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GRAPH PLOTTING:MONTE CARLO PROBLEM
C
C   GRAPH PLOTTING PROGRAM FOR MONTE CARLO CALCULATION
C   PLOTS GRAPHS OF DRIFT VELOCITY,MEAN ENERGY AND
C   K SPACE DISTRIBUTION FUNCTIONS ON VDU AND GRAPH PLOTTER
C
      REAL MNE1
      DIMENSION IT(21),F(10),VEL(10),MNE1(10),IT2(17)
     1  ,YINT(10,20),VEL1(10),IT3(13),XVAL(20),YVAL(20)
      COMMON/SCDTA/RV(160)
      DATA IT/21,'STATIC CHARACTERISTIC',5,'FIELD',8,'VELOCITY'/
      DATA IT2/11,'MEAN ENERGY',5,'FIELD',9,'MN ENERGY'/
      DATA IT3/14,'K DISTRIBUTION',1,'K',4,'F(K)'/
      CALL SEARCH(1,'GRAPPP',15)
C
C   READS TEST LABELS FOR CHOICE OF ACTION
C   FILE CONTAINS.
C                       STATIC
C                       ENERGY
C                       DSTRBN
C                       RERUNS
C                       COPIES
C
      READ(19,343)Y1
  343 FORMAT(A3)
      READ(19,343)Y2
      READ(19,343)Y3
      READ(19,343)Y4
      READ(19,343)Y5
      CALL SEARCH(4,0,15)
C
C   READ DATA FILES FROM PROGRAM CARLO FOR GRAPHICAL OUTPUT
C
      CALL SEARCH(1,'MDATA1',5)
      CALL SEARCH(1,'MDATA2',6)
      CALL SEARCH(1,'MDATA3',7)
      READ(9,801)NFG
  801 FORMAT(I2)
C
C   CALCULATES AXIS SIZES FOR GRAPHS
C
      NF=NFG
      FIX1=0.0
      FIX2=0.0
      CALL PAGE
      DO 100 I=1,NF
      READ(9,800)F(I)
      READ(10,800)VEL(I)
      IF(VEL(I).GT.FIX1) FIX1=VEL(I)
      READ(11,800)MNE1(I)
      IF(MNE1(I).GT.FIX2) FIX2=MNE1(I)
  800 FORMAT(E12.4)
C
C   INPUT OF EXPERIMENTAL VALUES FOR DRIFT VELOCITY TO
C   COMPARE WITH CALCULATED CURVE
C
      WRITE(1,910)F(I)
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  910 FORMAT(///,34HTYPE EXPERIMENTAL RESULT AT FIELD=,F4.2,2HKV)
      CALL ZREALD(VEL1(I))
      IF(VEL1(I).GT.FIX1) FIX1=VEL1(I)
  100 CONTINUE
      FIXX=F(NF)
C
C   INCLUDE ORIGIN AS POINT IN GRAPH
C
      NF1=NF+2
      DO 590 J=1,NF
      I=NF1-J
      K=NF-J+1
      VEL(I)=VEL(K)
      VEL1(I)=VEL1(K)
      MNE1(I)=MNE1(K)
      F(I)=F(K)
  590 CONTINUE
      F(1)=0.0
      VEL(1)=0.0
      VEL1(1)=0.0
      MNE1(1)=0.0
      NF=NF+1
C
C   CLOSE DATA FILES
C
      CALL SEARCH(4,0,5)
      CALL SEARCH(4,0,6)
      CALL SEARCH(4,0,7)
  888 CALL PAGE
C
C   MAKE SELECTION OF GRAPHS REQUIRED
C
      WRITE(1,288)
  288 FORMAT(///,10X,38HFOR STATIC CHARACTERISTIC TYPE STATIC///
     1,10X,38HFOR MEAN ENERGY VS. FIELD TYPE ENERGY///
     1,10X,38HFOR DISTRIBUTION FUNCTION TYPE DSTRBN///
     1,10X,38HFOR HARD COPIES OF GRAPHS TYPE COPIES///
     1,10X,38HTO RUN MONTE CARLO PROGRAM TYPE RERUNS///
     1,10X,38HFOR AN EXIT TO THE PROGRAM TYPE FINISH///)
      READ(1,343)X
      IF(X.EQ.Y1)GOTO 887
      IF(X.EQ.Y2)GOTO 886
      IF(X.EQ.Y3)GOTO 885
      IF(X.EQ.Y4)GOTO 883
      IF(X.EQ.Y5)GOTO 700
      GOTO 884
  700 CALL PAGE
C
C   CALLS GRAPH PLOTTER FOR HARD COPIES OF ALL GRAPHS.
