, E_2, E_3] \quad \vec{j} = [j_1, j_2, j_3]$$

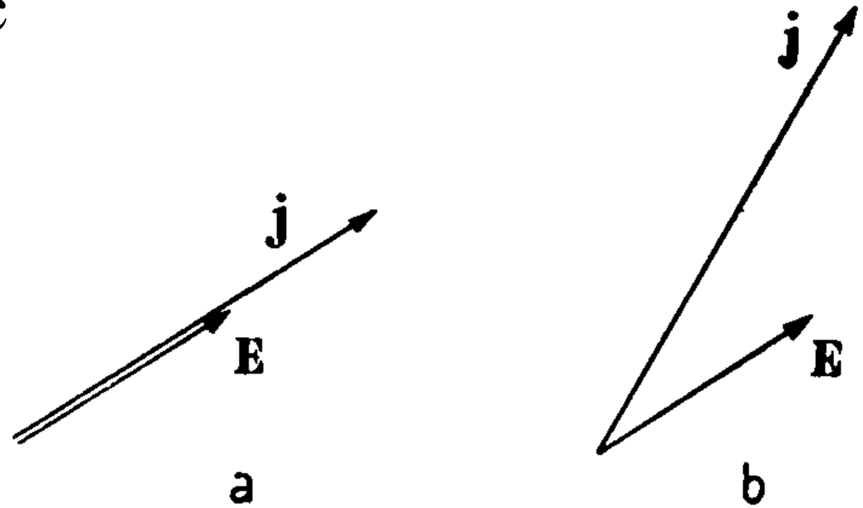
$$j_1 = \sigma E_1, \; j_2 = \sigma E_2, \; j_3 = \sigma E_3$$

  ii) if conductor is anisotropic

$$j_1 = \sigma_{11} E_1 + \sigma_{12} E_2 + \sigma_{13} E_3$$

$$j_2 = \sigma_{21} E_1 + \sigma_{22} E_2 + \sigma_{23} E_3$$

$$j_3 = \sigma_{31} E_1 + \sigma_{32} E_2 + \sigma_{33} E_3$$



isotropic anisotropic

Second Rank Tensor

- physical meaning of σ_{ij}

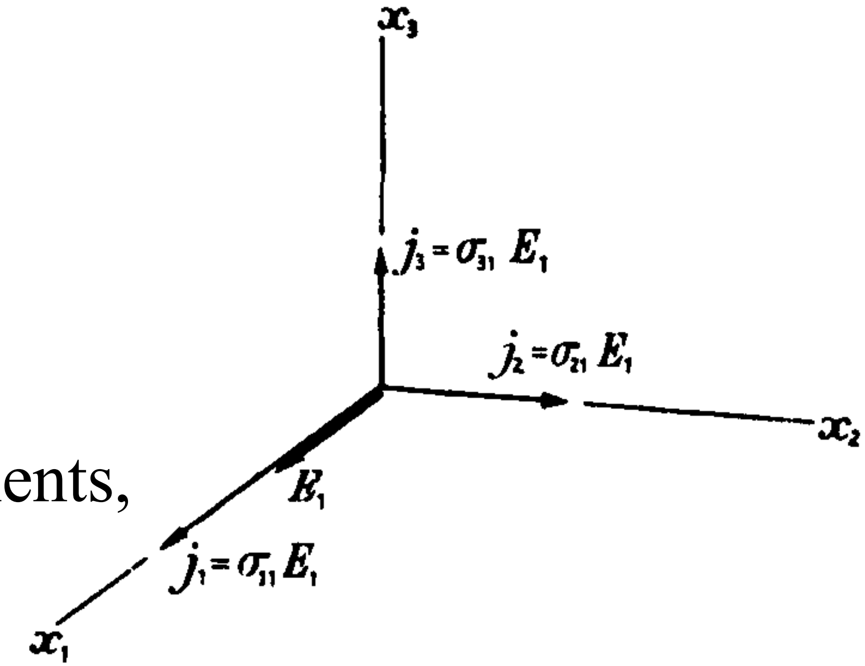
if field is applied along x_1, $\vec{E} = [E_1, 0, 0]$

$$j_1 = \sigma_{11} E_1 \quad j_2 = \sigma_{21} E_1 \quad j_3 = \sigma_{31} E_1$$

conductivity - nine components specified in a square array

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix}$$

second rank tensor, components, leading diagonal



* the number of subscripts equals the rank of tensor

Second Rank Tensor

in general

$$\vec{p} = [p_1, p_2, p_3] \quad \vec{q} = [q_1, q_2, q_3]$$

$$p_1 = T_{11}q_1 + T_{12}q_2 + T_{13}q_3$$

$$p_2 = T_{21}q_1 + T_{22}q_2 + T_{23}q_3$$

$$p_3 = T_{31}q_1 + T_{32}q_2 + T_{33}q_3$$

$$\begin{bmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{bmatrix}$$

Some examples of second-rank tensors relating two vectors

Tensor property	*Vector given or applied*	*Vector resulting or induced*
Electrical conductivity	electric field	electric current density
Thermal conductivity	(negative) temperature gradient	heat flow density
Permittivity	electric field	dielectric displacement
Dielectric susceptibility	,, ,,	,, polarization
Permeability	magnetic field	magnetic induction
Magnetic susceptibility	,, ,,	intensity of magnetization

Second Rank Tensor

$$p_1 = T_{11}q_1 + T_{12}q_2 + T_{13}q_3 = \sum_{j=1}^{3} T_{1j}q_j$$

$$p_2 = T_{21}q_1 + T_{22}q_2 + T_{23}q_3 = \sum_{j=1}^{3} T_{2j}q_j \qquad p_i = \sum_{j=1}^{3} T_{ij}q_j \;\; (i = 1, 2, 3)$$

$$p_3 = T_{31}q_1 + T_{32}q_2 + T_{33}q_3 = \sum_{j=1}^{3} T_{3j}q_j \qquad p_i = T_{ij}q_j (i = 1, 2, 3)$$

- Einstein summation convention: when a letter suffix occurs twice in the same term, summation with respect to that suffix is to be automatically understood.

j dummy suffix, i free suffix

$$p_i = T_{ij}q_j = T_{ik}q_k$$

Second Rank Tensor

-in an equation written in this notation, the free suffixs must be the same in all the terms on both sides of the equation: while the dummy suffixs must occur as pairs in each term.

ex)

$$A_{ij} + B_{ik}C_{kl}D_{lj} = E_{ik}F_{kj}$$

i, j free suffixs k, l dummy suffixs

$$(C_{kl}B_{ik}D_{lj} = B_{ik}C_{kl}D_{lj})$$

-in this book, the range of values of all letter suffixs is 1,2,3 unless some other things is specified.

