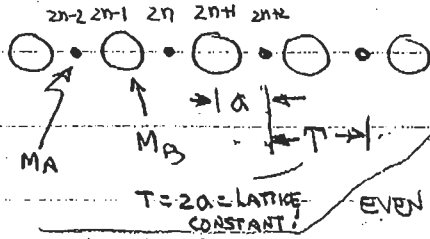


3.60 Symmetry, Structure and Tensor Properties of Materials

PROPAGATION OF WAVES ALONG ONE-DIMENSIONAL CRYSTAL WITH TWO KINDS OF ATOMS



CONSIDER A ONE-DIMENSIONAL CRYSTAL WITH 2 KINDS OF ATOMS $M_A \neq M_B$. NUMBER THE ATOMS ALONG THE CHAINS SUCH THAT A ATOMS ARE EVEN ($2n$), B ATOMS ODD ($2n+1$).

ONLY A SINGLE FORCE CONSTANT, β , REMAINS NECESSARY TO DESCRIBE NEAREST NEIGHBOR INTERACTIONS, AS AN A ATOM INTERACTS WITH B THE SAME WAY AS B WITH AN A.

IN SETTING UP A FORCE-BALANCE EQUATION WE MUST NOW WRITE A SEPARATE EQUATION FOR THE A AND B ATOMS — THEIR MASSES ARE DIFFERENT.

$$\begin{cases} M_A \frac{\partial^2 u_{2n}}{\partial t^2} = \beta (u_{2n+1} - 2u_{2n} + u_{2n-1}) \\ M_B \frac{\partial^2 u_{2n+1}}{\partial t^2} = \beta (u_{2n+2} - 2u_{2n+1} + u_{2n}) \end{cases}$$

LOOK FOR TRIAL SOLUTION

$$\begin{cases} u_{2n} = u_A e^{i(\omega t - k2na)} \\ u_{2n+1} = u_B e^{i[\omega t - k(2n+1)a]} \end{cases}$$

NO REASON TO ASSUME THE SAME AMPLITUDE FOR A & B ATOMS AS THEIR MASSES ARE DIFFERENT

SUBSTITUTING TRIAL SOLUTIONS INTO FORCE EQUATIONS:

$$\begin{cases} -M_A \omega^2 u_A e^{i(\omega t - 2nka)} = \beta \left\{ u_B e^{i[\omega t - (2n+1)ka]} - 2u_A e^{i[\omega t - 2nka]} + u_A e^{i[\omega t - (2n-1)ka]} \right\} \\ -M_B \omega^2 u_B e^{i[\omega t - (2n+1)ka]} = \beta \left\{ u_A e^{i[\omega t - (2n+2)ka]} - 2u_B e^{i[\omega t - (2n+1)ka]} + u_A e^{i[\omega t - 2nka]} \right\} \end{cases}$$

CANCELING COMMON TERMS

$$\begin{cases} -M_A \omega^2 u_A = \beta \left\{ u_B e^{+ika} - 2u_A + u_B e^{-ika} \right\} \\ -M_B \omega^2 u_B = \beta \left\{ u_A e^{+ika} - 2u_B + u_A e^{-ika} \right\} \end{cases}$$

NOTE THAT AMPLITUDES REMAIN IN EQS — THINGS ARE NOT QUITE AS TIDY AS BEFORE.

$$e^{ix} + e^{-ix} = 2 \cos x$$

$$\begin{cases} -M_A \omega^2 u_A = 2\beta u_B \cos ka - 2\beta u_A \\ -M_B \omega^2 u_B = 2\beta u_A \cos ka - 2\beta u_B \end{cases}$$

REARRANGING TERMS IN u_A & u_B

$$\begin{cases} (2\beta - M_A \omega^2) u_A - (2\beta \cos ka) u_B = 0 \\ -(2\beta \cos ka) u_A + (2\beta - M_B \omega^2) u_B = 0 \end{cases}$$

REGARD THE AMPLITUDES U_A & U_B AS UNKNOWN AND WE HAVE (? NO! NOT AGAIN!!) A SET OF LINEAR HOMOGENEOUS EQUATIONS FOR WHICH A NON-TRIVIAL SOLUTION EXISTS ONLY IF THE DETERMINANT OF COEFFICIENTS OF THE VARIABLES VANISHES:

$$\begin{vmatrix} (2\beta - M_A \omega^2) & -2\beta \cos ka \\ -2\beta \cos ka & (2\beta - M_B \omega^2) \end{vmatrix} = 0$$

NOTE - will give values of ω as a function of k as EIGENVALUES!

EXPANDING

$$(2\beta - M_A \omega^2)(2\beta - M_B \omega^2) - (-2\beta \cos ka)(-2\beta \cos ka) = 0$$

$$4\beta^2 - 2\beta \omega^2 (M_A + M_B) + M_A M_B \omega^4 - 4\beta^2 \cos^2 ka = 0$$

$$M_A M_B \omega^4 - 2\beta (M_A + M_B) \omega^2 + 4\beta^2 (1 - \cos^2 ka) = 0$$

$= \sin^2 ka$

$$\omega^4 - 2\beta \left(\frac{1}{M_A} + \frac{1}{M_B} \right) \omega^2 + \frac{4\beta^2}{M_A M_B} \sin^2 ka = 0$$

Solving, using BINOMIAL THEOREM $[ax^2 + bx + c = 0 \Rightarrow x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}]$

$$\omega^2 = \frac{2\beta \left(\frac{1}{M_A} + \frac{1}{M_B} \right)}{2} \pm \left\{ \frac{4\beta^2 \left(\frac{1}{M_A} + \frac{1}{M_B} \right)^2}{4} - \frac{4\beta^2 \sin^2 ka}{M_A M_B} \right\}^{\frac{1}{2}}$$

$$\omega^2 = \beta \left(\frac{1}{M_A} + \frac{1}{M_B} \right) \pm \beta \left\{ \left(\frac{1}{M_A} + \frac{1}{M_B} \right)^2 - \frac{4}{M_A M_B} \sin^2 ka \right\}^{\frac{1}{2}}$$

AGAIN WE HAVE THE CONDITION THAT ω BE A FUNCTION OF $k = \frac{2\pi}{\lambda}$. IF OUR PROPOSED SOLUTION IS TO BE ACCEPTABLE (SORRY GANG! THIS IS AS SIMPLE AS WE CAN MAKE IT!) THERE ARE TWO EIGENVALUES, ω^2 , FOR WHICH SOLUTIONS EXIST. EACH, WHEN SUBSTITUTED BACK INTO THE ORIGINAL EQUATION WOULD PROVIDE EQS FROM WHICH WE COULD SOLVE FOR U_A & U_B . THUS FOR A GIVEN k , THERE ARE NOW TWO DIFFERENT WAVES OF ANGULAR FREQUENCY ω WHICH MAY BE PROPAGATED IN THE CRYSTAL.

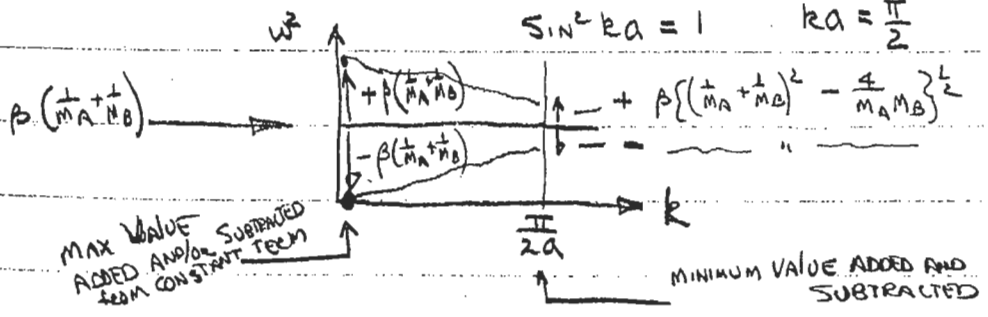
INTERPRETATION OF THE SOLUTIONS

NOTE THAT THE GENERAL FORM OF OUR RESULT THAT ω^2 IS A CONSTANT $\left(\beta \left(\frac{1}{M_A} + \frac{1}{M_B} \right) \right)$, TO WHICH WE EITHER ADD OR SUBTRACT A TERM WHICH IS GIVEN BY THE SQUARE ROOT OF A CONSTANT LESS: A TERM WHICH IS A FUNCTION OF k . ($\sin^2 ka$)
 THE MAXIMUM VALUE OF THE TERM WHICH WE ADD-OR-SUBTRACT OCCURS WHEN THE TERM WHICH IS A FN OF k IS A MINIMUM — NAMELY

$$\sin^2 ka = 0 \quad ka = 0 \quad k = 0$$

THE MINIMUM VALUE OF THE TERM WHICH WE ADD-OR-SUBTRACT OCCURS WHEN THE TERM WHICH IS A FN OF k IS A MAXIMUM — NAMELY

$$\sin^2 ka = 1 \quad ka = \frac{\pi}{2} \quad k = \frac{\pi}{2a}$$



(A) SOLUTIONS FOR SMALL k

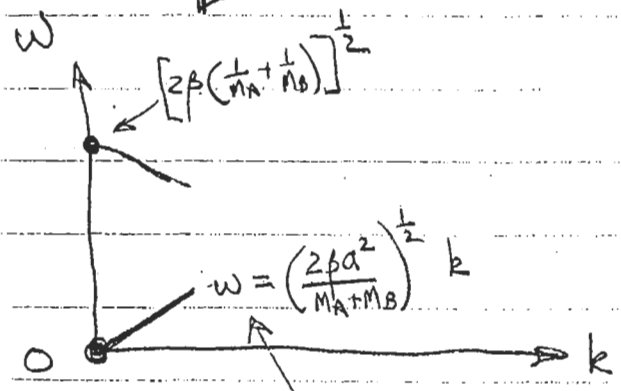
Solution with \oplus sign: AT $k=0$ $\omega^2 = \beta \left(\frac{1}{m_A} + \frac{1}{m_B} \right) \oplus \beta \left[\left(\frac{1}{m_A} + \frac{1}{m_B} \right)^2 - \frac{4}{m_A m_B} \sin^2 ka \right]^{\frac{1}{2}}$
 $\omega^2 = 2\beta \left(\frac{1}{m_A} + \frac{1}{m_B} \right)$

DECREASES FROM THIS MAXIMUM WITH INCREASING k , AS SIZE OF TERM ADDED BECOMES SMALLER.

Solution with \ominus sign: AT $k=0$ $\omega^2 = \beta \left(\frac{1}{m_A} + \frac{1}{m_B} \right) \ominus \beta \left[\left(\frac{1}{m_A} + \frac{1}{m_B} \right)^2 - \frac{4}{m_A m_B} \sin^2 ka \right]^{\frac{1}{2}}$
 $= 0$

NEAR $k=0$ $\omega^2 = \beta \left(\frac{1}{m_A} + \frac{1}{m_B} \right) \ominus \beta \left[\left(\frac{1}{m_A} + \frac{1}{m_B} \right)^2 - \frac{4}{m_A m_B} k^2 a^2 \right]^{\frac{1}{2}}$

SINX \approx X for small X
 if k is small AND THIS APPROXIMATION IS VALID, A TERM IN k^4 WOULD BE ABSOLUTELY MINISCULE SO WE COULD ADD IT TO THIS EXPRESSION WITHOUT ANY EFFECT.



$\omega^2 = \beta \left(\frac{1}{m_A} + \frac{1}{m_B} \right) \ominus \beta \left[\left(\frac{m_A + m_B}{m_A m_B} \right)^2 - \frac{4}{m_A m_B} (ka)^2 \right]^{\frac{1}{2}}$
 TERM IN k^4 TOO SMALL TO QUIBBLE ABOUT \rightarrow "4a^4 k^4" $\frac{1}{m_A + m_B}$
 $\approx \beta \left(\frac{1}{m_A} + \frac{1}{m_B} \right) \ominus \beta \left\{ \frac{m_A + m_B}{m_A m_B} - \frac{2a^2 k^2}{m_A + m_B} \right\}^{\frac{1}{2}}$
 $\approx \beta \left(\frac{m_A + m_B}{m_A m_B} \right) \ominus \beta \left(\frac{m_A + m_B}{m_A m_B} \right) + \beta \frac{2a^2 k^2}{m_A + m_B}$
 $\omega \approx \left(\frac{2\beta a^2}{m_A + m_B} \right)^{\frac{1}{2}} k$

VALUES OF AMPLITUDES

Solution with \oplus SIGN AT $k=0$
 $\left. \begin{aligned} (2\beta - m_A \omega^2) u_A - (2\beta \cos ka) u_B &= 0 \\ -(2\beta \cos ka) u_A + (2\beta - m_B \omega^2) u_B &= 0 \end{aligned} \right\} \Rightarrow \begin{cases} \left[2\beta - m_A \left[2\beta \left(\frac{1}{m_A} + \frac{1}{m_B} \right) \right] \right] u_A - 2\beta \cos ka u_B = 0 \\ -2\beta \cos ka u_A + \left[2\beta - m_B \left[2\beta \left(\frac{1}{m_A} + \frac{1}{m_B} \right) \right] \right] u_B = 0 \end{cases}$

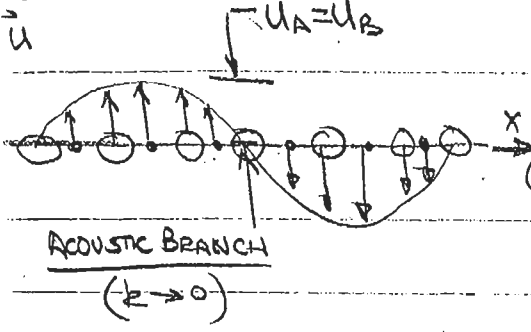
$\therefore \left\{ \begin{aligned} 2\beta \left[1 - m_A \left(\frac{m_A + m_B}{m_A m_B} \right) \right] u_A - 2\beta u_B &= 0 \\ -2\beta u_A + 2\beta \left[1 - m_B \left(\frac{m_A + m_B}{m_A m_B} \right) \right] u_B &= 0 \end{aligned} \right\} \Rightarrow \begin{cases} -m_A/m_B u_A - u_B = 0 \\ -u_A - m_B/m_A u_B = 0 \end{cases}$

THIS IS A MOTION IN WHICH THE AMPLITUDES OF A & B ARE INVERSELY PROPORTIONAL TO THE MASS OF THE ATOMS AND OPPOSITE IN SIGN. $\frac{u_A}{u_B} = -\frac{m_B}{m_A}$ $u_A \propto \frac{1}{m_A}$ $u_B \propto \frac{1}{m_B}$
 THE CENTER OF MASS OF THE UNIT CELL STAYS FIXED

Solution with \ominus sign at $k=0$

$$\left. \begin{aligned} (2\beta - M_A \omega^2) u_A - 2\beta \cos ka u_B &= 0 \\ (-2\beta \cos ka) u_A + (2\beta - M_B \omega^2) u_B &= 0 \end{aligned} \right\} \Rightarrow \begin{aligned} 2\beta u_A - 2\beta u_B &= 0 \\ -2\beta u_A + 2\beta u_B &= 0 \end{aligned}$$

$u_A = u_B$

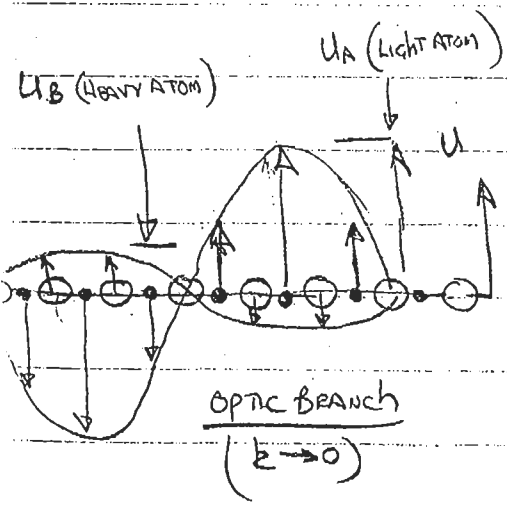


THIS WAS THE SITUATION FOR A NORMAL ELASTIC WAVE - A VOLUME ELEMENT (AND ALL ATOMS IN IT) HAS A CERTAIN AMPLITUDE.

WE OBTAINED, ABOVE THE RESULT (FOR SMALL k)

THAT $\omega \approx \left(\frac{2\beta a^2}{M_A + M_B} \right) k$
 i.e., THE VELOCITY OF THE WAVE $V = \left(\frac{2\beta a^2}{M_A + M_B} \right)^{\frac{1}{2}}$

IF $M_A = M_B = M$. THIS REDUCES TO $V = \left(\frac{\beta a^2}{M} \right)^{\frac{1}{2}}$



THE SAME AS PREVIOUSLY OBTAINED FOR A CONTINUUM OR FOR A CRYSTAL CONTAINING ONLY ONE TYPE ATOM. THIS IS A NORMAL ELASTIC WAVE OF THE SORT WHICH WOULD BE PRESENT IN PROPAGATION OF SOUND. THE SOLUTION WITH THE \ominus SIGN IS ACCORDINGLY CALLED THE ACOUSTIC BRANCH

THE SOLUTION WITH \oplus SIGN (FOR WHICH $\omega \neq 0$ AT $k=0$) FOR WHICH THE CENTER OF MASS OF THE CELL REMAINS FIXED HAS AMPLITUDES OF VIBRATION FOR THE TWO ATOMS WHICH ARE OPPOSITE IN SIGN. THIS SORT OF WAVE (TOTALLY UNACCOUNTED FOR IN THE CONTINUUM MODEL!) MIGHT WELL BE EXCITED IF AN ELECTROMAGNETIC FIELD WERE INCIDENT ON A IONIC CRYSTAL - IONS OF OPPOSITE CHARGE WOULD BE PULLED IN OPPOSING DIRECTIONS. THE SOLUTION WITH THE \oplus SIGN IS ACCORDINGLY CALLED THE OPTIC BRANCH

(B) SOLUTIONS FOR $k = k_{MAX}$

OTHER EXTREME IN SOLUTIONS OCCURS WHEN $\sin^2 ka$ REACHES MAXIMUM VALUE - NAMELY, $\sin ka = 1$ $ka = \frac{\pi}{2}$

$k_{MAX} = \frac{\pi}{2a}$

NOTE THAT FOR A 1-D XL WITH ONE KIND OF ATOM WE HAD EARLIER OBTAINED $k_{MAX} = \frac{\pi}{a}$. THE PRESENT RESULT LOOKS DIFFERENT UNTIL WE REALIZE THAT

$\left\{ \begin{aligned} T = a = \text{LATTICE CONSTANT WITH 1 KIND OF ATOM} \\ T = 2a = \text{LATTICE CONSTANT WITH 2 KINDS OF ATOM} \end{aligned} \right.$

$\therefore k_{MAX} = \frac{\pi}{T}$ IN BOTH

As $k \rightarrow k_{MAX}$

$$\omega^2 = \beta \left(\frac{1}{M_A} + \frac{1}{M_B} \right) \pm \beta \left\{ \left(\frac{1}{M_A} + \frac{1}{M_B} \right)^2 - \frac{4}{M_A M_B} \sin^2 ka \right\}^{\frac{1}{2}}$$

$$\omega^2 = \beta \left(\frac{1}{M_A} + \frac{1}{M_B} \right) \pm \beta \left\{ \left(\frac{1}{M_A^2} + \frac{1}{M_B^2} + \frac{2}{M_A M_B} \right) - \frac{4}{M_A M_B} \right\}^{\frac{1}{2}}$$

$$= \beta \left(\frac{1}{M_A} + \frac{1}{M_B} \right) \pm \beta \left\{ \frac{1}{M_A^2} + \frac{1}{M_B^2} - \frac{2}{M_A M_B} \right\}^{\frac{1}{2}} = \beta \left(\frac{1}{M_A} + \frac{1}{M_B} \right) \pm \beta \left\{ \left(\frac{1}{M_A} - \frac{1}{M_B} \right)^2 \right\}^{\frac{1}{2}}$$

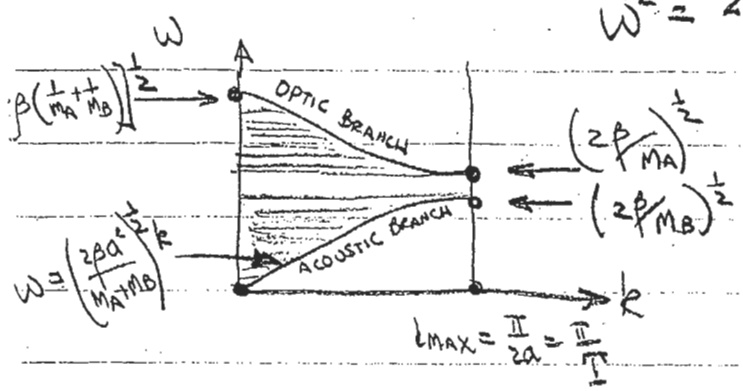
OR
$$\omega^2 = \beta \left(\frac{1}{M_A} + \frac{1}{M_B} \right) \pm \beta \left(\frac{1}{M_A} - \frac{1}{M_B} \right)$$

POSITIVE BRANCH (OPTIC BRANCH)

$$\omega^2 = \frac{2\beta}{M_A}$$

NEGATIVE SOLUTION (ACOUSTIC BRANCH)

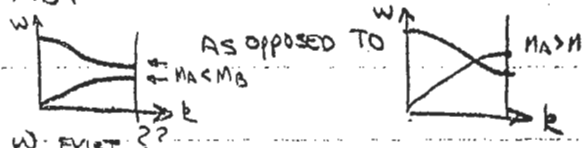
$$\omega^2 = \frac{2\beta}{M_B}$$



A FIRST UNEXPECTED RESULT OF THIS PROBLEM WAS THE PRESENCE OF THE OPTIC BRANCH (WHICH WOULD BE UNANTICIPATED IN THE CONTINUUM APPROACH) WE NOW SEE A SECOND UNEXPECTED FEATURE — NAMELY, THE PRESENCE OF A BAND OF FORBIDDEN INTERMEDIATE FREQUENCIES

$$\left(\frac{2\beta}{M_B} \right)^{\frac{1}{2}} < \omega < \left(\frac{2\beta}{M_A} \right)^{\frac{1}{2}} \text{ FOR WHICH NO ACCEPTABLE SOLUTION } \omega = f(k) \text{ IS DEFINED, AND WHICH THEREFORE ARE MODES WHICH CANNOT BE PROPAGATED IN THE CRYSTAL. [STIR ANY PRIMAERIAL RECOLLECTIONS OF 'FORBIDDEN' ENERGIES FOR ELECTRONS MOVING IN CRYSTALS ???]}$$

DISCUSSION. NOW HOLD ON A SEC, THE DISCRIMINATING STUDENT WILL EXPLOSTATE! IF THE PRECEDING PAGES ARE EXAMINED, WE HAVE NOWHERE SPECIFIED WHICH IS THE GREATER ATOMIC MASS, M_A OR M_B ! HOW THEN CAN WE SAY THAT ω AS A FUNCTION OF k DOES THIS



IS IT THEREFORE NECESSARY THAT A GAP IN ω EXIST??

WELL NOW, DISCRIMINATING STUDENT: IF THE TWO BRANCHES ARE TO CROSS AS IN THE SECOND SKETCH, THERE MUST BE SOME k FOR WHICH THE BRANCHES CROSS. THAT IS, LOOKING AT ω AS A FN OF k :

$$\omega^2 = \beta \left(\frac{1}{M_A} + \frac{1}{M_B} \right) \pm \beta \left\{ \left(\frac{1}{M_A} + \frac{1}{M_B} \right)^2 - \frac{4}{M_A M_B} \sin^2 ka \right\}^{\frac{1}{2}}$$

THIS TERM MUST, FOR SOME k , BE ZERO IF BRANCHES CROSS.

CAN WE PROVE
$$\left(\frac{1}{M_A} + \frac{1}{M_B} \right)^2 - \frac{4}{M_A M_B} \sin^2 ka \geq 0 \text{ ??}$$

MAX VALUE FOR SECOND TERM IS WHEN THIS = 1

$$\left(\frac{1}{M_A} + \frac{1}{M_B} \right)^2 - \frac{4}{M_A M_B} \geq 0 \text{ ?}$$

$$\frac{1}{M_A^2} + \frac{1}{M_B^2} + \frac{2}{M_A M_B} - \frac{4}{M_A M_B} \geq 0 \text{ ?}$$

$$\frac{1}{M_A^2} + \frac{1}{M_B^2} - \frac{2}{M_A M_B} = \left(\frac{1}{M_A} - \frac{1}{M_B} \right)^2 \geq 0 \text{ ?}$$

YES! ALWAYS TRUE! QED THERE IS A GAP IN ω .

[NOTE THAT THE REASON FOR THE PARADOX, RESOLVED ABOVE, IS THAT $(\frac{1}{M_A} - \frac{1}{M_B})^2 \equiv (\frac{1}{M_B} - \frac{1}{M_A})^2$. THE EXPRESSION WE ELECT TO USE AT THE BOTTOM OF Pg 4 DETERMINES WHETHER $\frac{1}{M_A}$ OR $\frac{1}{M_B}$ APPEARS AT k_{MAX} IN EACH BRANCH]

DISPLACEMENTS AT k_{MAX}

$$\begin{cases} (2\beta - M_A \omega^2) U_A - (2\beta \cos ka) U_B = 0 \\ -2\beta \cos ka U_A + (2\beta - M_B \omega^2) U_B = 0 \end{cases}$$

AT $k = k_{MAX}$ $\omega^2_{OPTIC} = \left(\frac{2\beta}{M_A}\right)^{\frac{1}{2}}$ $\omega^2_{ACOUSTIC} = \left(\frac{2\beta}{M_B}\right)^{\frac{1}{2}}$ WHERE $\frac{M_B}{M_A} > 1$, $k = \frac{\pi}{2a}$

$$\begin{cases} (2\beta - M_A \frac{2\beta}{M_A}) U_A - (2\beta \cos \frac{\pi}{2a} \cdot a) U_B = 0 \\ -2\beta \cos \frac{\pi}{2a} \cdot a U_A + (2\beta - M_B \frac{2\beta}{M_B}) U_B = 0 \end{cases}$$

$$\begin{cases} (-2\beta - 2\beta) U_A - 0 U_B = 0 \\ -0 U_A + (2\beta - 2\beta \frac{M_A}{M_A}) U_B = 0 \end{cases}$$

$$\begin{cases} 0 U_A - 0 U_B = 0 \\ 0 U_A + 2\beta(1 - \frac{M_B}{M_A}) U_B = 0 \end{cases}$$

$\Rightarrow U_B = 0$
FOR OPTIC MODE AT k_{MAX}

HEAVY ATOM STAYS MOTIONLESS, U_A FOR LIGHT ATOM IS ANY VALUE.

$$\begin{cases} (2\beta - M_A \frac{2\beta}{M_B}) U_A - (2\beta \cos \frac{\pi}{2a} \cdot a) U_B = 0 \\ (-2\beta \cos \frac{\pi}{2a} \cdot a) U_A + (2\beta - M_B \frac{2\beta}{M_B}) U_B = 0 \end{cases}$$

$$\begin{cases} 2\beta(1 - \frac{M_A}{M_B}) U_A - 0 U_B = 0 \\ 0 U_A + 0 U_B = 0 \end{cases}$$

$\Rightarrow U_A = 0$ $U_B = \text{ANYTHING}$

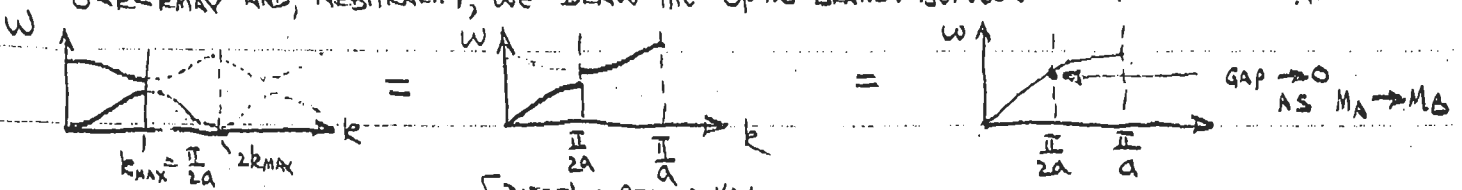
FOR ACOUSTIC MODE AT k_{MAX}
LIGHT ATOM STAYS MOTIONLESS.

CORRESPONDENCE TO THE IDENTICAL-ATOM PROBLEM

OUR SOLUTION TO THE TWO-ATOM-PER-CELL PROBLEM LOOKS VERY DIFFERENT FROM OUR EARLIER RESULT FOR A ONE-DIMENSIONAL CRYSTAL WITH ONE KIND OF ATOM — NAMELY WE HAVE FOUND THE PRESENCE OF A SECOND CLASS OF MODES — THE OPTIC BRANCH.

SUPPOSE NOW, THAT $M_B \rightarrow M_A$. THE PROBLEM THEN IS INDISTINGUISHABLE FROM THE 1-D. XI / ONE KIND OF ATOM PROBLEM. HOW DOES THE OPTIC BRANCH KNOW IT HAS TO DISAPPEAR WHEN $M_A = M_B$???

RECALL THAT ALL PHYSICALLY MEANINGFUL MODES EXIST FOR RANGES OF k WITHIN THE FIRST BRILLOUIN ZONE; LARGER VALUES OF k MAY BE SHIFTED TO WITHIN THE ZONE BY SUBTRACTING A Δk WHICH DOES NOT ALTER PHASE BETWEEN NEIGHBORING ATOMS. LET US REDRAW $\omega(k)$ SUCH THAT THE ACOUSTIC BRANCH IS DRAWN BETWEEN $0 < k < k_{MAX}$ AND, ARBITRARILY, WE DRAW THE OPTIC BRANCH BETWEEN $k_{MAX} < k < 2k_{MAX}$.

