STRESS ON SECONDARY SLIP SYSTEMS IN LiF <111>

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I. PROBLEM:

Plane waves are propagated through a crystal in a specified direction. Call this direction X_1' in a set of coordinates X_1', X_2', X_3'. Slip systems on which plastic deformation occurs are given. They are N_s in number and are identified by an index α. If the orientation of the X'-axes with respect to the crystal axes, X, is given, and if elastic constants in crystal coordinates C_{ijkl} are given, find the shear stress acting on each slip system. The coordinates X' are chosen so that propagation of a pure longitudinal disturbance is possible.

II. FORMAL SOLUTION*

1. Determine the coefficients A_{ij}' which govern the transformation of X coordinates to X' coordinates

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

$$A_{ij} = \vec{N}_i' \cdot \vec{N}_j$$

where $\vec{N}_i'$ and $\vec{N}_j$ are unit vectors along the X_i' and X_j axes, respectively.

2. Determine the coefficients ${}^{\alpha}A_{ij}''$ of transformation between the ${}^{\alpha}X''$ axes of the α slip system and the crystal coordinate, X.

$${}^{\alpha}X_i'' = {}^{\alpha}A_{ij}'' X_j$$

$${}^{\alpha}A_{ij}'' = {}^{\alpha}\vec{N}_i'' \cdot {}^{\alpha}\vec{N}_j$$

For comparison with J. N. Johnson, use the convention that

${}^{\alpha}X_3''$ is normal to the α slip-plane

${}^{\alpha}X_1''$ is parallel to the α slip direction.

* Reference: J. N. Johnson, J. Appl. Phys. 43, 2074 (1972).
J. N. Johnson, O. E. Jones and T. E. Michaels, J. Appl. Phys. 41, 2330 (1970).

3. Compute the coefficients of transformation, ${}^{\alpha}A''^{\prime}_{ij}$, between the X and ${}^{\alpha}X''$ axes

$${}^{\alpha}X''_{k} = {}^{\alpha}A''^{\prime}_{kj} \; X'_{j}$$

$${}^{\alpha}A''^{\prime}_{ij} = {}^{\alpha}\vec{N}''_{i} \cdot \vec{N}'_{j} = {}^{\alpha}a''_{il} a'_{jl}$$

4. Compute the elastic constants C'_{ijkl} in the laboratory coordinates, X':

$$C'_{ijkl} = A'_{im} \, A'_{jn} \, A'_{kp} \, A'_{lq} \, C_{mnpq}$$

Note: Normally the matrix constants C_{mn} are given.

C_{ijkl} can be determined by the following procedure:

if $i = j$ then $i = j = m$

if $i \neq j$ then $m = 9 - i - j$

so $C_{ijkl} = C_{mn}$ where $m = i$ if $i = j$

$m = 9 - i - j, \; i \neq j$

$n = k$ if $k = l$

$n = 9 - k - l$ if $k \neq l$

5. If strains are purely elastic, go to 6.

If strains are both elastic and plastic, assume that stresses are supported by elastic strains alone. Then let T = total strain, E = elastic strain and Π = plastic strain, with

$$T = E + \Pi \, .$$

Let S = stress and consider stress-strain relations for the laboratory coordinates:

$$S'_{ij} = C'_{ijkl} \, E'_{kl} = C'_{ijkl} T'_{kl} - C'_{ijkl} \, \Pi'_{kl}$$

Where Π'_{kl} is the total plastic strain component resulting from slip on the various active slip systems:

$$\Pi'_{kl} = \sum_{\alpha} {}^{\alpha}\Pi'_{kl}$$

where ${}^{\alpha}\Pi'_{kl}$ is the kl component of plastic strain in the X' system resulting from slip on the α-slip system. Plastic strain occurs only on the slip systems, and the only non-vanishing components of ${}^{\alpha}\Pi''_{kl}$ are ${}^{\alpha}\Pi''_{13} = {}^{\alpha}\Pi''_{31}$ because of the way in which the X" axes were chosen.

Define $\quad {}^{\alpha}\gamma/2 \equiv {}^{\alpha}\Pi''_{13} = {}^{\alpha}\Pi''_{31}$

(See internal report 75-01, Eq. (7).)

With this definition:

$$\begin{aligned} {}^{\alpha}\Pi''_{mn} &= (1/2)(\delta_{1m}\ \delta_{3n} + \delta_{3m}\ \delta_{1n})^{\alpha}\gamma \\ &= \frac{{}^{\alpha}\gamma}{2} \text{ if } m = 1 \text{ and } n = 3 \text{ or } m = 3 \text{ and } n = 1 \\ &= 0 \text{ otherwise} \end{aligned}$$

Then, since ${}^{\alpha}X''_i = {}^{\alpha}A''{}'_{ij}\ X'_j$

$$\begin{aligned} X'_j &= {}^{\alpha}X''_i\,{}^{\alpha}A''{}'_{ij} \\ {}^{\alpha}\Pi'_{kl} &= {}^{\alpha}\Pi''_{mn}\ {}^{\alpha}A''{}'_{mk}\ {}^{\alpha}A''{}'_{nl} \\ &= (1/2)^{\alpha}A''{}'_{mk}\ {}^{\alpha}A''{}'_{nl}\ (\delta_{1n}\ \delta_{3n} + \delta_{3m}\ \delta_{1n})^{\alpha}\gamma \\ \Pi'_{kl} &= (1/2)\sum_{\alpha}{}^{\alpha}A''{}'_{mk}\ {}^{\alpha}A''{}'_{nl}\ (\delta_{1m}\ \delta_{3n} + \delta_{3m}\ \delta_{1n})^{\alpha}\gamma \end{aligned}$$

Then

$$S'_{ij} = C'_{ijkl}\ T'_{kl} - (1/2)\sum_{\alpha} C'_{ijkl}\ {}^{\alpha}A''{}'_{mk}\ {}^{\alpha}A''{}'_{nl}\ (\delta_{1m}\ \delta_{3n} + \delta_{3m}\ \delta_{1n})^{\alpha}\gamma \qquad (1)$$

The stress on the slip system α is calculated in §7 below.

6. If strains are purely elastic, the only non-vanishing component of strain for a P-wave is T'_{11}. Then

$$\begin{aligned} S'_{ij} &= C'_{ij11}\ T'_{11} \\ &= \frac{C'_{ij11}}{C'_{1111}}\ S'_{11} \end{aligned}$$

Set $S'_{11} = 1$ and go to §7 to calculate the stress on slip systems.

For plane shear waves, the only non-vanishing components of strain are T'_{13}, T'_{31}, T'_{12}, T'_{21}. If the wave is polarized, either the first or second pair exists, but not the other, e.g. if

$$T'_{12} = T'_{21} = 0$$

$$S'_{13} = C'_{1313}\, T'_{13} + C'_{1331}\, T'_{31}$$

$$= 2\, C'_{1313}\, T'_{13}$$

$$S'_{mn} = 2\, C'_{mn13}\, T'_{13} = \frac{C'_{mn13}}{C'_{1313}}\, S'_{13}$$

Set $S'_{13} = \frac{1}{C'}$ and go to §7 to calculate the stress on slip systems

7. $$^{\alpha}S''_{13} = \text{stress on slip system } \alpha$$

$$= {}^{\alpha}A''{}'_{1m}\; {}^{\alpha}A''{}'_{3n}\; S'_{mn} \qquad (2)$$

where S'_{mn} is obtained from §5 or §6.

SUMMARY

In the elastic plane wave case the stresses on slip systems are multiples of the wave stress in the laboratory system and the proportionality constant is independent of strain. If plastic deformation exists, the ratio depends upon both total and plastic strain and must be calculated incrementally as the flow equations are solved.

