AM-75-002

(4 pages)

Interstratified Clays. I. Theoretical

Rodney Tettenhorst and Ralph E. Grim

The American Mineralogist

January - February 1975

Volume 60, Numbers 1-2

1a

```
C     A G-SQUARED PROGRAM FOR CU RADIATION
C     PROGRAM WRITTEN IN FORTRAN IV FOR IBM 360-75
C     PROGRAM WRITTEN MID 1973 AT OHIO STATE UNIVERSITY FOR MIXED LAYER STUDY
C     PROGRAM WRITTEN FOR "3-COMPONENTS" ONLY
C     PROGRAM WRITTEN FOR 11 SILICATE LAYERS--10 INTERLAYER REGIONS.
C     CARDS 5, 984, 979, 978, 970, 205, 206, 207, 208 SHOULD BE CHANGED IF A
C     DIFFERENT NUMBER OF SILICATE LAYERS/CRYSTALLITE IS DESIRED
C     LP FACTOR NOT INCLUDED
C     LIMIT OF CALCULATIONS IS SIN(THETA)/FLAMB = 0.35 OR 64 DEGREES 2-THETA
C     LITTLE F VALUES ARE COMPUTED USING A LINEAR INTERPOLATION ROUTINE WITH
C     VALUES TAKEN FROM THE INT TABLES, VOL 3, P 203
C     G-SQUARED CURVES ARE FURNISHED.
C     CARDS 701,702,703,704,801,802,803,804 AND DIMENSION STATEMENT MUST BE
C     CHANGED IF 2-THETA INCREMENT IS CHANGED
C     G**2 IS COMPUTED AT 0.05 DEGREES 2-THETA INCREMENTS
C     PLOTTING INTERVAL FOR CURVES IS TWO-TENTHS DEGREE 2-THETA
C     DATA FORMAT SPECIFICATIONS.
C     THE 1ST DATA CARD HAS A 5I5 FORMAT
C     COLS 1-5 CONTAIN # ATOM PLANES IN HALF OF THE END LAYER.
C     AN ATOM LOCATED AT EXACTLY HALF THE END CELL IS GIVEN A "P" OF ONE-HALF
C     ITS USUAL VALUE ON ITS ATOM SPECIFICATION CARD.  SEE BELOW
C     COLS 6-10 CONTAIN THE # OF ATOMS IN THE 10 ANGSTROM (A) LAYER.
C     COLS 11-15 CONTAIN # ATOMS IN THE 17 ANGSTROM (B) LAYER.
C     COLS 16-20 CONTAIN # ATOMS IN THE 13.5 ANGSTROM (C) LAYER.
C     ATOMS AT 0.0 AND "D" GET "P" VALUES OF ONE-HALF THE USUAL VALUE
C     ON THEIR ATOM SPECIFICATION CARDS.  SEE BELOW
C     # OF ATOM PLANES FOR ANY COMPONENT MUST BE < OR = 20
C     COLS 21-25 CONTAINS THE NUMBER OF JOBS (LAYER CONFIGURATIONS) TO BE DONE
C     # OF JOBS MUST BE < OR = TO 110
C     2ND CARD. SIN(THETA)/FLAMB VALUES FROM 0.0-0.35 IN AN 8F10.3 FORMAT
C     THE NEXT "NUMJOB" CARDS CONTAIN THE LAYER CONFIGURATIONS IN COLS 1-20
C     A LAYER CONFIGURATION, FOR EXAMPLE:  ABACBACAAC
C     "13TH-15TH-ETC"--UP TO NPE CARDS.  THE ATOMS IN HALF THE END LAYER
C     COLS 1-8.  THE NAME OF THE ATOM
C     COLS 10-19.  DISTANCE IN ANGSTROMS FROM ORIGIN ("Z").  NOT FRACT COORD.
C     COLS 20-29. NUMBER OF ATOMS PER PLANE PER UNIT CELL ("P"). F FIELD
C     COLS 30-39.  THE TEMPERATURE FACTOR ("BTEMP")
C     "14TH-16TH-ETC" CARDS
C     LITTLE "F" VALUES FOR EACH PRECEEDING CARD IN AN 8F10.3 FORMAT.
C     REPEAT THE PRECEDING FOR THE NPA CARDS.  THE # ATOMS IN THE "10 A" LAYER
C     REPEAT THE PRECEDING FOR THE NPB CARDS.  THE # ATOMS IN THE "17 A" LAYER
C     REPEAT THE PRECEDING FOR NPC CARDS.  THE # ATOMS IN THE "13.5 A" LAYER
      DIMENSION ATMA(20),ATMB(20),ATEMD(20),ATNA(20),ATNB(20),ATEND(20),