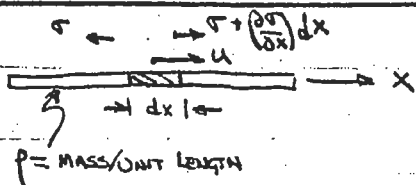


[DOES THIS REMIND YOU OF THE 1-D. XI PROBLEM ???]

3.60 Symmetry, Structure and Tensor Properties of Materials

A CRYSTAL IS NOT A CONTINUUM, BUT IS COMPOSED OF DISCREET ATOMS. HOW DOES THIS INFLUENCE THE PROPAGATION OF ELASTIC WAVES? WE WILL HERE CONSIDER ONLY A ONE DIMENSIONAL CRYSTAL IN ORDER TO KEEP THE ALGEBRA TRACTABLE. THIS IS NOT A SWINDLE! NO NEW NOTIONS ARE REQUIRED TO EXTEND THE DISCUSSION TO A TWO- OR THREE- DIMENSIONAL PROBLEM.

① WAVE PROPAGATION IN A CONTINUOUS ONE-DIMENSIONAL MEDIUM



$$\epsilon = \frac{\partial u}{\partial x} \quad \sigma = C \epsilon = C \frac{\partial u}{\partial x}$$

$$\underbrace{\rho dx}_m \frac{\partial^2 u}{\partial t^2} = \left[\sigma + \left(\frac{\partial \sigma}{\partial x} \right) dx \right] - \sigma$$

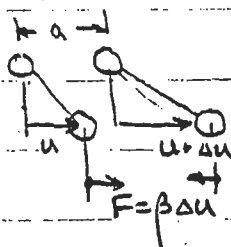
$$\rho \frac{\partial^2 u}{\partial t^2} = \frac{\partial \sigma}{\partial x} = C \frac{\partial^2 u}{\partial x^2}$$

$$\text{SOLUTION } u = u_0 e^{-2\pi i / \lambda (vt - x)}$$

SUBSTITUTION IN WAVE EQUATION GIVES

$$v = \sqrt{\frac{C}{\rho}}$$

CONSIDER A ONE-DIMENSIONAL CRYSTAL WITH ONE KIND OF ATOM OF MASS M SEPARATED BY LATTICE CONSTANT a . LET THE RESTORING FORCE WHICH ACTS WHEN AN ATOM IS DISPLACED BE DESCRIBED BY THE FORCE CONSTANT β SUCH THAT



$$F = \beta \Delta u$$

LET US NOW RELATE THE MACROSCOPIC PARAMETERS C AND ρ TO ATOMIC PARAMETERS.

$$\rho = \text{NO. OF ATOMS/UNIT LENGTH} \cdot M$$

$$\rho = \frac{1}{a} \cdot M$$

$$F = \beta \Delta u \quad \text{BUT } F = C \epsilon = C \frac{\Delta u}{a}$$

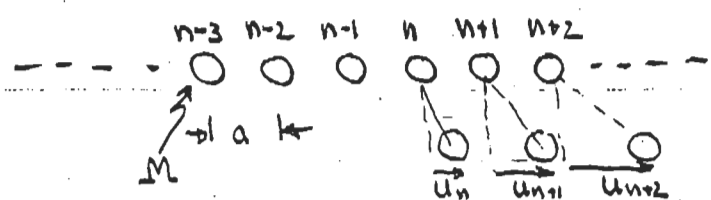
$$\therefore \frac{C}{a} = \beta$$

THE WAVE VELOCITY IN TERMS OF ATOMIC QUANTITIES IS

$$v = \sqrt{\frac{C}{\rho}} = \sqrt{\frac{\beta a^2}{M}} \quad \text{INDEPENDENT OF } \lambda$$

② WAVE MOTION ON A ROW OF IDENTICAL ATOMS

CONSIDER A CRYSTAL OF ONE DIMENSION CONTAINING ONE TYPE OF ATOM OF MASS M PER UNIT CELL a . NUMBER THE ATOMS;



LET AN ELASTIC WAVE PROPAGATE ALONG THE CHAIN. AT ONE INSTANT OF TIME EACH ATOM HAS A DISPLACEMENT u_n . CONSIDER ONLY NEAREST NEIGHBOR FORCES (BUT SEE DIGRESSIONS LATER)

WITH $F = \beta \Delta u$

$$\begin{aligned} \therefore F_n &= \beta(u_{n+1} - u_n) - \beta(u_n - u_{n-1}) \\ &= \beta(u_{n+1} - 2u_n + u_{n-1}) = M \frac{\partial^2 u_n}{\partial t^2} \end{aligned}$$

WE AGAIN LOOK FOR A WAVE SOLUTION OF THE FORM $u_n = u_0 e^{i(\omega t - kx)}$ BUT THIS EXACT FORM WILL NOT SUFFICE: x IS NO LONGER A CONTINUOUS VARIABLE. DISPLACEMENT IS DEFINED ONLY AT ATOM LOCATIONS.

LET $kx \rightarrow kna$ AND $u_n = u_0 e^{i(\omega t - kna)}$ IS AN ACCEPTABLE EXPRESSION [$u_{n+1} = u_0 e^{i[\omega t - k(n+1)a]}$ etc]

SUBSTITUTION OF THIS EXPRESSION IN THE EQUATION OF MOTION AS A TOTAL SOLUTION GIVES:

$$M u_0 (i\omega)^2 e^{i(\omega t - kna)} = \beta u_0 e^{i\omega t} [e^{-i[k(n+1)a]} - 2e^{-ikna} + e^{-i[k(n-1)a]}]$$

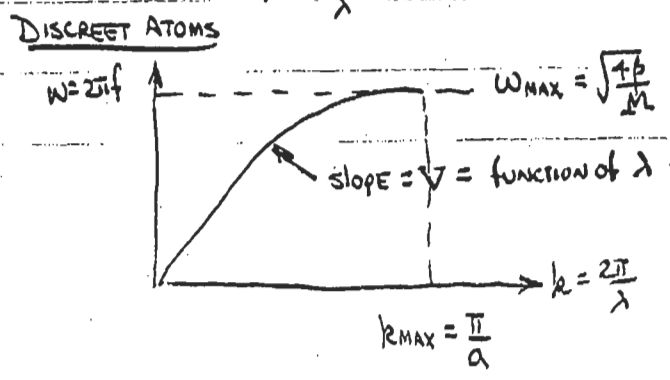
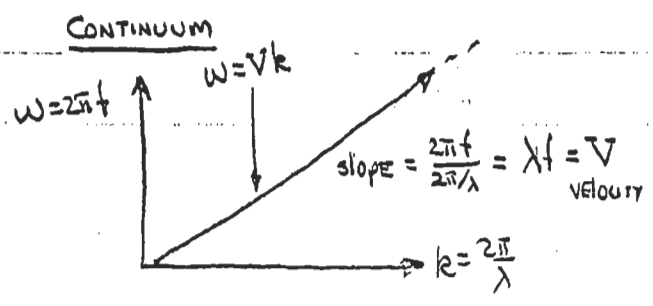
$$\begin{aligned} -M\omega^2 &= \beta \{ e^{-ika} - 2 + e^{+ika} \} \\ &= \beta (e^{-ika/2} - e^{+ika/2})^2 \end{aligned}$$

BUT $-\frac{1}{2}i(e^{ix} - e^{-ix}) = \sin x$

$$\therefore -M\omega^2 = \beta \left(-2 \sin \frac{ka}{2} \right)^2 = -4\beta \sin^2 \frac{ka}{2}$$

$$\omega = \left(\frac{4\beta}{M} \right)^{\frac{1}{2}} \sin \frac{ka}{2}$$

NOTE THAT $\omega = 2\pi f$ IS A FUNCTION OF $k = \frac{2\pi}{\lambda}$



FOR THE CONTINUUM, VELOCITY IS A CONSTANT $\sqrt{\frac{c}{\rho}}$, INDEPENDENT OF λ AND A WAVE OF ANY FREQUENCY OR ANY λ SHOULD BE PROPAGATABLE IN THE CRYSTAL
 TAKING INTO ACCOUNT THE DISCREET NATURE OF THE CRYSTAL WE FIND

- THERE IS A MAXIMUM ANGULAR FREQUENCY $\omega_{MAX} = \sqrt{\frac{4B}{M}}$ WHICH CAN BE PROPAGATED IN THE CRYSTAL
- VELOCITY IS A FUNCTION OF WAVELENGTH AND NOT A CONSTANT
 (NOTE THAT V SLOWS TO ZERO AT k_{MAX} !)

[ALL THIS IS RATHER UNEXPECTED! NOTE: NO RAZZLE-DAZZLE QUANTUM MECHANICS OR ANYTHING FANCY HERE! THIS IS PURELY CLASSICAL MECHANICS!]

DIGRESSION A DOES THIS RESULT REDUCE TO WHAT WE OBTAINED FOR THE CONTINUUM FOR WAVELENGTHS $\gg a$? THE WAVE SHOULDN'T BE ABLE TO TELL THAT ATOMS ARE THERE FOR THIS SITUATION!

$$\omega = \left(\frac{4B}{M}\right)^{\frac{1}{2}} \sin \frac{ka}{2}$$

FOR LARGE λ $k = \frac{2\pi}{\lambda}$ IS VERY SMALL $\therefore \sin \frac{ka}{2} \approx \frac{ka}{2}$

$$\begin{aligned} \text{THEN } \omega &\approx \left(\frac{4B}{M}\right)^{\frac{1}{2}} \frac{ka}{2} \\ &\approx \sqrt{\frac{Ba^2}{M}} k \end{aligned}$$

EXACTLY WHAT WE OBTAINED EARLIER!

WHAT IS "SMALL" k ?

CONSIDER $k_{MAX} = \frac{\pi}{a}$ a IS OF THE ORDER OF $\approx 10^{-8}$ CM

SO $k_{MAX} \approx 10^8$ CM⁻¹

CONSIDER A k ONLY 1% OF THE WAY TOWARDS k_{MAX} ,

IE $k \approx 10^6$ CM⁻¹. A TYPICAL VELOCITY OF AN ELASTIC WAVE IN

A SOLID IS $\approx 5 \cdot 10^5$ CM²/SEC

$$V = f\lambda = f \frac{2\pi}{k} \quad \text{SO } f = \frac{kV}{2\pi} = \frac{10^6 \cdot 5 \cdot 10^5}{2\pi}$$

$\approx 10^5$ MEGACYCLES, AN

ENORMOUSLY HIGH FREQUENCY!

INTERLUDE B IN A "REAL" 1-DIMENSIONAL CRYSTAL WE SHOULD CONSIDER INTERACTIONS BEYOND MERELY NEAREST-NEIGHBORS! HOW WILL THIS INFLUENCE THE RESULT?

IN THE FORCE BALANCE ON THE n^{TH} ATOM WE WROTE

$$M \frac{\partial^2 u_n}{\partial t^2} = F = \beta_1 (u_{n+1} - 2u_n + u_{n-1})$$

NOW INCLUDE THESE HIGHER-ORDER TERMS $\left\{ \begin{aligned} &+ \beta_2 (u_{n+2} - 2u_n + u_{n-2}) \\ &+ \beta_3 (u_{n+3} - 2u_n + u_{n-3}) + \dots \end{aligned} \right.$

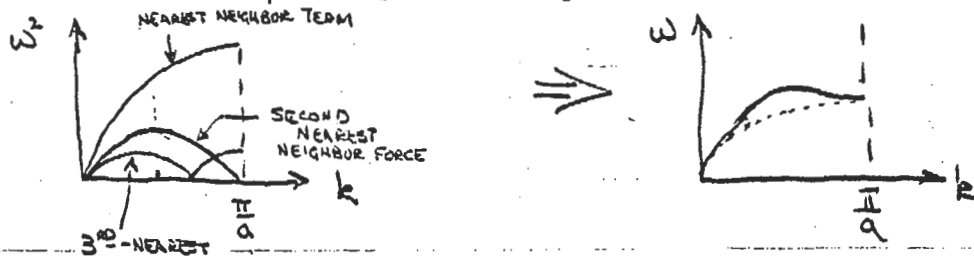
SUBSTITUTING OUR TRIAL SOLUTION:

$$-M\omega^2 = \beta_1 \{ e^{-ika} - 2 + e^{ika} \} + \beta_2 \{ e^{-i2ka} - 2 + e^{i2ka} \} + \beta_3 \{ e^{-i3ka} - 2 + e^{i3ka} \} + \dots$$

Each higher order term may now be condensed to give a \sin^2 term as before:

$$\omega^2 = \frac{4\beta_1}{M} \sin^2 \frac{ka}{2} + \frac{4\beta_2}{M} \sin^2 \frac{2ka}{2} + \frac{4\beta_3}{M} \sin^2 \frac{3ka}{2} + \dots$$

so that
$$\omega^2 = \sum_p \frac{4\beta_p}{M} \sin^2 \frac{pka}{2} \quad p = \text{AN INTEGER}$$



EFFECT OF HIGHER-NEIGHBOR INTERACTIONS IS TO IMPOSE SMALL PERTURBATIONS ON THE $\sin \frac{ka}{2}$ BEHAVIOR. THIS MIGHT APPEAR TO BE A MINOR HIGHER-ORDER EFFECT BUT IT IS ENORMOUSLY IMPORTANT IN CALCULATING SPECIFIC HEAT! (THE EXPRESSION WILL INVOLVE $\partial k / \partial \omega$ WHICH BLOWS UP AT THE POINT WHERE $\omega(k)$ HAS ZERO SLOPE!!)

= (FINIS DIGRESSIONS) =

LET US NOW EXAMINE THE MEANING OF THE WAVE WITH $k_{max} = \frac{\pi}{a}$ FOR WHICH ω ASSUMES THE MAXIMUM ANGULAR FREQUENCY FOR WHICH A VIBRATIONAL MODE MAY BE SUPPORTED BY THE CRYSTAL.

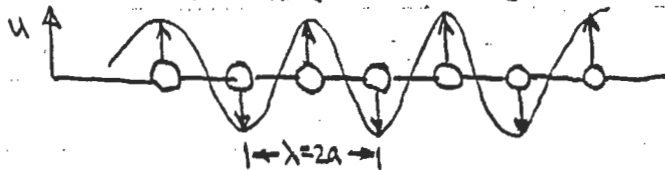
$$\omega = \sqrt{\frac{4\beta}{M}} \sin \frac{ka}{2} \quad \text{HAS MAXIMUM VALUE WHEN } \sin \frac{ka}{2} = 1$$

$$\frac{ka}{2} = \frac{\pi}{2}$$

$$\therefore k_{max} = \frac{\pi}{a}$$

THIS CORRESPONDS TO A WAVE WITH $\lambda_{min} = \frac{2\pi}{k_{max}} = \frac{2\pi a}{\pi} = \underline{\underline{2a}}$ AND, AS $\partial \omega / \partial k = v = 0$, A WAVE WITH ZERO VELOCITY.

LET'S PLOT THE DISPLACEMENT OF THE ATOMS FOR SUCH A WAVE AS A FUNCTION OF DISTANCE ALONG THE CHAIN AT ONE PARTICULAR INSTANT OF TIME

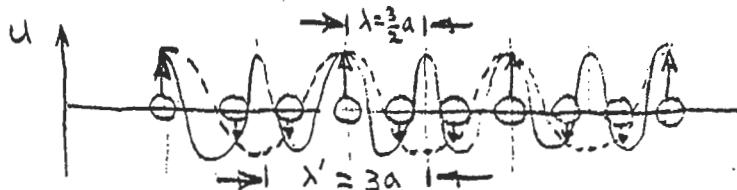
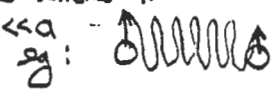


THE PATTERN OF DISPLACEMENTS ARE EQUAL BUT OPPOSITE IN DIRECTION.

THIS TURNS OUT TO BE THE SMALLEST WAVELENGTH ONE CAN DEFINE PHYSICALLY IN THE CRYSTAL! WHY? DISPLACEMENT MAY BE DEFINED ONLY AT THE LOCATIONS WHERE THE ATOMS SIT!

IT CLEARLY MAKES NO PHYSICAL SENSE TO TALK ABOUT A WAVE OF $\lambda \ll a$

A PATTERN OF DISPLACEMENTS WHICH WE MIGHT DRAW WITH $\lambda < 2a$ MAY BE EQUALLY WELL DEFINED IN TERMS OF SOME $\lambda' > 2a$. LET'S SHOW THIS SPECIFICALLY FOR $\lambda = \frac{3}{2}a$



SO THAT A WAVE WITH $\lambda = \frac{3}{2}a$ IS COMPLETELY INDISTINGUISHABLE FROM ONE WITH $\lambda' = 3a < 2a$!

WHAT IS THE REASON FOR THIS? WELL, ALL WE CAN REALLY TALK ABOUT WITH MEANING IS THE RELATIVE DISPLACEMENT OF NEIGHBORING ATOMS

$$\frac{u_n}{u_{n+1}} = \frac{u_0 e^{i(\omega t - k n a)}}{u_0 e^{i[\omega t - k(n+1)a]}} = e^{i k a}$$

WE CAN THEREFORE ADD OR SUBTRACT ANY INCREMENT TO k WHICH CHANGES PHASE OF $e^{i k a}$ BY 2π AND NOTHING WILL HAVE CHANGED. Δk SHOULD BE SUCH THAT

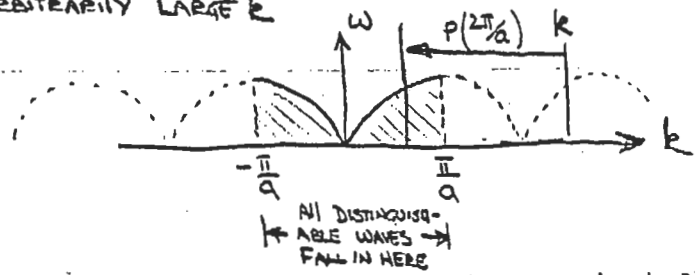
$$\Delta k a = 2\pi$$

$$\text{OR } \Delta k = \frac{2\pi}{a}$$

THUS IF k IS SUCH THAT $k > k_{\text{max}} = \frac{\pi}{a}$, WE CAN ALWAYS DEFINE WAVE IN TERMS OF A NEW k'

$$k' = k \pm p \left(\frac{2\pi}{a} \right) \quad (p = \text{AN INTEGER})$$

SUCH THAT $|k'| < \frac{\pi}{a}$, EVEN THOUGH, FORMALY, ONE HAS $\omega = \left(\frac{1}{M} \right)^{\frac{1}{2}} \sin \frac{k a}{2}$ DEFINED FOR ARBITRARILY LARGE k



[NOTICE THAT SOMETIMES, UPON SUBTRACTING OFF A MULTIPLE OF $2\pi/a$, ONE GETS A $|k'| < \frac{\pi}{a}$, BUT A VALUE WHICH IS NEGATIVE! A NEGATIVE k MERELY MEANS A WAVE WHICH IS TRAVELING IN THE OPPOSITE DIRECTION. IT IS AMUSING TO SHOW THIS TO ONESELF; YOU CAN DO IT WITH THE EXAMPLE SHOWN ABOVE IN WHICH

$$\lambda = \frac{2}{3} a \quad k = \frac{4}{3} \frac{\pi}{a}$$

$$X = 3a \quad k' = -\frac{2}{3} \frac{\pi}{a} = \frac{4}{3} \frac{\pi}{a} - \frac{6}{3} \frac{\pi}{a}$$

FINALLY, WHAT IS THE MEANING OF ZERO VELOCITY FOR THE WAVE WITH $k = k_{\text{max}} = \frac{\pi}{a}$?

$$u_n = u_0 e^{i(\omega t - k n a)}$$

SUBSTITUTING $k = \frac{\pi}{a}$

$$u_n = u_0 e^{i(\omega t - \frac{\pi}{a} n a)} = u_0 e^{i(\omega t)} e^{-i n \pi}$$

THIS REPRESENTS A STANDING WAVE; AMPLITUDE BUILDS UP AND DECAYS WITH TIME FOR A GIVEN ATOM BUT THE WAVE DOESN'T GO ANYWHERE!



SUCH A STANDING WAVE PATTERN WOULD BE PRODUCED BY TWO EQUAL WAVES MOVING IN OPPOSITE DIRECTIONS. THE NODES STAY FIXED! IN FACT, ONE CAN CONSIDER THIS AS ONE-DIMENSIONAL DIFFRACTION A LA BRAGG'S LAW

Path Diff = $2a = n\lambda$

$\therefore \lambda = 2a$ for $n=1$!!!

$k_{\text{max}} = \frac{\pi}{a}$ IS THEN NOTHING MORE THAN THE λ FOR WHICH DIFFRACTION OCCURS (CONSTRUCTIVE INTERFERENCE) THIS IS A PHENOMENON WHICH OCCURS WHEN EVER A WAVE (ELASTIC, X-RAY, ELECTRON DEBROGLIE WAVE) MOVES THROUGH A PERIODIC MEDIUM.

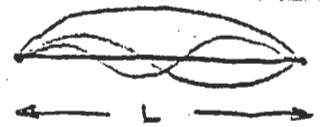
YOU PROBABLY ARE MORE FAMILIAR WITH THIS SITUATION IN CONNECTION WITH X-RAY DIFFRACTION OR ENERGY LEVELS OF ELECTRONS IN CRYSTALS BUT THEY ARE ALL THE SAME EFFECT

THE BOUNDARY TO k AT $k_{max} = \frac{\pi}{a}$ IS CALLED THE FIRST BRILLOUIN ZONE.

TOTAL NUMBER OF VIBRATIONAL MODES WHICH MAY BE SUPPORTED BY THE CRYSTAL

WE HAVE SHOWN THAT THERE IS A LOWER LIMIT, $\lambda_{min} = 2a$, TO THE WAVES WHICH MAY BE SUPPORTED BY A CRYSTAL COMPOSED OF DISCREET ATOMS.

FOR A FINITE-SIZED CHUNK OF CRYSTAL THERE WILL ALSO BE AN UPPER LIMIT TO λ DETERMINED BY THE DIMENSIONS OF THE SAMPLE. FOR A ONE-DIMENSIONAL CRYSTAL OF LENGTH L



$\lambda = 2L, L, \frac{2}{3}L \dots \dots \dots 2a$
 $\omega, \lambda = \frac{2L}{m}$ $m = \text{AN INTEGER} = 1, 2 \dots$

WHAT ARE THE VALUES OF k FOR THESE WAVES?

$k = \frac{2\pi}{\lambda} = \frac{2\pi}{2L}, \frac{2\pi}{L}, \frac{2\pi}{\frac{2}{3}L} \dots \dots \dots \frac{\pi}{a}$

$k = m \frac{\pi}{L}$

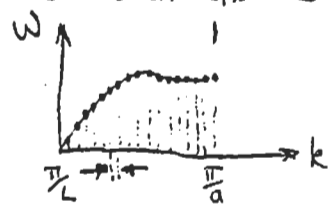
NOW, HOW MANY DISTINCT VIBRATIONAL MODES CAN THE CRYSTAL SUPPORT?

$m_{max} \frac{\pi}{L} = \frac{\pi}{a}$

$m_{max} = \frac{L}{a} \approx N$ THE NUMBER OF ATOMS IN THE CRYSTAL!

THEREFORE, OUR ONE DIMENSIONAL CRYSTAL WITH ONE KIND OF ATOM MAY SUPPORT A NUMBER OF VIBRATIONAL MODES WHICH IS EQUAL TO THE NUMBER OF ATOMS IN THE CRYSTAL

OUR PLOT OF ω AS A FUNCTION OF k SHOULD THEREFORE NOT BE REGARDED AS A CONTINUOUS FUNCTION, BUT RATHER A SET OF DISCRETE / CLOSELY-SPACED STATES - EACH SEPARATED EQUALLY BY AN AMOUNT $\Delta k = \frac{\pi}{L}$



3.60 Symmetry, Structure and Tensor Properties of Materials

PROPAGATION OF ELASTIC WAVES IN CRYSTALS

WE CONSIDER HERE ONLY A CRYSTAL OF CUBIC SYMMETRY. THE TREATMENT MAY BE READILY EXTENDED TO CRYSTALS OF LOWER SYMMETRY BUT AS THE NUMBER OF NON-ZERO TENSOR ELEMENTS WOULD BECOME LARGER, THE ALGEBRA WOULD BECOME CORRESPONDINGLY MORE TEDIOUS.

ALL CALCULATIONS WILL BE DONE IN ONE COORDINATE SYSTEM, SO LET'S USE THE MORE FAMILIAR x, y, z TO LABEL COORDINATES RATHER THAN SUBSCRIPTED VARIABLES.

LET US CONSIDER A VOLUME ELEMENT IN A SOLID AND SET UP A SET OF EQUATIONS WHICH WILL GIVE ITS DISPLACEMENTS u, v, w ALONG x, y, z RESPECTIVELY, AS A FUNCTION OF POSITION AND TIME

FOR A CUBIC CRYSTAL

$$(1) \begin{cases} \sigma_1 = c_{11} \epsilon_1 + c_{12} \epsilon_2 + c_{12} \epsilon_3 \\ \sigma_2 = c_{12} \epsilon_1 + c_{11} \epsilon_2 + c_{12} \epsilon_3 \\ \sigma_3 = c_{12} \epsilon_1 + c_{12} \epsilon_2 + c_{11} \epsilon_3 \\ \sigma_4 = c_{44} \epsilon_4 \\ \sigma_5 = c_{44} \epsilon_5 \\ \sigma_6 = c_{44} \epsilon_6 \end{cases}$$

(FOR A CRYSTAL OF LOWER SYMMETRY WE WOULD MERELY HAVE MORE TERMS)

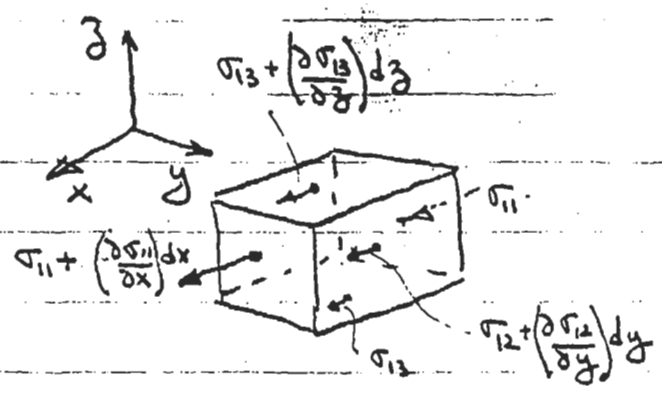
AS WE WANT AN EQUATION WHICH INVOLVES DISPLACEMENTS, SUBSTITUTE FOR ϵ_i ITS DEFINITION IN TERMS OF DISPLACEMENT, NAMELY

$$\begin{aligned} \epsilon_1 = \epsilon_{11} &= \frac{\partial u}{\partial x} & \epsilon_4 = \epsilon_{32} + \epsilon_{23} &= \frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \\ \epsilon_2 = \epsilon_{22} &= \frac{\partial v}{\partial y} & \epsilon_5 = \epsilon_{31} + \epsilon_{13} &= \frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \\ \epsilon_3 = \epsilon_{33} &= \frac{\partial w}{\partial z} & \epsilon_6 = \epsilon_{21} + \epsilon_{12} &= \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \end{aligned}$$

REPLACING ϵ_i BY THESE DEFINITIONS GIVES

$$(2) \begin{cases} \sigma_1 = c_{11} \frac{\partial u}{\partial x} + c_{12} \left(\frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) \\ \sigma_2 = c_{11} \frac{\partial v}{\partial y} + c_{12} \left(\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z} \right) \\ \sigma_3 = c_{11} \frac{\partial w}{\partial z} + c_{12} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \\ \sigma_4 = c_{44} \left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \right) \\ \sigma_5 = c_{44} \left(\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right) \\ \sigma_6 = c_{44} \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) \end{cases}$$

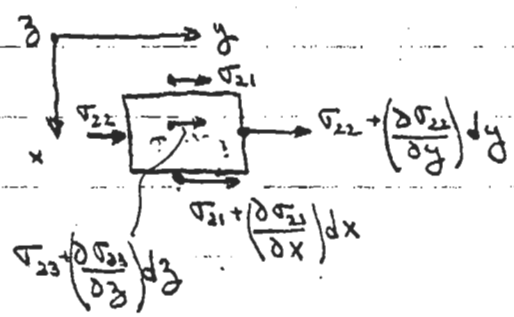
NOW CONSIDER A VOLUME ELEMENT IN THE SOLID WITH DENSITY ρ AND EDGES dx, dy, dz . FOR EACH DIRECTION (x, y & z) WE FIND THE NET FORCE ON THE ELEMENT ($\sigma \times$ AREA) AND SET IT EQUAL TO MASS \times ACCELERATION.



