

### 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

$$(1) \quad \left\{ \begin{array}{l} \sigma_1 = C_{11} \epsilon_1 + C_{12} \epsilon_2 + C_{12} \epsilon_3 \\ \sigma_2 = C_{12} \epsilon_1 + C_{11} \epsilon_2 + C_{12} \epsilon_3 \\ \sigma_3 = C_{12} \epsilon_1 + C_{12} \epsilon_2 + C_{11} \epsilon_3 \\ \sigma_4 = C_{44} \epsilon_4 \\ \sigma_5 = C_{44} \epsilon_5 \\ \sigma_6 = C_{44} \epsilon_6 \end{array} \right.$$

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

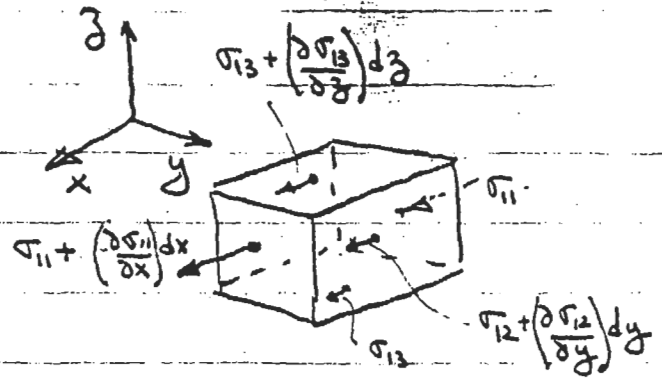
AS WE WANT AN EQUATION WHICH INVOLVES DISPLACEMENTS, SUBSTITUTE FOR  $\epsilon_i$  ITS DEFINITION IN TERMS OF DISPLACEMENT, NAMELY

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

REPLACING  $\epsilon_i$  BY THESE DEFINITIONS GIVES

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

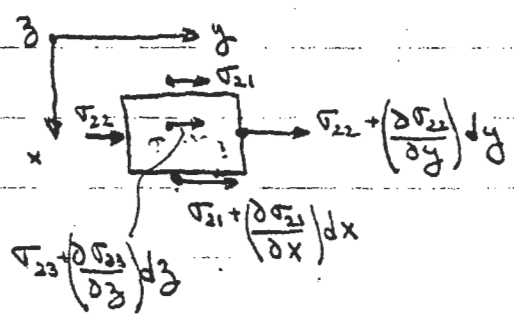
NOW CONSIDER A VOLUME ELEMENT IN THE SOLID WITH DENSITY  $\rho$  AND EDGES  $dx, dy, dz$ . FOR EACH DIRECTION ( $x, y, z$ ) WE FIND THE NET FORCE ON THE ELEMENT ( $\sigma \times \text{AREA}$ ) AND SET IT EQUAL TO MASS  $\times$  ACCELERATION.



FOR THE X-DIRECTION:

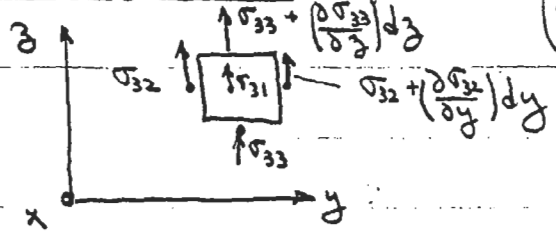
$$\underbrace{\left(\frac{\partial \sigma_{11}}{\partial x}\right) dx}_{\text{NET F/UNIT A}} \cdot \underbrace{dy dz}_{dA} + \underbrace{\left(\frac{\partial \sigma_{12}}{\partial y}\right) dy}_{\text{NET F/UNIT A}} \cdot \underbrace{dx dz}_{dA} + \underbrace{\left(\frac{\partial \sigma_{13}}{\partial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

SIMILARLY, FOR THE y DIRECTION



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

FOR THE z DIRECTION



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

COMBINING EQUATIONS AND REPLACING TENSOR DESCRIPTION OF  $\sigma_{ij}$  BY MATRIX ELEMENT  $\sigma_k$

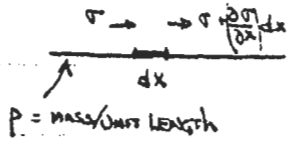
$$(3) \begin{cases} \frac{\partial \sigma_1}{\partial x} + \frac{\partial \sigma_6}{\partial y} + \frac{\partial \sigma_5}{\partial z} = \rho \frac{\partial^2 u}{\partial t^2} \\ \frac{\partial \sigma_6}{\partial x} + \frac{\partial \sigma_2}{\partial y} + \frac{\partial \sigma_4}{\partial z} = \rho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

SUBSTITUTING EXPRESSIONS FOR  $\sigma_i$  IN TERMS OF DERIVATIVES OF DISPLACEMENT [Eqs (2)]

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

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



$$e = \frac{\partial u}{\partial x} \quad \therefore \rho dx \frac{\partial^2 u}{\partial t^2} = \frac{\partial \sigma}{\partial x} dx$$

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

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

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

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

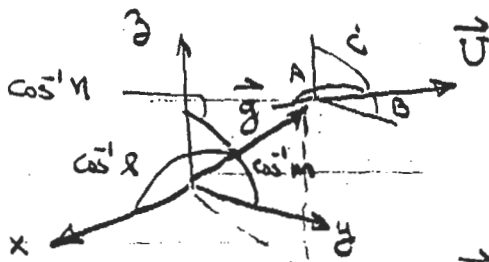
$$= \frac{2\pi}{\lambda} i (vt - x)$$

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

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

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

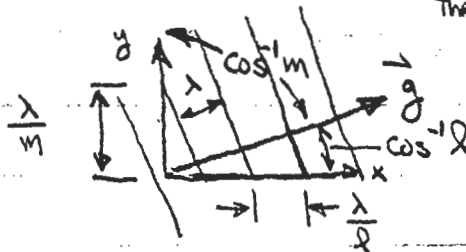


AN APPROPRIATE SOLUTION IS

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

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

with  $\begin{cases} u = UA \\ v = UB \\ w = UC \end{cases}$



LET US NOW SUBSTITUTE OUR TRIAL SOLUTION (5) INTO THE WAVE EQUATIONS (4). NOTE THAT  $\partial_{\partial x}(e^{ax}) = a e^{ax}$ , 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.

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

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.:

$$\begin{vmatrix} [C_{11}l^2 + C_{44}(m^2+n^2) - \rho v^2] & (C_{12}+C_{44})lm & (C_{12}+C_{44})ln \\ (C_{12}+C_{44})ml & [C_{11}m^2 + C_{44}(n^2+l^2) - \rho v^2] & (C_{12}+C_{44})mn \\ (C_{12}+C_{44})nl & (C_{12}+C_{44})nm & [C_{11}n^2 + C_{44}(l^2+m^2) - \rho v^2] \end{vmatrix} = 0$$

THIS IS AGAIN AN EIGENVALUE PROBLEM. EXPANDING THE DETERMINANT LEADS TO A 3<sup>RD</sup> ORDER EQUATION IN  $(\rho v^2)$  - 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  $l, m$ , AND  $n$ .

EACH OF THE THREE EIGENVALUES FOR  $\rho v^2$  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,  $\rho$
- 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