Transformation

$$p_1 = T_{11}q_1 + T_{12}q_2 + T_{13}q_3$$
$$p_2 = T_{21}q_1 + T_{22}q_2 + T_{23}q_3$$
$$p_3 = T_{31}q_1 + T_{32}q_2 + T_{33}q_3$$

- $q_j \rightarrow p_i$ (T_{ij} determine), arbitrary axes chosen
- different set of axes $\rightarrow$ different set of coefficients T_{ij}
- both sets of coefficents equally well represent the same physical quantity
- there must be some relation between them
- when we change the axes of reference, it is only our method of representing the property that changes; the property itself remains the same.

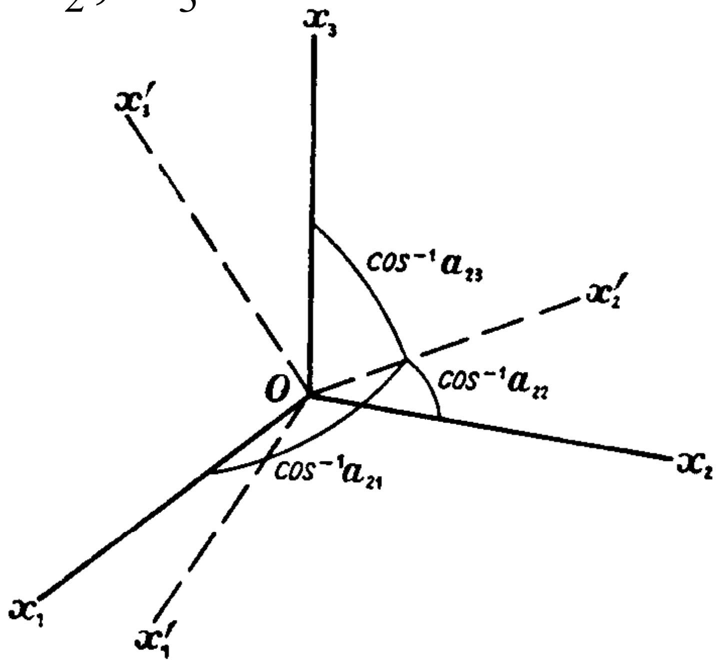
Transformation

- transformation of axes

a change from one set of mutually perpendicular axes to another set with same origin

first set: $x_1, x_2, x_3,$ second set: x'_1, x'_2, x'_3

angular relationship



$$
\begin{array}{c|ccc}
 & & \text{old} & \\
 & x_1 & x_2 & x_3 \\
\hline
x'_1 & a_{11} & a_{12} & a_{13} \\
\text{new} \quad x'_2 & a_{21} & a_{22} & a_{23} \\
x'_3 & a_{31} & a_{32} & a_{33}
\end{array}
$$

a_{ij} : cosine of the angle between x'_i and x_j (a_{ij}) : matrix

Direction Cosines, a_{ij}

- (a_{ij})-nine component- not independent
- only three independent quantities are needed to define the transformation.
- six independent relation between nine coefficients

$$a_{11}^2 + a_{12}^2 + a_{13}^2 = 1$$

$$a_{11}a_{21} + a_{12}a_{22} + a_{13}a_{23} = 0$$

$$a_{ik}a_{jk} = \delta_{ij} \quad (orthogonality\ relation)$$

Kronecker delta $\delta_{ij} = 1 \ (i = j)$

$0 \ (i \neq j)$

Transformation

- transformation of vector components

$\vec{p}$ $\quad p_1, p_2, p_3$ with respect to x_1, x_2, x_3

$\quad p'_1, p'_2, p'_3$ with respect to x'_1, x'_2, x'_3

$$p'_1 = p_1 \cos \widehat{x_1 x'_1} + p_2 \cos \widehat{x_2 x'_1} + p_3 \cos \widehat{x_3 x'_1}$$

$$= a_{11} p_1 + a_{12} p_2 + a_{13} p_3$$

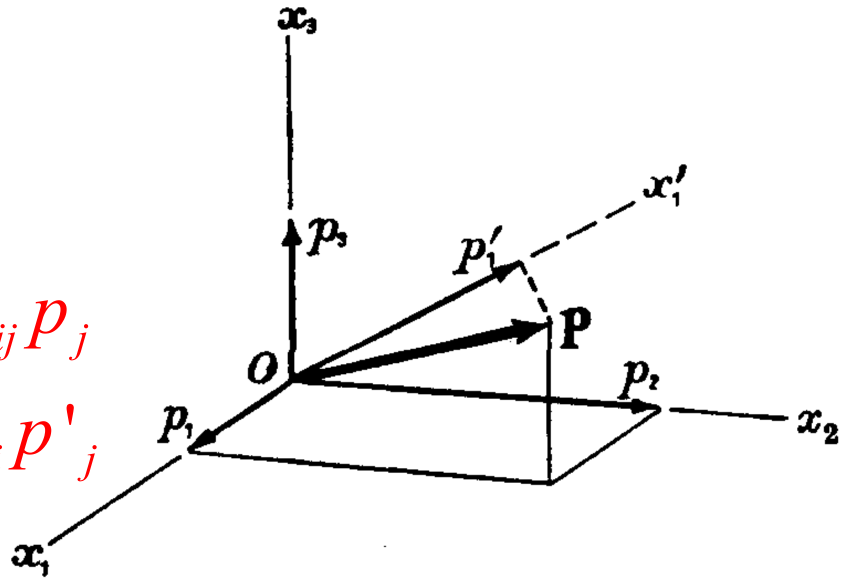
$$p'_2 = a_{21} p_1 + a_{22} p_2 + a_{23} p_3$$

$$p'_3 = a_{31} p_1 + a_{32} p_2 + a_{33} p_3$$

in dummy suffix notation

new in terms of old: $p'_i = a_{ij} p_j$

old in terms of new: $p_i = a_{ji} p'_j$



Transformation

- transformation of components of second rank tensor

$p_i = T_{ij} q_j$ with respect to x_1, x_2, x_3

$p'_i = T'_{ij} q'_j$ with respect to x'_1, x'_2, x'_3

$p' \rightarrow p \rightarrow q \rightarrow q'$ ($\rightarrow$: in terms of)