     1ZA(20),ZB(20),ZE(20),PA(20),PB(20),PE(20),BTMPA(20),BTMPB(20),BTMP
     2E(20),G(604),LINE(101),YE(20,10),YA(20,10),YB(20,10),XX(10),LAYER(
     311C,20),GSUM(604),G2(151,4),G2SUM(151,4),TTH(151,4),ATMC(20),ATNC(
     420),ZC(20),PC(20),BTMPC(20),YC(20,10)
      INTEGER BLANK,DOT,CIRCLE,SLASH,A,B,C
      DATA BLANK,DOT,CIRCLE,SLASH/1H ,1H.,1HO,1H-/
      DATA A,B,C/1HA,1HB,1HC/
  999 FORMAT('1','G**2 PROGRAM FOR 3-COMPONENT INTERSTRATIFIED CLAYS')
  996 FORMAT(5I5)
  993 FORMAT('0','THE ANGULAR RANGE COVERED IS 2 TO 32 DEGREES 2-THETA')
  992 FORMAT(2A4,1X,3F10.0)
  991 FORMAT(21X,4HATOM,12X,1HZ,12X,1HP,10X,5HBTEMP/)
  990 FORMAT(1H ,19X,2A4,4X,F8.3,6X,F7.3,8X,F5.2)
  989 FORMAT(110HO TWO THETA      G-SQUARED      TWO THETA      G-SQUARED
     1   TWO THETA      G-SQUARED      TWO THETA      G-SQUARED//)
  988 FORMAT(4(3X,F5.2,4X,E16.8))
  987 FORMAT(1H1,45X,9HG-SQUARED)
  986 FORMAT (1H0,101A1/////////)
  985 FORMAT(1H ,101A1)
```

```
984 FORMAT(10A1)
983 FORMAT(8F10.3)
982 FORMAT('0','DATA FOR THE "10-ANGSTROM" (A) LAYERS'/)
981 FORMAT('0','DATA FOR THE "17-ANGSTROM" (B) LAYERS'/)
979 FORMAT('0','BOTH ENDS OF THE 10 LAYER PARTICLE END ON'/)
978 FORMAT('0','PARTICLES HAVE 11 SILICATE LAYERS--10 INTERLAYER REGIO
   1NS')
977 FORMAT('0','DATA FOR THE "13.5-ANGSTROM" (C) LAYERS'/)
970 FORMAT('1','THE LAYER CONFIGURATION FOR THIS 10 LAYER PARTICLE IS
   1',10A1)
969 FORMAT('1','THE MEAN OF ALL OF THE PRECEEDING RUNS IS AS FOLLOWS')
968 FORMAT(26H0 TWO THETA       G-SQUARED//)
967 FORMAT(1H ,3X,F5.2,4X,E16.8)
    DO 2 I=1,604
    G(I)=0.0
  2 GSUM(I)=0.0
    DO 3 I1=1,151
    DO 3 I2=1,4
    G2(I1,I2)=0.0
    G2SUM(I1,I2)=0.0
  3 TTH(I1,I2)=0.0
    READ(5,996)NPE,NPA,NPB,NPC,NUMJOB
    READ(5,983)(XX(K),K=1,8)
    DO 5 II=1,NUMJOB
  5 READ(5,984)(LAYER(II,K),K=1,10)
    DO 9 N=1,NPE
    READ(5,992)ATEMD(N),ATEND(N),ZE(N),PE(N),BTMPE(N)
  9 READ(5,983)(YE(N,K),K=1,8)
    DO 11 N=1,NPA
    READ(5,992)ATMA(N),ATNA(N),ZA(N),PA(N),BTMPA(N)
 11 READ(5,983)(YA(N,K),K=1,8)
    DO 13 N=1,NPB
    READ(5,992)ATMB(N),ATNB(N),ZB(N),PB(N),BTMPB(N)
 13 READ(5,983)(YB(N,K),K=1,8)
    DO 14 N=1,NPC
    READ(5,992)ATMC(N),ATNC(N),ZC(N),PC(N),BTMPC(N)
 14 READ(5,983)(YC(N,K),K=1,8)
    WRITE(6,999)
    WRITE(6,993)
    WRITE(6,978)
    WRITE(6,979)
    WRITE(6,991)
    DO 15 N=1,NPE
 15 WRITE(6,990)ATEMD(N),ATEND(N),ZE(N),PE(N),BTMPE(N)
    WRITE(6,982)
    WRITE(6,991)
    DO 17 N=1,NPA
 17 WRITE(6,990)ATMA(N),ATNA(N),ZA(N),PA(N),BTMPA(N)
    WRITE(6,981)
    WRITE(6,991)
    DO 19 N=1,NPB
 19 WRITE(6,990)ATMB(N),ATNB(N),ZB(N),PB(N),BTMPB(N)
    WRITE(6,977)
    WRITE(6,991)
    DO 20 N=1,NPC
 20 WRITE(6,990)ATMC(N),ATNC(N),ZC(N),PC(N),BTMPC(N)
    RAD=3.14159/180.0
    DO 150 II=1,NUMJOB
205 WRITE(6,970)(LAYER(II,K),K=1,10)
    WRITE(6,989)
    GL=0.0
702 DO 70 I1=1,151