III. COMPUTATIONAL SCHEME

The object is to compute the stresses ${}^{\alpha}S''_{13}$. The formula to be evaluated is given by Eq. (2) of Section II.

Define: $$R^{\alpha}_{kl} = {}^{\alpha}A''^{\prime}_{mk}\ {}^{\alpha}A''^{\prime}_{nl}\ (\delta_{1m}\ \delta_{3n} + \delta_{3m}\ \delta_{1n}) \qquad (3.1)$$

$$U^{\alpha}_{ij} = C'_{ijkl}\ R^{\alpha}_{kl} \qquad (3.2)$$

$$Q'_{ij} = \sum_{\alpha} {}^{\alpha}\gamma U^{\alpha}_{ij} \qquad (3.3)$$

$$P'_{ij} = C'_{ijkl}\ T'_{kl} \qquad (3.4)$$

$$S'_{ij} = P'_{ij} - (1/2)Q'_{ij}$$

Then

$${}^{\alpha}S''_{13} = {}^{\alpha}A''^{\prime}_{1i}\ A''^{\prime}_{3j}\ S'_{ij}$$

Computations are done in the following sequence:

(i) $\quad {}^{\alpha}A''^{\prime}_{ij} = {}^{\alpha}A''_{il}\ A'_{jl}$

(ii) $\quad C'_{ijkl} = A'_{im}\ A'_{jn}\ A'_{kp}\ A'_{lq}\ C_{mnpq}$

(iii) $\quad R^{\alpha}_{kl}$ from Eq. (3.1)

(iv) $\quad U^{\alpha}_{ij}$ from Eq. (3.2)

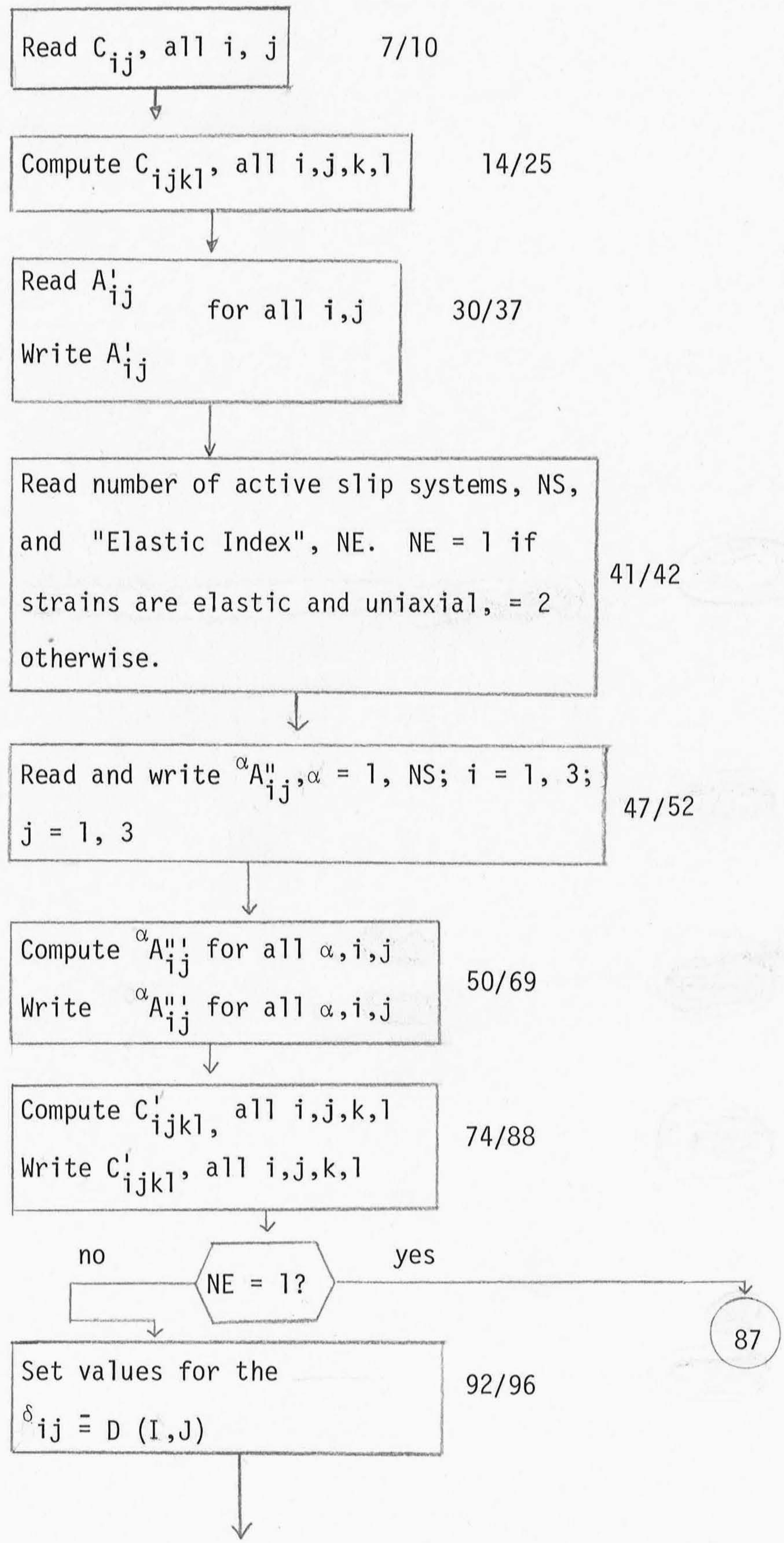
(v) $\quad Q'_{ij}$ from Eq. (3.3)

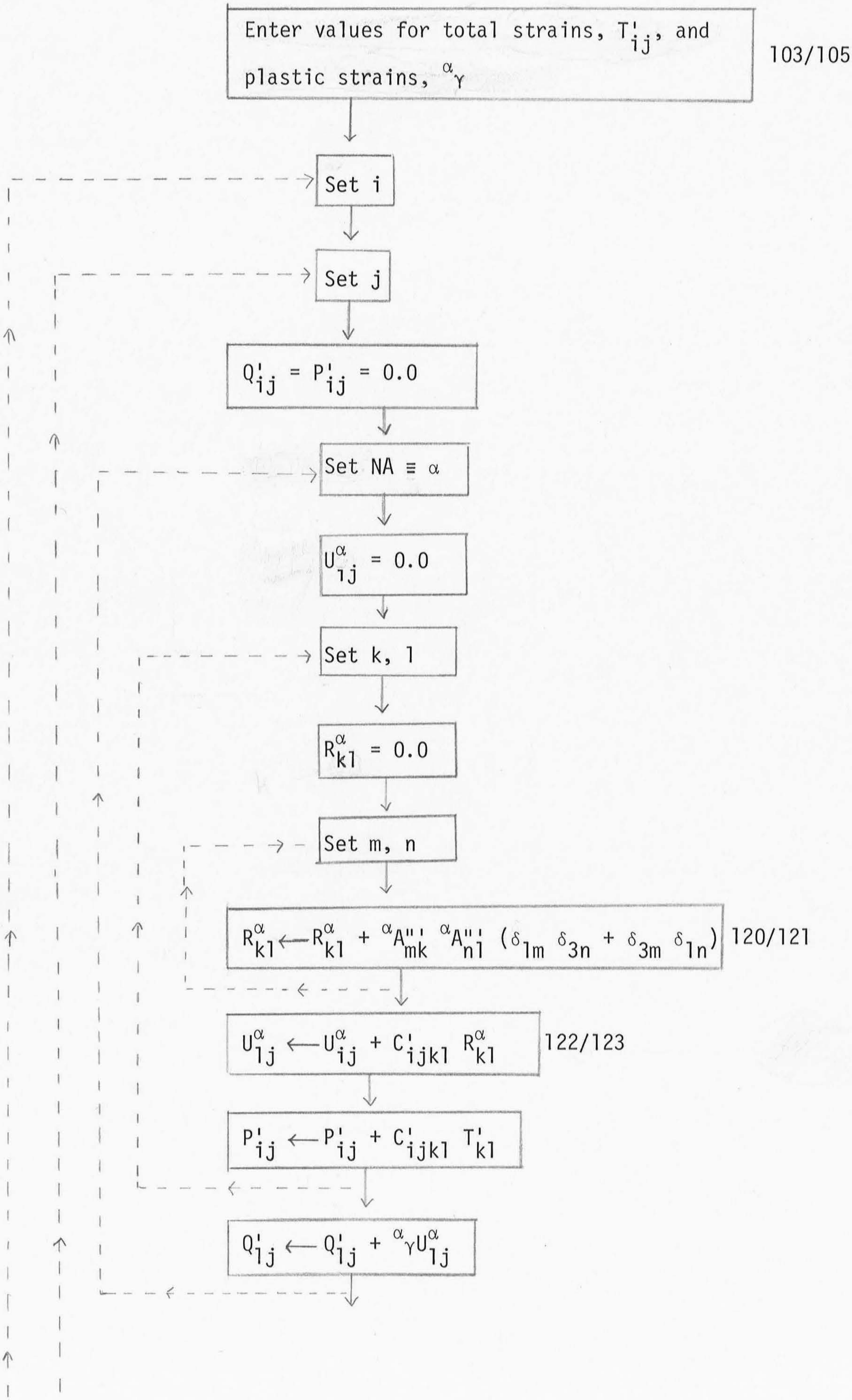
(vi) $\quad P'_{ij}$ from Eq. (3.4)