$p'_i = a_{ik} p_k \quad p_k = T_{kl} q_l \quad q_l = a_{jl} q'_j$

$p'_i = a_{ik} p_k = a_{ik} T_{kl} q_l = a_{ik} T_{kl} a_{jl} q'_j$

$p'_i = T'_{ij} q'_j$

$T'_{ij} = a_{ik} a_{jl} T_{kl}$

$T_{ij} = a_{ki} a_{lj} T'_{kl}$

Transformation

$$T'_{ij} = a_{ik}a_{jl}T_{kl} = a_{ik}a_{j1}T_{k1} + a_{ik}a_{j2}T_{k2} + a_{ik}a_{j3}T_{k3}$$
$$= a_{i1}a_{j1}T_{11} + a_{i1}a_{j2}T_{12} + a_{i1}a_{j3}T_{13}$$
$$+ a_{i2}a_{j1}T_{21} + a_{i2}a_{j2}T_{22} + a_{i2}a_{j3}T_{23}$$
$$+ a_{i3}a_{j1}T_{31} + a_{i3}a_{j2}T_{32} + a_{i3}a_{j3}T_{33}$$

Transformation laws for tensors

Name	*Rank of tensor*	*Transformation law*	
		New in terms of old	*Old in terms of new*
Scalar	0	$\phi' = \phi$	$\phi = \phi'$
Vector	1	$p'_i = a_{ij}p_j$	$p_i = a_{ji}p'_j$
—	2	$T'_{ij} = a_{ik}a_{jl}T_{kl}$	$T_{ij} = a_{ki}a_{lj}T'_{kl}$
—	3	$T'_{ijk} = a_{il}a_{jm}a_{kn}T_{lmn}$	$T_{ijk} = a_{li}a_{mj}a_{nk}T'_{lmn}$
—	4	$T'_{ijkl} = a_{im}a_{jn}a_{ko}a_{lp}T_{mnop}$	$T_{ijkl} = a_{mi}a_{nj}a_{ok}a_{pl}T'_{mnop}$

Definition of a Tensor

-a physical quantity which, with respect to a set of axes x_i, has nine components T_{ij} that transform according to equations $T'_{ij} = a_{ik}a_{jl}T_{kl}$

-a second rank tensor- physical quantity existing in its own right, and quite independent of the particular choice of axes

-when we change the axes, the physical quantity does not change, but only our method of representing it.

- (a_{ij}): array of coefficient relating two set of axes

- symmetric $T_{ij} = T_{ji}$
  anti-symmetric (skew-symmetric) $T_{ij} = -T_{ji}$

Representation Quadric

- geometrical representation of a **second rank tensor**
- consider the equation

$$S_{ij}x_ix_j = 1 \qquad S_{ij}\text{:coefficients}$$

$$S_{11}x_1^2 + S_{12}x_1x_2 + S_{13}x_1x_3$$
$$+S_{21}x_2x_1 + S_{22}x_2^2 + S_{23}x_2x_3$$
$$+S_{31}x_3x_1 + S_{32}x_3x_2 + S_{33}x_3^2 = 1$$

- if $S_{ij} = S_{ji}$ (for 2차 rank 대칭 tensor)

$$S_{11}x_1^2 + S_{22}x_2^2 + S_{33}x_3^2 + 2S_{23}x_2x_3 + 2S_{31}x_3x_1 + 2S_{12}x_1x_2 = 1$$

- general equation of a second-degree surface(2차곡면) (quadric) referred to its center as origin

Representation Quadric

- transformed to new axes Ox'_i

  $x_i = a_{ki}x'_k \quad x_j = a_{lj}x'_l$

  $S_{ij}a_{ki}a_{lj}x'_k\, x'_l = 1$

  $S'_{kl}\, x'_k\, x'_l = 1$ where $S'_{kl} = a_{ki}a_{lj}S_{ij}$

- compared with second rank tensor transformation law

  $T'_{ij} = a_{ik}a_{jl}T_{kl}$ (identical)

  if $S_{ij} = S_{ji}$

  coefficient S_{ij} of the quadric transform like the components

  of a symmetrical tensor of the second tank.

Representation Quadric

- a representation quadric can be used to describe any symmetrical second-rank tensor, and in particular, it can be used to describe any crystal property which is given by such a tensor (전기전도도, 유전율, 투자율)

- principal axes

principal axes- three directions at right angles such that $S_{ij}x_i x_j = 1$ takes the simpler form

$$S_1 x_1^2 + S_2 x_2^2 + S_3 x_3^2 = 1$$

Representation Quadric

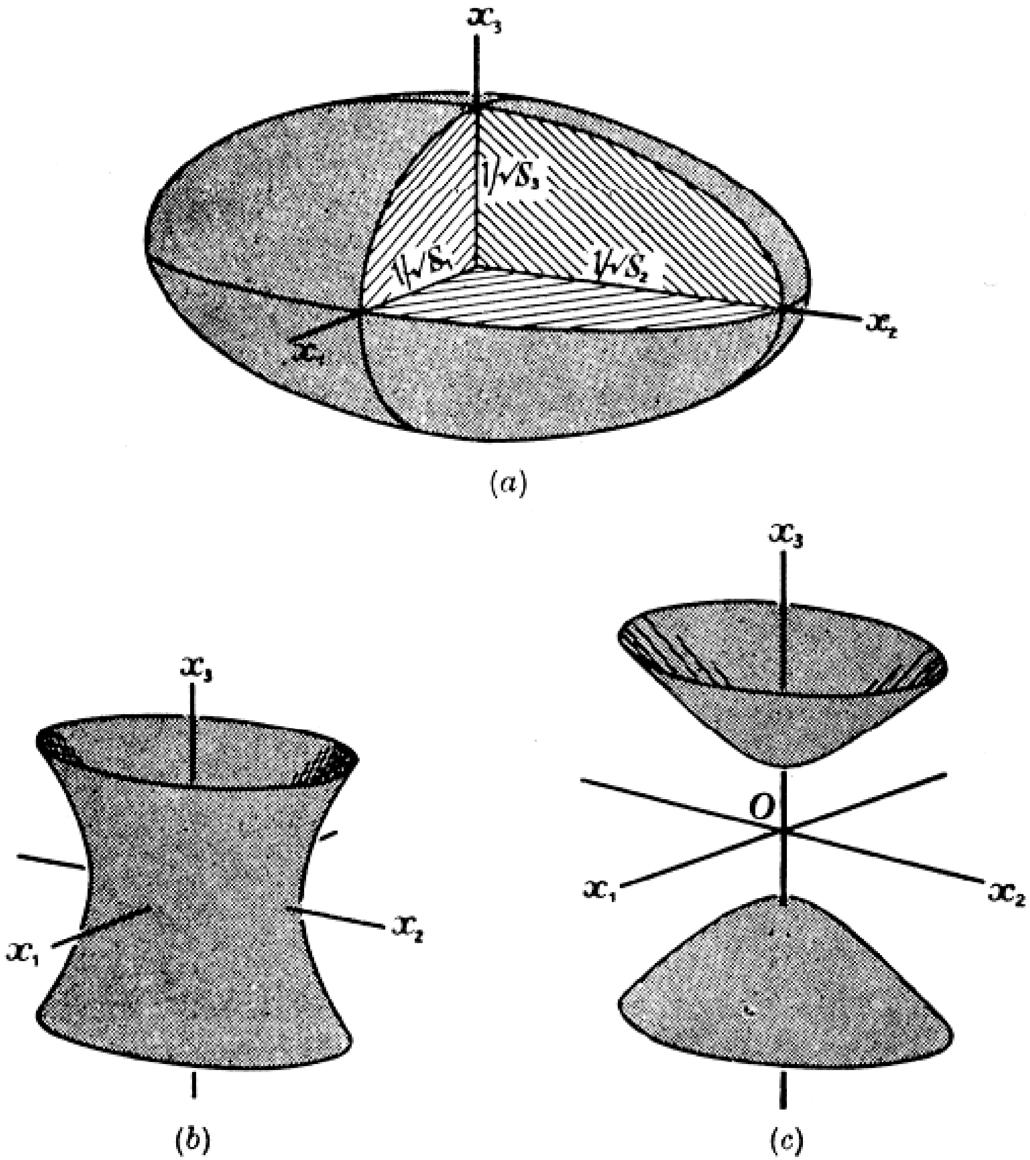
$$\left[S_{ij}\right] = \begin{bmatrix} S_{11} & S_{21} & S_{31} \\ S_{21} & S_{22} & S_{23} \\ S_{31} & S_{32} & S_{33} \end{bmatrix} \rightarrow \begin{bmatrix} S_1 & 0 & 0 \\ 0 & S_2 & 0 \\ 0 & 0 & S_3 \end{bmatrix}$$