FOR THE X-DIRECTION:

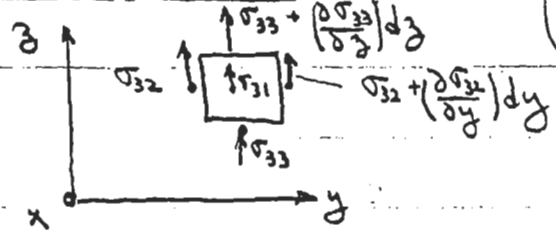
$$\underbrace{\left(\frac{\partial \sigma_{11}}{\partial x}\right) dx}_{\text{NET F/UNIT A}} \cdot \underbrace{dy dz}_{dA} + \underbrace{\left(\frac{\partial \sigma_{12}}{\partial y}\right) dy}_{\text{NET F/UNIT A}} \cdot \underbrace{dx dz}_{dA} + \underbrace{\left(\frac{\partial \sigma_{13}}{\partial z}\right) dz}_{\text{NET F/UNIT A}} \cdot \underbrace{dx dy}_{dA} = \underbrace{\rho dx dy dz}_{dV} \left(\frac{\partial^2 u}{\partial t^2}\right)$$

SIMILARLY, FOR THE y DIRECTION



$$\left(\frac{\partial \sigma_{22}}{\partial y}\right) dy \cdot dx dz + \left(\frac{\partial \sigma_{21}}{\partial x}\right) dx \cdot dy dz + \left(\frac{\partial \sigma_{23}}{\partial z}\right) dz \cdot dx dy = \rho dx dy dz \left(\frac{\partial^2 v}{\partial t^2}\right)$$

FOR THE z DIRECTION



$$\left(\frac{\partial \sigma_{33}}{\partial z}\right) dz \cdot dx dy + \left(\frac{\partial \sigma_{31}}{\partial x}\right) dx \cdot dy dz + \left(\frac{\partial \sigma_{32}}{\partial y}\right) dy \cdot dx dz = \rho dx dy dz \left(\frac{\partial^2 w}{\partial t^2}\right)$$

COMBINING EQUATIONS AND REPLACING TENSOR DESCRIPTION OF σ_{ij} BY MATRIX ELEMENT σ_k

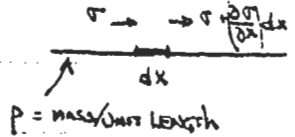
$$(3) \begin{cases} \frac{\partial \sigma_1}{\partial x} + \frac{\partial \sigma_6}{\partial y} + \frac{\partial \sigma_5}{\partial z} = \rho \frac{\partial^2 u}{\partial t^2} \\ \frac{\partial \sigma_6}{\partial x} + \frac{\partial \sigma_2}{\partial y} + \frac{\partial \sigma_4}{\partial z} = \rho \frac{\partial^2 v}{\partial t^2} \\ \frac{\partial \sigma_5}{\partial x} + \frac{\partial \sigma_4}{\partial y} + \frac{\partial \sigma_3}{\partial z} = \rho \frac{\partial^2 w}{\partial t^2} \end{cases}$$

SUBSTITUTING EXPRESSIONS FOR σ_i IN TERMS OF DERIVATIVES OF DISPLACEMENT [EQS (2)]

$$(4) \begin{cases} C_{11} \frac{\partial^2 u}{\partial x^2} + C_{12} \left(\frac{\partial^2 v}{\partial x \partial y} + \frac{\partial^2 w}{\partial x \partial z} \right) + C_{44} \left(\frac{\partial^2 v}{\partial x \partial y} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 w}{\partial x \partial z} + \frac{\partial^2 u}{\partial z^2} \right) = \rho \frac{\partial^2 u}{\partial t^2} \\ C_{11} \frac{\partial^2 v}{\partial y^2} + C_{12} \left(\frac{\partial^2 u}{\partial x \partial y} + \frac{\partial^2 w}{\partial y \partial z} \right) + C_{44} \left(\frac{\partial^2 u}{\partial x \partial y} + \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 w}{\partial y \partial z} + \frac{\partial^2 v}{\partial z^2} \right) = \rho \frac{\partial^2 v}{\partial t^2} \\ C_{11} \frac{\partial^2 w}{\partial z^2} + C_{12} \left(\frac{\partial^2 u}{\partial x \partial z} + \frac{\partial^2 v}{\partial y \partial z} \right) + C_{44} \left(\frac{\partial^2 u}{\partial x \partial z} + \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 v}{\partial y \partial z} + \frac{\partial^2 w}{\partial y^2} \right) = \rho \frac{\partial^2 w}{\partial t^2} \end{cases}$$

EQUATIONS (4) REPRESENT THE EQUATIONS GOVERNING DISPLACEMENT OF THE VOLUME ELEMENT!
 WHILE ALL THIS LOOKS RATHER FORMIDABLE, NOTE THAT THIS IS NOTHING MORE THAN A PLAIN OLD WAVE EQUATION [STIFFNESS TIMES SECOND PARTIAL DERIVATIVE OF DISPLACEMENT WITH POSITION ON THE LEFT, DENSITY AND SECOND PARTIAL DERIVATIVE OF DISPLACEMENT WITH TIME ON THE RIGHT]
 ACCORDINGLY, WE LOOK FOR A SOLUTION IN THE FORM OF A TRAVELING WAVE - GENERALIZED APPROPRIATELY FOR A THREE-DIMENSIONAL PROBLEM.

RECALL THE ONE-DIMENSIONAL WAVE PROBLEM



$$\epsilon = \frac{\partial u}{\partial x} \quad \therefore \underbrace{\rho dx}_{m} \frac{\partial^2 u}{\partial t^2} = \frac{\partial \sigma}{\partial x} dx$$

$$\sigma = c \epsilon \quad = c \frac{\partial^2 u}{\partial x^2}$$

SOLUTION IS $u = u_0 e^{i(\omega t - kx)}$

$$\omega = 2\pi f \quad k = \frac{2\pi}{\lambda}$$

$$f \lambda = v \text{ VELOCITY OF WAVE} = \sqrt{\frac{E}{\rho}}$$

THE TERM IN THE EXPONENT MAY THEREFORE BE WRITTEN IN ALTERNATIVE FORMS

$$i(\omega t - kx) = i \left(2\pi f t - \frac{2\pi}{\lambda} x \right)$$

$$= 2\pi i \left(\frac{v}{\lambda} t - \frac{2\pi}{\lambda} x \right)$$

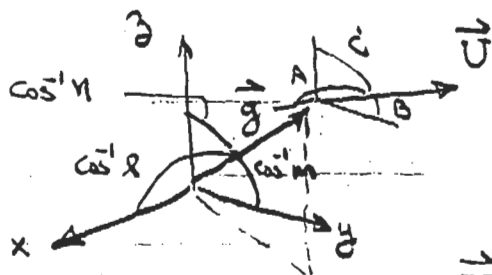
$$= \frac{2\pi}{\lambda} i (v t - x)$$

(i.e., AS x CHANGES FROM x TO $x + \lambda$ PHASE CHANGES BY 2π
 AS t CHANGES FROM t TO $t + \frac{\lambda}{v}$ PHASE CHANGES BY 2π)

TO CAST THE WAVE EQUATION IN A THREE-DIMENSIONAL FORM, LET A UNIT VECTOR \vec{g} WITH DIRECTION COSINES l, m, n DEFINE THE DIRECTION IN THE CRYSTAL IN WHICH THE WAVE PROPAGATES.

LET THE DISPLACEMENT OF THE VOLUME ELEMENT BE $\vec{U}(x, y, z, t)$. THERE IS NO REASON WHY THE DISPLACEMENT \vec{U} NEED BE IN THE DIRECTION OF \vec{g} . THEREFORE, LET THE DIRECTION COSINES OF \vec{U} BE DEFINED BY A, B, C . THE COMPONENTS OF DISPLACEMENT FOR WHICH WE HAVE EQUATIONS ARE ACCORDINGLY

$$u = |U| A \quad v = |U| B \quad w = |U| C$$

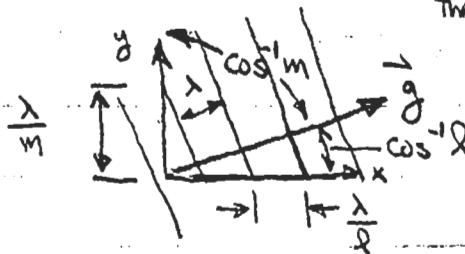


AN APPROPRIATE SOLUTION IS

$$\vec{U} = \vec{U}_0 e^{i \frac{2\pi}{\lambda} (vt - lx - my - nz)} \quad (5)$$

(NOTICE THAT PUTTING THE DIRECTION COSINE IN FRONT OF x, y, z MEANS THAT AS WE MOVE ALONG x , FOR EXAMPLE, PHASE GOES THROUGH 2π AS WE GO A DISTANCE λ/l)

with $\begin{cases} u = U A \\ v = U B \\ w = U C \end{cases}$



LET US NOW SUBSTITUTE OUR TRIAL SOLUTION (5) INTO THE WAVE EQUATIONS (4). NOTE THAT $\partial_x(e^{ax}) = a e^{ax}$. THEREFORE EVERY TERM IN (4), UPON SUBSTITUTION OF (5) WILL CONTAIN A COMMON FACTOR $i \left(\frac{2\pi}{\lambda}\right) U_0 e^{-i \frac{2\pi}{\lambda} (vt - lx - my - nz)}$ WHICH WILL CANCEL OUT. — SO LET'S NOT BOTHER TO WRITE IT.

$$\begin{cases} C_{11} l^2 + C_{12} (l m + m n) + C_{44} (l m + m^2 + C l n + n^2) = \rho v^2 A \\ C_{11} m^2 + C_{12} (l m + C m n) + C_{44} (l m + B l^2 + C m n + B n^2) = \rho v^2 B \\ C_{11} n^2 + C_{12} (l n + B m n) + C_{44} (l n + C l^2 + B m n + C m^2) = \rho v^2 C \end{cases}$$

REARRANGING & COLLECTING TERMS IN $A, B \& C$

$$(6) \begin{cases} [C_{11} l^2 + C_{44} (m^2 + n^2) - \rho v^2] A + (C_{12} + C_{44}) (l m B + l n C) = 0 \\ [C_{11} m^2 + C_{44} (n^2 + l^2) - \rho v^2] B + (C_{12} + C_{44}) (m n C + m l A) = 0 \\ [C_{11} n^2 + C_{44} (l^2 + m^2) - \rho v^2] C + (C_{12} + C_{44}) (n l A + n m B) = 0 \end{cases}$$

OUR SOLUTION MUST SATISFY THIS SET OF EQUATIONS IF IT IS TO BE AN ACCEPTABLE SOLUTION!

WHICH ARE THE INDEPENDENT AND WHICH THE DEPENDENT VARIABLES?

— THE CRYSTAL GIVES US THE STIFFNESSES $C_{11}, C_{12} \& C_{44}$.

— YOU PICK THE DIRECTION IN WHICH YOU WISH TO PROPAGATE THE WAVE, SO l, m, n MAY BE SELECTED FOR A DIRECTION OF INTEREST

— THE VELOCITY OF THE WAVE, v , AND THE DIRECTION COSINES $A, B \& C$ OF THE DISPLACEMENT VECTOR \vec{U} ARE UNKNOWN VARIABLES.

LET US REGARD THE DIRECTION COSINES A, B & C AS VARIABLES. EQUATIONS (6) REPRESENT A SET OF THREE LINEAR HOMOGENEOUS EQUATIONS. ONE SOLUTION IS $A=B=C=0$ (THIS IS NOT ONLY A TRIVIAL SOLUTION, BUT AN IMPOSSIBLE ONE, AS $A^2+B^2+C^2=1$ MUST ALSO BE SATISFIED) A NON-TRIVIAL SOLUTION EXISTS ONLY IF THE DETERMINANT OF THE COEFFICIENTS OF A, B & C IS ZERO, i.e.:

$$\begin{vmatrix} [C_{11}l^2 + C_{44}(m^2+n^2) - \rho V^2] & (C_{12}+C_{44})l m & (C_{12}+C_{44})l n \\ (C_{12}+C_{44})m l & [C_{11}m^2 + C_{44}(n^2+l^2) - \rho V^2] & (C_{12}+C_{44})m n \\ (C_{12}+C_{44})n l & (C_{12}+C_{44})n m & [C_{11}n^2 + C_{44}(l^2+m^2) - \rho V^2] \end{vmatrix} = 0$$

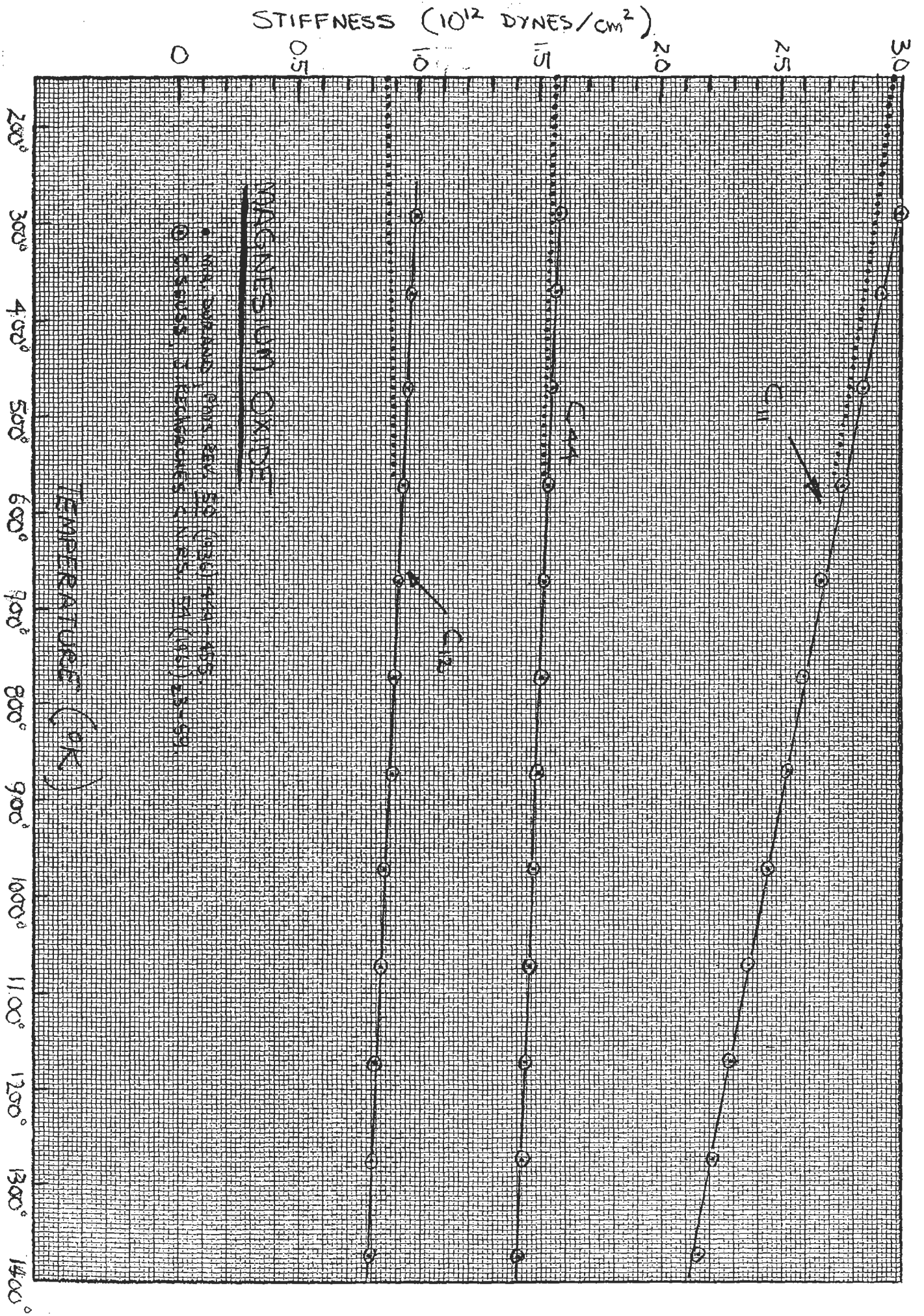
THIS IS AGAIN AN EIGENVALUE PROBLEM. EXPANDING THE DETERMINANT LEADS TO A 3RD ORDER EQUATION IN (ρV^2) - THESE ARE THE EIGENVALUES AND THERE WILL BE THREE OF THEM. AN ACCEPTABLE SOLUTION EXISTS ONLY FOR THESE THREE VELOCITIES; THEY ARE FUNCTIONS OF THE STIFFNESS AND l, m, n .

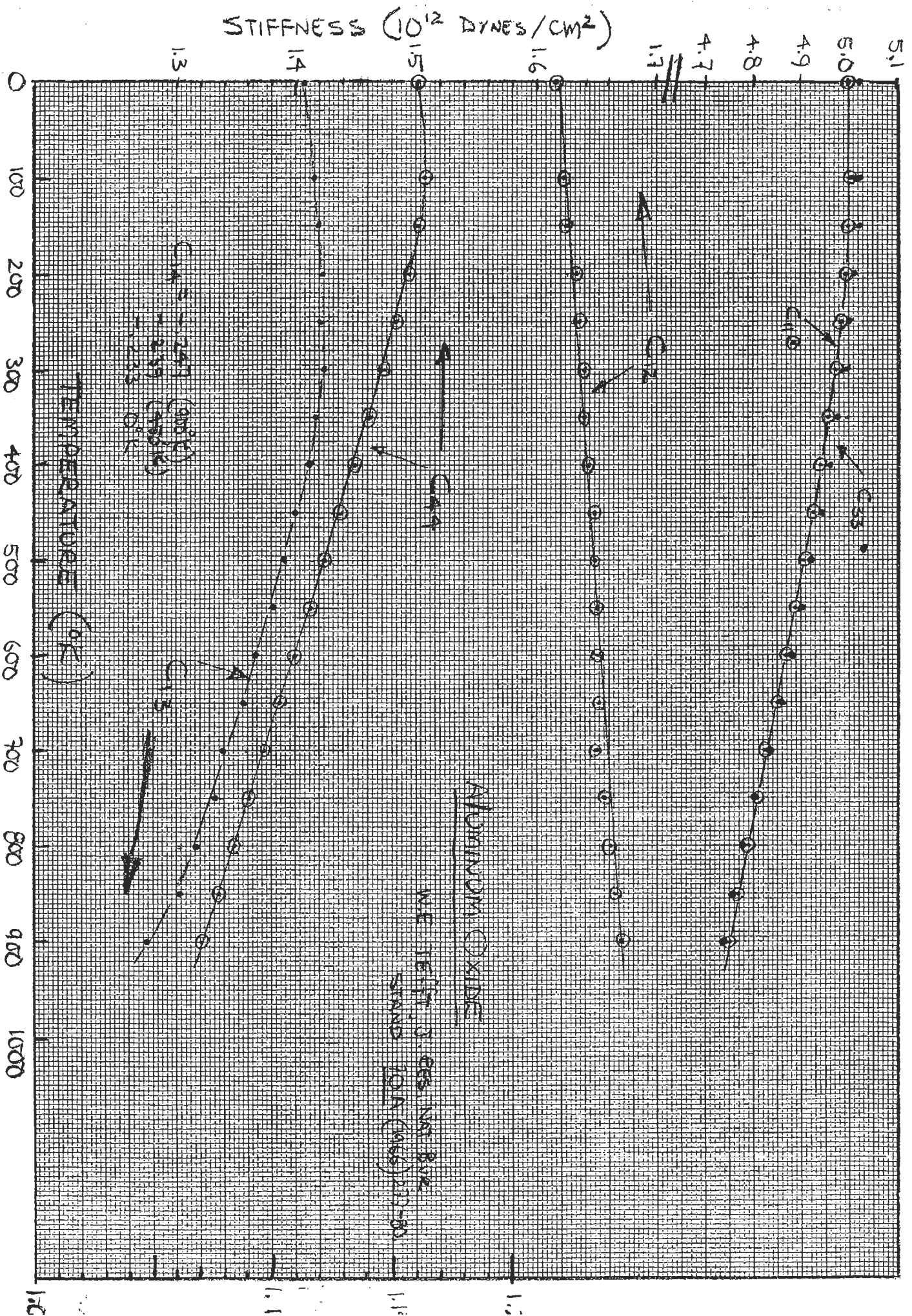
EACH OF THE THREE EIGENVALUES FOR ρV^2 MAY BE SUBSTITUTED, IN TURN, BACK INTO THE ORIGINAL EQUATIONS (6) WHICH MAY THEN BE SOLVED FOR THE DIRECTION COSINES A, B, C OF THE DISPLACEMENT VECTOR.

THE ESSENTIAL FEATURES OF THE RESULT ARE:

- THERE ARE 3 DIFFERENT TYPES OF WAVES WHICH MAY BE PROPAGATED ALONG ANY GIVEN DIRECTION IN THE CRYSTAL
- THE VELOCITY OF THESE WAVES ARE DIFFERENT AND ARE FUNCTIONS OF DIRECTION IN THE CRYSTAL (l, m, n), THE STIFFNESSES C_{ij} , AND DENSITY, ρ
- THE DIRECTION OF THE DISPLACEMENT AMPLITUDE \vec{U} OF THE WAVE (A, B, C) IS NOT ARBITRARY, BUT IS FIXED BY DIRECTION OF PROPAGATION (l, m, n) AND C_{ij} ; MOREOVER, IT WILL BE DIFFERENT FOR THE THREE TYPES OF WAVES.

NOTE THAT EQUATIONS (6) WILL TAKE ON MUCH SIMPLER FORM AND BE MORE AMENABLE TO DIRECT SOLUTION FOR SPECIAL DIRECTIONS IN THE CRYSTAL





3.60 Symmetry, Structure and Tensor Properties of Materials

CONVENTIONS FOR RELABELING STRESS, STRAIN, STIFFNESS + COMPLIANCE

IN MATRIX NOTATION

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} \longrightarrow \begin{bmatrix} \sigma_1 & \sigma_6 & \sigma_5 \\ \sigma_6 & \sigma_2 & \sigma_4 \\ \sigma_5 & \sigma_4 & \sigma_3 \end{bmatrix} \quad \text{ie } \sigma_m \equiv \sigma_{ij}$$

$$\begin{bmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} \\ \epsilon_{21} & \epsilon_{22} & \epsilon_{23} \\ \epsilon_{31} & \epsilon_{32} & \epsilon_{33} \end{bmatrix} \longrightarrow \begin{bmatrix} \epsilon_1 & \frac{1}{2}\epsilon_6 & \frac{1}{2}\epsilon_5 \\ \frac{1}{2}\epsilon_6 & \epsilon_2 & \frac{1}{2}\epsilon_4 \\ \frac{1}{2}\epsilon_5 & \frac{1}{2}\epsilon_4 & \epsilon_3 \end{bmatrix} \quad \text{ie } \epsilon_m \equiv \begin{cases} \epsilon_{ij} & i=j \\ \frac{1}{2}\epsilon_{ij} & i \neq j \end{cases}$$

$$C_{ijkl} \equiv C_{ijrk} \equiv C_{mn} \quad \text{ie, NO FACTORS OF 2 OR 4 INVOLVED}$$

$$\left\{ \begin{array}{l} S_{ijkl} \equiv S_{ijrk} \equiv S_{mn} \quad \text{for } m \text{ AND } n \neq 4, 5, 6 \\ S_{ijkl} \equiv S_{ijrk} \equiv \frac{1}{2}S_{mn} \quad \text{for } m \text{ OR } n = 4, 5, 6 \\ S_{ijkl} \equiv S_{ijrk} \equiv \frac{1}{4}S_{mn} \quad \text{for } m \text{ AND } n = 4, 5, 6 \end{array} \right.$$

CONDENSATION FROM TENSOR TO MATRIX NOTATION & VICE VERSA

(MORAL: YOU CAN'T WIN, BUT IF YOU PLAY IT RIGHT YOU CAN COME OUT EVEN)

A STRAIN IN TERMS OF STRESS

WRITING ONE REPRESENTATIVE LINE IN TENSOR NOTATION:

TENSOR:
$$\epsilon_{23} = S_{2311} \sigma_{11} + S_{2322} \sigma_{22} + \dots + S_{2321} \sigma_{21} + S_{2312} \sigma_{12}$$

$\downarrow \epsilon_{23} \equiv \frac{1}{2} \epsilon_4 \quad \sigma_{11} \equiv \sigma_1 \quad \sigma_{22} \equiv \sigma_2 \quad \sigma_{21} \equiv \sigma_6 \quad \sigma_{12} \equiv \sigma_6$

$\frac{1}{2} \epsilon_4 = S_{2311} \sigma_1 + S_{2322} \sigma_2 + \dots + S_{2321} \sigma_6 + S_{2312} \sigma_6$

$\downarrow S_{2311} \equiv \frac{1}{2} S_{41} \quad S_{2322} \equiv \frac{1}{2} S_{42} \quad S_{2321} \equiv \frac{1}{4} S_{46} \quad S_{2312} \equiv \frac{1}{4} S_{46}$

$\frac{1}{2} \epsilon_4 = \frac{1}{2} S_{41} \sigma_1 + \frac{1}{2} S_{42} \sigma_2 + \dots + \frac{1}{4} S_{46} \sigma_6 + \frac{1}{4} S_{46} \sigma_6$

$\frac{1}{2} \epsilon_4 = \frac{1}{2} S_{41} \sigma_1 + \frac{1}{2} S_{42} \sigma_2 + \dots + \frac{1}{2} S_{46} \sigma_6$

MATRIX:
$$\therefore \epsilon_4 = S_{41} \sigma_1 + S_{42} \sigma_2 + \dots + S_{46} \sigma_6$$

$\downarrow S_{41} \equiv 2S_{2311} \quad S_{42} \equiv 2S_{2322} \quad S_{46} \left(\frac{1}{2} \sigma_6 \right) + S_{46} \left(\frac{1}{2} \sigma_6 \right) \downarrow S_{46} \equiv 4S_{2321} \equiv 4S_{2312}$

$\epsilon_4 = 2S_{2311} \sigma_1 + 2S_{2322} \sigma_2 + \dots + 4S_{2321} \frac{1}{2} \sigma_6 + 4S_{2312} \frac{1}{2} \sigma_6$

$\downarrow \epsilon_4 \equiv 2\epsilon_{23} \equiv 2\epsilon_{32} \quad \sigma_1 \equiv \sigma_{11} \quad \sigma_2 \equiv \sigma_{22} \quad \sigma_6 \equiv \sigma_{21} \equiv \sigma_{12}$

$2\epsilon_{23} = 2S_{2311} \sigma_{11} + 2S_{2322} \sigma_{22} + \dots + 4S_{2321} \frac{1}{2} \sigma_{21} + 4S_{2312} \frac{1}{2} \sigma_{12}$

$2\epsilon_{23} = 2S_{2311} \sigma_{11} + 2S_{2322} \sigma_{22} + \dots + 2S_{2321} \sigma_{21} + 2S_{2312} \sigma_{12}$

TENSOR:
$$\therefore \epsilon_{23} = S_{2311} \sigma_{11} + S_{2322} \sigma_{22} + \dots + S_{2321} \sigma_{21} + S_{2312} \sigma_{12}$$

B STRESS IN TERMS OF STRAIN

WRITING ONE REPRESENTATIVE LINE IN TENSOR NOTATION:

TENSOR: $\sigma_{21} = C_{2111} \epsilon_{11} + C_{2122} \epsilon_{22} + \dots + C_{2123} \epsilon_{23} + C_{2132} \epsilon_{32} + \dots$

\downarrow $\epsilon_1 \equiv \epsilon_{11}$ \downarrow $\epsilon_2 \equiv \epsilon_{22}$ \downarrow $\epsilon_{23} \equiv \frac{1}{2} \epsilon_4$ \downarrow $\epsilon_{32} \equiv \frac{1}{2} \epsilon_4$
 $\sigma_{21} \equiv \sigma_6$

$\sigma_6 = C_{2111} \epsilon_1 + C_{2122} \epsilon_2 + \dots + C_{2123} \frac{1}{2} \epsilon_4 + C_{2132} \frac{1}{2} \epsilon_4 + \dots$

$C_{ij} \epsilon_j \equiv C_{jik} \epsilon_k \equiv C_{ijl} \epsilon_l \equiv C_{mnl}$

$\sigma_6 = C_{61} \epsilon_1 + C_{62} \epsilon_2 + \dots + C_{64} \frac{1}{2} \epsilon_4 + C_{64} \frac{1}{2} \epsilon_4 + \dots$

MATRIX: $\sigma_6 = C_{61} \epsilon_1 + C_{62} \epsilon_2 + \dots + C_{64} \epsilon_4 + \dots$

\swarrow \searrow

$\sigma_6 = C_{61} \epsilon_1 + C_{62} \epsilon_2 + \dots + C_{64} \left(\frac{1}{2} \epsilon_4\right) + C_{64} \left(\frac{1}{2} \epsilon_4\right)$

\downarrow $\epsilon_{11} \equiv \epsilon_1$ \downarrow $\epsilon_{22} \equiv \epsilon_2$ \downarrow $\epsilon_{23} \equiv \epsilon_{32} \equiv \frac{1}{2} \epsilon_4$

$\sigma_6 = C_{61} \epsilon_{11} + C_{62} \epsilon_{22} + \dots + C_{64} \epsilon_{23} + C_{64} \epsilon_{32} + \dots$

\downarrow $C_{mnl} \equiv C_{ijkl} \equiv C_{jikl} \equiv C_{ijl} \epsilon_l$

TENSOR: $\sigma_{21} = C_{2111} \epsilon_{11} + C_{2122} \epsilon_{22} + \dots + C_{2123} \epsilon_{23} + C_{2132} \epsilon_{32} + \dots$

3.60 Symmetry, Structure and Tensor Properties of Materials

SYMMETRY RESTRICTIONS FOR 4TH RANK PROPERTY TENSORS

TRICLINIC

$$\begin{matrix}
 S_{11} & S_{12} & S_{13} & S_{14} & S_{15} & S_{16} \\
 & S_{22} & S_{23} & S_{24} & S_{25} & S_{26} \\
 & & S_{33} & S_{34} & S_{35} & S_{36} \\
 & & & S_{44} & S_{45} & S_{46} \\
 & & & & S_{55} & S_{56} \\
 & & & & & S_{66}
 \end{matrix}$$