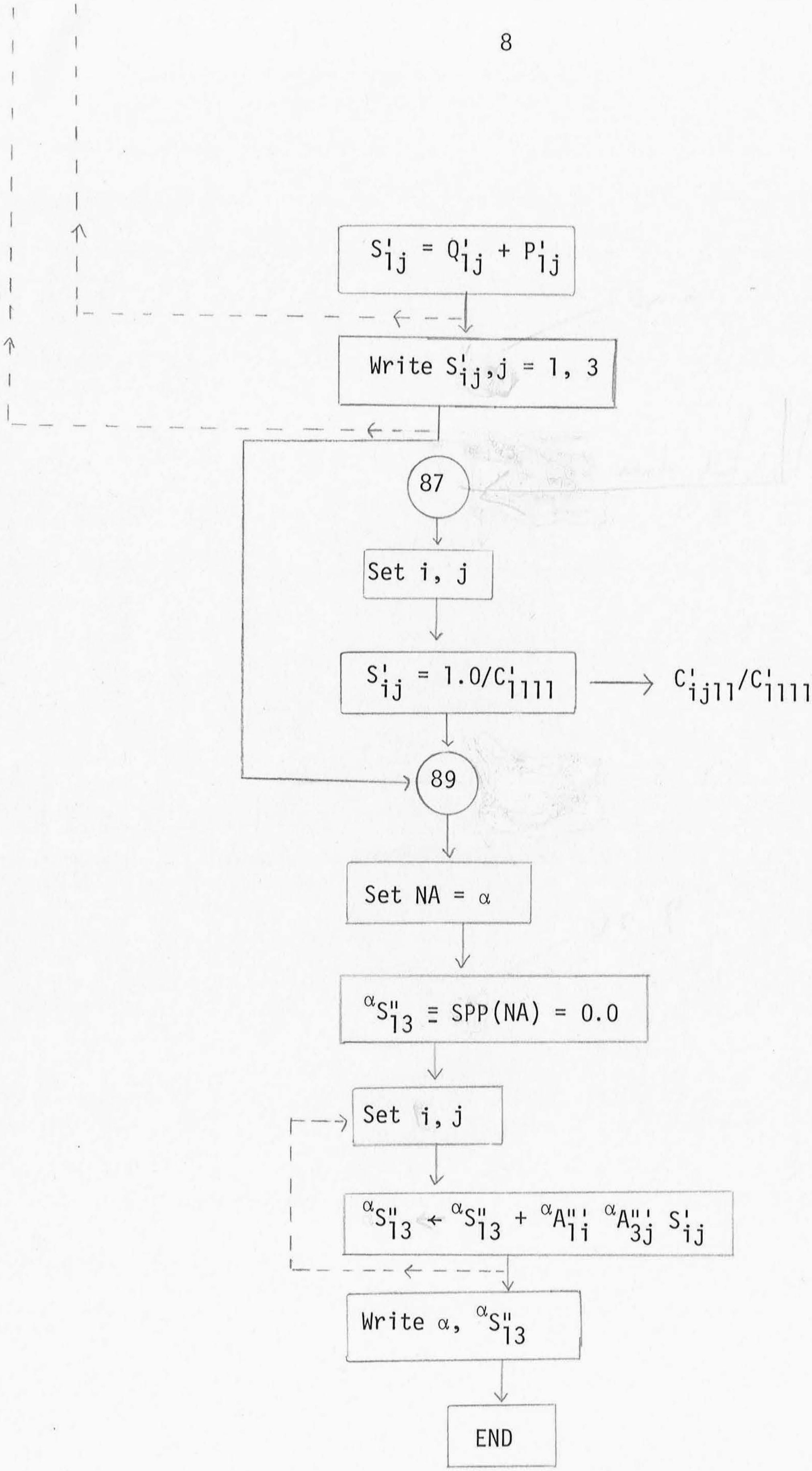
$\quad S'_{ij}$, ${}^{\alpha}S''_{13}$ for each α

If strain is assumed to be totally elastic, as in an elastic precursor, steps (iii) - (vi) are passed and S'_{ij} is set equal to C'_{ij11} / C'_{1111}. Computation of ${}^{\alpha}S''_{13}$ than proceeds as before. The result is the ratio of shear stress on the slip system to S'_{11}.

IV. FLOW CHART




Enter values for total strains, T'_{ij}, and plastic strains, ${}^{\alpha}\gamma$
103/105
Set i
Set j
$Q'_{ij} = P'_{ij} = 0.0$
Set NA ≡ α
$U^{\alpha}_{ij} = 0.0$
Set k, l
$R^{\alpha}_{kl} = 0.0$
Set m, n
$R^{\alpha}_{kl} \leftarrow R^{\alpha}_{kl} + {}^{\alpha}A'''_{mk}\ {}^{\alpha}A'''_{nl}\ (\delta_{1m}\ \delta_{3n} + \delta_{3m}\ \delta_{1n})$
120/121
$U^{\alpha}_{lj} \leftarrow U^{\alpha}_{ij} + C'_{ijkl}\ R^{\alpha}_{kl}$
122/123
$P'_{ij} \leftarrow P'_{ij} + C'_{ijkl}\ T'_{kl}$
$Q'_{lj} \leftarrow Q'_{lj} + {}^{\alpha}\gamma U^{\alpha}_{lj}$


S'ij = Q'ij + P'ij
Write S'ij, j = 1, 3
87
Set i, j
S'ij = 1.0/C'1111
C'ij11/C'1111
89
Set NA = α
αS"13 ≡ SPP(NA) = 0.0
Set i, j
αS"13 ← αS"13 + αA"1i αA"3j S'ij
Write α, αS"13
END