```

```
      DO 70 I2=1,4
      I=4*(I1-1)+I2
  703 M=25*I+975
      THETA=M/1000.0
      TTH(I1,I2)=THETA*2.0
      THR=THETA*RAD
      SINTH=SIN(THR)
      SSS=8.15055*SINTH
      SQ=SINTH/1.54178
      SQ2 = SQ**2
      K = 1
   21 IF(XX(K)-SQ)22,26,24
   22 K = K + 1
      GO TO 21
   24 K = K - 1
   26 PF=(SQ-XX(K))/(XX(K+1)-XX(K))
      AA=0.0
      BB=0.0
      DO 35 J=1,NPE
      FT =(YE(J,K) - PF*(YE(J,K) - YE(J,K+1)))*PE(J)*EXP(-BTMPE(J)*SQ2)
      ARG=SSS*ZE(J)
      AA=AA+FT*COS(ARG)
   35 BB=BB+FT*SIN(ARG)
      Q=0.0
      N=1
   36 IF(LAYER(II,N).EQ.B)GO TO 39
   37 IF(LAYER(II,N).EQ.C)GO TO 63
   38 DO 40 J=1,NPA
      FT =(YA(J,K) - PF*(YA(J,K) - YA(J,K+1)))*PA(J)*EXP(-BTMPA(J)*SQ2)
      ARG=SSS*(ZA(J)+Q)
      AA=AA+FT*COS(ARG)
   40 BB=BB+FT*SIN(ARG)
      Q=Q+ZA(NPA)
      N=N+1
  206 IF(N.GT.10)GO TO 65
      IF(LAYER(II,N).EQ.A)GO TO 38
      IF(LAYER(II,N).EQ.C)GO TO 63
   39 DO 41 J=1,NPB
      FT =(YB(J,K) - PF*(YB(J,K) - YB(J,K+1)))*PB(J)*EXP(-BTMPB(J)*SQ2)
      ARG=SSS*(ZB(J)+Q)
      AA=AA+FT*COS(ARG)
   41 BB=BB+FT*SIN(ARG)
      Q=Q+ZB(NPB)
      N=N+1
  207 IF(N.GT.10)GO TO 65
      IF(LAYER(II,N).EQ.A)GO TO 38
      IF(LAYER(II,N).EQ.B)GO TO 39
   63 DO 64 J=1,NPC
      FT =(YC(J,K) - PF*(YC(J,K) - YC(J,K+1)))*PC(J)*EXP(-BTMPC(J)*SQ2)
      ARG=SSS*(ZC(J)+Q)
      AA=AA+FT*COS(ARG)
   64 BB=BB+FT*SIN(ARG)
      Q=Q+ZC(NPC)
      N=N+1
  208 IF(N.LE.10)GO TO 36
   65 DO 68 J=1,NPE
      FT =(YE(J,K) - PF*(YE(J,K) - YE(J,K+1)))*PE(J)*EXP(-BTMPE(J)*SQ2)
      ARG=SSS*(Q+ABS(ZE(J)))
      AA=AA+FT*COS(ARG)
   68 BB=BB+FT*SIN(ARG)
      G2(I1,I2)=AA**2+BB**2
      G2SUM(I1,I2)=G2SUM(I1,I2)+G2(I1,I2)
```

```
      IF(GL.GE.G2(I1,I2))GO TO 70
      GL=G2(I1,I2)
   70 CONTINUE
   75 WRITE(6,988)(((TTH(I1,I2),G2(I1,I2)),I2=1,4),I1=1,151)
      DO 77 I1=1,151
      DO 77 I2=1,4
      I=4*(I1-1)+I2
      G(I)=G2(I1,I2)
   77 GSUM(I)=G2SUM(I1,I2)
   79 WRITE(6,987)
      DO 80 L=1,101
   80 LINE(L)=DOT
      WRITE(6,986)LINE
      DO 90 L=1,101
   90 LINE(L)=BLANK
  701 DO 120 I=1,601,4
      L=100.0*(G(I)/GL)+1.5
      LINE(L)=CIRCLE
  704 IF(MOD(I,40).EQ.1)LINE(1)=SLASH
      WRITE(6,985)LINE
      LINE(L)=BLANK
  120 LINE(1)=BLANK
  150 CONTINUE
      DO 160 I=1,601
  160 GSUM(I)=GSUM(I)/NUMJOB
      GLSUM=0.0
      WRITE(6,969)
      WRITE(6,968)
  802 DO 170 I=1,601
  803 M=25*I+975
      THETA=M/1000.0
      TWOTH=THETA*2.0
      IF(GLSUM.GE.GSUM(I))GO TO 170
      GLSUM=GSUM(I)
  170 WRITE(6,967)TWOTH,GSUM(I)
      WRITE(6,987)
      DO 180 L=1,101
  180 LINE(L)=DOT
      WRITE(6,986)LINE
      DO 190 L=1,101
  190 LINE(L)=BLANK
  801 DO 200 I=1,601,4
      L=100.0*(GSUM(I)/GLSUM)+1.5
      LINE(L)=CIRCLE
  804 IF(MOD(I,40).EQ.1)LINE(1)=SLASH
      WRITE(6,985)LINE
      LINE(L)=BLANK
  200 LINE(1)=BLANK
      STOP
      END
```