S_1, S_2, S_3 : principal components

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = 1$$

representation quadric- semi axes $\dfrac{1}{\sqrt{\mathrm{S}_1}}, \dfrac{1}{\sqrt{\mathrm{S}_2}}, \dfrac{1}{\sqrt{\mathrm{S}_3}}$

Representation Quadric



The representation quadric for the tensor $[S_{ij}]$, as (a) an ellipsoid, (b) a hyperboloid of one sheet, and (c) a hyperboloid of two sheets.

Representation Quadric

- in a symmetric tensor refered to arbitrary axes, the number of independent components is six.
- if the tensor is refered to its principal axes, the number of independent components is reduced to three.
- the number of degree of freedom is nevertheless still six, for three independent quantities are needed to specify the directions of the axes, and three to fix the magnitudes of the principal components.

Representation Quadric (2차 곡면)

- simplification of equations when referred to pricipal axes

  $p_i = S_{ij} q_j$ (T_{ij} replaced by symmetric S_{ij})

  $p_1 = S_1 q_1,\ p_2 = S_2 q_2,\ p_3 = S_3 q_3$

- for example, consider electrical conductivity

  $j_1 = \sigma_1 E_1,\ j_2 = \sigma_2 E_2,\ j_3 = \sigma_3 E_3$

  ($\sigma_1, \sigma_2, \sigma_3$: principal conductivities)

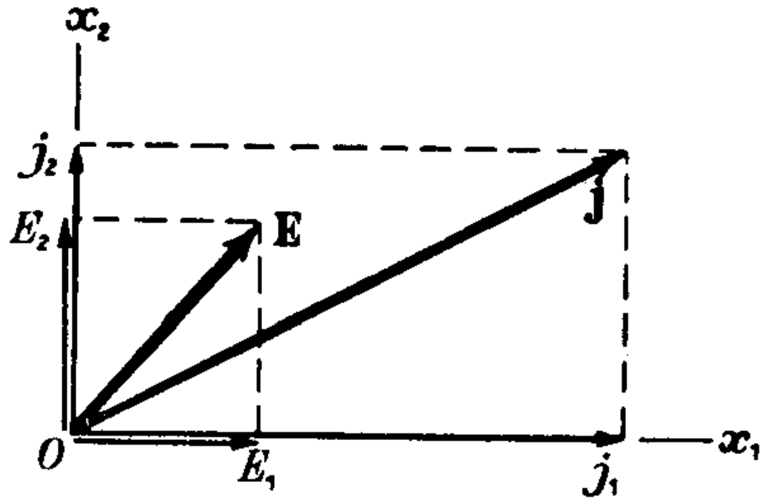
- if $\vec{E}$ is parallel to Ox_1, so $E_2 = E_3 = 0$

  $j_2 = j_3 = 0$ $\vec{\mathrm{j}}$ is parallel to Ox_1

- if $\vec{E} = [E_1, E_2, 0]$,

  $j_1 = \sigma_1 E_1,\ j_2 = \sigma_2 E_2,\ j_3 = 0$

  $\vec{E}$ and $\vec{j}$ not parallel



Effect of Crystal Symmetry on Crystal Properties

- Neumann's Principle

  the symmetry elements of any physical properties of a crystal must include the symmetry elements of the point group of the crystal
- physical properties may, and often do, possess more symmetry than the point group.
- ex1) cubic crystals - optically isotropic

  physical property (isotropic) possesses the symmetry elements of all the cubic point groups.

Effect of Crystal Symmetry on Crystal Properties

- ex2) trigonal system (tourmaline, 3*m*) - optical properties

  (variation of refractive index with direction - indicatrix)

  indicatrix for 3*m*- ellipsoid of revolution about triad axis (optic axis)

  ellipsoid of revolution- vertical triad axis

  three vertical planes of symmetry

  (extra- center of symmetry, other symmetry elements)
- the symmetry of a physical property

  a relation between certain measurable quantities associated with the crystal

Effect of Crystal Symmetry on Crystal Properties

- all second-rank tensor properties are centrosymmetric.