V. Program Listing. #TRANS3 on USER GXD

```
$JOB
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION TP(3,3), GAMMA(6)
      DIMENSION APP (6,3,3), AP(3,3), C(3,3,3,3)
      DIMENSION APPP(6,3,3), CP(3,3,3,3), R(6,3,3)
      DIMENSION U(6,3,3), QP(3,3), PP(3,3)
      DIMENSION SP(3,3), CM(6,6),D(3,3), SPP(6)
C     READ ELASTIC CONSTANTS IN MATRIX FORM FOR CRYSTAL COORDINATES
      DO 1 I=1,6
      READ (5,200)(CM(I,J), J=1,6)
  200 FORMAT (6F8.5)
    1 CONTINUE
      DO 61 I=1,6
      WRITE (6,110)I,(CM(I,J),J=1,6)
  110 FORMAT (2X,I2,6F8.5)
   61 CONTINUE
C
C     SET ELASTIC CONSTANTS IN TENSOR FORM
C
      DO 2 I=1,3
      DO 2 J=1,3
      DO 2 K=1,3
      DO 2 L=1,3
      IF(I.EQ.J)GO TO 3
      M=9-I-J
      GO TO 22
    3 M=I
   22 IF(K.EQ.L)GO TO 21
      N=9-K-L
      GO TO 4
   21 N=K
    4 C(I,J,K,L)=CM(M,N)
    2 CONTINUE
      WRITE (6,170)
      DO 71 I=1,3
      DO 71 J=1,3
      DO 71 K=1,3
      WRITE (6,100)I,J,K,(C(I,J,K,L),L=1,3)
   71 CONTINUE
  170 FORMAT (15X,'C(I,J,K,L)'/3X,'I J K',10X,'L=',
     *'1',12X,'L=2',12X,'L=3')
C
C     READ TRANSFORMATION MATRIX FROM X TO X-PRIME
C     I.E. X(I)-PRIME=AP(I,J)*X(I)
C
      DO 20 I=1,3
      READ (5,201)(AP(I,J), J=1,3)
  201 FORMAT (3F15.7)
      WRITE (6,103) I, (AP(I,J),J=1,3)
  103 FORMAT (2X, I2, 3F15.7)
   20 CONTINUE
C     IF NE=1, TP(I,J)=0 UNLESS I = J = (ELASTIC)
C     READ NS, THE NO. OF ACTIVE SLIP SYSTEMS, AND NE
C
      READ (5,209) NS, NE
  209 FORMAT (2I2)
C
C     READ TRANSFORMATION MATRICES FROM X TO X-DOUBLE PRIME
C     FOR EACH SLIP SYSTEM, ALPHA.  NA DENOTES THE SYSTEM ALPHA.
C
```

```
   31 CONTINUE
      READ (5,201)(GAMMA(NA),NA=1,NS)
C
C     CALCULATE STRESSES IN LAB (PRIMED) COORDINATES,SP(I,J)
C
      DO 33 I=1,3
      DO 32 J=1,3
      QP(I,J)=0.0
      PP(I,J)=0.0
      DO 42 NA=1,NS
      U(NA,I,J)=0.0
      DO 41 K=1,3
      DO 41 L=1,3
      R(NA,K,L)=0.0
      DO 40 M=1,3
      DO 40 N=1,3
   40 R(NA,K,L)=R(NA,K,L)+APPP(NA,M,K)*
     +APPP(NA,N,L)*(D(1,M)*D(3,N)+D(3,M)*D(1,N))
      U(NA,I,J)=U(NA,I,J)+CP(I,J,K,L)*
     +R(NA,K,L)
   41 PP(I,J)=PP(I,J)+CP(I,J,K,L)*TP(K,L)
   42 QP(I,J)=QP(I,J)+GAMMA(NA)*U(NA,I,J)
      SP(I,J)=PP(I,J)-0.5*QP(I,J)
   32 CONTINUE
      WRITE (6,104)I,(SP(I,J),J=1,3)
   33 CONTINUE
C
C     CALCULATE SHEAR STRESS ON EACH SLIP
C     SYSTEM S''(NA,1,3)
C
      GO TO 89
   87 DO 88 I=1,3
      DO 88 J=1,3
   88 SP(I,J)=CP(I,J,1,1)/CP(1,1,1,1)
   89 CONTINUE
      WRITE (6,108)
  108 FORMAT (2X,'SP(I,J)')
      DO 35 I=1,3
   35 WRITE (6,103)I,(SP(I,J),J=1,3)
      DO 44 NA=1,6
      SPP(NA)=0.0
      DO 43 I=1,3
      DO 43 J=1,3
      SPP(NA)=SPP(NA)+APPP(NA,1,I)*APPP(NA,3,J)
     +*SP(I,J)
   43 CONTINUE
      WRITE (6,107) NA,SPP(NA)
  107 FORMAT (2X,'NA=', I2, 'SPP(NA)= ',F14.7)
   44 CONTINUE
      STOP
      END
```

```
      DO 30 NA=1,NS
      DO 30 I=1,3
      READ (5,201)(APP(NA,I,J),J=1,3)
      WRITE (6,104) NA,I, (APP(NA,I,J), J=1,3)
  104 FORMAT (2X, 2I2, 3F15.7)
   30 CONTINUE
C
C     COMPUT A''', THE TRANSFORMATION MATRIX BETWEEN X'
C     AND X'': X''(I)=A'''(I,J)*X'(J) FOR EACH
C     SLIP SYSTEM ALPHA=NA
C
      DO 9 NA=1, NS
      DO 10 I=1,3
      DO 8 J=1,3
      APPP(NA,I,J)=0.0
      DO 5 L=1,3
      APPP(NA,I,J)=APPP(NA,I,J)+APP(NA,I,L)*AP(J,L)
    5 CONTINUE
    8 CONTINUE
      WRITE (6,102) NA,I,(APPP(NA,I,J), J=1,3)
  102 FORMAT (2X,2I2,3F15.7)
   10 CONTINUE
    9 CONTINUE
C
C     CALCULATE ELASTIC CONSTANTS, CP(I,J,K,L), IN
C     PRIMED (LABORATORY) COORDINATES
C
      DO 6 IP=1,3
      DO 6 JP=1,3
      DO 6 KP=1,3
      DO 11 LP=1,3
      CP(IP,JP,KP,LP)=0.0
      DO 7 I=1,3
      DO 7 J=1,3
      DO 7 K=1,3
      DO 77 L=1,3
      CONST1=AP(IP,I)*AP(JP,J)*AP(KP,K)*AP(LP,L)*C(I,J,K,L)
      CP(IP,JP,KP,LP)=CP(IP,JP,KP,LP)+CONST1
   77 CONTINUE
    7 CONTINUE
   11 CONTINUE
      WRITE(6,100) IP,JP,KP,(CP(IP,JP,KP,LP), LP=1,3)
    6 CONTINUE
      IF (NE.EQ.1) GO TO 87
  100 FORMAT (2X,3I2,3F14.7)
C
C     SET VALUES FOR THE KRONECKER DELTA, D(M,N)
C
      DO 12 M=1,3
      DO 12 N=1,3
   12 D(M,N)=0.0
      DO 13 M=1,3
   13 D(M,M)=1.0
C
C     SET VALUES FOR THE TOTAL STRAIN IN
C     LABORATORY COORDINATES, TP(K,L), AND PLASTIC
C     STRAIN FOR EACH SLIP SYSTEM, GAM(NA)
C
      DO 31 K=1,3
      READ (5,201)(TP(K,L),L=1,3)
```

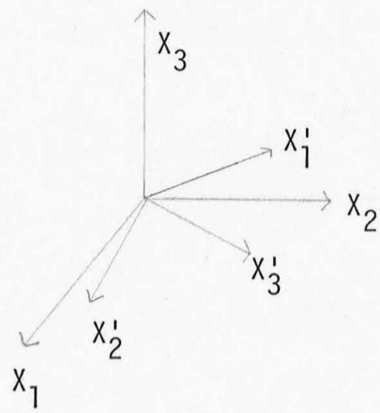
VI. EXAMPLE: COMPRESSIONAL WAVES TRAVELLING IN A <111> DIRECTION THROUGH LiF.