(21)

MONOCLINIC
(2 || X₃)

$$\begin{matrix}
 S_{11} & S_{12} & S_{13} & 0 & 0 & S_{16} \\
 & S_{22} & S_{23} & 0 & 0 & S_{26} \\
 & & S_{33} & 0 & 0 & S_{36} \\
 & & & S_{44} & S_{45} & 0 \\
 & & & & S_{55} & 0 \\
 & & & & & S_{66}
 \end{matrix}$$

(13)

ORTHORHOMBIC (2 || X₁, X₂, X₃)

$$\begin{matrix}
 S_{11} & S_{12} & S_{13} & 0 & 0 & 0 \\
 & S_{22} & S_{23} & 0 & 0 & 0 \\
 & & S_{33} & 0 & 0 & 0 \\
 & & & S_{44} & 0 & 0 \\
 & & & & S_{55} & 0 \\
 & & & & & S_{66}
 \end{matrix}$$

(9)

TETRAGONAL (4, $\bar{4}$, $\frac{4}{m}$)

$$\begin{matrix}
 S_{11} & S_{12} & S_{13} & 0 & 0 & S_{16} \\
 & S_{11} & S_{13} & 0 & 0 & -S_{16} \\
 & & S_{33} & 0 & 0 & 0 \\
 & & & S_{44} & 0 & 0 \\
 & & & & S_{44} & 0 \\
 & & & & & S_{66}
 \end{matrix}$$

(7)

TETRAGONAL (4₂₂, 4_{mm}, $\bar{4}2m$, $\frac{4}{m}mm$)

$$\begin{matrix}
 S_{11} & S_{12} & S_{13} & 0 & 0 & 0 \\
 & S_{11} & S_{13} & 0 & 0 & 0 \\
 & & S_{33} & 0 & 0 & 0 \\
 & & & S_{44} & 0 & 0 \\
 & & & & S_{44} & 0 \\
 & & & & & S_{66}
 \end{matrix}$$

(6)

CUBIC

$$\begin{matrix}
 S_{11} & S_{12} & S_{12} & 0 & 0 & 0 \\
 & S_{11} & S_{12} & 0 & 0 & 0 \\
 & & S_{11} & 0 & 0 & 0 \\
 & & & S_{44} & 0 & 0 \\
 & & & & S_{44} & 0 \\
 & & & & & S_{44}
 \end{matrix}$$

(3)

3.60 Symmetry, Structure and Tensor Properties of Materials

SYMMETRY RESTRICTIONS FOR 4TH RANK PROPERTY TENSORS

Triclinic

$$\begin{matrix}
 S_{11} & S_{12} & S_{13} & S_{14} & S_{15} & S_{16} \\
 & S_{22} & S_{23} & S_{24} & S_{25} & S_{26} \\
 & & S_{33} & S_{34} & S_{35} & S_{36} \\
 & & & S_{44} & S_{45} & S_{46} \\
 & & & & S_{55} & S_{56} \\
 & & & & & S_{66}
 \end{matrix}$$

(21)

MONOCLINIC
(2 || X₃)

$$\begin{matrix}
 S_{11} & S_{12} & S_{13} & 0 & 0 & S_{16} \\
 & S_{22} & S_{23} & 0 & 0 & S_{26} \\
 & & S_{33} & 0 & 0 & S_{36} \\
 & & & S_{44} & S_{45} & 0 \\
 & & & & S_{55} & 0 \\
 & & & & & S_{66}
 \end{matrix}$$

(13)

ORTHORHOMBIC (2 || X₁, X₂, X₃)

$$\begin{matrix}
 S_{11} & S_{12} & S_{13} & 0 & 0 & 0 \\
 & S_{22} & S_{23} & 0 & 0 & 0 \\
 & & S_{33} & 0 & 0 & 0 \\
 & & & S_{44} & 0 & 0 \\
 & & & & S_{55} & 0 \\
 & & & & & S_{66}
 \end{matrix}$$

(9)

TETRAGONAL (4, $\bar{4}$, $\frac{4}{m}$)

$$\begin{matrix}
 S_{11} & S_{12} & S_{13} & 0 & 0 & S_{16} \\
 & S_{11} & S_{13} & 0 & 0 & -S_{16} \\
 & & S_{33} & 0 & 0 & 0 \\
 & & & S_{44} & 0 & 0 \\
 & & & & S_{44} & 0 \\
 & & & & & S_{66}
 \end{matrix}$$

(7)

TETRAGONAL (4₂₂, 4_{mm}, $\bar{4}$ _{2m}, $\frac{4}{m}$ _{mmm})

$$\begin{matrix}
 S_{11} & S_{12} & S_{13} & 0 & 0 & 0 \\
 & S_{11} & S_{13} & 0 & 0 & 0 \\
 & & S_{33} & 0 & 0 & 0 \\
 & & & S_{44} & 0 & 0 \\
 & & & & S_{44} & 0 \\
 & & & & & S_{66}
 \end{matrix}$$

(6)

CUBIC

$$\begin{matrix}
 S_{11} & S_{12} & S_{12} & 0 & 0 & 0 \\
 & S_{11} & S_{12} & 0 & 0 & 0 \\
 & & S_{11} & 0 & 0 & 0 \\
 & & & S_{44} & 0 & 0 \\
 & & & & S_{44} & 0 \\
 & & & & & S_{44}
 \end{matrix}$$

(3)

HEXAGONAL

TRIGONAL (3, $\bar{3}$)

$$S_{11} \ S_{12} \ S_{13} \ S_{14} \ S_{15} \ 0$$

$$S_{11} \ S_{13} \ -S_{14} \ -S_{15} \ 0$$

$$S_{33} \ 0 \ 0 \ 0$$

$$S_{44} \ 0 \ -2S_{15}$$

$$S_{44} \ 2S_{14}$$

$$(2S_{11} - 2S_{12})$$

(7)

TRIGONAL (32, 3m, $\bar{3}m$)

$$S_{11} \ S_{12} \ S_{13} \ S_{14} \ 0 \ 0$$

$$S_{11} \ S_{13} \ -S_{14} \ 0 \ 0$$

$$S_{33} \ 0 \ 0 \ 0$$

$$S_{44} \ 0 \ 0$$

$$S_{44} \ 2S_{14}$$

$$(2S_{11} - 2S_{12})$$

(6)

HEXAGONAL (6, $\bar{6}$, 6/m, 622, 6mm, $\bar{6}m2$, 6/mmm)

$$S_{11} \ S_{12} \ S_{13} \ 0 \ 0 \ 0$$

$$S_{11} \ S_{13} \ 0 \ 0 \ 0$$

$$S_{33} \ 0 \ 0 \ 0$$

$$S_{44} \ 0 \ 0$$

$$S_{44} \ 0$$

$$(2S_{11} - 2S_{12})$$

(5)

ISOTROPIC

$$S_{11} \ S_{12} \ S_{12} \ 0 \ 0 \ 0$$

$$S_{11} \ S_{12} \ 0 \ 0 \ 0$$

$$S_{11} \ 0 \ 0 \ 0$$

$$2(S_{11} - S_{12}) \ 0 \ 0$$

$$2(S_{11} - S_{12}) \ 0$$

$$2(S_{11} - S_{12})$$

(2)

$$2C_{44} = (C_{11} - C_{12})$$

$$\frac{1}{2}S_{44} = (S_{11} - S_{12})$$

CAUCHY RELATION

(1) CENTRAL FORCES

(2) EACH ATOM AT CENTER OF SYMMETRY

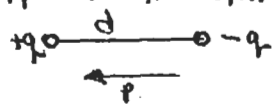
(3) NO INITIAL STRESS

$$C_{12} = C_{44}$$

3.60 Symmetry, Structure and Tensor Properties of Materials

SOME BASIC RELATIONS IN ELECTROMAGNETISM

DIPOLE MOMENT: CONSIDER A PAIR OF POINT CHARGES OF EQUAL MAGNITUDE BUT OPPOSITE SIGN SEPARATED BY A DISTANCE d



THE DIPOLE MOMENT IS DEFINED AS $|\vec{p}| = q \cdot d$

IT IS ASSIGNED A VECTOR SENSE - PARALLEL TO \vec{d} AND POINTING FROM THE NEGATIVE CHARGE TOWARD THE POSITIVE CHARGE

(IT IS A USEFUL DEFINITION BECAUSE THE VECTOR SENSE AND THE COMBINATION OF q AND d TOGETHER APPEAR IN CONSIDERATIONS SUCH AS THE ELECTRIC FIELD \vec{E} CREATED IN THE REGION AROUND THE DIPOLE OR IN COMPUTING THE TORQUE ON A DIPOLE WHEN IT IS PLACED IN AN ELECTRIC FIELD.)

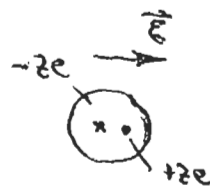
DIPOLAS CAN BE EITHER

PERMANENT



OR INDUCED

(a) ATOM IN ELECTRIC FIELD



$$\vec{p} \propto \vec{E}$$

$$\equiv \alpha \vec{E}$$

ELECTRONIC POLARIZABILITY

OR INDUCED (b) - IONS IN A STRUCTURE



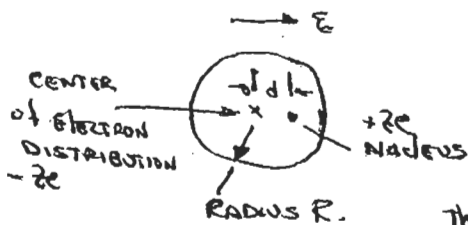
(ACTUALLY, A TENSOR!)

$$P_i = \alpha_{ij} E_j$$

$$P_i = \alpha_i E_i$$

IONIC POLARIZABILITY

LET'S CONSIDER A VERY SIMPLIFIED MODEL FOR THE DIELECTRIC POLARIZABILITY



WE REPRESENT THE ELECTRON CLOUD BY A SPHERE OF RADIUS R THAT HAS A UNIFORM CONCENTRATION OF ELECTRONS THROUGHOUT ITS VOLUME. ALSO, WE ASSUME THAT, WHEN THE ELECTRIC FIELD ACTS TO DISPLACE THE NUCLEUS AND THE ELECTRONS, THE SPHERICAL DISTRIBUTION OF ELECTRONS IS NOT DEFORMED

THE CENTER OF THE ELECTRON DISTRIBUTION AND THE NUCLEUS WILL SEPARATE UNTIL THE FORCE ON THE CHARGES EXERTED BY THE ELECTRIC FIELD IS JUST BALANCED BY THE ATTRACTION BETWEEN NUCLEUS AND ELECTRONS.

The Dipole Moment is $zed = p$

THE FORCE ON THE CHARGES EXERTED BY THE ELECTRIC FIELD E IS

$$F = ze \vec{E} \quad (\vec{E} \text{ IS FORCE PER UNIT } + \text{ CHARGE})$$



DRAW A CIRCLE OF RADIUS d (THE SEPARATION OF THE CENTER OF THE ELECTRON

DISTRIBUTION AND THE NUCLEUS) ABOUT THE CENTER OF THE ELECTRON SPHERE. THEN THE FORCE BETWEEN THE ELECTRONS AND NUCLEUS, IS (BY COULOMB'S LAW)

$$F = \frac{1}{4\pi\epsilon_0} \frac{ze \cdot Q}{d^2} \quad \text{WHERE } Q \text{ IS THE CHARGE INSIDE THE SPHERE OF RADIUS } d.$$

(WE USE THE FACT THAT A CHARGE PLACED WITHIN

A UNIFORMLY-CHARGED SPHERE EXPERIENCES NO FORCE AT ANY POSITION

$$Q \text{ WILL BE } \frac{4}{3}\pi d^3 \cdot \frac{ze}{\frac{4}{3}\pi R^3}$$

EQUATING THESE ELECTROSTATIC FORCES

$$zeE = \frac{1}{4\pi\epsilon_0} \frac{ze \cdot Q}{d^2} = \frac{1}{4\pi\epsilon_0} \frac{ze}{d^2} \cdot \left(\frac{d^3}{R^3} \cdot ze \right)$$

Solving for d

$$d = \frac{4\pi\epsilon_0 R^3}{ze} E$$

AND THE DIPOLE MOMENT zed

$$\text{is } p = \frac{4\pi\epsilon_0 R^3}{ze} \cdot ze E$$

From which $\vec{P} = 4\pi\epsilon_0 R^3 \vec{E}$

AND THE ELECTRONIC POLARIZABILITY IS

$$\alpha = 4\pi\epsilon_0 R^3$$

THIS VERY SIMPLIFIED MODEL IS INSTRUCTIVE AND AMUSING FOR TWO REASONS.

- (1) IT PREDICTS THAT THE INDUCED DIPOLE MOMENT IS PREDICTED TO BE PROPORTIONAL TO \vec{E}
- (2) THE ELECTRONIC POLARIZABILITY IS SHOWN TO BE PROPORTIONAL TO THE VOLUME OF THE ATOM: BIG ATOMS ARE MUSHIER, WHICH IS IN FACT THE CASE. (I^+ HAS THE LARGEST IONIC POLARIZABILITY OF ANY CATION)

POLARIZABILITIES ARE RELATED TO INDEX OF REFRACTION, n , BY THE LORENZ-LORENTZ EQUATION

$$\frac{n^2 - 1}{n^2 + 2} = \frac{4\pi}{3} \sum N_i \alpha_i \quad \text{WHERE } N_i \text{ IS NUMBER OF SPECIES } i \text{ PER UNIT VOLUME}$$

OR, IN ANOTHER FORM

$$\frac{M}{\rho} \frac{n^2 - 1}{n^2 + 2} = \frac{4\pi}{3} L \alpha \quad \text{WHERE } \begin{cases} M = \text{MOLECULAR WEIGHT} \\ \rho = \text{DENSITY} \\ L = \text{AVOGADRO'S NUMBER} \\ \alpha = \text{POLARIZABILITY PER "MOLECULE"} \end{cases}$$

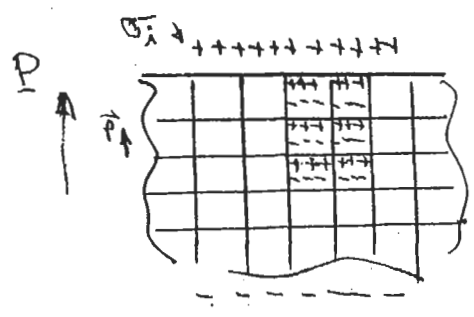
THE DIELECTRIC CONSTANT OF A MATERIAL, ϵ , IS RELATED TO INDEX OF REFRACTION BY $\epsilon = n^2$

THE ABOVE RELATIONS MAY, THEREFORE, BE WRITTEN IN TERMS OF ϵ (UPON WHICH THEY BECOME KNOWN AS THE CLAUSIUS-MOSSOTTI EQUATIONS)

A SET OF ELECTRONIC POLARIZABILITIES FOR IONS HAVE BEEN DETERMINED ON THIS BASIS BY TESSMAN, KAHN AND SHOCKLEY (PHYS. REV. 92 890 (1953).)

MATTER IN BULK

The Dipole moment per unit volume is designated by P and has units of $\frac{\text{Charge} \cdot \text{Length}}{\text{Length}^3} = \frac{\text{Charge}}{\text{Unit Area}}$



Let each of the atomic dipoles above be represented by a cubic cell of edge δ with induced charges on its surface

The Dipole moment on each atom is

$$p = q_i \delta \quad \text{where } q_i \text{ is the induced charge}$$

The number of cells/unit volume is

$$n = \frac{\text{Unit Volume}}{\text{Vol./cell}} = \frac{1}{\delta^3}$$

so the Dipole moment per unit volume, P

$$P = n p = \frac{1}{\delta^3} \cdot q_i \delta$$

$$P = \frac{q_i}{\delta^2} \quad \text{AN INDUCED CHARGE/UNIT AREA}$$

While this model may seem overly simple and crude the details of the "cells" do not matter because charge everywhere cancels internally and remains un-neutralized only on the surface of the specimen

so Polarization, P , Dipole moment/unit vol. is equally numerically and physically to an induced charge/unit area

PIEZOELECTRICITY

PIEZOELECTRICITY (literally "PRESSURE ELECTRICITY") IS AN IMPORTANT PROPERTY THAT MUST BE DESCRIBED IN TERMS OF A THIRD-RANK TENSOR. THE PROPERTY IS THE BASIS OF A NUMBER OF DEVICES RANGING FROM TRANSDUCERS, SENSORS AND ACTUATORS THROUGH AUDIO EQUIPMENT DOWN TO EVERYDAY DEVICES SUCH AS CIGARETTE LIGHTERS

THERE ARE SEVERAL DISTINCT PIEZOELECTRIC PHENOMENA AND WE SHALL DESCRIBE EACH IN TURN.

THE DIRECT PIEZOELECTRIC EFFECT DESCRIBES A DIPOLE MOMENT PER UNIT VOLUME (POLARIZATION, P) THAT IS CREATED WHEN A MATERIAL IS SUBJECTED TO AN APPLIED STRESS. THE ORIGIN OF THE PROPERTY CAN BE QUITE SIMPLE IN SOME MATERIALS. IN AN IONIC MATERIAL THE CREATION OF DEFORMATION THROUGH APPLICATION OF A STRESS MOVES CHARGED IONS RELATIVE TO ONE ANOTHER AND THEREBY CREATES LOCAL DIPOLE MOMENTS. (IT IS POSSIBLE TO CALCULATE THE MAGNITUDE OF THE PROPERTY FOR SIMPLE STRUCTURES IF ONE KNOWS THE ELASTIC PROPERTIES)

WE WILL FOLLOW THE SIMPLE ASSUMPTIONS THAT WE MADE FOR SECOND-RANK TENSORS - NAMELY, WE WILL ASSUME A LINEAR RESPONSE AND, SECOND, THAT EVERY COMPONENT OF THE GENERALIZED DISPLACEMENT IS GIVEN BY A LINEAR COMBINATION OF EACH COMPONENT OF THE GENERALIZED FORCE. FOR THE DIRECT PIEZOELECTRIC EFFECT THIS MEANS WE WRITE EACH COMPONENT OF THE POLARIZATION VECTOR AS A LINEAR COMBINATION OF EACH OF THE NINE COMPONENTS OF THE STRESS TENSOR

$$P_i = d_{ijk} \sigma_{jk}$$

P_i IS A VECTOR (TENSOR OF FIRST RANK) AND TRANSFORMS ACCORDING TO THE LAW FOR VECTORS

$$P'_i = C_{ir} P_r \text{ WHERE } C_{ir} \text{ ARE THE DIRECTION COSINES FOR THE CHANGE OF AXES.}$$

σ_{jk} IS A TENSOR OF SECOND RANK AND TRANSFORMS ACCORDING TO THE LAW FOR 2ND RANK TENSORS

$$\sigma'_{jk} = C_{jr} C_{km} \sigma_{rm}$$

FROM THIS IT FOLLOWS THAT d_{ijk} WILL TRANSFORM ACCORDING TO

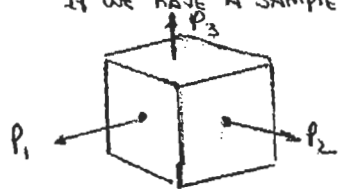
$$d'_{ijk} = C_{ir} C_{jm} C_{kn} d_{rmn} \text{ AND IS, THEREFORE, A TENSOR OF THIRD RANK}$$

THE ELEMENTS d_{ijk} ARE CALLED THE PIEZOELECTRIC MODULI AND ARE THE COEFFICIENTS IN THREE EQUATIONS FOR P_1, P_2, P_3 THAT INVOLVE ALL NINE ELEMENTS OF STRESS

$$\begin{cases} P_1 = d_{111}\sigma_{11} + d_{122}\sigma_{22} + d_{133}\sigma_{33} + d_{123}\sigma_{23} + d_{132}\sigma_{32} + d_{113}\sigma_{13} + d_{131}\sigma_{31} + d_{112}\sigma_{12} \\ P_2 = d_{211}\sigma_{11} + \dots \\ P_3 = \dots \end{cases} \quad \begin{matrix} \text{3 EQS} \\ \downarrow \\ \text{9 VARIABLES} \end{matrix} \quad \therefore d_{ijk} \text{ IS AN ARRAY OF } 3 \times 9 = 27 (!) \text{ ELEMENTS}$$

FROM THE PRECEDING LECTURE WE SAW THAT A CONSEQUENCE OF POLARIZATION WAS AN INDUCED SURFACE CHARGE AND THAT POLARIZATION (DIPOLE MOMENT/UNIT VOL) IS NUMERICALLY EQUAL TO \vec{P}

IF WE HAVE A SAMPLE IN WHICH A POLARIZATION HAS BEEN INDUCED IN SOME GENERAL DIRECTION RELATIVE TO SURFACES NORMAL TO OUR REFERENCE



AXES x_1, x_2, x_3 , THE x_1 COMPONENT OF \vec{P}, P_1 , WILL BE EQUAL TO THE CHARGE PER UNIT AREA ON THE SURFACE NORMAL TO x_1 , P_2 THE CHARGE PER UNIT AREA ON A SURFACE NORMAL TO x_2 -- ETC. NOTE THAT WE CAN, THROUGH THE GEOMETRY OF

THE SAMPLE, CREATE A SPECIMEN THAT EMPHASIZES ONE CHARGE DENSITY OVER ANOTHER - FOR EXAMPLE A VERY THIN PLATE IN THE x_1, x_2 PLANE WILL PRIMARILY

MEASURE P_3 — BIG SURFACE X CHARGE PER UNIT AREA = BIG CHARGE.

\vec{P} MEASURES CHARGE/UNIT AREA (Coulombs/m²) AND σ_{ij} IS FORCE/UNIT AREA (NEWTONS/m²)
 THEREFORE, P (Coulombs/m²) = $d \sigma$ (NEWTONS/m²) THE UNITS OF d_{ijk} ARE $\frac{\text{Coulombs}}{\text{NEWTON}}$

CHARGE PER UNIT FORCE.

IF THE CHARGE INDUCED ON A SURFACE IS POSITIVE THEN P_i IS POSITIVE (RECALL THAT, ON AN ATOMIC SCALE DIPOLE MOMENT IS A VECTOR DIRECTED FROM THE (-) CHARGE TO THE (+) CHARGE ALONG THE VECTOR SEPARATING THE CHARGES) IF THE INDUCED DIPOLE MOMENT IS ONE THAT CREATES (+) CHARGE ON A SURFACE THAT MACROSCOPICALLY, A POSITIVE \vec{P} IS ONE THAT IS PARALLEL TO THE INDUCED DIPOLE MOMENTS.

NOTE THAT THE NATURE OF THE RELATION $P_i = d_{ijk} \sigma_{jk}$ SAYS THAT IF P IS, SAY, (+) FOR A GIVEN STATE OF STRESS (i.e. POSITIVE CHARGE ON THE SURFACE OUT OF WHICH \vec{P} IS DIRECTED) THEN REVERSING THE SIGN OF σ (e.g. GOING FROM TENSILE TO COMPRESSIVE) CHANGES THE SIGN OF THE INDUCED SURFACE CHARGE AND THE DIRECTION OF P .

CONVERSION TO MATRIX NOTATION

LET US EXAMINE ONE LINE OF THE TENSOR RELATION BETWEEN P_i AND σ_{jk} . FOR EXAMPLE

$$P_i = d_{i11} \sigma_{11} + d_{i22} \sigma_{22} + d_{i33} \sigma_{33} + d_{i23} \sigma_{23} + d_{i32} \sigma_{32} + d_{i31} \sigma_{31} + d_{i13} \sigma_{13} + d_{i12} \sigma_{12} + d_{i21} \sigma_{21}$$

A FEATURE OF THIS RELATION IS THAT THE SECOND TWO SUBSCRIPTS ON d_{ijk} ALWAYS ACT IN PAIRS. THIS RAISES A QUESTION OF WHETHER WE SHOULD KEEP THIS AWKWARD TENSOR NOTATION.

(THE NOTATION, IN FACT, GROWS INCREASINGLY CUMBERSOME AS THE RANK OF THE TENSOR INCREASES!) WHY DON'T WE SIMPLIFY LIFE BY USING A SINGLE SYMBOL TO REPRESENT THE RELATION BETWEEN POLARIZATION AND STRESS?

TO ANSWER THAT QUESTION — IF WE MOVE TO A TWO-SUBSCRIPT NOTATION WE HAVE LOST THE INDICES ON THE TENSOR ELEMENTS AND NO LONGER HAVE THE INFORMATION NEEDED TO TRANSFORM FROM ONE COORDINATE SYSTEM TO ANOTHER. IN SHORT, WE WILL HAVE A MATRIX RELATION AND NOT A TENSOR EXPRESSION. THIS IS OF SMALL CONCERN TO A DEVICE ENGINEER WHOSE WORK INVOLVES, SAY, WORKING WITH QUARTZ WAFERS THAT ARE CUT IN A PARTICULAR, NEVER-CHANGING CRYSTALLOGRAPHIC ORIENTATION. IF THE NEED ARISES TO REFER THE PROPERTIES TO A DIFFERENT COORDINATE SYSTEM, HOWEVER, WE MUST BE CONSTANTLY PREPARED TO RESUBJECT THE FULL THREE SUBSCRIPT TENSOR NOTATION.

THE NUMBERS THAT DESCRIBE PIEZOELECTRIC BEHAVIOR ARE, HOWEVER, INVARIABLY REPORTED IN MATRIX FORM REFERRED TO REFERENCE AXES WHOSE RELATION TO CRYSTALLOGRAPHIC AXES AND SYMMETRY ELEMENTS IS ESTABLISHED BY NOMENCLATURE COMMITTEES OF RELEVANT PROFESSIONAL SOCIETIES.

THE CONVENTION FOR SWITCHING THE LAST TWO INDICES TO A SINGLE SYMBOL IS EASY TO REMEMBER FROM THE FOLLOWING: TAKE A PATH THROUGH THE STRESS TENSOR AS FOLLOWS:



WITH THIS CONVENTION WE CAN BEGIN TO WRITE TENSOR: $P_i = d_{i11} \sigma_{11} + d_{i22} \sigma_{22} + d_{i33} \sigma_{33} +$ } whoops! NOW WE HAVE A PROBLEM !!
 MATRIX $P_i = d_{i1} \sigma_1 + d_{i2} \sigma_2 + d_{i3} \sigma_3$

WHEN WE ENCOUNTER THE OFF-DIAGONAL ELEMENTS of SHEAR STRESS WE HAVE TWO ELEMENTS THAT CARRY THE SAME TWO SUBSCRIPTS. MOREOVER, WHEN $i \neq j$ $\sigma_{ij} = \sigma_{ji}$ AND YOU CANNOT HAVE ONE WITHOUT THE OTHER IF THE BODY IS IN MECHANICAL EQUILIBRIUM.

THEFORE, ATTEMPTING TO CONTINUE

TENSOR: $P_i = \dots + d_{123} \sigma_{23} + d_{132} \sigma_{32} + d_{131} \sigma_{31} + d_{113} \sigma_{13} + d_{112} \sigma_{12} + d_{121} \sigma_{21}$
 MATRIX: $d_{14} \sigma_4 + d_{14} \sigma_4 + d_{15} \sigma_5 + d_{15} \sigma_5 + d_{16} \sigma_6 + d_{16} \sigma_6$

THIS IS TERRIBLE!! WE CAN'T APPLY A σ_{23} WITHOUT AN EQUAL σ_{32} - SO, HOW ARE WE TO MEASURE d_{123} AND d_{132} INDEPENDENTLY? ARE THEY EQUAL ($d_{123} = d_{132}$)? HOW CAN WE TELL? ARE WE GOING TO HAVE TO MODIFY OUR NOTATION SUCH THAT WE CAN KEEP d_{132} AND d_{123} DISTINGUISHABLE? IF SO, WE ARE BACK TO A 3x9 ARRAY OF ELEMENTS AND THERE IS NO POINT OR GAIN IN GOING FROM TENSOR TO MATRIX NOTATION. IF WE CAN'T MEASURE d_{132} AND d_{123} SEPARATELY, SHALL WE ASSUME THAT THEY ARE EQUAL? WHY NOT, IF WE CAN ONLY EXPERIMENTALLY MEASURE THEIR COMBINATION??

BUT THEN DO WE WRITE

$$d_{123} \sigma_{23} + d_{132} \sigma_{32} \Rightarrow d_{14} \sigma_4 + d_{14} \sigma_4 = 2d_{14} \sigma_4 \quad ??$$

IN OTHER WORDS DO WE SAY $P_i = d_{ij} \sigma_j$ FOR $j = 1, 2, 3$

BUT $P_i = 2d_{ij} \sigma_j$ FOR $j = 4, 5, 6$ FINE MATRIX THAT WOULD BE!!

THERE IS EFFICIENCY IN A MATRIX RELATION, HOWEVER, AND IT IS SENSIBLE TO WRITE $P_i = d_{ij} \sigma_j$ FOR $i = 1, 2, 3$ AND $j = 1, 2, 3$ PLUS $4, 5, 6$

THE ONLY WAY TO DO THIS IS TO ABSORB THE FACTOR OF 2 IN DEFINING THE MATRIX PIEZOELECTRIC MODULI AND SAY $d_{ijk} \equiv d_{ij}$ IF $j = k = 1, 2$ OR 3
 BUT $d_{ijk} + d_{ikj} \equiv d_{ij}$ IF $j = 4, 5, 6$

(THIS PROBLEM OF HIDING A FACTOR 2 GETS PROGRESSIVELY WORSE WITH HIGHER-RANK TENSORS!)