  $p_i = T_{ij} q_j$

  $-p_i = T_{ij}(-q_j)$ $\quad T_{ij}$: unchanged
- symmetric second-rank tensor- 6 independent components
- symmetry of crystal reduces the number of independent components
- consider representation quadric for symmetric second rank tensor

The effect of crystal symmetry on properties represented by symmetrical second-rank tensors

Optical classification	*System*	*Characteristic symmetry* (see p. 280)†	*Nature of representation quadric and its orientation*	*Number of independent coefficients*	*Tensor referred to axes in the conventional orientation*‡
Isotropic (anaxial)	Cubic	4 3-fold axes	*Sphere*	1	$\begin{bmatrix} S & 0 & 0 \\ 0 & S & 0 \\ 0 & 0 & S \end{bmatrix}$
Uniaxial	Tetragonal Hexagonal Trigonal	1 4-fold axis 1 6-fold axis 1 3-fold axis	*Quadric of revolution* about the principal symmetry axis $(x_3)(z)$	2	$\begin{bmatrix} S_1 & 0 & 0 \\ 0 & S_1 & 0 \\ 0 & 0 & S_3 \end{bmatrix}$
Biaxial	Orthorhombic	3 mutually perpendicular 2-fold axes; no axes of higher order	*General quadric* with axes (x_1, x_2, x_3) ‖ to the diad axes (x, y, z)	3	$\begin{bmatrix} S_1 & 0 & 0 \\ 0 & S_2 & 0 \\ 0 & 0 & S_3 \end{bmatrix}$
	Monoclinic	1 2-fold axis	*General quadric* with one axis (x_2) ‖ to the diad axis (y)	4	$\begin{bmatrix} S_{11} & 0 & S_{31} \\ 0 & S_2 & 0 \\ S_{31} & 0 & S_{33} \end{bmatrix}$
	Triclinic	A centre of symmetry or no symmetry	*General quadric.* No fixed relation to crystallographic axes	6	$\begin{bmatrix} S_{11} & S_{12} & S_{31} \\ S_{12} & S_{22} & S_{23} \\ S_{31} & S_{23} & S_{33} \end{bmatrix}$

Anisotropic Diffusion of Ni in Olivine

Fick's first law

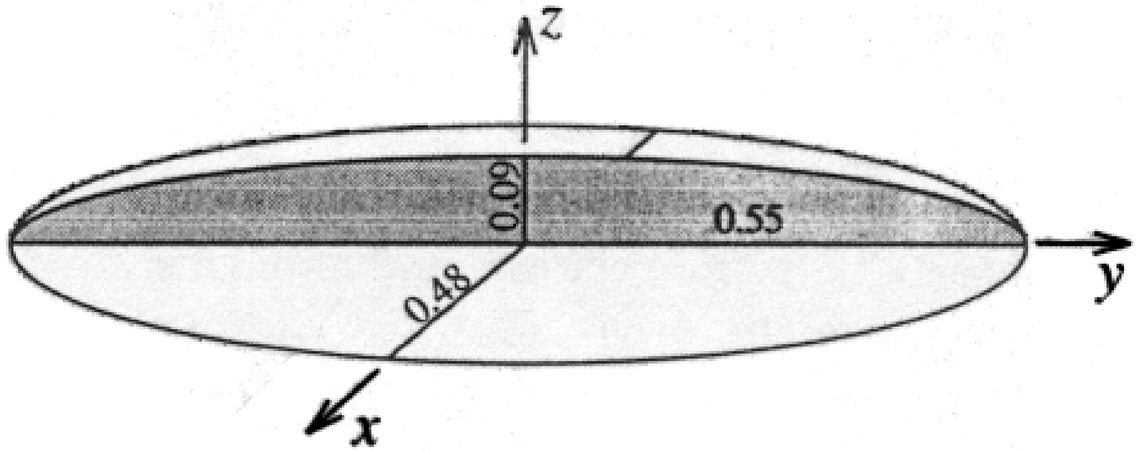
$$J_i = -D_{ij} \frac{\partial c}{\partial x_j}$$

ex) Ni diffusion in olivine($(Mg,Fe)_2SiO_4$, orthorhombic)

at 1150°C

D_x=4.40x10^{-14}cm^2/s, D_y=3.35x10^{-14}cm^2/s, D_z=124x10^{-14}cm^2/s

$$\mathrm{a:b:c} = \frac{1}{\sqrt{D_x}} : \frac{1}{\sqrt{D_y}} : \frac{1}{\sqrt{D_z}} = 0.48 : 0.55 : 0.09$$



Magnitude of a Property in a Given Direction

- defintion

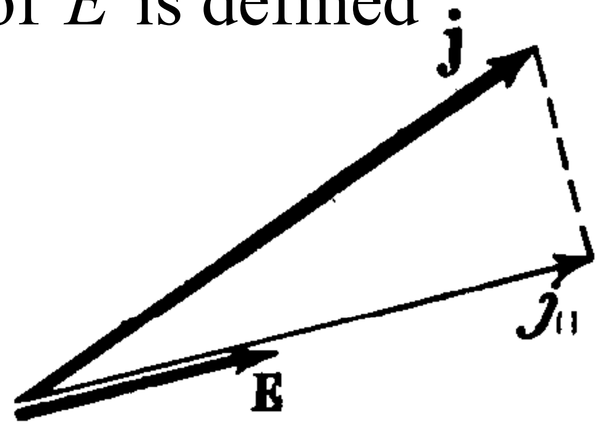
  in general, if $p_i = S_{ij} q_j$, the magnitude S of the property $[S_{ij}]$ in a certain direction is obtained by applying $\vec{q}$ in that direction and measuring $p_{||} / q$,

  where $p_{||}$ is the componet of $\vec{p}$ parallel to $\vec{q}$

- ex) electrical conductivity

  the conductivity σ in the direction of $\vec{E}$ is defined to be the component of $\vec{j}$ parallel to $\vec{E}$ divided by E,

  that is, $j_{||} / E$



Magnitude of a Property in a Given Direction

- analytical expression

(i) referred to principal axes

direction cosine: l_1, l_2, l_3

$\vec{\mathrm{E}} = [l_1 E,\ l_2 E,\ l_3 E]$ $\quad\quad$ $\vec{\mathrm{j}} = [\sigma_1 l_1 E,\ \sigma_2 l_2 E,\ \sigma_3 l_3 E]$