6.1 Determination of a'_{ij}.

The X' coordinates are chosen with the X'_1 axis parallel to a <111> direction and the X'_2 and X'_3 axes symmetrically disposed with respect to the X_3 axis. The former condition gives for the unit vector in the $+X'_1$ direction:

$$\vec{n}'_1 = \frac{1}{\sqrt{3}}(\vec{n}_1 + \vec{n}_2 + \vec{n}_3) = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right) \qquad (6.1)$$

With the X'_2 and X'_3 axes as shown in the figure, the following relations exist among the a'_{ij}:



$$\vec{n}'_1 \cdot \vec{n}_2 = a'_{21} = \vec{n}'_3 \cdot \vec{n}_2 = a'_{32} > 0$$

$$\vec{n}'_2 \cdot \vec{n}_2 = a'_{22} = \vec{n}'_3 \cdot \vec{n}'_1 = a'_{31} < 0$$

$$\vec{n}'_2 \cdot \vec{n}_3 = a'_{23} = \vec{n}'_3 \cdot \vec{n}_3 = a'_{33} < 0$$

The transformation matrix is

$$a'_{ij} = \begin{pmatrix} 1/\sqrt{3} & 1/\sqrt{3} & 1/\sqrt{3} \\ a'_{21} & a'_{22} & a'_{23} \\ a'_{22} & a'_{21} & a'_{23} \end{pmatrix} \qquad (6.2)$$

Since $\vec{n}'_2 \cdot \vec{n}'_1 = \vec{n}'_3 \cdot \vec{n}'_2 = 0$, $\vec{n}'_2 \cdot \vec{n}'_2 = 1$, the following equations hold and can be solved for a'_{21}, a'_{22}, a'_{23}:

$$a'_{21} + a'_{22} + a'_{23} = 0$$

$$2a'_{21}a'_{22} + a'^{2}_{23} = 0$$

$$a'^{2}_{21} + a'^{2}_{22} + a'^{2}_{23} = 1$$

With the condition $a'_{21} > 0$, these give

$$a'_{21} = \frac{1}{2}\left(1 + \frac{1}{\sqrt{3}}\right) \quad , \quad a'_{22} = -\frac{1}{2}\left(1 - \frac{1}{\sqrt{3}}\right) \quad , \quad a'_{23} = -\frac{1}{\sqrt{3}}$$

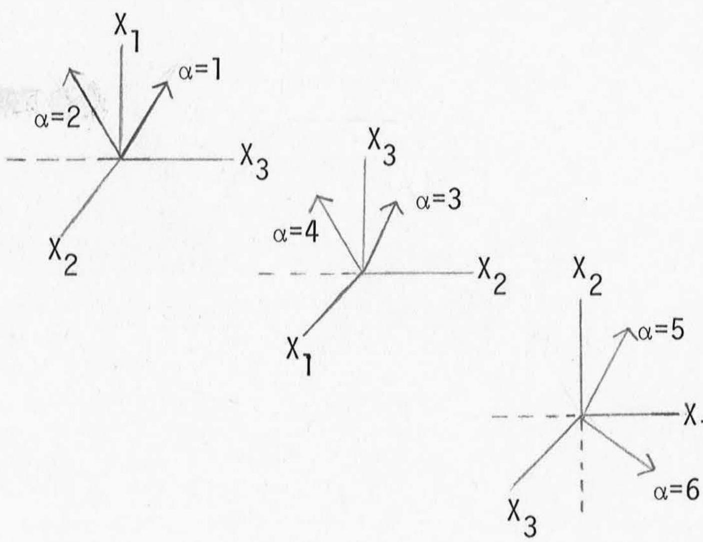
$$a'_{31} = -\frac{1}{2}\left(1 - \frac{1}{\sqrt{3}}\right) \quad , \quad a'_{32} = \frac{1}{2}\left(1 + \frac{1}{\sqrt{3}}\right) \quad , \quad a'_{33} = -\frac{1}{\sqrt{3}} \qquad (6.3)$$

6.2 Secondary Slip Systems.

The primary slip systems in LiF are [110]<110> (see Internal Report 75-01) and it has been shown by others that when propagation is in a <111> direction the stresses on these slip systems vanish. Except for the possibility of slip by heterogeneous stresses, one then expects secondary slip to occur. Secondary slip systems have been identified as [100]<110>; they can be enumerated as follows with the help of the figures on the right:

Table 6.1

α	Secondary Slip System
1	$[010]\langle 101\rangle$
2	$[010]\langle 10\bar{1}\rangle$
3	$[100]\langle 011\rangle$
4	$[100]\langle 0\bar{1}1\rangle$
5	$[001]\langle 110\rangle$
6	$[001]\langle 1\bar{1}0\rangle$



This set is not unique. There are six equivalent systems obtained by reversing directions. The choice of sign will influence the sign of the calculated resolved shear stress, otherwise it will have no effect on the results.

When strain is uniaxial in the <111> direction, stresses in the X' coordinates are

$$S'_{11} \equiv \sigma'_1 = C'_{11}T'_{11}$$

$$S'_{22} = S'_{33} = C'_{21}T'_{11} = \frac{C'_{12}}{C'_{11}} \cdot S'_{11}$$

or

$$\overleftrightarrow{S'} = S'_{11}\vec{1}'_1\vec{1}'_1 + S'_{22}(\vec{1}'_2\vec{1}'_2 + \vec{1}'_3\vec{1}'_3) \qquad (6.4)$$

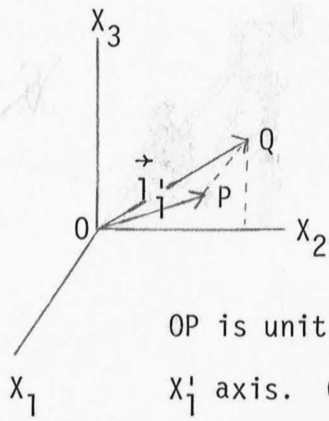
Calculate the stress on the [100]<011> slip system. Slip occurs along the line OQ in the figure. Stress at O is $\overleftrightarrow{S}'$ given by Eq. (6.4). The force per unit area acting on the X_2,X_3 plane is

$$\vec{f} = \vec{1}_1 \cdot \overleftrightarrow{S}' \qquad (6.5)$$

and the component of this force acting in the direction OQ is

$$\tau = \widehat{OQ}\cdot\vec{f} = \frac{1}{\sqrt{2}}(\hat{1}_2 + \hat{1}_3)\cdot\vec{f}$$

$$= \frac{1}{\sqrt{2}}(\hat{1}_2 + \hat{1}_3)\cdot\hat{1}_1\cdot\overleftrightarrow{S}' \qquad (6.6)$$



OP is unit vector, $\vec{1}_1'$, along X_1' axis. OQ is its projection on the X_2,X_3 plane.

