

AM-75-002

(4 pages)

Interstratified Clays. I. Theoretical

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The American Mineralogist

January - February 1975

Volume 60, Numbers 1-2

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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 PRECEDING 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
C   DIMENSION ATMA(20),ATMB(20),ATEMD(20),ATNA(20),ATNB(20),ATEND(20),
C   1ZA(20),ZB(20),ZE(20),PA(20),PB(20),PE(20),BTMPA(20),BTMPB(20),BTMP
C   2E(20),G(604),LINE(101),YE(20,10),YA(20,10),YB(20,10),XX(10),LAYER(
C   3110,20),GSUM(604),G2(151,4),G2SUM(151,4),TTH(151,4),ATMC(20),ATNC(
C   420),ZC(20),PC(20),BTMPC(20),YC(20,10)
C   INTEGER BLANK,DOT,CIRCLE,SLASH,A,B,C
C   DATA BLANK,DOT,CIRCLE,SLASH/1H,1H.,1H0,1H-/
C   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(110H0 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)

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984 FORMAT(10A1)
983 FORMAT(HF10.3)
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
INS')
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

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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)

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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
TWOIH=THETA*2.0
IF(GLSUM.GE.GSUM(I))GO TO 170
GLSUM=GSUM(I)
170 WRITE(6,967)TWOIH,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

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