component of $\vec{j}$ parallel to $\vec{E}$

$$j_{||} = l_1^2 \sigma_1 E + l_2^2 \sigma_2 E + l_3^2 \sigma_3 E$$

magnitude of conductivity in the direction l_i

$$\sigma = l_1^2 \sigma_1 + l_2^2 \sigma_2 + l_3^2 \sigma_3$$

Magnitude of a Property in a Given Direction

- analytical expression

(ii) referred to general axes

l_i : direction cosine of $\vec{E}$ referred to general axes

$E_i = El_i$

component of $\vec{j}$ parallel to $\vec{E}$

$\vec{j} \bullet \vec{E} / E$ in suffix notation $j_i E_i / E$

conductivity in the direction l_i

$$\sigma = \frac{j_i E_i}{E^2} = \frac{\sigma_{ij} E_j E_i}{E^2}$$

$$\sigma = \sigma_{ij} l_i l_j$$

Geometrical Properties of Representation Quadric

- length of the radius vector

let P be a general point on the ellipsoid: $\sigma_{ij} x_i x_j = 1$

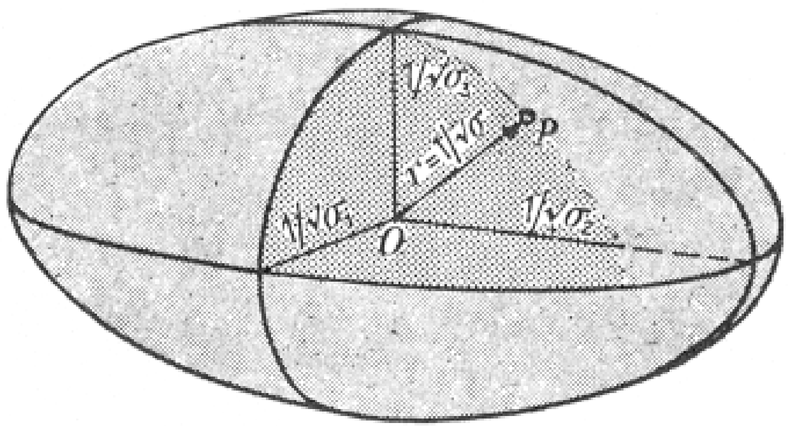
direction cosines of OP: l_i $\quad x_i = r l_i$ where $OP = r$

$$r^2 \sigma_{ij} l_i l_j = 1 \quad (\sigma = \sigma_{ij} l_i l_j)$$

$$\sigma = 1/r^2 \qquad r = 1/\sqrt{\sigma}$$

special cases- radius vectors in the directions of semi-axes

of lengths $1/\sqrt{\sigma_1}$, $1/\sqrt{\sigma_2}$, $1/\sqrt{\sigma_3}$



Geometrical Properties of Representation Quadric

- in general, any symmetric second-rank tensor property S_{ij}

$$S = 1/r^2 \qquad r = 1/\sqrt{S}$$

- the length r of any radius vector of representation quadric is equal to the reciprocal of square root of magnitude S of the property in that direction

Geometrical Properties of Quadric Representation

- radius-normal property

Ox_i principal axes of σ_{ij}

$\vec{E} = [l_1 E,\ l_2 E,\ l_3 E]$ $\vec{j} = [\sigma_1 l_1 E,\ \sigma_2 l_2 E,\ \sigma_3 l_3 E]$

direction cosines of $\vec{j}$ are proportional to

$$\sigma_1 l_1,\ \sigma_2 l_2,\ \sigma_3 l_3$$

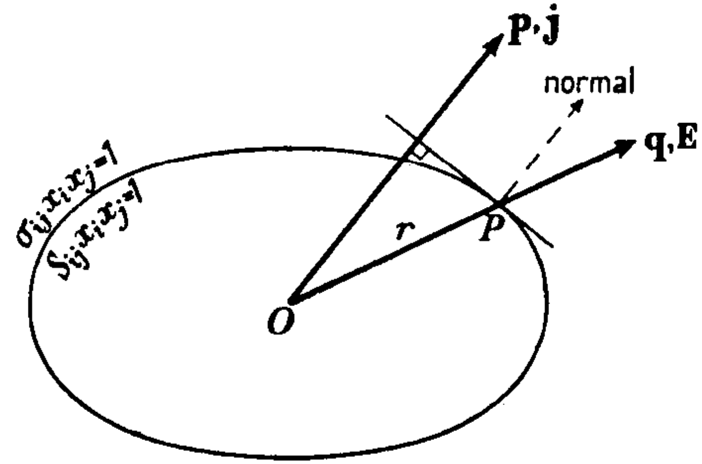
if P is a point on $\sigma_1 x_1^2 + \sigma_2 x_2^2 + \sigma_3 x_3^2 = 1$

such that OP is parallel to $\vec{E}$

$P = (rl_1, rl_2, rl_3)$ where $OP = r$

tangent plane at P

$rl_1\sigma_1 x_1 + rl_2\sigma_2 x_2 + rl_3\sigma_3 x_3 = 1$



Tangent Plane:

- **Theorem:** The tangent to the surface F(x, y, z) =c at the point of (x_0, y_0, z_0) is given by

$$\frac{\partial F}{\partial x}(x - x_0) + \frac{\partial F}{\partial y}(y - y_0) + \frac{\partial F}{\partial z}(z - z_0) = 0$$

Proof: This is a simple example of gthe use of vector geometry. Given that (x0, y0, z0) lies on the surface, and so in the tangent, then for any other point (x, y, z) in the tangent plane, the vector (x-x0, y-y0, z-z0) must lie in the tangent plane, and so must be normal to the normal to the curve (i.e. to ∇F

Thus (x-x0, y-y0, z-z0) and ∇F are perpendicular, and that requirement is the equation which gives the tangent plane.

Geometrical Properties of Representation Quadric

- radius-normal property

normal at P has direction cosines proportional to

$$l_1\sigma_1,\ l_2\sigma_2,\ l_3\sigma_3$$

hence normal at P is parallel to $\vec{j}$

if $p_i = S_{ij}q_j$, the direction of $\vec{p}$ for a given $\vec{q}$ may be found by first drawing, parallel to $\vec{q}$ a radius vector OP of the representation quadric, and then taking the normal to the quadric at P.

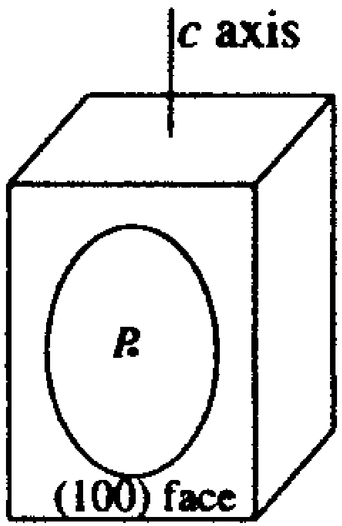
Heat Flow in a Crystal

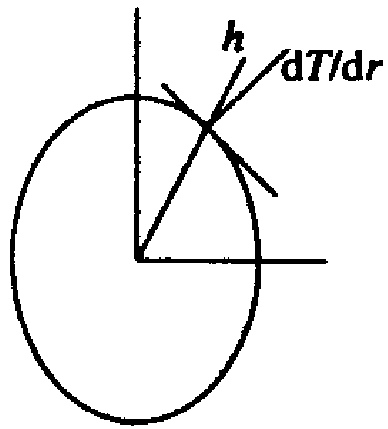
- a point source of heat on the face of a crystal of a tetragonal mineral (uniaxial)

isothermal surface: (001) plane- circle, (100) plane- ellipse

heat flow-radially away from P, thernal gradient-normal to isothermal surface

heat flow ⇒ thermal gradient (in general, not parallel)