BY GOING TO MATRIX NOTATION WE HAVE GONE FROM $3 \times 9 = 27$ TENSOR ELEMENTS TO $3 \times 6 = 18$ MATRIX ELEMENTS

THE CONVERSE PIEZOELECTRIC EFFECT

THIS IS, SEEMINGLY, A DIFFERENT TYPE OF 3RD RANK TENSOR PROPERTY. IT DESCRIBES THE FACT THAT IF ONE APPLIES AN ELECTRIC FIELD TO A CRYSTAL A STATE OF STRAIN IS INDUCED. THIS IS PERHAPS NOT SURPRISING: IN AN IONIC CRYSTAL AN ELECTRIC FIELD WOULD PULL POSITIVE IONS IN ONE DIRECTION AND ANIONS IN THE OPPOSITE DIRECTION AND THIS IS SURELY NOT UNEXPECTED.

WE COULD WRITE THEREFORE $\epsilon_{ijk} = T_{jk} \epsilon_i$ WHICH WOULD BE A SET

OF NINE EQUATIONS $\xrightarrow{9}$ IN THREE VARIABLES, THE COMPONENTS OF ϵ
 \downarrow THUS A $9 \times 3 = 27$ ELEMENTS IN THE ARRAY

(STILL A THIRD RANK TENSOR - THREE SUBSCRIPTS - AND STILL THE SAME LAW OF TRANSFORMATION)

WHAT IS SURPRISING - VERY SURPRISING, IN FACT, IS THAT THE SAME ARRAY OF COEFFICIENTS SERVE TO DESCRIBE BOTH THE DIRECT AND THE CONVERSE PIEZOELECTRIC EFFECTS!!

TO BE ABLE TO WRITE THE CONVERSE PIEZOELECTRIC EFFECT IN TERMS OF THE PIEZOELECTRIC MODULI, HOWEVER, ONE MUST BEND THE CONVENTIONS FOR SUMMATIONS OVER REPEATED SUBSCRIPTS A LITTLE BIT AND WRITE $\epsilon_{ijk} = d_{jik} \epsilon_i$ (NOTE THE REVERSED ORDER OF THE SUBSCRIPTS.) THIS RELATION COMES

FROM A THERMODYNAMIC ARGUMENT AND NOT FROM TENSOR FORMALISM

THERE IS ONE INTERESTING CONSEQUENCE OF THE CONVERSE PIEZOELECTRIC EFFECT THAT HAS BEARING ON THE AMBIGUITIES THAT WE ENCOUNTERED IN GOING FROM TENSOR TO MATRIX NOTATION IN THE CASE OF THE DIRECT PIEZOELECTRIC EFFECT. WRITING OUT A FEW LINES OF THE EQUATIONS

$$\begin{aligned} \epsilon_{11} &= d_{11} \epsilon_1 + d_{21} \epsilon_2 + d_{31} \epsilon_3 \\ \epsilon_{22} &= d_{12} \epsilon_1 + d_{22} \epsilon_2 + d_{32} \epsilon_3 \\ \epsilon_{33} &= d_{13} \epsilon_1 + d_{23} \epsilon_2 + d_{33} \epsilon_3 \\ &\vdots \\ \epsilon_{23} &= d_{123} \epsilon_1 + d_{223} \epsilon_2 + d_{323} \epsilon_3 \\ \epsilon_{32} &= d_{132} \epsilon_1 + d_{232} \epsilon_2 + d_{332} \epsilon_3 \end{aligned}$$

THESE THREE EQUATIONS GIVE AN ANSWER TO A QUESTION THAT WE HAVE NOT YET ASKED: CAN APPLICATION OF AN ELECTRIC FIELD CAUSE A VOLUME CHANGE? $\epsilon_{11} + \epsilon_{22} + \epsilon_{33} = \text{TRACE of the STRAIN TENSOR} = \Delta V$ IF THE TERMS ON THE RIGHT ARE ZERO FOR ANY ϵ_i THERE CAN BE NO VOLUME CHANGE!!

BUT $\epsilon_{23} = \epsilon_{32}$ BY DEFINITION OF THE STRAIN TENSOR!

IF WE WERE TO APPLY AN ELECTRIC FIELD WITH ONLY AN ϵ_1 COMPONENT

$$\left. \begin{aligned} \epsilon_{23} &= d_{123} \epsilon_1 \\ \epsilon_{32} &= d_{132} \epsilon_1 \end{aligned} \right\} \text{ BUT } \epsilon_{23} = \epsilon_{32} \therefore d_{123} = d_{132} \text{ THEREFORE, ALTHOUGH}$$

WE COULD NOT MEASURE d_{ijk} AND d_{ikj} INDIVIDUALLY ON THE BASIS OF THE DIRECT PIEZOELECTRIC EFFECT WE CAN DO SO IN THE CONVERSE PIEZOELECTRIC EFFECT. THUS $d_{ijk} = d_{ikj}$

UNFORTUNATELY, THE NASTY FACTOR OF 2 THAT WE ENCOUNTERED IN THE DIRECT PIEZOELECTRIC EFFECT NOW REAPPEARS TO CAUSE TROUBLE AGAIN. WE HAD WRITTEN

$$P_i = d_{ij} \sigma_j \text{ IN MATRIX FORM. IN ORDER TO DO SO WE HAD TO ASSURE}$$

A FACTOR OF TWO WHEN WE WROTE, FOR EXAMPLE,

$$\begin{aligned} P_1 &= \dots + d_{123} \sigma_3 + d_{132} \sigma_2 + d_{131} \sigma_1 + d_{113} \sigma_3 + d_{121} \sigma_2 + d_{112} \sigma_1 \\ &= d_{123} \sigma_4 + d_{132} \sigma_4 + d_{131} \sigma_5 + d_{113} \sigma_5 + d_{121} \sigma_6 + d_{112} \sigma_6 \\ &= (d_{123} + d_{132}) \sigma_4 + (d_{131} + d_{113}) \sigma_5 + (d_{121} + d_{112}) \sigma_6 \end{aligned}$$

WE OBSERVED THAT WE COULD NOT APPLY A σ_{32} WITHOUT APPLYING AN IDENTICAL σ_{23} AND SO IT SEEMED THAT WE COULDN'T MEASURE d_{123} AND d_{132} INDIVIDUALLY. IT THEREFORE SEEMED REASONABLE TO WMP THEM TOGETHER INTO A SINGLE MATRIX ELEMENT.

WE NOW KNOW THAT $d_{123} = d_{132}$ AS A RESULT OF THE CONVERSE PIEZOELECTRIC EFFECT! WE CAN THEREFORE WRITE

$$P_1 = \dots + 2d_{123} \sigma_4 + 2d_{113} \sigma_5 + 2d_{112} \sigma_6$$

AND THEN DEFINED $d_{14} \sigma_4 + d_{15} \sigma_5 + d_{16} \sigma_6$

THEREFORE $\begin{cases} d_{123} = d_{132} = \frac{1}{2} d_{14} \\ d_{113} = d_{131} = \frac{1}{2} d_{15} \\ d_{112} = d_{121} = \frac{1}{2} d_{16} \end{cases}$

NOW WE ENCOUNTER TROUBLE! IF WE NOW ATTEMPT TO WRITE THE CONVERSE EFFECT IN MATRIX FORM

$$\begin{aligned} \epsilon_{23} &= d_{123} \epsilon_1 + d_{223} \epsilon_2 + d_{323} \epsilon_3 \\ \epsilon_{32} &= \frac{1}{2} d_{14} \epsilon_1 + \frac{1}{2} d_{24} \epsilon_2 + \frac{1}{2} d_{34} \epsilon_3 \end{aligned}$$

AND NOW WE CANNOT WRITE A MATRIX RELATION WITHOUT SOME TERMS HAVING A FACTOR $\frac{1}{2}$ AND SOME NOT! WE MUST HIDE THE FACTOR 2 SOMEPLACE ELSE AND THE ONLY PLACE LEFT IS IN THE DEFINITION OF MATRIX STRAIN

WE ARE THUS FORCED TO WRITE

$$\begin{bmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} \\ \epsilon_{21} & \epsilon_{22} & \epsilon_{23} \\ \epsilon_{31} & \epsilon_{32} & \epsilon_{33} \end{bmatrix} \rightarrow \begin{bmatrix} \epsilon_1 & \frac{1}{2}\epsilon_6 & \frac{1}{2}\epsilon_5 \\ \frac{1}{2}\epsilon_6 & \epsilon_2 & \frac{1}{2}\epsilon_4 \\ \frac{1}{2}\epsilon_5 & \frac{1}{2}\epsilon_4 & \epsilon_3 \end{bmatrix}$$

SYMMETRY RESTRICTIONS ON PIEZOELECTRIC MODULI (d_{ij})

WE HAVE BECOME FAMILIAR WITH THE PROCEDURE FOR DERIVING THESE CONSTRAINTS IN CONSIDERING SECOND RANK TENSORS. THE PROCESS IS EXACTLY ANALOGOUS FOR THIRD-RANK TENSORS EXCEPT THAT WE MUST, FIRST, CONVERT FROM MATRIX FORM TO TENSOR FORM IN ORDER TO HAVE ALL THREE PROPER SUBSCRIPTS FOR d_{ijk} . AND, SECOND, THERE ARE MORE DIRECTION COSINES IN THE SUMMATION FOR THE TRANSFORMED ELEMENT ($d'_{ijk} = C_{i\alpha} C_{j\beta} C_{k\gamma} d_{\alpha\beta\gamma}$) AND THERE ARE A GREAT MANY ELEMENTS TO BE TRANSFORMED AND A GREAT MANY MORE TERMS IN EACH SUMMATION.

LET'S PERFORM A TRANSFORMATION FOR TWO ELEMENTS JUST TO REMIND OURSELVES HOW IT WORKS

(a) d_{13} IN A MONOCLINIC CRYSTAL WITH SYMMETRY 2 (ORIENTED ALONG x_3)

$d_{13} \equiv d_{133}$ USING THE METHOD OF DIRECT INSPECTION $x_1, x_2, x_3 \rightarrow -x_1, -x_2, x_3$

$$\frac{d_{ijk}}{d_{133}} \frac{x_i x_j x_k}{x_1 x_2 x_3} = \frac{x'_i x'_j x'_k}{x'_1 x'_2 x'_3} = \frac{d'_{ijk}}{d_{133}} = +d_{133} = 0$$

IF TENSOR IS TO STAY INVARIANT

$\therefore d_{133} = 0$

(b) d_{13} IN A MONOCLINIC CRYSTAL WITH SYMMETRY M (ORIENTED $\perp x_3$)

$d_{13} \equiv d_{133}$

TRANSFORMATION OF AXES IS $x_1, x_2, x_3 \rightarrow x_1, x_2, -x_3$

$$\frac{d_{ijk}}{d_{133}} \frac{x_i x_j x_k}{x_1 x_2 x_3} = \frac{x'_i x'_j x'_k}{x'_1 x'_2 x'_3} = x_1 x_2 (-x_3) = -d_{133} \equiv d_{133} \text{ NO CONSTRAINT}$$

NOTICE THAT CRYSTALS OF SYMMETRY 2 AND M ARE BOTH MONOCLINIC AND YET THE CONSTRAINTS ON d_{133} ARE QUITE DIFFERENT (UNLIKE EVEN-RANK TENSORS FOR WHICH ALL MONOCLINIC CRYSTALS MUST DISPLAY THE SAME CONSTRAINTS)

SYMMETRY RESTRICTIONS ON PIEZOELECTRIC MODULI (d_{ij})

CENTROSYMMETRIC SYMMETRY: All $d_{ij} \equiv 0$

($T, 2/m, 2/m 2/m 2/m, 4/m, 4/m 2/m 2/m, \bar{3}, \bar{3} 2/m, 6/m, 6/m 2/m 2/m, 2/m \bar{3}, 2/m \bar{3} 2/m$)

TRICLINIC (1)

$d_{11} \ d_{12} \ d_{13} \ d_{14} \ d_{15} \ d_{16}$

$d_{21} \ d_{22} \ d_{23} \ d_{24} \ d_{25} \ d_{26}$

$d_{31} \ d_{32} \ d_{33} \ d_{34} \ d_{35} \ d_{36}$

(18)

MONOCLINIC 2 (11 x_3)

$0 \ 0 \ 0 \ d_{14} \ d_{15} \ 0$

$0 \ 0 \ 0 \ d_{24} \ d_{25} \ 0$

$d_{31} \ d_{32} \ d_{33} \ 0 \ 0 \ d_{36}$

(8)

m (1 x_3)

$d_{11} \ d_{12} \ d_{13} \ 0 \ 0 \ d_{16}$

$d_{21} \ d_{22} \ d_{23} \ 0 \ 0 \ d_{26}$

$0 \ 0 \ 0 \ d_{34} \ d_{35} \ 0$

(10)

ORTHORHOMBIC

222 ($11x_1, x_2, x_3$)

$$\begin{array}{ccccccc}
 0 & 0 & 0 & d_{14} & 0 & 0 & \\
 0 & 0 & 0 & 0 & d_{15} & 0 & \textcircled{3} \\
 0 & 0 & 0 & 0 & 0 & d_{36} &
 \end{array}$$

2mm ($211x_3$)

$$\begin{array}{ccccccc}
 0 & 0 & 0 & 0 & d_{15} & 0 & \\
 0 & 0 & 0 & d_{24} & 0 & 0 & \textcircled{5} \\
 d_{31} & d_{32} & d_{33} & 0 & 0 & 0 &
 \end{array}$$

TETRAAGONAL

4 ($11x_3$)

$$\begin{array}{ccccccc}
 0 & 0 & 0 & d_{14} & d_{15} & 0 & \\
 0 & 0 & 0 & d_{15} & -d_{14} & 0 & \textcircled{4} \\
 d_{31} & d_{31} & d_{33} & 0 & 0 & 0 &
 \end{array}$$

4

$$\begin{array}{ccccccc}
 0 & 0 & 0 & d_{14} & d_{15} & 0 & \\
 0 & 0 & 0 & -d_{15} & d_{14} & 0 & \textcircled{4} \\
 d_{31} & -d_{31} & 0 & 0 & 0 & d_{16} &
 \end{array}$$

422 ($411x_3$)

$$\begin{array}{ccccccc}
 0 & 0 & 0 & d_{14} & 0 & 0 & \\
 0 & 0 & 0 & 0 & -d_{14} & 0 & \textcircled{1} \\
 0 & 0 & 0 & 0 & 0 & 0 &
 \end{array}$$

4mm ($411x_3$)

$$\begin{array}{ccccccc}
 0 & 0 & 0 & 0 & d_{15} & 0 & \\
 0 & 0 & 0 & d_{15} & 0 & 0 & \textcircled{3} \\
 d_{31} & d_{31} & d_{33} & 0 & 0 & 0 &
 \end{array}$$

42m ($411x_3, 211x_1$)

$$\begin{array}{ccccccc}
 0 & 0 & 0 & d_{14} & 0 & 0 & \\
 0 & 0 & 0 & 0 & d_{14} & 0 & \textcircled{2} \\
 0 & 0 & 0 & 0 & 0 & d_{36} &
 \end{array}$$

CUBIC

432

$$\begin{array}{ccccccc}
 0 & 0 & 0 & 0 & 0 & 0 & \textcircled{0} \\
 0 & 0 & 0 & 0 & 0 & 0 & \\
 0 & 0 & 0 & 0 & 0 & 0 & \\
 \text{All moduli ARE ZERO!} & & & & & &
 \end{array}$$

43m AND 23

$$\begin{array}{ccccccc}
 0 & 0 & 0 & d_{14} & 0 & 0 & \\
 0 & 0 & 0 & 0 & d_{14} & 0 & \textcircled{1} \\
 0 & 0 & 0 & 0 & 0 & d_{14} &
 \end{array}$$

HEXAGONAL

3 (1x3)

$$\begin{matrix} d_{11} & -d_{11} & 0 & d_{14} & d_{15} & +2d_{21} \\ d_{21} & -d_{21} & 0 & d_{15} & -d_{14} & -2d_{11} \\ d_{31} & d_{31} & d_{33} & 0 & 0 & 0 \end{matrix} \quad (6)$$

32 (3x3, 2x1)

$$\begin{matrix} d_{11} & -d_{11} & 0 & d_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -d_{14} & -2d_{11} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{matrix} \quad (2)$$

3M (3x3, m1x1)

$$\begin{matrix} 0 & 0 & 0 & 0 & d_{15} & 2d_{21} \\ d_{21} & -d_{21} & 0 & d_{15} & 0 & 0 \\ d_{31} & d_{31} & d_{33} & 0 & 0 & 0 \end{matrix} \quad (4)$$

6

$$\begin{matrix} 0 & 0 & 0 & d_{14} & d_{15} & 0 \\ 0 & 0 & 0 & d_{15} & -d_{14} & 0 \\ d_{31} & d_{31} & d_{33} & 0 & 0 & 0 \end{matrix} \quad (4)$$

SAME AS FOR 4

6MM

$$\begin{matrix} 0 & 0 & 0 & 0 & d_{15} & 0 \\ 0 & 0 & 0 & d_{15} & 0 & 0 \\ d_{31} & d_{31} & d_{33} & 0 & 0 & 0 \end{matrix} \quad (3)$$

SAME RESULT AS FOR 4MM

622

$$\begin{matrix} 0 & 0 & 0 & d_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -d_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{matrix} \quad (1)$$

SAME RESULT AS FOR 422

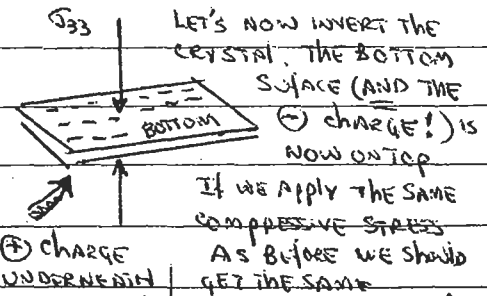
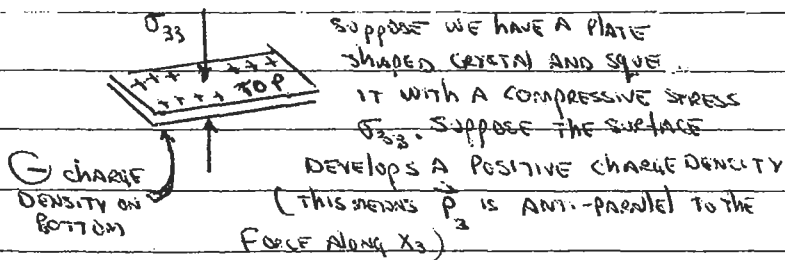
6 = 3/m

$$\begin{matrix} d_{11} & -d_{11} & 0 & 0 & 0 & 2d_{21} \\ d_{21} & -d_{21} & 0 & 0 & 0 & -2d_{11} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{matrix} \quad (2)$$

6m2 (m1x1)

$$\begin{matrix} 0 & 0 & 0 & 0 & 0 & 2d_{21} \\ d_{21} & -d_{21} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{matrix} \quad (1)$$

THE REASON FOR SOME OF THE ABOVE CONSTRAINTS CAN BE UNDERSTOOD FROM A SIMPLE PHYSICAL ARGUMENT. FOR EXAMPLE, IF A CRYSTAL POSSESSES INVERSION SYMMETRY IT CANNOT BE PIEZOELECTRIC (ALL $d_{ij} \equiv 0$)



Result as before if the crystal is left unchanged by inversion. But the polarity of the charge is changed and has not remained invariant. The result is impossible.

OTHER PIEZOELECTRIC EFFECTS

THERE ARE TWO OTHER PIEZOELECTRIC EFFECTS THAT WE CAN MENTION. THEY ARE NOT DIGNIFIED WITH SPECIAL NAMES OF A SPECIFIC "EFFECT".

IF WE APPLY A STRESS TO INDUCE A POLARIZATION (THE "DIRECT PIEZOELECTRIC EFFECT") WE WILL ALSO INDUCE A STRAIN AS A CONSEQUENCE OF THAT STRESS. THEREFORE, WE COULD WRITE A RELATION BETWEEN INDUCED POLARIZATION AND STRAIN

$$P_i = e_{ijk} \epsilon_{jk}$$

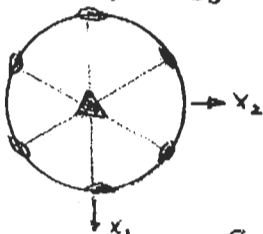
SIMILARLY, IN THE CONVERSE PIEZOELECTRIC EFFECT, IF AN ELECTRIC FIELD INDUCES A STATE OF STRAIN, THE MATERIAL MUST ALSO BE UNDER STRESS AND

$$\sigma_{ij} = -e_{ijk} \epsilon_i \quad \text{NOTE, AGAIN THE TRANSPOSED ORDER OF SUBSCRIPTS}$$

RELATIVE TO CONVENTION IN TENSOR NOTATION, THE RELATIONSHIP BETWEEN e_{ijk} AND $-e_{ijr}$ AGAIN FOLLOWS FROM THERMODYNAMIC PRINCIPLES AND NOT FROM SYMMETRY REQUIREMENTS.

EXAMPLES OF PIEZOELECTRIC MATERIALS

① QUARTZ (SiO_2) POINT GROUP 32



THE "STANDARD" REFERENCE AXES ARE AS SHOWN. THE MATRIX OF PIEZOELECTRIC MODULI IS

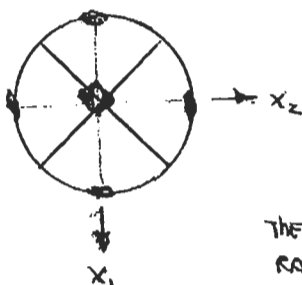
$$d_{ij} = \begin{bmatrix} -2.3 & 2.3 & 0 & -0.67 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.67 & 4.6 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \times 10^{-12} \text{ COUL/NEWTON}$$

QUARTZ IS NOT AN ESPECIALLY STRONG PIEZOELECTRIC MATERIAL.

SUPPOSE WE APPLY A FIELD OF 100 VOLTS/CM = 10^4 V/M ALONG THE 2-FOLD AXIS DIRECTED ALONG x_1 . THEN, FROM THE CONVERSE PIEZOELECTRIC EFFECT $\epsilon_1 = d_{11} \epsilon_1 = -2.3 \cdot 10^{-12} \cdot 10^4 = -2.3 \cdot 10^{-8}$ NOT A VERY LARGE STRAIN!

WHAT MAKES QUARTZ USEFUL AS A PIEZOELECTRIC MATERIAL IS ITS LOW COST, CHEMICAL STABILITY, AND VERY GOOD MECHANICAL PROPERTY. A MATERIAL THAT WILL EARN ITS LIVING BEING SQUEEZED CANNOT BE SOFT AND EASILY DEFORMED!

② AMMONIUM DIHYDROGEN PHOSPHATE (ADP) POINT GROUP $\bar{4}2m$



$$d_{ij} = \begin{bmatrix} 0 & 0 & 0 & 1.7 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.7 & 0 \\ 0 & 0 & 0 & 0 & 0 & 51.7 \end{bmatrix} 10^{-12} \text{ COUL/NEWTON}$$

NOTE THE VERY LARGE VALUE OF d_{33} - MORE THAN 10 TIMES THE LARGEST MODULUS IN QUARTZ. THE MATERIAL, UNFORTUNATELY, IS RATHER SOFT AND IS ATTACKED BY MOISTURE.

there is an exciting new family of piezoelectric materials that has been discovered very recently. they are perovskite-related ceramics that have piezoelectric moduli over an order of magnitude larger than anything previously known. $0.955 \text{ Pb}(2\text{Ni}_3\text{Nb}_3\text{O}_3 - 0.95 \text{ PbTiO}_3$ has $d_{33} > 2000 \text{ pC/newton}$. [for literature see J. Yin, B. Jiang and W. Cao, IEEE Trans. on Ultrasonics, Ferroelectrics and Frequency Control 47 [1] JAN 2000, 285-291.]

some of these materials have shown strains up to 0.85% !!!

$\rho = \rho_{CO} = 10^{-12}$ STATED ANOTHER WAY, $2000 \cdot 10^{12} \text{ Coulomb/newton}$ is $10^3 \times d_{11}$ for quartz!

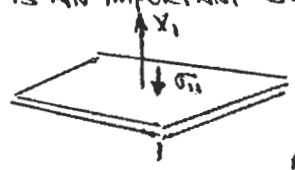
REPRESENTATION SURFACES

unfortunately, it is not possible to create any representation surface (such as the representation quadric for second-rank tensors) that gives a view of how higher-rank tensor properties. consider the converse piezoelectric effect. we apply an electric field in a given direction (that part is easy! we handled that question for second rank tensor properties!) but then what results is a strain - a tensor! how do we represent that as a function of the direction of \vec{E} ? there are six independent elements of strain!! should we try to visualize simultaneously six different representation quadrics? this is hardly useful!

what we can do, however, is to apply a vector or something like a uniaxial stress that is specialized but for which "direction" is unambiguously specified. we then examine - perhaps through a sample of specialized geometry such as a rod or plate - one of the components of the generalized displacement we can then ask how this component of displacement varies with the direction of the generalized force or some component thereof.

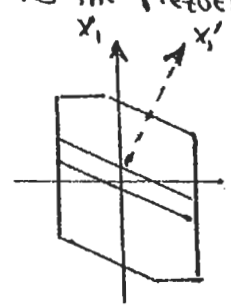
THE LONGITUDINAL PIEZOELECTRIC EFFECT

this is an important scalar modulus. we cut a very thin plate of the material. define its normal as the direction of x_1 . we then apply a uniaxial stress σ_1 along x_1 . this will, in general create a polarization \vec{P} in a general orientation. surface



charge density will thus be induced on all surfaces of the plate but, as the surface normal to x_1 is much larger in area than the very thin areas parallel to x_1 , most of the total charge on the plate will be due to the charge density on the large surface normal to x_1 . the geometry of the plate, therefore, means that upon applying a compressive stress σ_1 , we measure the polarization component P_1 . the quantity relating the two variables is defined as the longitudinal piezoelectric modulus and it is obviously the same quantity as the piezoelectric modulus d_{11}

$$P_1 = d \sigma_1 = d_{11} \sigma_1$$



we can now ask the following question: if I were to cut a similar plate from the crystal with its normal in a different direction, along x_1' , say, how will the longitudinal piezoelectric modulus change? we would apply a similar compressive stress along x_1' so this would be σ_1' and measure the component P_1' along x_1'

THE EXPERIMENT WOULD BE

$$P_i' = d_{ij}' \sigma_j'$$

WE ARE ASKING, THEREFORE, FOR THE VALUE OF d_{ij}' AS A FUNCTION OF THE ORIENTATION OF X_1' , THE NORMAL TO THE PLATE.

THE WAY ONE SOLVES THIS PROBLEM IS THE SAME FOR ALL SCALAR MODULI THAT REPRESENT BEHAVIOR OF HIGHER-RANK TENSOR PROPERTIES:

- (1) CONVERT THE MATRIX ELEMENTS TO PROPER TENSOR SUBSCRIPTS AND REMOVE FACTORS OF 2
- (2) REPLACE THE SUBSCRIPTS ON ANY ELEMENT THAT WE HAVE WRITTEN INCORRECTLY TO EMPHASIZE AN EQUALITY
- (3) PERFORM THE TRANSFORMATION OF THE TENSOR ELEMENT USING $d_{ijk}' = C_{i2} C_{jm} C_{kn} d_{lmn}$
- (4) RESTORE THE EQUALITIES BETWEEN ELEMENTS
- (5) COLLAPSE THE SUBSCRIPTS BACK TO MATRIX FORM.