Define $\hat{1}_j'\cdot\hat{1}_k \equiv a_{jk}'$. Then $\hat{1}_j' = a_{jk}'\hat{1}_k$

$$\hat{S}' = S_{11}'a_{1k}'a_{1j}'\hat{1}_k\hat{1}_j \quad + \quad S_{22}'(a_{2k}'a_{2j}' + a_{3k}'a_{3j}')\hat{1}_k\hat{1}_j$$

$$\tau = \frac{1}{\sqrt{2}}(\hat{1}_2 + \hat{1}_3)\cdot(\hat{1}_1\cdot\overleftrightarrow{S}') = [S_{11}'a_{11}'a_{1j}'\hat{1}_j + S_{22}'(a_{21}'a_{2j}' + a_{31}'a_{3j}')\hat{1}_j]\cdot\frac{1}{\sqrt{2}}(\hat{1}_2 + \hat{1}_3) \qquad (6.7)$$

$$\tau = \frac{1}{\sqrt{2}}[S_{11}'a_{11}'(a_{12}' + a_{13}') + S_{22}'(a_{21}'a_{22}' + a_{31}'a_{32}') + S_{22}'(a_{21}'a_{23}' + a_{31}'a_{33}')] \qquad (6.8)$$

Using the transformation matrix as given by Eqs. (6.2) and (6.3), Eq. (6.8) becomes

$$\tau = \frac{1}{\sqrt{2}}[S_{11}'a_{11}'(a_{12}' + a_{13}') + S_{22}'(a_{21}'a_{22}' + a_{21}'a_{22}' + a_{21}'a_{23}' + a_{22}'a_{23}')]$$

$$\tau = \frac{1}{\sqrt{2}}[S_{11}'\cdot 2(a_{11}')^2 + S_{22}'(2a_{21}'a_{22}' + (a_{21}' + a_{22}')a_{23}')]$$

Numerical values are $a_{11}' = 1/\sqrt{3}$, $a_{23}' = -1/\sqrt{3}$

$$a_{21}' = \frac{1}{2}(1 + 1/\sqrt{3}), \qquad a_{22}' = -\frac{1}{2} + \frac{1}{2\sqrt{3}}$$

Then $a_{21}'a_{22}' = -\frac{1}{6}$ $\qquad a_{21}' + a_{22}' = \frac{1}{\sqrt{3}}$

so

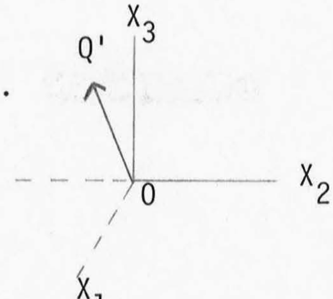
$$\tau = \frac{2}{3\sqrt{2}} S''_{11}(1 - \frac{S'_{22}}{S'_{11}}) \qquad (6.10)$$

or, since $S'_{22}/S'_{11} = C'_{12}/C'_{11}$,

$$\frac{\tau}{S''_{11}} = \frac{2}{3\sqrt{2}}(1 - \frac{C'_{12}}{C'_{11}}) \qquad (6.11)$$

$$= \frac{2}{3\sqrt{2}}\left[1 - \frac{\frac{1}{3}(C_{11} + 2C_{12} - 2C_{44})}{\frac{1}{3}(C_{11} + 2C_{12} + 4C_{44})}\right] = 0.38786$$

The second slip system on the [100] plane is shown in the figure. The direction of slip is OQ', parallel to



$$\vec{n}' = -\hat{1}_2 + \hat{1}_3$$

If $\hat{1}_2$ in Eq. (6.7) is replaced by $-\hat{1}_2$, Eq. (6.8) is replaced by

$$\tau' = \frac{1}{\sqrt{2}}[S'_{11}a'_{11}(-a'_{12} + a'_{13}) + S'_{22}(-a'_{21}a'_{22} - a'_{31}a'_{32} + a'_{21}a'_{23} + a'_{31}a'_{33})]$$

$$= \frac{1}{\sqrt{2}}S'_{22}(-a'_{21}a'_{22} - a'_{22}a'_{21} + a'_{21}a'_{23} + a'_{22}a'_{23})$$

$$= 0$$

This result is in accord with the fact that OQ' lies in the [111] plane, ie normal to the X'_1 axis.

Similarly, of the other two slip planes [010] and [001], each contains one slip direction which lies parallel to the projection of the <111> vector and a second which is perpendicular. Because of the symmetry the resolved shear stress on each of the former systems is given by Eq. (6.10). That in the normal system is zero. So there are three active slip systems

[100]<011>

[010]<101>

[001]<110>

And on each of these the ratio of resolved shear stress to S'_{11} is

$$\tau/S'_{11} = \frac{2\sqrt{2}\, C_{44}}{C_{11} + 2C_{12} + 4C_{44}} = .38781$$

A tabulation of the transformation coefficients ${}^{\alpha}a''_{ij}$ is required for computation. These are given in Table 6.2 where 0.707107 is a decimal approximation to $1/\sqrt{2}$.

Table 6.2

Coordinates and Transformation Matrices for Secondary Slip Systems in LiF

$$[010]\langle 101\rangle, \qquad \alpha = 1, \qquad {}^{1}a''_{ij} = \begin{pmatrix} .707107 & 0 & .707107 \\ .707107 & 0 & -.707107 \\ 0 & 1 & 0 \end{pmatrix}$$

$$[010]\langle 10\bar{1}\rangle, \qquad \alpha = 2, \qquad {}^{2}a''_{ij} = \begin{pmatrix} .707107 & 0 & -.707107 \\ -.707107 & 0 & -.707107 \\ 0 & 1 & 0 \end{pmatrix}$$

$$[100]\langle 011\rangle, \qquad \alpha = 3, \qquad {}^{3}a''_{ij} = \begin{pmatrix} 0 & .707107 & .707107 \\ 0 & -.707107 & .707107 \\ 1 & 0 & 0 \end{pmatrix}$$

$$[100]\langle 0\bar{1}1\rangle, \qquad \alpha = 4, \qquad {}^{4}a''_{ij} = \begin{pmatrix} 0 & -.707107 & .707107 \\ 0 & -.707107 & -.707107 \\ 1 & 0 & 0 \end{pmatrix}$$

$$[001]\langle 110\rangle, \qquad \alpha = 5, \qquad {}^{5}a''_{ij} = \begin{pmatrix} .707107 & .707107 & 0 \\ -.707107 & .707107 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$[001]\langle 1\bar{1}0\rangle, \qquad \alpha \quad 6, \qquad {}^{6}a''_{ij} = \begin{pmatrix} .707107 & -.707107 & 0 \\ .707107 & .707107 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

X''_1 = slip direction

X''_3 = normal to slip plane

X''_2 = $a''_{ij}X_j$

6.3 Computation of the Matrices ${}^{\alpha}a''_{ij}$.

Since $${}^{\alpha}X'''_{i} = {}^{\alpha}a''_{ij}X_{j}$$

$$X'_{k} = a'_{ij}X_{j} ,$$

it follows that

$$X_{j} = X'_{k}a'_{kj}$$

$${}^{\alpha}X'''_{i} = {}^{\alpha}a''_{ij}a'_{kj}X'_{k} \equiv {}^{\alpha}a'''_{ik}X'_{k}$$

$${}^{\alpha}a'''_{ik} = {}^{\alpha}a''_{ij}a'_{kj} \tag{6.12}$$

Straightforward application of this rule to the matrices given by Eqs. (6.2) and (6.3) and by the first entry in Table 6.2 yields for $\alpha = 1$,

$${}^{1}a'''_{ij} = \begin{pmatrix} \frac{2}{\sqrt{6}} & \frac{1}{2\sqrt{2}}(1 - \frac{1}{\sqrt{3}}) & -\frac{1}{2\sqrt{2}}(1 + \frac{1}{\sqrt{3}}) \\ 0 & \frac{1}{2\sqrt{2}}(1 + \sqrt{3}) & -\frac{1}{2\sqrt{2}}(1 - \sqrt{3}) \\ \frac{1}{\sqrt{3}} & -\frac{1}{2}(1 - \frac{1}{\sqrt{3}}) & \frac{1}{2}(1 + \frac{1}{\sqrt{3}}) \end{pmatrix}$$

$$= \begin{pmatrix} .81650 & .14943 & -.55768 \\ 0 & .96593 & .25882 \\ .55735 & -.21132 & .78868 \end{pmatrix}$$