-the resistivity along the c-axis is less than that normal to it

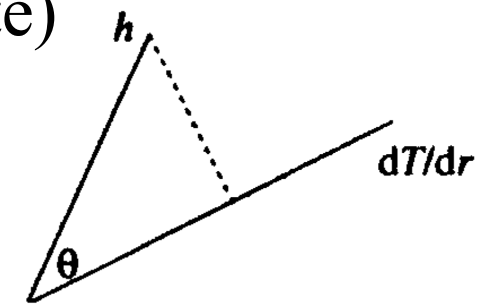
Heat Flow in a Crystal

- resistivity $\dfrac{\partial T}{\partial x_i} = -r_{ij} h_j$

$$r = \frac{dT / dr \cos\theta}{h}$$ (long rod experiment)

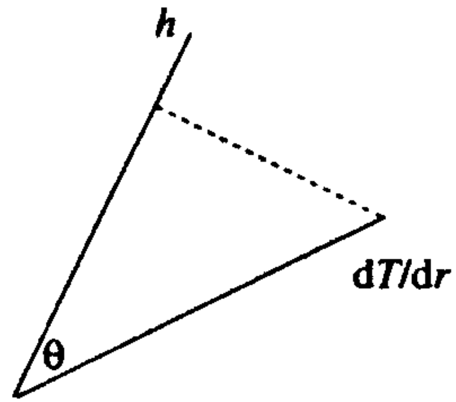
- conductivity $h_i = -k_{ij} \dfrac{\partial T}{\partial x_j}$

$$k = \frac{h \cos\theta}{dT / dr}$$ (thin flat plate)