FOR THE LONGITUDINAL PIEZOELECTRIC MODULUS

$$d_{111} = d_{111} \text{ IN TENSOR NOTATION}$$

$$\text{AND THE CHANGE WE ARE MAKING IS TO A } d_{111}' = C_{i2} C_{jm} C_{kn} d_{lmn}$$

THE DIRECTION COSINES INVOLVED ARE SIMPLY THE DIRECTION COSINES OF X_1' (WE DON'T CARE ANYTHING ABOUT X_2' AND X_3' AND DON'T NEED THEM!) LET US THEREFORE REPLACE $C_{i2} C_{jm} C_{kn}$ BY MERELY THE DIRECTION COSINES OF THE SINGLE DIRECTION, X_1' WITH WHICH WE ARE CONCERNED AND CHANGE $C_{i2} C_{jm} C_{kn} \rightarrow l_2 l_m l_n$.

$$\text{SO } d_{111}' = d_{111} = l_2 l_m l_n d_{lmn}$$

LET'S DO THIS SUMMATION FOR QUARTZ, POINT GROUP 32

THE FORM OF THE PIEZOELECTRIC MODULUS TENSOR IS

$$d_{ij}' = \begin{bmatrix} d_{11} & -d_{11} & 0 & d_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -d_{14} & -2d_{11} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

BUT THE PROPER FORM OF THE MATRIX WITHOUT EQUALITIES INSERTED IS

$$\begin{bmatrix} d_{11} & d_{12} & 0 & d_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & d_{25} & d_{26} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \text{ WHERE } \begin{cases} d_{22} = -d_{11} \\ d_{25} = -d_{14} \\ d_{26} = -2d_{11} \end{cases}$$

CONVERTING TO A TENSOR (AND MERELY EXTRACTING THE NON-ZERO ELEMENTS

$$d_{111} \quad d_{122} \quad \underbrace{d_{123} \quad d_{132}}_{\text{NOTE THAT } d_{14} \text{ IS THE SUM OF TWO MATRIX ELEMENTS}} \quad \underbrace{d_{213} \quad d_{231}} \quad \underbrace{d_{212} \quad d_{221}}$$

PERFORMING THE TRANSFORMATION

$$\begin{aligned} d_{111}' &= l_1 l_1 l_1 d_{111} + l_1 l_2 l_2 d_{122} + l_1 l_2 l_3 d_{123} + l_1 l_3 l_2 d_{132} \\ &\quad + l_2 l_1 l_3 d_{213} + l_2 l_3 l_1 d_{231} + l_2 l_1 l_2 d_{212} + l_2 l_2 l_1 d_{221} \\ &= l_1^3 d_{111} + l_1 l_2^2 (d_{122} + d_{212} + d_{221}) + l_1 l_2 l_3 (d_{213} + d_{231} + d_{123} + d_{132}) \end{aligned}$$

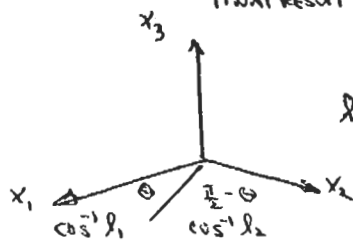
RESTORING MATRIX NOTATION

$$d_{111}' = l_1^3 d_{11} + l_1 l_2^2 (d_{12} + d_{26}) + l_1 l_2 l_3 (d_{25} + d_{14})$$

INSERTING THE EQUALITIES BETWEEN ELEMENTS

$$\begin{aligned} d_{111}' &= l_1^3 d_{11} + l_1 l_2^2 [-d_{11} + (-2d_{11})] + l_1 l_2 l_3 (\cancel{-d_{14}} + \cancel{d_{14}}) \\ &= (l_1^3 - 3 l_1 l_2^2) d_{11} \end{aligned}$$

Final result is $d = d'_{111} = (\rho_1^3 - 3\rho_1\rho_2^2) d_{11}$ ρ_3 DOES NOT APPEAR!



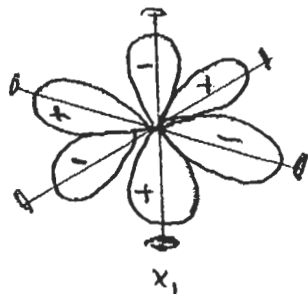
Let $\rho_1 = \cos \theta$
 $\rho_2 = \sin \theta$

THE x_1, x_2 PLANE

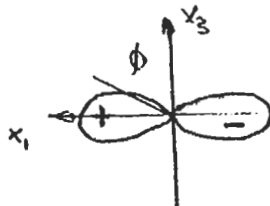
$$d = d_{11} \cos \theta (\cos^2 \theta - 3\sin^2 \theta)$$

THIS IS A "WELL KNOWN" (?) IDENTITY

$$d = d_{11} \cos 3\theta$$



NOTE THAT THE SURFACE CONFORMS TO SYMMETRY 3C!



IN x_1, x_3 PLANE

$$d'_{111} = \rho_1^3 d_{11}$$

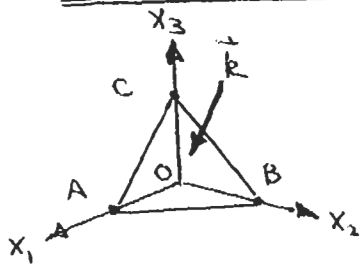
$$d'_{111} = d_{11} \cos^3 \phi$$

THIS IS A UNIVERSAL SURFACE FOR 3RD RANK PROPERTIES FOR SYMMETRY 3C!



3.60 Symmetry, Structure and Tensor Properties of Materials

THE STRESS TENSOR



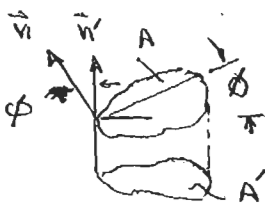
CONSIDER A FORCE-DENSITY VECTOR \vec{k} (FORCE PER UNIT AREA) ACTING ON THE EXTERNAL SURFACE ABC OF A VOLUME ELEMENT OABC. WE ASSUME THIS VOLUME ELEMENT IS IN EQUILIBRIUM (NO LINEAR OR ANGULAR ACCELERATION) THE EXTERNAL FORCE DENSITY \vec{k} THAT PUSHES ON THE SOLID MUST, THEREFORE, BE BALANCED BY THE MATERIAL INSIDE THE VOLUME ELEMENT PUSHING BACK AGAINST THE FORCE.

LET US SET UP RELATIONS THAT BALANCE EXTERNAL AND INTERNAL FORCES IN THE x_1, x_2, x_3 DIRECTIONS AS $\vec{k} = k_1, k_2, k_3$ IS A FORCE DENSITY, WE MUST MULTIPLY BY AN AREA TO GET FORCE.

ALONG x_1 $k_1 \cdot \text{AREA ABC} = \sigma_{11} \cdot \text{AREA BOC} + \sigma_{12} \cdot \text{AREA AOC} + \sigma_{13} \cdot \text{AREA AOB}$

(x_2 is \perp AOC)

WE HAVE PUT IN QUANTITIES σ , FORCES PER UNIT AREA, WITH TWO SUBSCRIPTS. THE FIRST IS THE DIRECTION IN WHICH THE FORCE DENSITY ACTS, THE SECOND SPECIFIES THE NORMAL TO THE INTERNAL SURFACE ON WHICH THE FORCE DENSITY ACTS. THUS σ_{ij} IS THE FORCE PER UNIT AREA ACTING ALONG x_i ON AN INTERNAL SURFACE WHOSE NORMAL IS x_j .



LET US DIVIDE THROUGH BY AREA ABC

$$k_1 = \sigma_{11} \frac{\text{AREA BOC}}{\text{AREA ABC}} + \sigma_{12} \frac{\text{AREA AOC}}{\text{AREA ABC}} + \sigma_{13} \frac{\text{AREA AOB}}{\text{AREA ABC}}$$

IF WE HAVE AN AREA A IN ONE PLANE AND PROJECT IT ONTO A SURFACE IN A PLANE THAT MAKES AN ANGLE ϕ WITH RESPECT TO THE FIRST, THE NEW AREA $A' = A \cos \phi$

NOTE THAT ϕ IS THE SAME THING AS THE ANGLE BETWEEN THE NORMAL TO THE ORIGINAL SURFACE \vec{n} AND THE NORMAL TO THE NEW SURFACE \vec{n}' . LOOKING AT OUR EQUATION FOR k_1 , ABOVE

$\frac{\text{AREA BOC}}{\text{AREA ABC}} = \cos$ of ANGLE BETWEEN THE NORMAL TO THE SURFACE ABC AND THE NORMAL TO BOC, WHICH IS x_1 — AND, THE COSINE OF THE ANGLE BETWEEN ANY VECTOR AND x_1 IS DEFINED AS THE DIRECTION COSINE OF THAT VECTOR

$\therefore \frac{\text{AREA BOC}}{\text{AREA ABC}} = l_1$ A DIRECTION COSINE OF THE NORMAL TO THE SURFACE ABC

Similarly $\frac{\text{AREA AOC}}{\text{AREA ABC}} = l_2$ $\frac{\text{AREA AOB}}{\text{AREA ABC}} = l_3$

IT FOLLOWS THAT THE REMAINING EQUATIONS, BALANCING FORCES IN THE x_2 AND x_3 DIRECTIONS

ARE

$$\begin{cases} k_1 = \sigma_{11} l_1 + \sigma_{12} l_2 + \sigma_{13} l_3 \\ k_2 = \sigma_{21} l_1 + \sigma_{22} l_2 + \sigma_{23} l_3 \\ k_3 = \sigma_{31} l_1 + \sigma_{32} l_2 + \sigma_{33} l_3 \\ k_i = \sigma_{ij} l_j \end{cases}$$

THE NINE COEFFICIENTS σ_{ij} ARE CALLED THE ELEMENTS OF STRESS

$\vec{k} = k_1, k_2, k_3$ IS A VECTOR. WE KNOW THE LAW FOR TRANSFORMATION OF A VECTOR UPON CHANGE OF COORDINATE SYSTEM)

SPECIFIED BY $x'_i = C_{ij} x_j$. NAMELY $k'_i = C_{ij} k_j$

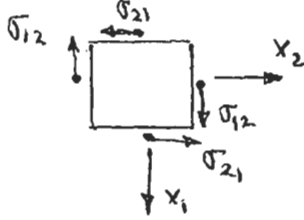
THE ELEMENTS l_j CONSTITUTE A VECTOR — THIS IS \vec{n} A UNIT VECTOR NORMAL TO THE EXTERNAL SURFACE ABC. THE COMPONENTS $n'_i = l'_i$; THUS BECOME $l'_i = C_{ij} l_j$

THE COEFFICIENTS σ_{ij} MUST TRANSFORM LIKE A TENSOR AND, ACCORDINGLY, σ_{ij} IS A TENSOR

THE SIGN OF AN ELEMENT OF STRESS CAN BE + OR - , WE DEFINE THE FOLLOWING CONVENTION
 A POSITIVE ELEMENT OF STRESS σ_{ij} IS WHEN THE MATERIAL OUTSIDE THE VOLUME ELEMENT ACTS ON THE MATERIAL INSIDE THE VOLUME ELEMENT TO PRODUCE A FORCE PER UNIT AREA IN THE $+x_i$ DIRECTION ON A SURFACE WHOSE NORMAL IS $+x_j$ (OR $-x_i$ AND $-x_j$)

IF THE SOLID IS IN EQUILIBRIUM THE STRESS TENSOR MUST BE SYMMETRIC

CONSIDER THE ELEMENTS OF STRESS σ_{12} AND σ_{21}



σ_{12} AND THE SAME σ_{12} ON THE OPPOSITE SIDE OF THE VOLUME ELEMENT CREATE A COUPLE THAT WOULD ACT TO PRODUCE AN ANGULAR ACCELERATION. σ_{21} IS THE ONLY COUPLE THAT CAN BALANCE σ_{12} .

$\therefore \sigma_{12} = \sigma_{21}$ AND $\boxed{\sigma_{ij} = \sigma_{ji}}$ FOR EQUILIBRIUM.

AS STRESS IS A SECOND-RANK TENSOR, WE CAN DEFINE A STRESS QUADRIC

$\boxed{\sigma_{ij} x_i x_j = 1}$

EVERYTHING THAT WE HAVE SAID ABOUT THE REPRESENTATION QUADRIC APPLIES TO THE STRESS QUADRIC.

(a) REFERENCE AXES CAN BE CHANGED $x_1, x_2, x_3 \rightarrow x'_1, x'_2, x'_3$ TO PLACE THE TENSOR IN A DIAGONAL FORM

(b) USING $\sigma_{ij} l_i l_j = \sigma$ WE CAN COMPUTE THE VALUE OF STRESS IN A PARTICULAR DIRECTION.

WE'LL HAVE TO THINK A MOMENT TO SEE WHAT THAT MEANS! THE "APPLIED VECTOR" IN $k_i = \sigma_{ij} l_j$ IS THE SET OF DIRECTION COSINES OF THE NORMAL TO THE SURFACE. THE

"GENERALIZED DISPLACEMENT" IS \vec{k} THE IMPOSED FORCE DENSITY.

WHAT $\sigma_{ij} l_i l_j$ PROVIDES IS $\frac{k_{11}}{\text{UNIT NORMAL}} = \frac{k_{11}}{|n|} = k_{11}$ THIS IS THE FORCE PER UNIT AREA

THAT IS PARALLEL TO THE NORMAL TO THE SURFACE THAT IS TRANSMITTED ACROSS THIS SURFACE

IN OTHER WORDS THE TENSILE COMPONENT OF THE TRANSMITTED STRESS.

(c) SOME SPECIAL FORMS OF THE STRESS TENSOR WHEN IN DIAGONAL FORM

$\begin{bmatrix} \sigma & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$

UNIAXIAL STRESS

$\begin{bmatrix} \sigma_{11} & 0 & 0 \\ 0 & \sigma_{22} & 0 \\ 0 & 0 & 0 \end{bmatrix}$

BIAXIAL STRESS

$\begin{bmatrix} \sigma_{11} & 0 & 0 \\ 0 & \sigma_{22} & 0 \\ 0 & 0 & \sigma_{33} \end{bmatrix}$

TRIAxIAL STRESS

$\begin{bmatrix} -p & 0 & 0 \\ 0 & -p & 0 \\ 0 & 0 & -p \end{bmatrix}$

HYDROSTATIC PRESSURE

$\begin{bmatrix} \sigma & 0 & 0 \\ 0 & -\sigma & 0 \\ 0 & 0 & 0 \end{bmatrix}$

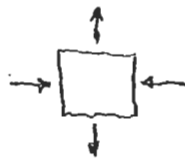
SHEAR STRESS

ROTATE AXES
45°

$\begin{bmatrix} 0 & \sigma' & 0 \\ \sigma' & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$

NOTE:

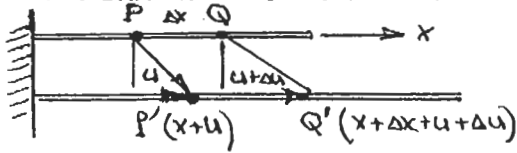
$\sigma' \neq \sigma$



STRESS IS A FIELD TENSOR NOT A PROPERTY TENSOR!

STRAIN

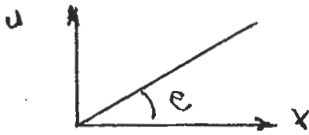
LET US INTRODUCE THE CONCEPT OF STRAIN WITH A ONE-DIMENSIONAL EXAMPLE. LET US CONSIDER AN ELASTIC BAND ATTACHED TO A WALL.



IF WE EXERT A FORCE ON THE ELASTIC BAND, POINT P AT LOCATION x BEFORE THE DEFORMATION, UNDERGOES A DISPLACEMENT u TO POINT P' AT $(x+u)$

A POINT Q AT DISTANCE Δx FROM P IS ALSO DISPLACED: IT MOVES A DISTANCE $u + \Delta u$ AND IS THUS DISPLACED TO $Q'(x + \Delta x + u + \Delta u)$

IF WE PLOT u AS A FUNCTION OF DISTANCE ALONG THE ELASTIC BAND WE FIND THAT u WILL INCREASE LINEARLY WITH x . THIS IS TERMED HOMOGENEOUS DEFORMATION THE SLOPE OF THE PLOT IS LINEAR AND $\frac{\partial u}{\partial x} = e$



LET'S RETURN TO OUR POINTS P & Q . IT IS NOT DISPLACEMENT THAT

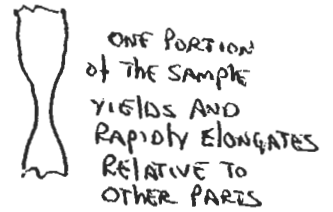
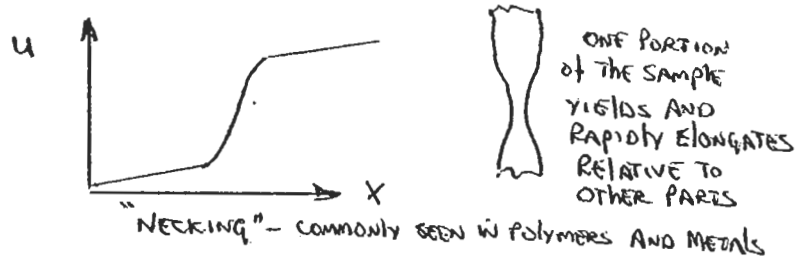
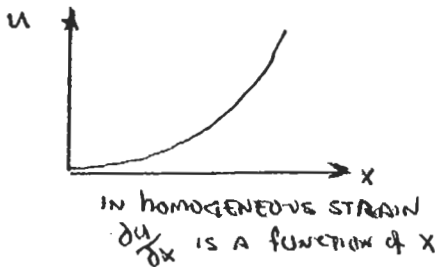
INTERESTS US AS MUCH AS RELATIVE DISPLACEMENT AS THIS CAUSES CHANGES IN LENGTH AND FORCES WITHIN THE MATERIAL

$$\begin{cases} P(x) \text{ HAS BEEN MAPPED TO } P'(x+u) = P'(x+ex) = P'[x(1+e)] \\ Q(x+\Delta x) \rightarrow Q'[(x+\Delta x)+(u+\Delta u)] = Q'[x+\Delta x + e(x+\Delta x)] = Q'[x+\Delta x(1+e)] \end{cases}$$

$$\therefore P'Q' = \Delta x(1+e)$$

$$\text{RELATIVE CHANGE OF LENGTH IS } \frac{\Delta x(1+e) - \Delta x}{\Delta x} = e = \frac{\Delta u}{\Delta x} \equiv \text{STRAIN (DIMENSIONLESS)}$$

BEFORE CONTINUING, WE SHOULD PAUSE TO NOTE THAT THE REAL WORLD DISPLAYS TYPES OF STRAIN IN ADDITION TO HOMOGENEOUS STRAIN



EXTENSION TO THREE DIMENSIONS

IN THE ABOVE EXPRESSION FOR ONE DIMENSION WE STARTED BY SAYING $u = ex$ ($\frac{\partial u}{\partial x} = e$) BUT THEN SHOWED THAT CHANGES IN LENGTH BEHAVE THE SAME WAY $\frac{\Delta u}{\Delta x} = e = \text{FRACTIONAL CHANGE IN LENGTH OF LINE SEGMENT}$

WHAT WE ESSENTIALLY SAID WAS THAT \vec{u} IS PROPORTIONAL TO POSITION

TO EXPRESS THE FRACTIONAL CHANGE OF LENGTH IN DIFFERENT DIRECTIONS IN THREE DIMENSIONS LET'S ASSUME THAT \vec{u} IS PROPORTIONAL TO (BUT NOT NECESSARILY PARALLEL TO) POSITION IN THE MATERIAL, \vec{x} .

WE CAN THEN WRITE

$$\begin{cases} u_1 = \frac{\partial u_1}{\partial x_1} x_1 + \frac{\partial u_1}{\partial x_2} x_2 + \frac{\partial u_1}{\partial x_3} x_3 \\ u_2 = \frac{\partial u_2}{\partial x_1} x_1 + \frac{\partial u_2}{\partial x_2} x_2 + \frac{\partial u_2}{\partial x_3} x_3 \\ u_3 = \frac{\partial u_3}{\partial x_1} x_1 + \frac{\partial u_3}{\partial x_2} x_2 + \frac{\partial u_3}{\partial x_3} x_3 \end{cases}$$

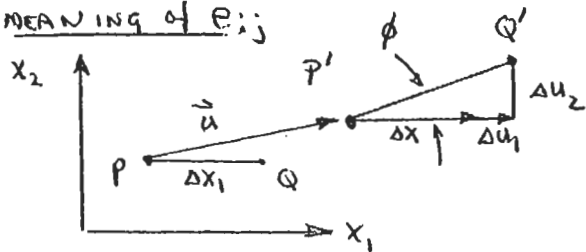
OR $u_i = \frac{\partial u_i}{\partial x_j} x_j$

OR IN TERMS OF DIFFERENCES IN DISPLACEMENT

$$\begin{cases} \Delta u_1 = \frac{\partial u_1}{\partial x_1} \Delta x_1 + \frac{\partial u_1}{\partial x_2} \Delta x_2 + \frac{\partial u_1}{\partial x_3} \Delta x_3 \\ \vdots \\ \text{OR } \Delta u_i = \frac{\partial u_i}{\partial x_j} \Delta x_j \end{cases}$$

LET'S DEFINE $\frac{\partial u_i}{\partial x_j} = e_{ij}$

MEANING OF e_{ij}



LET US CONSIDER A LINE SEGMENT PQ OF LENGTH Δx_1 , THAT IS INITIALLY PARALLEL TO x_1

$$\begin{cases} \Delta u_1 = \frac{\partial u_1}{\partial x_1} \Delta x_1 = e_{11} \Delta x_1 \\ \Delta u_2 = \frac{\partial u_2}{\partial x_1} \Delta x_1 = e_{21} \Delta x_1 \end{cases}$$

SELECTION OF PQ AS INITIALLY PARALLEL TO x_1 MEANS THERE IS NO CONTRIBUTION Δx_2 . THIS KEEPS THINGS SIMPLE

THE LINE SEGMENT $PQ = \Delta x_1$ HAS CHANGED LENGTH AND HAS ROTATED DIRECTION.

THE CHANGE OF LENGTH IS $\{(\Delta x + \Delta u_1)^2 + \Delta u_2^2\}^{\frac{1}{2}} \approx \Delta x + \Delta u_1$ OR, MORE RIGOROUSLY

IT THE CHANGE OF LENGTH IN $P'Q'$ RESOLVED ALONG x_1 ,

$$\therefore e_{11} = \frac{\Delta u_1}{\Delta x_1} = \text{TENSILE STRAIN ALONG } x_1$$

THE LINE SEGMENT $P'Q'$ HAS ALSO ROTATED AN AMOUNT ϕ

$$e_{21} = \frac{\Delta u_2}{\Delta x_1} = \text{TENSILE STRAIN ALONG } x_2$$

$$\tan \phi = \frac{\Delta u_2}{\Delta x_1 + \Delta u_1} \approx \frac{\Delta u_2}{\Delta x_1} = e_{21} \approx \phi \quad \text{if } e_{21} \text{ IS SMALL AN } \tan \phi \approx \phi$$

$\therefore e_{21}$ = ANGLE OF ROTATION OF LINE SEGMENT INITIALLY ALONG x_1 , IN THE DIRECTION OF x_2

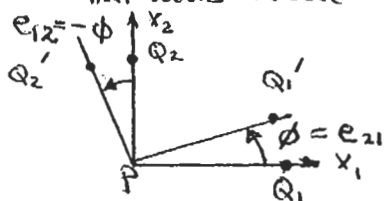
OR, GENERAL

$$e_{ij} = \frac{\partial u_i}{\partial x_j} \approx \text{ANGLE OF ROTATION OF LINE SEGMENT ALONG } x_j \text{ IN THE DIRECTION OF AXIS } x_i$$

PROPER DEFINITION OF A SATISFACTORY MEASURE OF STRAIN

CONSIDER, IN A 2-DIMENSIONAL SPACE, A STATE OF "STRAIN" IN WHICH $e_{12} = -e_{21}$ $e_{ii} = 0$

THAT WOULD PRODUCE DISPLACEMENTS IN WHICH A LINE PQ_1 , INITIALLY ALONG x_1 , IS ROTATED TOWARD x_2 BY AN ANGLE $\phi \approx e_{12}$

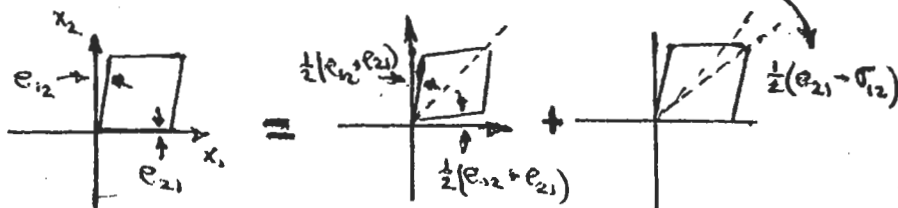
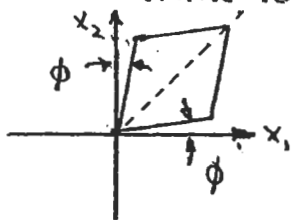


CONSIDER A LINE PQ_2 INITIALLY ALONG x_2 . IF e_{12} IS $-e_{21}$

IT ROTATES $-\phi$ TO A NEW LOCATION PQ_2' (IT $+e_{ij}$; ROTATES A LINE ALONG x_j TOWARD x_i ; THEN A NEGATIVE e_{ij} ; ROTATES A LINE ALONG x_j AWAY FROM x_i)

WOULD ONE CALL THIS A "DEFORMATION"? NO! IT LOOKS PRETTY MUCH LIKE ROTATION ABOUT x_3 WITH OUT ANY STRAIN AT ALL!

INDEED, IF YOU PICKED UP WHAT HAD BEEN INITIALLY A CUBE OF MATERIAL AND WANTED TO PLACE IT IN A POSITION SO THAT ANGLES SUCH AS e_{21} AND e_{12} REALLY DID PROVIDE A MEASURE OF DEFORMATION, YOU WOULD PROBABLY, BY INSPIRED, PLACE THE DEFORMED BLOCK RELATIVE TO THE REFERENCE AXES SUCH THAT $e_{ij} = e_{ji}$. IN OTHER WORDS, IF $e_{21} \neq e_{12}$, YOU WOULD ROTATE THE BODY UNTIL IT WAS



THIS IS A NEW CONCEPT: ADDITION OF TENSORS!

LET US TAKE THE TENSOR e_{ij} AND DIVIDE IT INTO TWO PARTS

$$e_{ij} = e_{ij} + w_{ij} \quad \text{with} \quad \begin{cases} e_{ij} \equiv \frac{1}{2}(e_{ij} + e_{ji}) \\ w_{ij} \equiv \frac{1}{2}(e_{ij} - e_{ji}) \end{cases}$$

$$e_{ij} = e_{ij} + w_{ij} = \frac{1}{2}(2e_{ij})$$

THE TENSOR w_{ij} WILL, FROM THE WAY IN WHICH IT WAS DEFINED, HAVE $w_{ii} = 0$ AND $w_{ij} = -w_{ji}$. IT IS AN "ANTISYMMETRIC TENSOR"

PROOF THAT PURE ROTATION WITH NO STRAIN CORRESPONDS AN ANTI-SYMMETRIC e_{ij}

IF e_{ij} RELATES A DISPLACEMENT VECTOR u_i TO A POSITION IN THE SOLID $\vec{R} = (x_1, x_2, x_3)$ AND e_{ij} CORRESPONDS TO PURE RIGID BODY ROTATION, THEN A CHARACTERISTIC OF u_i THEN A CHARACTERISTIC OF \vec{u} IS THAT IT IS EVERYWHERE $\perp \vec{R}$ REGARDLESS OF THE COORDINATES x_1, x_2, x_3 TO WHICH \vec{R} EXTENDS FOR THIS TO BE TRUE $\vec{u} \cdot \vec{R} = 0$ (NOTE: STRAW IS ASSUMED TO BE SMALL!)
OR $u_i R_i = 0$ $u_i = e_{ij} x_j$
 $(e_{ij} x_j x_i) = 0$ $R_i = x_i$

EXPANDING THE ABOVE EXPRESSION

$$e_{11} x_1^2 + e_{22} x_2^2 + e_{33} x_3^2 + (e_{13} + e_{31}) x_1 x_3 + (e_{23} + e_{32}) x_2 x_3 + (e_{12} + e_{21}) x_1 x_2 = 0$$

FOR THIS TO BE TRUE FOR ALL x_i , THE COEFFICIENTS OF $x_i x_j$ MUST INDIVIDUALLY VANISH!

$$\therefore e_{11} = e_{22} = e_{33} = 0 \quad \begin{cases} e_{13} + e_{31} = 0 \\ e_{23} + e_{32} = 0 \\ e_{12} + e_{21} = 0 \end{cases} \quad \begin{cases} e_{13} = -e_{31} \\ e_{23} = -e_{32} \\ e_{12} = -e_{21} \end{cases}$$

THEREFORE RIGID BODY ROTATION CORRESPONDS TO

$$\begin{bmatrix} 0 & e_{12} & e_{13} \\ -e_{12} & 0 & e_{23} \\ -e_{31} & -e_{32} & 0 \end{bmatrix} \quad \text{QED!}$$

TO DEFINE TRUE STRAIN e_{ij} - THAT IS, REAL DEFORMATION, WE THEREFORE SPLIT A GENERAL e_{ij} INTO TWO PARTS $e_{ij} = e_{ij} + w_{ij}$ WITH $e_{ij} = \frac{1}{2}(e_{ij} + e_{ji})$ $w_{ij} = \frac{1}{2}(e_{ij} - e_{ji})$

THE FINAL RESULT IS, FOR TRUE DEFORMATION

$$u_i = e_{ij} x_j \quad u_i \text{ IS A DISPLACEMENT VECTOR, } x_i \text{ IS A POSITION VECTOR.}$$

u_i AND x_i BOTH TRANSFORM ACCORDING TO THE LAW FOR 1ST RANK TENSORS, THEREFORE

e_{ij} IS A TENSOR, THE STRAIN TENSOR, OF 2ND RANK.