6.4 Transformation of Elastic Constants to <111> Coordinates.

The elastic constants transform as a fourth order tensor. Since $X'_{i} = a'_{ij}X_{j}$, then

$$C'_{ijkl} = a'_{im}a'_{jn}a'_{kp}a'_{lq}\, C_{mnpq} \tag{6.13}$$

For the cubic system the matrix array of elastic constants is

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

This implies that many of the tensor components, C_{mnpq}, vanish. With the symmetry conditions $C_{ijkl} = C_{jikl} = C_{ijlk} = C_{klij}$ and with the convention that tensor subscripts 11 go to matrix subscripts 1, 22 → 2, 33 → 3, 23 → 4, 13 → 5, 12 → 6, we have the following set of non-vanishing tensor components:

$$\begin{aligned} &C_{1111} = C_{11}, \quad C_{2222} = C_{11}, \quad C_{3333} = C_{11} \\ &C_{1122} = C_{1133} = C_{2233} = C_{2211} = C_{3311} = C_{3322} = C_{12} \\ &C_{1212} = C_{1221} = C_{1313} = C_{1331} = C_{2112} = C_{2121} = C_{44} \\ &C_{2323} = C_{2332} = C_{3113} = C_{3131} = C_{3223} = C_{3232} = C_{44} \end{aligned} \tag{6.14}$$

Calculation of the C'_{ijkl} consists of successive application of Eq. (6.13), using the values given in Eq. (6.14). For example

$$\begin{aligned} C'_{2212} = {} & C_{11}(a'^{3}_{21}a'_{11} + a'^{3}_{22}a'_{12} + a'^{3}_{23}a'_{13}) + C_{12}(a'^{2}_{21}a'_{12}a'_{22} + a'^{2}_{21}a'_{13}a'_{23} \\ & + a'^{2}_{22}a'_{13}a'_{23} + a'^{2}_{22}a'_{11}a'_{21} + a'^{2}_{23}a'_{11}a'_{21} + a'^{2}_{23}a'_{12}a'_{22}) + C_{44}(a'_{21}a'_{11}a'^{2}_{22} \\ & + a'^{2}_{21}a'_{22}a'_{12} + a'^{2}_{23}a'_{21}a'_{11} + a'^{2}_{21}a'_{23}a'_{13} + a'^{2}_{22}a'_{21}a'_{11} + a'^{2}_{21}a'_{22}a'_{12} \\ & + a'^{2}_{23}a'_{22}a'_{12} + a'^{2}_{22}a'_{23}a'_{13} + a'^{2}_{23}a'_{21}a'_{11} + a'^{2}_{21}a'_{23}a'_{13} + a'^{2}_{23}a'_{22}a'_{12} \\ & + a'^{2}_{22}a'_{23}a'_{13}) \end{aligned} \tag{6.15}$$

Since $a'_{31} = a'_{21} = a'_{11}$, $a'_{31} = a'_{22}$, $a'_{32} = a'_{21}$, $a'_{23} = a'_{33} = -a'_{11}$, Eq. (6.15) can be reduced to simpler form:

$$C'_{2212} = a'_{11}C_{11}(a'^{\,3}_{21} + a'^{\,3}_{22} + a'^{\,3}_{23}) - a'_{11}C_{12}(a'^{\,3}_{21} + a'^{\,3}_{22} + a'^{\,3}_{23})$$
$$- 2a'_{11}C_{44}(a'^{\,3}_{21} + a'^{\,3}_{22} + a'^{\,3}_{23})$$

where the condition $a'_{21} + a'_{22} + a'_{23} = 0$ has been used. This can be further simplified to yield

$$C'_{2212} = a'_{11}(C_{11} - C_{12} - 2C_{44})(a'^{\,3}_{21} + a'^{\,3}_{22} + a'^{\,3}_{23}) \tag{6.16}$$

From Eq. (6.3) it is evident that

$$a'_{21} = \frac{1}{2}(1 - a'_{23}), \quad a'_{22} = -\frac{1}{2}(1 + a'_{23}) \tag{6.17}$$

Substitution of (6.17) into (6.16) yields

$$C'_{2212} = a'_{11}(C_{11} - C_{12} - 2C_{44})\cdot\frac{3a'_{23}}{4}(a'^{\,2}_{23} - 1) \tag{6.18}$$

With $a'_{11} = 1/\sqrt{3}$, $a'_{23} = -1/\sqrt{3}$, $C_{11} = 1.14$, $C_{12} = .477$, $C_{44} = .636$, this becomes

$$C'_{2212} = C'_{26} = \frac{1}{6}(C_{11} - C_{12} - 2C_{44})$$
$$= -.1015$$

With this procedure, the following array is calculated

$$\begin{matrix} C'_{11} & C'_{12} & C'_{12} & 0 & 0 & 0 \\ & C'_{22} & C'_{23} & 0 & C'_{25} & -C'_{25} \\ & & C'_{22} & 0 & -C'_{25} & C'_{25} \\ & & & C'_{44} & C'_{25} & C'_{25} \\ & & & & C'_{55} & 0 \\ & & & & & C'_{55} \end{matrix}$$

where
$$C'_{11} = \frac{1}{3}(C_{11} + 2C_{12} + 4C_{44})$$
$$C'_{12} = \frac{1}{3}(C_{11} + 2C_{12} - 2C_{44})$$
$$C'_{22} = \frac{1}{2}(C_{11} + C_{12} + 2C_{44})$$
$$C'_{26} = \frac{1}{6}(C_{11} - C_{12} - 2C_{44})$$

Transformation formulae for the remaining three coefficients haven't been calculated. Numerical values for all, with $C_{11} = 1.14$, $C_{12} = .477$, $C_{44} = .636$ megabar, are given in Table 6.3.

Table 6.3

Transformed Elastic Constants for LiF, megabar.

$C'_{11} = 1.5460$	$C'_{12} = .2740$	
$C'_{22} = 1.4445$	$C'_{23} = .3755$	$C'_{25} = .1015$
$C'_{44} = .5345$	$C'_{55} = .4330$	

6.5 Data for the Computer Program

(i) Tabulate the C_{ij} in crystal coordinates: six rows with FORMAT (6F8.5) for each row:

C_{11} C_{12} C_{13} C_{14} C_{15} C_{16}

C_{21} C_{22} C_{23} C_{24} C_{25} C_{26}

etc.

(ii) Tabulate $a'_{ij} \equiv$ AP(I,J) in three rows with FORMAT (3F15.7):

a'_{11} a'_{12} a'_{13}

etc.

(iii) NS = No. of active slip systems (6) and NE = 1 or 2.

(iv) Tabulate the a''_{ij} for α = 1, NS with FORMAT (3F15.7):

$$
\begin{matrix}
{}^1a''_{11} & {}^1a''_{12} & {}^1a''_{13} \\
{}^1a''_{21} & {}^1a''_{22} & {}^1a''_{23} \\
{}^1a''_{31} & {}^1a''_{32} & {}^1a''_{33} \\
{}^2a''_{11} & {}^2a''_{12} & {}^2a''_{13}
\end{matrix}
$$

etc.

(v) If plastic strains are allowed, tabulate the total strains, T'_{ij}, in a 3x3 matrix with FORMAT (3F15.7)

$$
\begin{matrix}
T'_{11} & T'_{12} & T'_{13} \\
T'_{21} & T'_{22} & T'_{23}
\end{matrix}
$$

\- - - - - - -

(vi) If plastic strains are allowed, tabulate the plastic strains ${}^{\alpha}\gamma$. FORMAT (3F15.7).

$$
\begin{matrix}
{}^1\gamma & {}^2\gamma & {}^3\gamma \\
{}^4\gamma & {}^5\gamma & {}^6\gamma
\end{matrix}
$$

etc.

A listing of data for the sample problem is given in Table 6.4. Numerical output is given in Table 6.5.