Conductivity

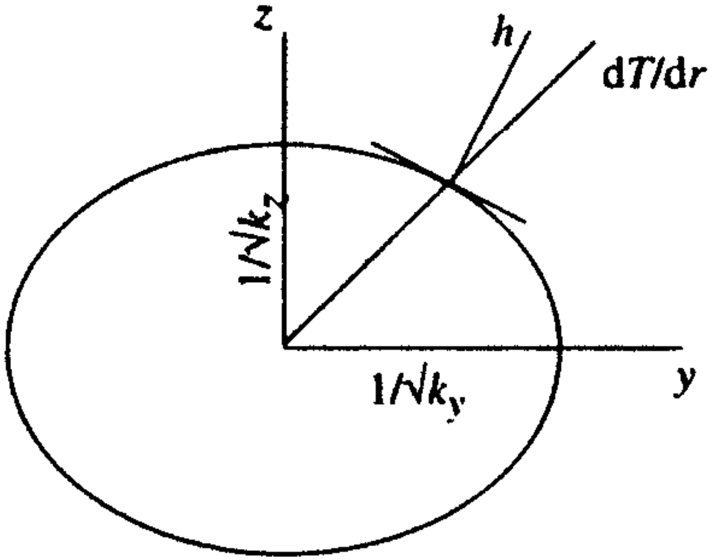
$$k = \frac{h \cos\theta}{dT/dr}$$



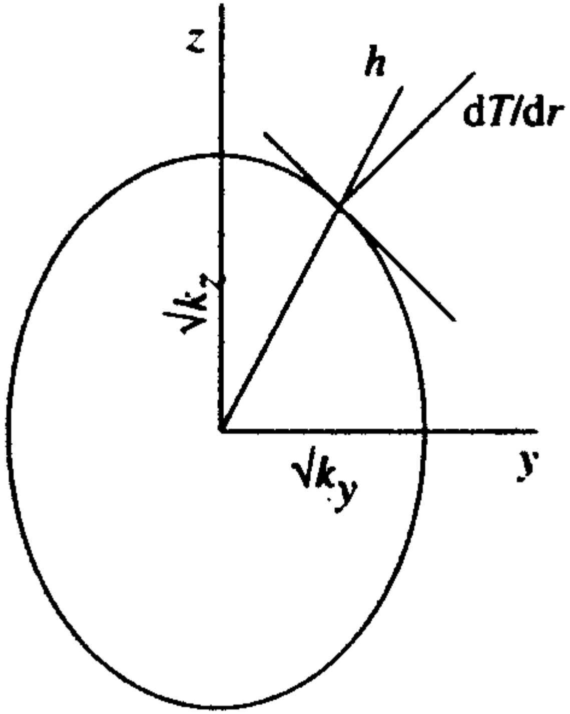
Resistivity

$$r = \frac{dT/dr \cos\theta}{h}$$

Heat Flow in a Crystal



Conductivity surface



Resistivity surface

Along the principal axes $1/r = k$

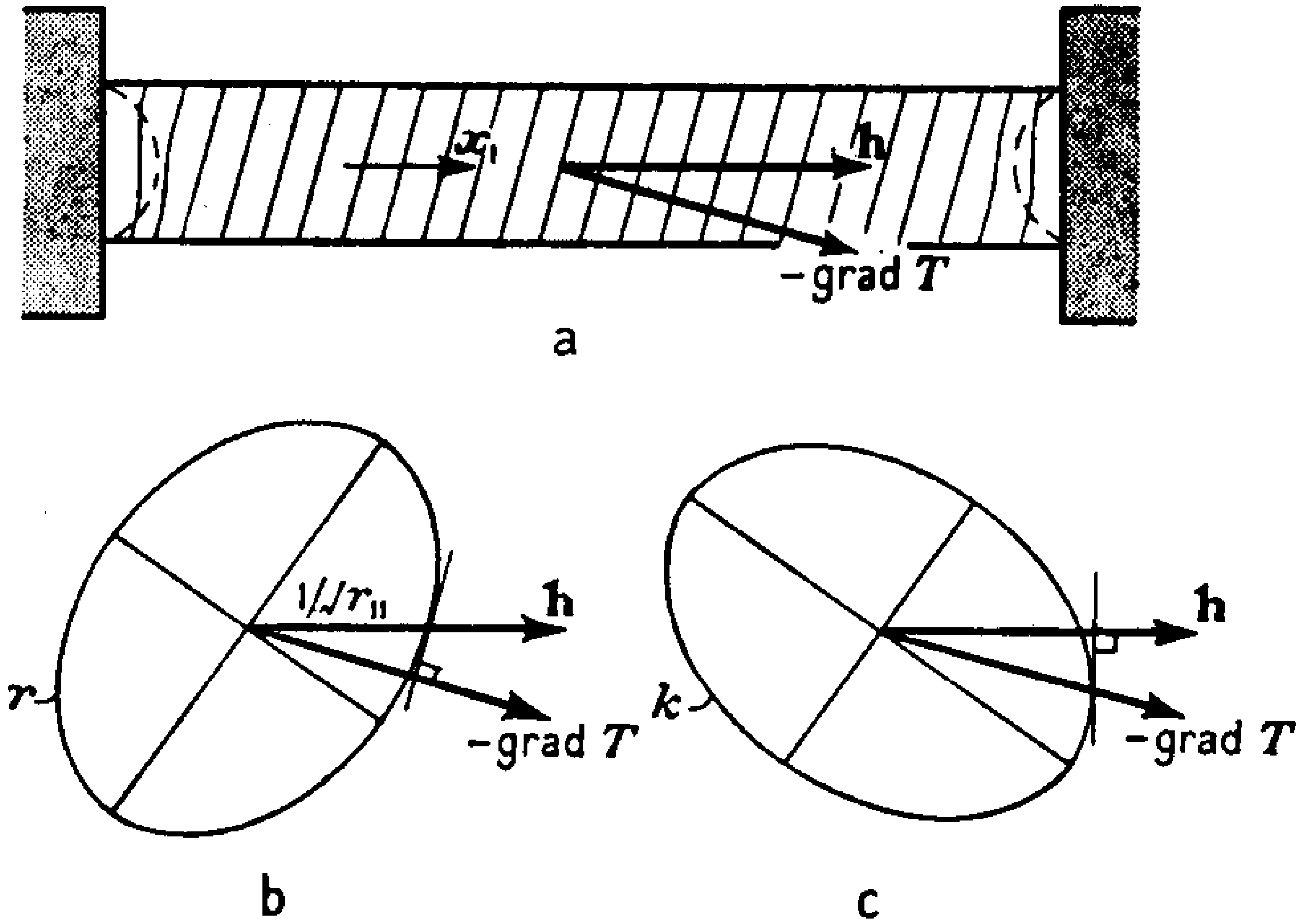


FIG. 11.2. Heat flow down a long rod. The directions of $-\text{grad}\ T$ and **h** *in relation to (a) the rod, (b) the resistivity ellipsoid*, and (c) the conductivity ellipsoid.

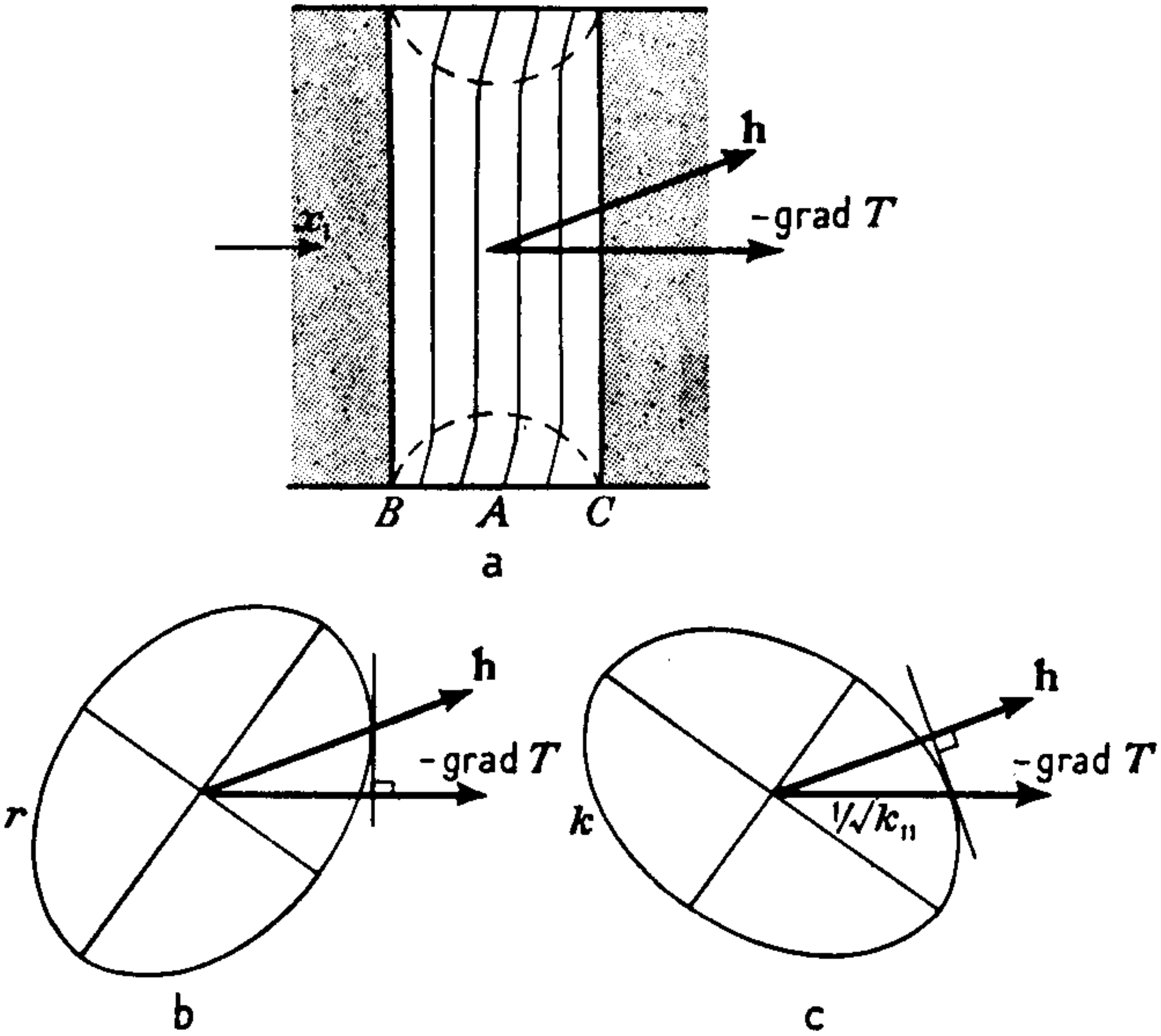


Fig. 11.1. Heat flow across a flat plate between good conductors. The directions of $-\text{grad}\, T$ and $\mathbf{h}$ in relation to (*a*) the plate, (*b*) the resistivity ellipsoid, and (*c*) the conductivity ellipsoid.