ALL OF THE PROPERTIES THAT WE HAVE ASCRIBED TO TENSORS IN PREVIOUS DISCUSSION THEREFORE APPLY TO THE STRAIN TENSOR

→ THE ELEMENTS OF STRAIN DEPEND ON THE COORDINATE SYSTEM TO WHICH THEY ARE REFERRED. UPON CHANGE OF REFERENCE AXES $x_1, x_2, x_3 \rightarrow x'_1, x'_2, x'_3$ DESCRIBED BY $[C_{is}]$, $e'_{ij} = C_{i\alpha} C_{j\beta} e_{\alpha\beta}$

→ The "value of strain" in a given direction defined by direction cosines l_i is $\epsilon = \epsilon_{ij} l_i l_j$. What does it mean? Turning to our definition of value of a property in a given direction,

$$\text{if } q_i = a_i; p_i \quad a = a_i l_i l_j = \frac{q_{11}}{|R|}$$

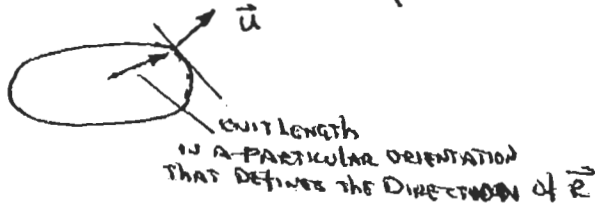
in the present case $\epsilon = \frac{u_{11}}{|R|}$ — it is the component of \vec{u} in the

direction of \vec{R} , or the TENSILE displacement per unit length of R

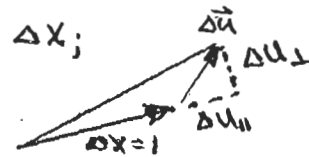
→ A strain quadric $\epsilon_{ij} x_i x_j = 1$ can be defined and has all of the properties that we ascribed to the representation quadric — including those that are valid only for symmetric tensors (as we have defined ϵ_{ij} as symmetric)

→ The strain quadric, accordingly, has a radius that is $1/\sqrt{\epsilon}$ in the direction of the radius

The "radius normal" property works because ϵ_{ij} is symmetric



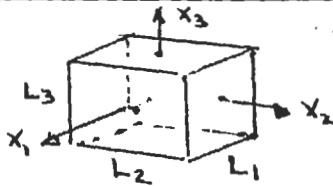
$$\Delta u_x = \epsilon_{ij} \Delta x_j$$



THE INITIAL LINE SEGMENT IS ROTATED AND CHANGES LENGTH $\epsilon_{ij} l_i l_j$; GIVES ϵ_{11} PER UNIT Δx AND IS CALLED THE STRETCH IN THAT DIRECTION

→ A STRAIN TENSOR IN GENERAL FORM CAN BE CONVERTED TO A DIAGONAL FORM BY FINDING THE EIGENVALUES AND EIGENVECTORS AND REFERRING THE TENSOR TO THE NEW PRINCIPAL AXES.

VOLUME CHANGE ASSOCIATED WITH DEFORMATION



CONSIDER A VOLUME ELEMENT, A BOX WITH EDGES L_1, L_2, L_3

TO KEEP THINGS SIMPLE, LET'S ASSUME THAT WE HAVE TAKEN THE REFERENCE AXES ALONG THE PRINCIPAL AXES OF THE STRAIN QUADRIC SO THAT THE STRAIN TENSOR IS DIAGONAL

$$\text{AFTER DEFORMATION} \begin{cases} L_1 \rightarrow L_1 (1 + \epsilon_{11}) \\ L_2 \rightarrow L_2 (1 + \epsilon_{22}) \\ L_3 \rightarrow L_3 (1 + \epsilon_{33}) \end{cases} \quad \begin{bmatrix} \epsilon_{11} & 0 & 0 \\ 0 & \epsilon_{22} & 0 \\ 0 & 0 & \epsilon_{33} \end{bmatrix}$$

THEN, IF $V = L_1 L_2 L_3$

$$\begin{aligned} V' &= V + \Delta V = L_1 (1 + \epsilon_{11}) \cdot L_2 (1 + \epsilon_{22}) \cdot L_3 (1 + \epsilon_{33}) \\ &= L_1 L_2 L_3 (1 + \epsilon_{11} + \epsilon_{22} + \epsilon_{33} + \epsilon_{11} \epsilon_{22} + \epsilon_{11} \epsilon_{33} + \epsilon_{22} \epsilon_{33} + \epsilon_{11} \epsilon_{22} \epsilon_{33}) \end{aligned}$$

AS STRAINS ARE SMALL, NEGLECT HIGHER-ORDER TERMS

$$\therefore V + \Delta V \approx L_1 L_2 L_3 (1 + \epsilon_{11} + \epsilon_{22} + \epsilon_{33})$$

$$V + \Delta V = V + \underbrace{V(\epsilon_{11} + \epsilon_{22} + \epsilon_{33})}_{\Delta V}$$

$$\boxed{\frac{\Delta V}{V} = \epsilon_{11} + \epsilon_{22} + \epsilon_{33}}$$

THIS IS THE FRACTIONAL CHANGE IN VOLUME CAUSED BY DEFORMATION — CALLED THE DILATION

WE SHOWED THAT THE FRACTIONAL VOLUME CHANGE UPON DEFORMATION IS

$\epsilon_{11} + \epsilon_{22} + \epsilon_{33}$. BECAUSE $\Delta V/V$ IS A SCALAR QUANTITY, WE WOULD NOT EXPECT THE DILATION TO CHANGE UPON CHANGE OF REFERENCE AXES. INDEED, IT DOES NOT. THIS SUM OF DIAGONAL ELEMENTS FOR A SECOND-RANK TENSOR IS A GENERALLY-DEFINED QUANTITY FOR TENSORS AND IS CALLED THE TRACE OF THE TENSOR

$$\text{TRACE} = T = a_{11} + a_{22} + a_{33}$$

IT HAS THE PROPERTY THAT IT REMAINS INVARIANT UPON ANY CHANGE OF REFERENCE AXES.

(THIS IS STRAIGHTFORWARD TO PROVE: ADD TOGETHER $a'_{11} = c_{1l} c_{1m} a_{lm} + c_{2l} c_{2m} a_{lm} + c_{3l} c_{3m} a_{lm} = (c_{1l} c_{1m} + c_{2l} c_{2m} + c_{3l} c_{3m}) a_{lm}$

$= 0 \quad l \neq m$
 $= 1 \quad l = m$ } from the ORTHOGONALITY PROPERTIES OF THE DIRECTION COSINE MATRIX

$\therefore T' = a_{11} + a_{22} + a_{33} \quad \text{QED}$)

SOME SPECIAL FORMS OF THE DIAGONALIZED STRAIN TENSOR

PLANE STRAIN

$$\begin{bmatrix} \epsilon_{11} & 0 & 0 \\ 0 & \epsilon_{22} & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

"PURE SHEAR" (SPECIAL CASE OF PLANE STRAIN)

$$\begin{bmatrix} -\epsilon_{11} & 0 & 0 \\ 0 & \epsilon_{11} & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

ROTATE AXES BY 45°

$$\begin{bmatrix} 0 & \epsilon' & 0 \\ \epsilon' & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

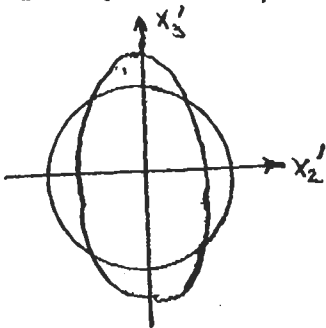
NOTE THAT TRACE $= 0$ SHEAR CAUSES NO VOLUME CHANGES!

SOME OTHER NON-TENSOR DEFINITIONS INVOLVING STRAIN

"Simple Shear"



ONE SOMETIMES SEES REFERENCE TO THE "STRAIN ELLIPSOID"



CONSIDER A SPECIMEN INITIALLY IN THE FORM OF A SPHERE OF UNIT RADIUS

$$x_1^2 + x_2^2 + x_3^2 = 1$$

AFTER DEFORMATION (TAKING x_1', x_2', x_3' ALONG PRINCIPAL AXES)

$$\begin{cases} x_1' = x_1 (1 + \epsilon_{11}) \\ x_2' = x_2 (1 + \epsilon_{22}) \\ x_3' = x_3 (1 + \epsilon_{33}) \end{cases}$$

THE EQUATION OF THE SURFACE AFTER DEFORMATION WILL BE

$$\frac{x_1'^2}{(1 + \epsilon_{11})^2} + \frac{x_2'^2}{(1 + \epsilon_{22})^2} + \frac{x_3'^2}{(1 + \epsilon_{33})^2} = 1$$

THIS IS THE "STRAIN ELLIPSOID" (IT IS NOT THE STRAIN QUADRIC!!)

3.60 Symmetry, Structure and Tensor Properties of Materials

SOME SOLUTIONS TO THIRD-ORDER EQUATIONS

BASIC EQUATION: $y^3 + py^2 + qy + r = 0$

TO CONVERT TO "NORMAL FORM" LET $y = x - p/3$

THEN $x^3 + ax + b = 0$

WITH $\begin{cases} a \equiv \frac{1}{3}(3q - p^2) \\ b \equiv \frac{1}{27}(2p^3 - 9pq + 27r) \end{cases}$

SOLUTIONS:

$$x_1 = A + B$$

$$x_2, x_3 = -\frac{1}{2}(A+B) \pm i\sqrt{\frac{3}{2}}(A-B)$$

WHERE:

$$A = \left\{ -\frac{b}{2} + \left(\frac{b^2}{4} + \frac{a^3}{27} \right)^{\frac{1}{2}} \right\}^{\frac{1}{3}}$$

$$B = \left\{ -\frac{b}{2} - \left(\frac{b^2}{4} + \frac{a^3}{27} \right)^{\frac{1}{2}} \right\}^{\frac{1}{3}}$$

IF p, q, r ARE REAL, THEN IF:

$$\begin{cases} \frac{b^2}{4} + \frac{a^3}{27} > 0 & \text{THERE ARE 1 REAL, 2 CONJUGATE IMAGINARY ROOTS} \\ \frac{b^2}{4} + \frac{a^3}{27} = 0 & \text{" " 3 REAL ROOTS, TWO OF WHICH ARE EQUAL} \\ \frac{b^2}{4} + \frac{a^3}{27} < 0 & \text{" " 3 REAL, UNEQUAL ROOTS} \end{cases}$$

UNFORTUNATELY, THE THIRD CASE IS THE ONE MOST FREQUENTLY ENCOUNTERED IN PRESENT APPLICATIONS. IN THIS INSTANCE THE ABOVE RELATIONS ARE OF LITTLE USE (NOTE THE TERM $(\frac{b^2}{4} + \frac{a^3}{27})^{\frac{1}{2}}$ IN THE DEFINITION OF THE PARAMETERS A AND B ABOVE)

THE THREE FOLLOWING ALTERNATIVE EXPRESSIONS FOR THE ROOTS MAY THEN BE USEFUL:

IF $\frac{b^2}{4} + \frac{a^3}{27} < 0$:

$$x_k = -2 \frac{b}{|b|} \left(\frac{-a}{3} \right)^{\frac{1}{2}} \cos\left(\frac{\phi}{3} + 120^\circ \cdot k\right) \quad k=0,1,2$$

with $\cos \phi = \left[\frac{b^2}{4} \cdot \left(\frac{-27}{a^3} \right) \right]^{\frac{1}{2}}$

IF $\frac{b^2}{4} + \frac{a^3}{27} = 0$

$$\text{ROOTS ARE: } -2 \frac{b}{|b|} \left(\frac{-a}{3} \right)^{\frac{1}{2}}, \quad \frac{b}{|b|} \left(\frac{-a}{3} \right)^{\frac{1}{2}} \text{ TWICE}$$

IF $\frac{b^2}{4} + \frac{a^3}{27} > 0$

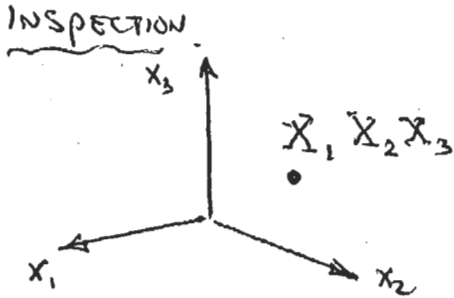
$$\text{THE REAL ROOT IS } x = 2 \frac{b}{|b|} \left(\frac{a}{3} \right)^{\frac{1}{2}} \text{ CTN } 2\phi$$

with $\tan \phi = \left(\tan \psi \right)^{\frac{1}{3}}$
 AND $\text{CTN } 2\phi = \left(\frac{b^2}{4} \cdot \frac{27}{a^3} \right)^{\frac{1}{2}}$

3.60 Symmetry, Structure and Tensor Properties of Materials

THE METHOD OF DIRECT INSPECTION

A USEFUL ALGORITHM EXISTS THROUGH WHICH ONE CAN DEDUCE THE VALUE OF A TRANSFORMED TENSOR ELEMENT BY INSPECTION, A METHOD CALLED (APPROPRIATELY ENOUGH) THE METHOD OF DIRECT INSPECTION.



LET'S CONSIDER A POINT (COULD BE THE TERMINAL POINT OF A VECTOR WITH COORDINATES X_1, X_2, X_3 (WE USE UPPER CASE SYMBOLS TO DISTINGUISH COORDINATES FROM THE LABELS ATTACHED TO OUR REFERENCE AXES))

LET'S NOW EXAMINE THE VALUE OF THE PRODUCT OF A PAIR OF THESE COORDINATES $X_i X_j$. IF WE CHANGE REFERENCE AXES TO A NEW SET OF BASIS VECTORS x'_1, x'_2, x'_3 , THE VALUE OF THE PRODUCT WILL CHANGE. LET'S EVALUATE THE NEW VALUE OF THE PRODUCT $X'_i X'_j$ (C'MON, YOU PROTEST! I DON'T EVEN SEE WHY YOU TOOK THE PRODUCT IN THE FIRST PLACE!! WHY SHOULD I CARE WHAT THE NEW VALUE MIGHT BE ?? HOLD ON! ALL WILL BE REVEALED DIRECTLY.)

THE NEW VALUE OF THE PRODUCT $X'_i X'_j$ WILL BE

$$X'_i X'_j = (C_{ir} X_r) \cdot (C_{jm} X_m) \\ = C_{ir} C_{jm} X_r X_m \quad \text{--- SO WHAT ??}$$

WELL, THE LAW FOR TRANSFORMATION FOR A TENSOR OF SECOND RANK

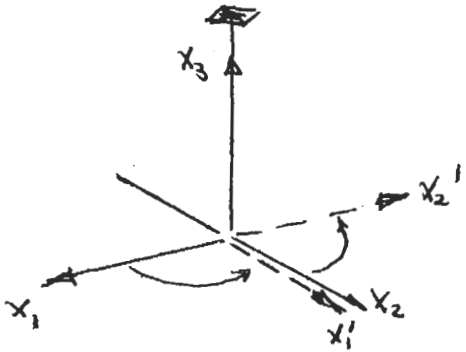
IS

$$a'_{ij} = C_{ir} C_{jm} a_{rm}$$

WHICH IS ANALOGOUS TO THE WAY IN WHICH THE PRODUCT OF COORDINATES TRANSFORMS (IT IS NOT IDENTICAL !! INTERCHANGING C_{ir} AND C_{jm} DOES NOT CHANGE THE VALUE OF THE PRODUCT OF THE COORDINATES — BUT DOING SO FOR a'_{ij} GIVES A COMPLETELY DIFFERENT EXPRESSION!)

THEREFORE THE ELEMENTS OF A TENSOR TRANSFORM, UPON A CHANGE OF REFERENCE AXES, IN EXACTLY THE SAME WAY AS THE PRODUCT OF CORRESPONDING COORDINATES PROVIDED WE MAINTAIN THE CORRECT ORDER OF TERMS

LET'S PROVIDE AN EXAMPLE AS THIS COOKBOOK RECIPE IS DECEPTIVELY SIMPLE. LET'S CONSIDER (ANTICIPATING AN APPLICATION OF THIS FORMALISM THAT IS SOON TO COME) A 4-FOLD ROTATION OF 90° ABOUT X_3



$$\begin{cases} X_1' = X_2 \\ X_2' = -X_1 \\ X_3' = X_3 \end{cases}$$

IF WE WISH TO DETERMINE THE NEW VALUE FOR, SAY, a_{12}' AFTER THIS CHANGE OF AXES

WE EVALUATE

$$X_1' X_2' = X_2 (-X_1)$$

IF THE TENSOR ELEMENTS TRANSFORM LIKE THE PRODUCT OF COORDINATES, WE CAN SAY BY INSPECTION THAT

$$a_{12}' = -a_{21}$$

THAT IS, UPON THIS CHANGE OF AXES, THE NUMBER THAT APPEARS IN THE 1-2 BOX OF THE NEW TENSOR a_{ij}' IS THE NEGATIVE OF THE VALUE THAT APPEARED IN THE 2-1 BOX OF a_{ij}

THE METHOD IS DIRECTLY APPLICABLE TO TENSORS OF HIGHER RANK

IF WE WISH TO DETERMINE THE NEW VALUE OF, SAY, THE ELASTIC COMPLIANCE ELEMENT S_{1213} WE WOULD EXAMINE THE TRANSFORMATION OF THE PRODUCT $X_1 X_2 X_1 X_3$

FOR THE ABOVE CHANGE OF REFERENCE AXES

$$X_1' X_2' X_1' X_3' \rightarrow X_2 (-X_1) X_2 X_3$$

THE VALUE OF S_{1213}' IS THUS $-S_{2123}$

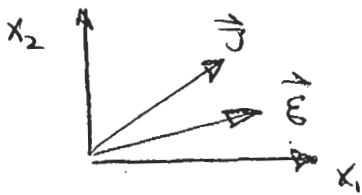
[WOULD YOU BELIEVE THAT WE HAVE JUST PERFORMED A QUADRUPLE SUMMATION THAT CONTAINED 81 TERMS !! ??]

THE VALUE OF A SECOND-RANK TENSOR PROPERTY IN A GIVEN DIRECTION

LET'S CONSIDER A PROPERTY SUCH AS ELECTRICAL CONDUCTIVITY, A SECOND-RANK TENSOR THAT RELATES A CURRENT DENSITY VECTOR, \vec{J} , TO AN APPLIED ELECTRIC FIELD

$$J_i \text{ (CHARGE/UNIT AREA/UNIT TIME)} = \sigma_{ij} E_j \text{ (VOLTS/UNIT LENGTH)}$$

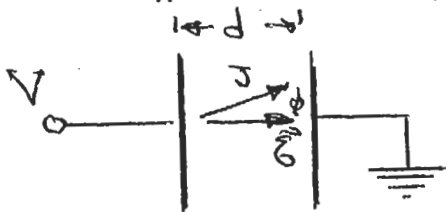
THE EXPERIMENT WE PERFORM MIGHT BE TO SUBJECT A CRYSTAL TO THE ELECTRIC FIELD \vec{E} AND THEN DETERMINE \vec{J} . \vec{J} WILL NOT, IN GENERAL, BE PARALLEL TO \vec{E}



WHEN WE MEASURE σ (A SCALAR QUANTITY!) THEN, TO WHAT "DIRECTION" DOES IT PERTAIN? THE DIRECTION OF \vec{J} ? THE DIRECTION OF \vec{E} ?

OR SHOULD WE SPLIT THE DIFFERENCE AND SAY THE "DIRECTION" IS MIDWAY BETWEEN THE TWO VECTORS?

WELL, LET'S CONSIDER IN DETAIL WHAT WE MIGHT DO IN AN ACTUAL EXPERIMENT. SAY WE WANT TO MEASURE σ ALONG THE $[111]$ DIRECTION. WHAT WE WOULD DO IS TO CUT A PLATE NORMAL TO $[111]$, ATTACH ELECTRODES AND APPLY A VOLTAGE, V , PROVIDING A FIELD, $E = V/d$



THE FIELD \vec{E} IS DIRECTED BETWEEN THE ELECTRODES - i.e., ALONG $[111]$ SO CLEARLY $\sigma_{[111]}$ WILL BE THE VALUE OF THE

"GENERALIZED FORCE", IS APPLIED.

WHAT, THEN, IS THE VALUE OF σ ? $|\vec{J}|/|\vec{E}|$ RIGHT? WRONG!

WHAT WE MEASURE AS THE FLUX OF CHARGE PARALLEL TO \vec{E} AS WE MEASURE THE CHARGE/UNIT AREA PER UNIT TIME THAT PASSES BETWEEN ELECTRODES

$$\text{THUS } \sigma = \frac{J_{\parallel}}{|\vec{E}|} = \frac{|\vec{J}| \cos \phi}{|\vec{E}|} = \frac{\vec{J} \cdot \vec{E}}{|\vec{E}|^2}$$

$$\sigma = \frac{\vec{J} \cdot \vec{E}}{|\vec{E}|^2}$$

WE CAN NOW WRITE THIS EXPRESSION IN TERMS OF THE CONDUCTIVITY TENSOR

$$\sigma = \frac{\vec{J} \cdot \vec{E}}{|\vec{E}|^2} = \frac{J_i E_i}{|\vec{E}|^2}$$

$$\text{AS } \vec{J} \cdot \vec{E} = J_1 E_1 + J_2 E_2 + J_3 E_3$$

$$= \frac{\sigma_{ij} E_j E_i}{|\vec{E}|^2}$$

E_i IS $|\vec{E}| l_i$ WHERE l_1, l_2, l_3 ARE THE DIRECTION COSINES OF THE ORIENTATION IN WHICH WE APPLY \vec{E}

$$\sigma = \frac{\sigma_{ij} l_i l_j |\vec{E}| |\vec{E}|}{|\vec{E}|^2}$$

SO THE VALUE OF σ IN A DIRECTION SPECIFIED BY DIRECTION COSINES l_i

IS

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

$$= \sigma_{11} l_1^2 + \sigma_{22} l_2^2 + \sigma_{33} l_3^2 + (\sigma_{12} + \sigma_{21}) l_1 l_2 + (\sigma_{13} + \sigma_{31}) l_1 l_3 + (\sigma_{23} + \sigma_{32}) l_2 l_3$$

WE CAN IMMEDIATELY USE THIS EXPRESSION TO PROVIDE A PHYSICAL INTERPRETATION OF SOME OF THE ELEMENTS IN A SECOND-RANK TENSOR.

LET'S ASK THE VALUE OF σ THAT WOULD BE MEASURED ALONG X_1 ,

THE DIRECTION COSINES OF X_1 ARE $1, 0, 0$

$$\therefore \sigma = \sigma_{11} 1^2 + \sigma_{22} 0^2 + \sigma_{33} 0^2 + (\sigma_{12} + \sigma_{21}) 1 \cdot 0$$

$$+ (\sigma_{13} + \sigma_{31}) 1 \cdot 0 + (\sigma_{23} + \sigma_{32}) 0 \cdot 0$$

$$\boxed{\sigma = \sigma_{11}}$$

THUS THE DIAGONAL ELEMENTS σ_{ii} IN A SECOND RANK TENSOR REPRESENT THE VALUES OF THE PROPERTY THAT ONE WOULD MEASURE ALONG X_1, X_2 OR X_3 , RESPECTIVELY.

"SYMMETRIC" TENSORS (AN UNFORTUNATE TERM)

A TENSOR σ_{ij} IS SAID TO BE "SYMMETRIC" IF $\sigma_{ij} \equiv \sigma_{ji}$

THIS EQUALITY COMES FROM ENERGY AND THERMODYNAMIC ARGUMENTS (AND NOT FROM CRYSTALLOGRAPHIC SYMMETRY!) THE EQUALITY MUST BE ESTABLISHED PROPERTY BY PROPERTY. MOST SECOND RANK PROPERTY TENSORS ARE SYMMETRIC, BUT NOT ALL! (THERMOELECTRICITY IS ONE EXAMPLE)

THE REPRESENTATION QUADRIC

WE CAN USE THE ELEMENTS OF A SECOND-RANK TENSOR TO DEFINE A SURFACE

$$a_{ij} X_i X_j = 1$$

THE SURFACE IS A QUADRATIC FORM AND CAN REPRESENT EITHER

AN ELLIPSOID

AN HYPERBOLOID OF ONE SHEET

AN HYPERBOLOID OF TWO SHEETS

AN IMAGINARILY ELLIPSOID

THE EQUATION IS CALLED A "REPRESENTATION" SURFACE BECAUSE IT CONTAINS JUST ABOUT EVERYTHING ONE MIGHT LIKE TO KNOW ABOUT A SECOND RANK TENSOR. IN A PARTICULAR DIRECTION SPECIFIED BY DIRECTION COSINES l_i A RADIUS VECTOR \vec{R} , FROM THE ORIGIN OUT TO THE SURFACE OF THE QUADRIC TERMINATES AT A POINT

$$X_1 = |R| l_1$$

$$X_2 = |R| l_2$$

$$X_3 = |R| l_3$$

THIS POINT SATISFIED THE EQUATION OF THE QUADRIC, SO

$$a_{ij} |R| l_i |R| l_j = 1$$

$$|R|^2 = \frac{1}{a_{ij} l_i l_j}$$

BUT THE DENOMINATOR IN THE TERM AT RIGHT IS THE VALUE OF THE PROPERTY, a , ALONG THE DIRECTION SPECIFIED BY l_1, l_2, l_3

THEREFORE THE RADIUS IN A GIVEN DIRECTION OF THE QUADRIC IS THE RECIPROCAL OF THE SQUARE ROOT OF THE PROPERTY IN THAT DIRECTION $|R| = \frac{1}{\sqrt{a}}$ OR, CONVERSELY, $a = \frac{1}{|R|^2}$

THEREFORE, THE VARIATION OF A SECOND-RANK TENSOR PROPERTY VARIES SMOOTHLY WITH DIRECTION, WITH NO LUMPS, DIMPLES OR LOBES EVEN THOUGH SUCH VARIATION MIGHT BE COMPATIBLE WITH CRYSTAL SYMMETRY!

3.60 Symmetry, Structure and Tensor Properties of Materials

TENSOR PROPERTIES OF CRYSTALS AND ANISOTROPY

WHEN WE SPEAK OF A "PROPERTY" OF A MATERIAL WE MEAN — MAKING A DEFINITION IN FORMAL TERMS — THE RESPONSE OF A MATERIAL TO A SPECIFIC CHANGE IN A GIVEN SET OF CONDITIONS THAT RELATES INDEPENDENT AND DEPENDENT QUANTITIES IN A PARTICULAR PROCESS

WE SOMETIMES COLLECT PROPERTIES INTO SPECIFIC CATEGORIES

- eg • MECHANICAL
• ELECTRICAL

OTHER PROPERTIES ARE NOT QUITE SO SIMPLE TO CLASSIFY

- • COMPOSITE AND QUALITATIVE PROPERTIES
 - eg • A "FUZZY" FABRIC (SURFACE TEXTURE, REFLECTIVITY, FIBER RIGIDITY)
 - "SINTERABILITY" OF A CERAMIC POWDER (PARTICLE SIZE, SURFACE ENERGY, DIFFUSIVITY, VAPOR PRESSURE)
- • NON SINGLE-VALUED PROPERTIES (HYSTERISIS)
 - POLARIZATION OF A FERROELECTRIC MATERIAL
 - MAGNETIZATION OF A FERROMAGNETIC MATERIAL
- • PROPERTIES DETERMINED BY TESTS THAT ARE INHERENTLY NON-REVERSIBLE (THE PROPERTY MAY BE MEASURED FOR A SAMPLE THAT NO LONGER EXISTS!)
 - YIELD STRENGTH
 - FRACTURE TOUGHNESS
 - STREAK COLOR
- • STRUCTURE-SENSITIVE PROPERTIES
PROPERTY DEPENDS ON DENSITY OR DISTRIBUTION OF DEFECTS

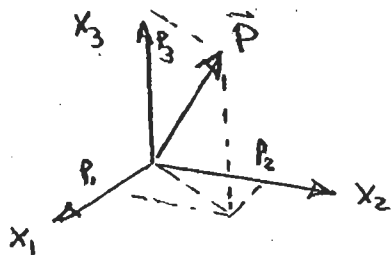
OUR PRESENT DISCUSSION WILL DEAL WITH EQUILIBRIUM PROPERTIES THAT ARE RIGOROUSLY DEFINED AND MEASURABLE.

Our "PROPERTY" will express a response of the material to a generalized "FORCE" by a generalized "DISPLACEMENT"

EXAMPLES: "FORCES": T (TEMPERATURE) E (ELECTRIC FIELD), σ (STRESS)
"DISPLACEMENT": S (ENTROPY) D (DISPLACEMENT), ϵ (STRAIN)

TENSORS

LET US SUPPOSE THAT OUR GENERALIZED FORCE IS A VECTOR, \vec{P} , WHOSE COMPONENTS ARE P_1 , P_2 AND P_3 RELATIVE TO A CARTESIAN (NOT CRYSTALLOGRAPHIC!!) COORDINATE SYSTEM x_1, x_2, x_3



THE RESPONSE OR "DISPLACEMENT" OF THE MATERIAL IS OFTEN A VECTOR \vec{q} .

IN MANY CASES WE CAN ASSUME $P \propto q$ AND WRITE $P = a q$

THIS MAY BE TRUE, BUT IS USUALLY VALID ONLY FOR "SMALL" q , AND WHAT CONSTITUTES "SMALL" DEPENDS ON THE PROPERTY.

EXAMPLE ① THE ELECTRICAL CONDUCTIVITY σ OF A CERAMIC DIELECTRIC MATERIAL RELATES CURRENT DENSITY J (CHARGE PER UNIT AREA PER UNIT TIME) TO AN APPLIED ELECTRIC FIELD, E (VOLTS/UNIT LENGTH) ACCORDING TO $J = \sigma E$. BUT — MAKE E SUFFICIENTLY LARGE AND DIELECTRIC BREAKDOWN RESULTS

EXAMPLE ② THE MAGNETIC SUSCEPTIBILITY χ RELATES THE MAGNETIZATION, M (MAGNETIC MOMENT PER UNIT VOLUME) TO APPLIED MAGNETIC FIELD H . FOR A DILUTE SOLUTION OF FE ATOMS IN A SILICATE GLASS $M = \chi H$ BUT, IF THE MAGNETIC FIELD IS SUFFICIENTLY LARGE, THE MAGNETIC MOMENT OF EVERY FE ATOM IS DRAGGED INTO ALIGNMENT WITH H AND ONE IS UNABLE TO SQUEEZE ANY MORE MAGNETIZATION OUT OF THE MATERIAL!