Table 6.4

Input for Sample Problem

```
1.14000 0.47700 0.47700
0.47700 1.14000 0.47700
0.47700 0.47700 1.14000
                        0.63600
                                0.63600
                                        0.63600
      .57735              .57735              .57735
      .788675            -.211325            -.57735
     -.211325             .788675            -.57735
6 1
      .707107                                 .707107
      .707107                                -.707107
                         1.
      .707107                                -.707107
     -.707107                                -.707107
                         1.
                          .707107             .707107
                         -.707107             .707107
     1.
                         -.707107             .707107
                         -.707107            -.707107
     1.
     .707107             .707107
    -.707107             .707107
                                            1.
     .707107            -.707107
     .707107             .707107
                                            1.
```

Table 6.5

Output for Sample Problem

$DATA

1	1.14000	0.47700	0.47700	0.00000	0.00000	0.00000	
2	0.47700	1.14000	0.47700	0.00000	0.00000	0.00000	
3	0.47700	0.47700	1.14000	0.00000	0.00000	0.00000	C_{mn}
4	0.00000	0.00000	0.00000	0.63600	0.00000	0.00000	
5	0.00000	0.00000	0.00000	0.00000	0.63600	0.00000	
6	0.00000	0.00000	0.00000	0.00000	0.00000	0.63600	

C(I,J,K,L)

I	J	K	L=1	L=2	L=3	
1	1	1	1.1400000	0.0000000	0.0000000	
1	1	2	0.0000000	0.4770000	0.0000000	
1	1	3	0.0000000	0.0000000	0.4770000	
1	2	1	0.0000000	0.6360000	0.0000000	
1	2	2	0.6360000	0.0000000	0.0000000	
1	2	3	0.0000000	0.0000000	0.0000000	
1	3	1	0.0000000	0.0000000	0.6360000	
1	3	2	0.0000000	0.0000000	0.0000000	
1	3	3	0.6360000	0.0000000	0.0000000	
2	1	1	0.0000000	0.6360000	0.0000000	
2	1	2	0.6360000	0.0000000	0.0000000	
2	1	3	0.0000000	0.0000000	0.0000000	C_{mnpq}
2	2	1	0.4770000	0.0000000	0.0000000	
2	2	2	0.0000000	1.1400000	0.0000000	
2	2	3	0.0000000	0.0000000	0.4770000	
2	3	1	0.0000000	0.0000000	0.0000000	
2	3	2	0.0000000	0.0000000	0.6360000	
2	3	3	0.0000000	0.6360000	0.0000000	
3	1	1	0.0000000	0.0000000	0.6360000	
3	1	2	0.0000000	0.0000000	0.0000000	
3	1	3	0.6360000	0.0000000	0.0000000	
3	2	1	0.0000000	0.0000000	0.0000000	
3	2	2	0.0000000	0.0000000	0.6360000	
3	2	3	0.0000000	0.6360000	0.0000000	
3	3	1	0.4770000	0.0000000	0.0000000	
3	3	2	0.0000000	0.4770000	0.0000000	
3	3	3	0.0000000	0.0000000	1.1400000	
1			0.5773500	0.5773500	0.5773500	
2			0.7886750	-0.2113250	-0.5773500	a'_{ij}
3			-0.2113250	0.7886750	-0.5773500	
1	1		0.7071070	0.0000000	0.7071070	
1	2		0.7071070	0.0000000	-0.7071070	
1	3		0.0000000	1.0000000	0.0000000	
2	1		0.7071070	0.0000000	-0.7071070	
2	2		-0.7071070	0.0000000	-0.7071070	
2	3		0.0000000	1.0000000	0.0000000	
3	1		0.0000000	0.7071070	0.7071070	
3	2		0.0000000	-0.7071070	0.7071070	
3	3		1.0000000	0.0000000	0.0000000	
4	1		0.0000000	-0.7071070	0.7071070	
4	2		0.0000000	-0.7071070	-0.7071070	${}^{\alpha}a''_{ij}$
4	3		1.0000000	0.0000000	0.0000000	
5	1		0.7071070	0.7071070	0.0000000	
5	2		-0.7071070	0.7071070	0.0000000	
5	3		0.0000000	0.0000000	1.0000000	
6	1		0.7071070	-0.7071070	0.0000000	
6	2		0.7071070	0.7071070	0.0000000	
6	3		0.0000000	0.0000000	1.0000000	
1	1		0.8164965	0.1494294	-0.5576776	
1	2		0.0000000	0.9659258	0.2588188	
1	3		0.5773500	-0.2113250	0.7886750	
2	1		0.0000000	0.9659258	0.2588188	${}^{\alpha}a'''_{ij}$
2	2		-0.8164965	-0.1494294	0.5576776	
2	3		0.5773500	-0.2113250	0.7886750	
3	1		0.8164965	-0.5576776	0.1494294	
3	2		0.0000000	-0.2588188	-0.9659258	
3	3		0.5773500	0.7886750	-0.2113250	
4	1		0.0000000	-0.2588188	-0.9659258	
4	2		-0.8164965	0.5576776	-0.1494294	

Table 6.5 contd.

4 3	0.5773500	0.7886750	-0.2113250	
5 1	0.8164965	0.4082482	0.4082482	
5 2	0.0000000	-0.7071070	0.7071070	
5 3	0.5773500	-0.5773500	-0.5773500	
6 1	0.0000000	0.7071070	-0.7071070	
6 2	0.8164965	0.4082482	0.4082482	
6 3	0.5773500	-0.5773500	-0.5773500	
1 1 1	1.5459971	-0.0000000	-0.0000000	
1 1 2	-0.0000000	0.2739996	-0.0000001	
1 1 3	-0.0000000	-0.0000001	0.2739996	
1 2 1	-0.0000000	0.4329994	-0.0000002	
1 2 2	0.4329994	-0.1015000	0.1014999	
1 2 3	-0.0000002	0.1014999	0.1014999	
1 3 1	0.0000000	-0.0000002	0.4329994	
1 3 2	-0.0000002	0.1014999	0.1014999	
1 3 3	0.4329994	0.1014999	-0.1015000	
2 1 1	-0.0000000	0.4329994	-0.0000002	
2 1 2	0.4329994	-0.1015000	0.1014999	
2 1 3	-0.0000002	0.1014999	0.1014999	C'_{ijkl}
2 2 1	0.2739996	-0.1015000	0.1014999	
2 2 2	-0.1015000	1.4444987	-0.0000007	
2 2 3	0.1014999	-0.0000007	0.3754996	
2 3 1	-0.0000001	0.1014999	0.1014999	
2 3 2	0.1014999	-0.0000007	0.5344995	
2 3 3	0.1014999	0.5344995	-0.0000007	
3 1 1	0.0000000	-0.0000002	0.4329994	
3 1 2	-0.0000002	0.1014999	0.1014999	
3 1 3	0.4329994	0.1014999	-0.1015000	
3 2 1	-0.0000001	0.1014999	0.1014999	
3 2 2	0.1014999	-0.0000007	0.5344995	
3 2 3	0.1014999	0.5344995	-0.0000007	
3 3 1	0.2739996	0.1014999	-0.1015000	
3 3 2	0.1014999	0.3754996	-0.0000007	
3 3 3	-0.1015000	-0.0000007	1.4444987	
SP(I,J)				
1	1.0000000	-0.0000000	0.0000000	
2	-0.0000000	0.1772316	-0.0000001	S'_{ij}
3	0.0000000	-0.0000001	0.1772316	
NA=	1SPP(NA)=	0.3878564		
NA=	2SPP(NA)=	-0.0000001		
NA=	3SPP(NA)=	0.3878564		${}^{\alpha}S''_{31}$
NA=	4SPP(NA)=	0.0000001		
NA=	5SPP(NA)=	0.3878565		
NA=	6SPP(NA)=	0.0000000		

${}^{\alpha}S''_{31}$ is stress on the slip system α