WE CAN RETAIN THE EXPECTATION THAT $|\vec{p}\rangle$ WILL BE PROPORTIONAL TO $|\vec{q}\rangle$ BUT RELAX THE ASSUMPTION THAT $\vec{p} \parallel \vec{q}$ BY ASSUMING THAT EACH COMPONENT OF \vec{p} IS GIVEN BY A LINEAR COMBINATION OF EVERY COMPONENT OF \vec{q} . THAT IS, A RELATION OF THE FORM

$$\begin{cases} p_1 = a_{11} q_1 + a_{12} q_2 + a_{13} q_3 \\ p_2 = a_{21} q_1 + a_{22} q_2 + a_{23} q_3 \\ p_3 = a_{31} q_1 + a_{32} q_2 + a_{33} q_3 \end{cases}$$

WE CAN SUMMARIZE THE SET OF EQUATIONS WITH

$$p_i = \sum_{j=1}^3 a_{ij} q_j$$

THE FIRST SUBSCRIPT, i , HAS MEANING: IT SPECIFIES WHICH COMPONENT p_i THAT ONE IS EVALUATING. THE SECOND SUBSCRIPT j IS AN INDEX OF SUMMATION, SOMETIMES

REFERRED TO AS A "DUMMY INDEX".

WE WILL SHORTLY ENCOUNTER DOUBLE, TRIPLE OR QUADRUPLE (!) SUMMATIONS AND WILL VERY QUICKLY TIRE OF THE NEED TO CONSTANTLY WRITE \sum 'S LET US THEREFORE WRITE, SIMPLY

$$p_i = a_{ij} q_j$$

AND TAKE SUCH AN EXPRESSION TO MEAN THAT SUMMATION FROM 1 TO 3 OF ANY REPEATED INDEX (IN THIS EXAMPLE j) IS AUTOMATICALLY UNDERSTOOD

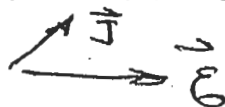
THIS IS REFERRED TO AS THE EINSTEIN CONVENTION

THE ARRAY OF COEFFICIENTS a_{ij} CONSTITUTES A TENSOR OF SECOND RANK (TWO SUBSCRIPTS) AND CAN RELATE TWO VECTORS (AS IN OUR EXAMPLES OF ELECTRONIC POLARIZABILITY AND THERMAL CONDUCTIVITY) OR CAN RELATE A SCALAR AND A SECOND RANK TENSOR (FOR EXAMPLE, THERMAL EXPANSION, α , RELATING STRAIN, ϵ_{ij} , AND TEMPERATURE CHANGE, ΔT , ACCORDING TO $\epsilon_{ij} = \alpha_{ij} \Delta T$)

THERE IS A SECOND ASSUMPTION BUILT INTO THE RELATION $\vec{p} = \alpha \vec{q}$ BECAUSE BOTH \vec{p} AND \vec{q} MAY BE VECTORS:

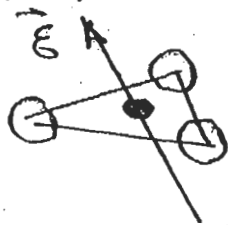
$$\vec{p} = \alpha \vec{q}$$

WE ARE THUS ASSUMING THAT \vec{p} AND \vec{q} ARE PARALLEL! WHY NOT??!
LET'S NOT BE SILLY! WHO WOULD CLAIM THAT IF WE APPLY AN ELECTRIC FIELD \vec{E} TO A MATERIAL THAT THE CURRENT RUNS OFF IN A DIFFERENT DIRECTION!!



WELL, WE SHOULD PERHAPS NOT MAKE THIS ASSUMPTION TOO SWIFTLY.

- CONSIDER THE ELECTRIC DIPOLE MOMENT \vec{p} THAT IS INDUCED ON A TIGHTLY-BOUND TRIANGULAR GROUP OF IONS IN A CRYSTAL



IN RESPONSE TO AN APPLIED ELECTRIC FIELD \vec{E} . THE PROPERTY RELATING THE TWO VECTORS IS THE ELECTRONIC POLARIZABILITY α

$$\vec{p} = \alpha \vec{E} \quad \text{BUT, WOULD WE EXPECT THE ELECTRON CLOUD}$$

ON THE IONS TO BE DISPLACED AS EASILY WITHIN THE PLANE OF THE GROUP AS IN A DIRECTION NORMAL TO IT?? WELL, MAYBE NOT. -----

- CONSIDER THE THERMAL CONDUCTIVITY OF A SINGLE CRYSTAL OF A LAYER STRUCTURE, k . THERMAL CONDUCTIVITY RELATES HEAT-FLOW DENSITY TO AN APPLIED TEMPERATURE GRADIENT. k DEPENDS ON THE VELOCITY OF PHONONS IN THE STRUCTURE AND THIS CAN BE SEVERAL ORDERS OF MAGNITUDE LARGER IN THE PLANE OF THE LAYER THAN NORMAL TO THEM.

a_j , A VECTOR, IS A FIRST-RANK TENSOR AND SOME PROPERTIES ARE TENSORS OF FIRST RANK. AN EXAMPLE IS THE PYROELECTRICITY TENSOR THAT RELATES AN INDUCED POLARIZATION P_i (DIPOLE MOMENT PER UNIT VOLUME) TO A SCALAR CHANGE IN TEMPERATURE, ΔT

AN ARRAY OF 3×9 OR 9×3 COEFFICIENTS a_{ijk} THAT EITHER RELATES A SECOND-RANK TENSOR TO A VECTOR, OR A VECTOR TO AN APPLIED SECOND-RANK TENSOR AS THE GENERALIZED FORCE CONSTITUTES A THIRD RANK TENSOR. EXAMPLES

- STRAIN E_{ij} INDUCED BY AN APPLIED ELECTRIC FIELD E_k (THE CONVERSE PIEZOELECTRIC EFFECT)

$$E_{ij} = a_{ijk} E_k$$

- POLARIZATION P_i (DIPOLE MOMENT PER UNIT VOLUME) INDUCED BY AN APPLIED STRESS T_{jk}

$$P_i = a_{ijk} T_{jk}$$

(THE DIRECT PIEZOELECTRIC EFFECT)

FOURTH-RANK TENSORS APPEAR IN ELASTICITY AS THE COEFFICIENTS THAT RELATE STRESS T_{ij} AND STRAIN E_{kl}

THE STIFFNESSES C_{ijkl} RELATE STRESS AND STRAIN

$$T_{ij} = C_{ijkl} E_{kl} \quad (\text{A } 9 \times 9 \text{ ARRAY OF 81 ELEMENTS!!})$$

THE COMPLIANCES S_{ijkl} RELATE STRAIN TO STRESS

$$E_{ij} = S_{ijkl} T_{kl}$$

YET HIGHER-RANK TENSORS ARE REQUIRED TO DESCRIBE OTHER PROPERTIES — EG, THE CHANGE OF ELASTIC PROPERTIES WITH APPLIED PRESSURE !!

TRANSFORMATION OF TENSORS

THERE ARE TWO IMPLICATIONS OF THE PRESUMABLY-SATISFACTORY RELATION THAT WE HAVE PROPOSED TO RELATE TWO VECTORS

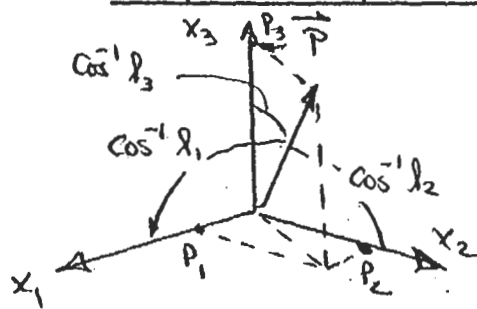
$$P_i = a_{ij} q_j$$

THE FIRST IS THAT THERE IS NO REASON TO EXPECT ALL NINE ELEMENTS a_{ij} TO HAVE THE SAME NUMERICAL VALUES.

- THEREFORE THE COMPONENTS P_i AND THE MAGNITUDE OF \vec{P} WILL CHANGE AS WE CHANGE THE ORIENTATION OF THE APPLIED VECTOR \vec{q} (BECAUSE THE COMPONENTS OF \vec{q} , q_1, q_2, q_3 DEPEND IN SIZE ON THE ORIENTATION OF \vec{q}). ACCORDINGLY, THE PROPERTY DESCRIBED BY a_{ij} WILL BE ANISOTROPIC! ITS VALUE WILL CHANGE WITH THE ORIENTATION OF THE APPLIED VECTOR.

- THE VALUES OF THE APPLIED VECTOR \vec{q} (q_1, q_2, q_3) AS WELL AS THE RESULTING VECTOR \vec{p} (p_1, p_2, p_3) DEPEND ON THE COORDINATE SYSTEM X_1, X_2, X_3 THAT WE USE TO DESCRIBE THE VECTORS. THE VECTORS ARE REAL, FIXED IN SPACE, BUT IF WE CHANGE X_1, X_2, X_3 TO SOME NEW AXES X'_1, X'_2, X'_3 THE NUMBERS P_i AND q_i CHANGE TO NEW VALUES. IF P_i AND q_i CHANGE THEN THE TENSOR ELEMENTS a_{ij} WILL ALSO CHANGE WITH CHANGE IN THE COORDINATE SYSTEM!

COMPONENTS OF A VECTOR



LET'S CONSIDER A VECTOR OF MAGNITUDE $|\vec{P}|$ THAT IS DIRECTED IN A PARTICULAR ORIENTATION THAT WE CAN SPECIFY BY MEANS OF THE ANGLES θ_1 , θ_2 & θ_3 THAT IT MAKE WITH REFERENCE AXES x_1 , x_2 , x_3

THE THREE COMPONENTS OF THE VECTOR ALONG THESE AXES WILL BE

$$\text{GIVEN BY } \begin{cases} P_1 = |\vec{P}| \cos \theta_1 \equiv |\vec{P}| l_1 \\ P_2 = |\vec{P}| \cos \theta_2 \equiv |\vec{P}| l_2 \\ P_3 = |\vec{P}| \cos \theta_3 \equiv |\vec{P}| l_3 \end{cases}$$

THE QUANTITIES $\cos \theta_i$ WILL OCCUR IN SO MUCH THAT WE ARE ABOUT TO DO THAT WE WILL INTRODUCE A SEPARATE SYMBOL l_i FOR THEM THAT WE WILL DIRECTLY USE TO SPECIFY AN ORIENTATION. WE WILL REFER TO THESE QUANTITIES AS DIRECTION COSINES IN THE SPECIAL CASE IN WHICH \vec{P} IS A VECTOR OF UNIT MAGNITUDE \vec{u} , WHERE $|\vec{u}| \equiv 1$, THE ABOVE SET OF EQUATIONS REDUCES TO

$$\begin{cases} u_1 = |\vec{u}| l_1 = l_1 \\ u_2 = |\vec{u}| l_2 = l_2 \\ u_3 = |\vec{u}| l_3 = l_3 \end{cases}$$

THIS MEANS THAT WE CAN REGARD THE DIRECTION COSINES AS THE COMPONENTS OF A UNIT VECTOR THAT IS ORIENTED ALONG THE DIRECTION SPECIFIED BY l_i

THE MAGNITUDE OF THIS UNIT VECTOR IS GIVEN BY

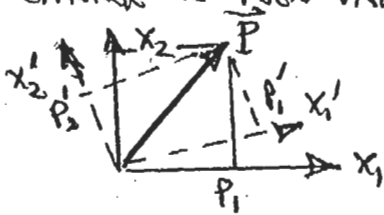
$$u_1^2 + u_2^2 + u_3^2 = |\vec{u}|^2 = 1 = (|\vec{u}| l_1)^2 + (|\vec{u}| l_2)^2 + (|\vec{u}| l_3)^2$$

$$\boxed{1 = l_1^2 + l_2^2 + l_3^2}$$

THE SUM OF THE SQUARES OF DIRECTION COSINES IS, THEREFORE, ALWAYS UNITY! ONLY TWO ARE INDEPENDENT. (NOTE HOWEVER, THAT THE SIGN OF THE THIRD DIRECTION COSINE MAY BE EITHER \oplus OR \ominus)

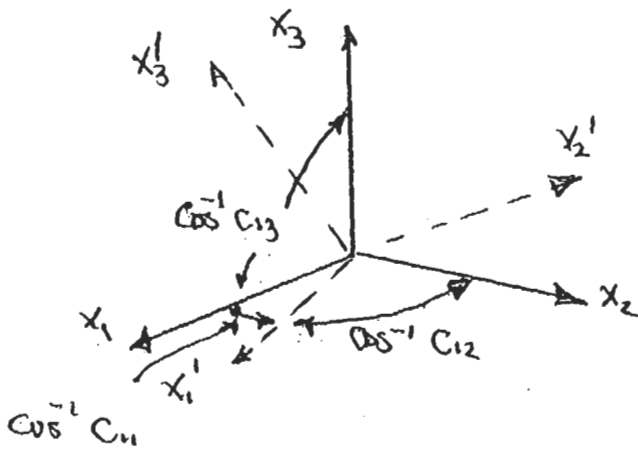
SPECIFICATION OF A CHANGE IN COORDINATE SYSTEM

If we change from a first coordinate system x_1, x_2, x_3 to a new set of axes x'_1, x'_2, x'_3 the components of a vector \vec{P} , P_i , will change to new values P'_i . This is apparent from the two-dimensional



EXAMPLE SKETCHED TO THE LEFT. THE VECTOR \vec{P} IS REAL AND REMAINS MAJESTICALLY IMMOBILE IN SPACE. THE COMPONENTS P_1, P_2 OR P'_1, P'_2 HOWEVER, DEPEND ON OUR CHOICE OF COORDINATE

SYSTEM. TO SPECIFY A CHANGE IN COORDINATE SYSTEM IT IS NECESSARY TO PROVIDE THE DIRECTION COSINES FOR ALL THREE OF THE NEW AXES x'_1, x'_2, x'_3 RELATIVE TO THE ORIGINAL SET OF AXES x_1, x_2, x_3 . THIS WILL REQUIRE A 3×3 ARRAY OF DIRECTION COSINES THAT WE WILL DEFINE AS C_{ij} WHERE C_{ij} IS DEFINED AS THE COSINE OF THE ANGLE BETWEEN THE NEW AXIS x'_i AND THE ORIGINAL REFERENCE AXIS x_j .



AND	x_1	x_2	x_3
x'_1	C_{11}	C_{12}	C_{13}
x'_2	C_{21}	C_{22}	C_{23}
x'_3	C_{31}	C_{32}	C_{33}

Cos of ANGLE BETWEEN

RELATIONS AMONG THE COEFFICIENTS IN THE DIRECTION COSINE

SCHEME FOR A CHANGE IN COORDINATE SYSTEM

WE HAVE SET UP A 3×3 MATRIX OF DIRECTION COSINES THAT SPECIFIES THE RELATION BETWEEN THE AXES OF NEW COORDINATE SYSTEM X'_i AND AN ORIGINAL SET OF AXES X_i :

$$\begin{cases} X'_1 = C_{11} X_1 + C_{12} X_2 + C_{13} X_3 \\ X'_2 = C_{21} X_1 + C_{22} X_2 + C_{23} X_3 \\ X'_3 = C_{31} X_1 + C_{32} X_2 + C_{33} X_3 \end{cases}$$

OR $[X'_i] = [C_{ij}] [X_j]$
IN MATRIX NOTATION

OR SIMPLY

$$X'_i = C_{ij} X_j$$

WHERE WE HAVE USED THE EINSTEIN CONVENTION IN WHICH SUMMATION FROM 1 TO 3 IS AUTOMATICALLY UNDERSTOOD IN ANY PRODUCT WITH REPEATED SUBSCRIPTS (IN THIS CASE, THE INDEX 'j')

A GREAT MANY RELATIONS EXIST AMONG THE DIRECTION COSINES C_{ij} ; AS WE HAVE SEEN THAT DIRECTION COSINES CAN BE INTERPRETED AS THE THREE COMPONENTS OF A UNIT VECTOR POINTING IN A PARTICULAR DIRECTION. FROM WHICH:

(1) THE DIRECTION COSINES IN ANY ROW - FOR EXAMPLE

$$X'_1 = C_{11} X_1 + C_{12} X_2 + C_{13} X_3$$

PROVIDES THE ORIENTATION OF THE NEW AXIS X'_1 AND C_{11} IS THE COSINE OF THE ANGLE BETWEEN X'_1 AND X_1 , C_{12} THE ^{COSINE OF THE} ANGLE BETWEEN X'_1 AND X_2 AND C_{13} THE COSINE OF THE ANGLE BETWEEN X'_1 AND X_3 . IN OTHER WORDS C_{ij} REPRESENT THE COMPONENTS OF A UNIT VECTOR ALONG X'_1 RELATIVE TO THE ORIGINAL AXES X_j .

THEREFORE, THE SUM OF THEIR SQUARES $C_{11}^2 + C_{12}^2 + C_{13}^2$ MUST BE 1!

BY SIMILAR ANALYSIS WE CAN SAY THE SUM OF THE SQUARES OF THE ELEMENTS IN ANY ROW OF THE MATRIX C_{ij} IS UNITY!

(2) LET'S EXAMINE THE MEANING OF THE ELEMENTS OF ANY COLUMN IN

$[C_{ij}]$ - FOR EXAMPLE, $\begin{matrix} C_{12} \\ C_{22} \\ C_{32} \end{matrix}$

C_{12} IS THE COSINES OF THE ANGLE BETWEEN X'_1 AND X_2
 C_{22} " " " " " " " " X'_2 AND X_2
 C_{32} " " " " " " " " X'_3 AND X_2

THESE ARE THE DIRECTION COSINES OF X_2 IN THE ORIGINAL COORDINATE SYSTEM. THE SUM OF THEIR SQUARES MUST BE UNITY AND, IN GENERAL THE SUM OF THE SQUARES OF ELEMENTS IN ANY COLUMN IS UNITY

NOTE, HOWEVER, THAT THE RELATIONS IN (1) AND (2) HAVE LIMITATIONS: THEY INVOLVE THE SQUARES OF THE COSINES AND THEREFORE CANNOT BE USED TO DETERMINE THEIR SIGNS (WHICH, BEING COSINES, CAN BE \oplus OR \ominus)

(3) IF THE ROW C_{1j} IN THE DIRECTION COSINE MATRIX REPRESENTS THE COMPONENTS THE DIRECTION COSINES OF X'_1 RELATIVE TO X_1, X_2, X_3 AND, IF THE ROW C_{2j} REPRESENTS THE DIRECTION COSINES OF X'_2 RELATIVE TO X_1, X_2, X_3 WE HAVE AT HAND THE COMPONENTS OF TWO UNIT VECTORS WHICH, IN CARTESIAN COORDINATE SYSTEMS, MUST BE ORTHOGONAL! THEREFORE, THE SCALAR (OR "DOT") PRODUCT OF THESE TWO VECTORS HAS TO BE ZERO!

$$\text{THUS } C_{11} \cdot C_{21} + C_{12} \cdot C_{22} + C_{13} \cdot C_{23} = 0$$

AND THE SUM OF THE PRODUCTS OF CORRESPONDING ELEMENTS IN ANY PAIR OF ROWS IN C_{ij} MUST BE ZERO

(4) BY SIMILAR ARGUMENT, COLUMNS C_{i1} AND C_{i2} REPRESENT THE COMPONENTS OF X_1 AND X_2 RELATIVE TO THE NEW COORDINATE SYSTEM X'_1, X'_2, X'_3 AND THE SUM OF THE PRODUCTS OF CORRESPONDING ELEMENTS IN ANY PAIR OF COLUMNS IN C_{ij} MUST BE ZERO

(5) THE TRANSFORMATION OF AXES $X_1, X_2, X_3 \rightarrow X'_1, X'_2, X'_3$ INVOLVES NO DISTORTION AND IS TERMED A "MEASURE PRESERVING" TRANSFORMATION. THE MATRIX $[C_{ij}]$ IS WHAT IS TERMED A UNITARY MATRIX AND HAS SEVERAL PROPERTIES, USEFUL IN PROBLEMS, THAT WE WILL STATE WITHOUT PROOF

- THE VALUE OF THE DETERMINANT $|C_{ij}| = \pm 1$
+1 IF THE NEW COORDINATE SYSTEM HAS NOT CHANGED CHIRALITY (THAT IS, RIGHT-HANDED \rightarrow RIGHT HANDED OR LEFT HANDED \rightarrow LEFT HANDED) AND -1 IF THE CHIRALITY IS CHANGED (RIGHT \rightarrow LEFT HANDED OR LEFT \rightarrow RIGHT HANDED)

• ANOTHER VERY USEFUL, LABOR-SAVING PROPERTY OF UNITARY MATRICES CONCERNS THE REVERSE TRANSFORMATION, THAT IS, IF

$$X_i' = C_{ij} X_j$$

WHAT IF WE CHANGE OUR MIND AND WANT TO GO BACK FROM THE NEW COORDINATE SYSTEM TO THE ORIGINAL ONE? THAT RELATION IS SPECIFIED BY THE RELATION

$$X_i = [C_{ij}]^{-1} X_j'$$

WHERE $[C_{ij}]^{-1}$ IS THE INVERSE MATRIX. FOR SIMPLE TRANSFORMATIONS OF AXES ONE CAN OFTEN WRITE X_i IN TERMS OF X_j' BY INSPECTION AND PICK OFF THE ELEMENTS OF $[C_{ij}]^{-1}$ DIRECTLY.

ONE CAN ALSO EVALUATE $[C_{ij}]^{-1}$ MORE GENERALLY, BUT -----

THIS INVOLVES AN UNPLEASANT AMOUNT OF EVALUATION OF 3x3 DETERMINANTS FOR A TOTAL OF NINE ELEMENTS!

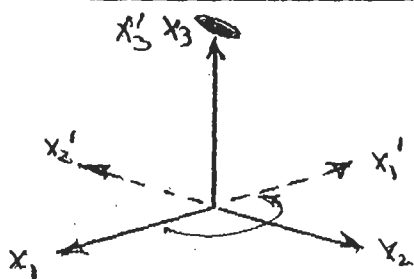
THE GREAT ASSISTANCE OF A UNITARY MATRIX IN THIS SITUATION

IS THAT $[C_{ij}]^{-1} = [C_{ji}]$

NOTE THAT $[C_{ji}]$ IS SIMPLY THE 3x3 ARRAY OF COEFFICIENTS FLIPPED ACROSS THE DIAGONAL THAT RUNS FROM UPPER LEFT TO LOWER RIGHT. THIS IS CALLED THE TRANSPOSE OF THE MATRIX $[C_{ij}]$ AND IS WRITTEN EITHER $[C_{ij}]^{\sim}$ OR $[C_{ij}]^T$ BY VARIOUS WRITERS. (WE SHALL USE THE FORMER NOTATION.)

OBVIOUSLY SPECIFYING $[C_{ij}]^{\sim}$ IS SOMETHING THAT WE CAN DO IN A TWINKLING OF THE EYE BY COMPARISON WITH THE EVALUATION OF NINE RATIOS OF 3x3 DETERMINANTS !!

MOMENT OF REASSURANCE



ALL THIS MAY SEEM RATHER DAUNTING, BUT WE SHALL SHORTLY USE THIS FORMALISM TO OBTAIN CONSTRAINTS IMPOSED ON PROPERTY TENSORS BY CRYSTAL SYMMETRY. FOR A 2-FOLD AXIS, FOR EXAMPLE,

$$\begin{cases} x_1' = -x_1 \\ x_2' = -x_2 \\ x_3' = x_3 \end{cases}$$

SO FOR THIS TRANSFORMATION $[C_{ij}] = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

STILL MORE TRANSFORMATION MACHINERY

TRANSFORMATION OF A SECOND RANK TENSOR

SUPPOSE A GENERALIZED VECTOR DISPLACEMENT, q_i , IS RELATED TO A GENERALIZED VECTOR FORCE, p_j , BY A SECOND RANK TENSOR a_{ij} :

$$q_i = a_{ij} p_j$$

IF THE COORDINATE SYSTEM X_i RELATIVE TO WHICH THE COMPONENTS OF \vec{q} AND \vec{p} ARE DEFINED IS CHANGED TO SOME NEW SET OF BASIS VECTORS X'_i SPECIFIED BY THE DIRECTION COSINE SCHEME $[C_{ij}]$, THEN THE COMPONENTS OF \vec{q} AND \vec{p} TAKE ON NEW NUMERICAL VALUES q'_i AND p'_j . OUR TENSOR RELATION, HOWEVER, SAYS THAT EACH COMPONENT OF \vec{q} IS GIVEN BY A LINEAR COMBINATION OF ALL THREE COMPONENTS OF \vec{p} . IF THE COMPONENTS OF \vec{q} AND \vec{p} HAVE CHANGED THEIR NUMERICAL VALUES, THE ELEMENTS OF THE TENSOR WHICH RELATES THEM MUST ALSO CHANGE TO SOME NEW VALUES SUCH THAT

$$q'_i = a'_{ij} p'_j$$

HOW MAY a'_{ij} BE EVALUATED IN TERMS OF THE ORIGINAL ELEMENTS a_{ij} AND THE DIRECTION COSINE SCHEME $[C_{ij}]$ WHICH SPECIFIES THE CHANGE OF REFERENCE AXES?

LET'S BEGIN BY WRITING THE NEW COMPONENTS q'_i IN TERMS OF THE ORIGINAL COMPONENTS q_j

$$q'_i = C_{im} q_m$$

q_m IS DETERMINED BY THE TENSOR RELATION WHICH, FOR THE m^{th} COMPONENT OF \vec{p} , SPECIFIES $q_m = a_{ml} p_l$. THUS

$$q'_i = C_{im} [a_{ml} p_l]$$

NOW, IN ORDER TO OBTAIN AN EXPRESSION WHICH HAS q' ON THE LEFT AND p' ON THE RIGHT, LET'S WRITE p_l IN TERMS OF THE NEW COMPONENTS OF \vec{p} . IF $[p'_l] = [C_{lj}][p_j]$

THEN $[p_l] = [C_{lj}]^{-1} [p'_j] = [C_{lj}] [p'_j] = [C_{jl}] [p'_j]$ AS THE INVERSE OF A UNITARY MATRIX IS EQUAL TO THE TRANSPOSE OF THE MATRIX. SUBSTITUTING $C_{jl} p'_j$ FOR p_l WE OBTAIN

$$q'_i = C_{im} [a_{ml} (C_{jl} p'_j)]$$

THE ABOVE EXPRESSION REPRESENTS A TRIPLE SUMMATION (OVER $j, l \& m$, AS THESE SUBSCRIPTS ARE REPEATED) OF A PRODUCT OF FOUR QUANTITIES. WE MAY PERFORM THE SUMMATION IN ANY ORDER WE WISH AND, SIMILARLY, ARRANGE THE PRODUCT IN ANY

DESIRED ORDER. THEREFORE, LETS WRITE BY REARRANGEMENT

$$q'_i = [C_{im} C_{jl} a_{ml}] p'_j$$

BUT, BY DEFINITION,

$$q'_i = a'_{ij} p'_j$$

THUS

$$a'_{ij} = C_{im} C_{jl} a_{ml}$$

THIS EXPRESSION IS A DOUBLE SUMMATION OVER m & l ; THUS EACH ELEMENT IN THE NEW TENSOR $[a'_{ij}]$ IS GIVEN BY A LINEAR COMBINATION OF EVERY ONE OF THE NINE ELEMENTS OF THE ORIGINAL TENSOR $[a_{ml}]$

NOTE THAT m & l HAVE NO PHYSICAL SIGNIFICANCE AND FUNCTION MERELY AS INDICES OF SUMMATION; THEY ARE "DUMMY INDICES". THE INDICES i & j , IN CONTRAST, (WHICH APPEAR, RESPECTIVELY, AS THE FIRST INDEX IN THE TWO ELEMENTS OF THE DIRECTION COSINE MATRIX AND THE PRODUCT) DO HAVE ABSOLUTE SIGNIFICANCE; THEY ARE SPECIFIED BY THE SUBSCRIPTS OF THE PARTICULAR TRANSFORMED TENSOR ELEMENT a'_{ij} WHICH ONE WISHES TO EVALUATE.

TRANSFORMATION OF HIGHER-RANK TENSORS

THE ABOVE RESULT MAY BE EXTENDED, USING SIMILAR REASONING, TO THE LAW FOR TRANSFORMATION OF A TENSOR OF ANY RANK. THE RESULT IS

$$a'_{ijkl\dots} = C_{iI} C_{jJ} C_{kK} C_{lL} \dots a_{IJKL\dots}$$

i, j, k, l, \dots ARE "REAL":
DETERMINED BY THE ELEMENT
YOU WISH TO EVALUATE.

THE NUMBER OF DIRECTION
COSINES IN THE COEFFICIENT IS EQUAL
TO THE RANK OF THE TENSOR.

I, J, K, L, \dots ARE "DUMMY"
INDICES OF SUMMATION.

NOTE THAT, INDEPENDENT OF THE RANK OF THE TENSOR, EACH NEW, TRANSFORMED ELEMENT IS GIVEN BY A LINEAR COMBINATION OF EVERY ELEMENT OF THE ORIGINAL TENSOR.

THE COEFFICIENT IN FRONT OF EACH ORIGINAL ELEMENT IS A PRODUCT OF DIRECTION COSINES, EQUAL IN NUMBER TO THE RANK OF THE TENSOR.

THUS, GENERAL TRANSFORMATION OF, SAY, THE ELASTIC STIFFNESSES (A 4TH RANK TENSOR) REQUIRES A SUMMATION OF A PRODUCT OF FIVE TERMS FOR ALL $9 \times 9 = 81$ ELEMENTS OF THE TENSOR, AND REPETITION OF THE PROCESS 81 TIMES FOR THE NEW ELEMENTS! $(5 \times 81) \cdot 81 = 32,805$ TERMS!