C
C   'CALL A4' COMMAND SPECIFIES AN A4 FORMAT FOR GRAPHS.
C
      CALL A4
C
C   PLOTS DRIFT VELOCITY/FIELD GRAPHS
C
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      CALL FIXAXS(0.0,FIXX,0.0,FIX1)
      CALL FGPLT(F,VEL,NF,3,3,1,0,IT,6)
      CALL FGPLT(F,VEL1,NF,3,4,1,1,IT,6)
C
C   SIGNALS COMPLETION TO VDU AND SOUNDS BUZZER
C
      WRITE(1,701)
  701 FORMAT(////,25X,23HVELOCITY PLOT COMPLETED,/)
      CALL T1OU(7)
C
C   PLOTS MEAN ENERGY/FIELD GRAPH
C
      CALL FIXAXS(0.0,FIXX,0.0,FIX2)
      CALL FGPLT(F,MNE1,NF,3,3,1,0,IT2,6)
C
C   SIGNALS COMPLETION TO VDU AND SOUNDS BUZZER.
C
      WRITE(1,702)
  702 FORMAT(/,25X,26HMEAN ENERGY PLOT COMPLETED,/)
      CALL T1OU(7)
      KK=1
C
C   GOES TO LABEL 889 TO CALCULATE GRAPH AXES FOR
C   DISTRIBUTION PLOT KK=1 ENABLES RETURN TO LABEL 703.
C
      GOTO 889
  703 CALL SEARCH(4,0,8)
C
C   PLOTS K SPACE DISTRIBUTION FUNCTION AT EACH FIELD
C
      DO 705 I=1,NF
      DO 704 K=1,20
      YVAL(K)=YINT(I,K)
  704 CONTINUE
      JG=0
      IF(I.NE.1)JG=1
      CALL FGPLT(XVAL,YVAL,20,3,I,1,JG,IT3,6)
C
C   SIGNALS COMPLETION TO VDU AND SOUNDS BUZZER
C
      WRITE(1,706)I
  706 FORMAT(/,25X,19HDISTRIBUTION CURVE ,I2,10H COMPLETED,/)
      CALL T1OU(7)
  705 CONTINUE
      GOTO 888
C
C   PLOTS VELOCITY/FIELD GRAPHS ON VDU
C
C   CALCULATED CURVE
C
  887 CALL T4010
      CALL FIXAXS(0.0,FIXX,0.0,FIX1)
      CALL FGPLT(F,VEL,NF,3,3,1,0,IT,5)
C
C   SOUNDS BUZZER AND WAITS FOR CARRIAGE RETURN
C
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      CALL CHAMOD
      CALL T1OUK(7)
      CALL ZREALD(A)
C
C   PLOTS EXPERIMENTAL VELOCITY/FIELD CURVE ON SAME GRAPH
C
      CALL FGPLT(F,VEL1,NF,3,4,1,1,IT,5)
C
C   SOUNDS BUZZER AND WAITS FOR CARRIAGE RETURN
C
      CALL CHAMOD
      CALL T1OUK(7)
      CALL ZREALD(A)
      GOTO 888
C
C   PLOTS MEAN ENERGY/FIELD CURVE ON VDU
C
  886 CALL FIXAXS(0.0,FIXX,0.0,FIX2)
      CALL FGPLT(F,MNE1,NF,3,3,1,0,IT2,5)
C
C   SOUNDS BUZZER AND WAITS FOR CARRIAGE RETURN
C
      CALL CHAMOD
      CALL T1OUK(7)
      CALL ZREALD(A)
      GOTO 888
C
C   CALCULATES AXIS SIZE FOR DISTRIBUTION FUNCTION PLOT
C
  885 KK=0
  889 CALL SEARCH(1,'MDATA4',8)
      NF=NFG
      DO 38 I=1,20
      READ(12,31)XVAL(I)
   31 FORMAT(E12.4)
   38 CONTINUE
      FIX3=0.0
      DO 56 I=1,NF
      DO 56 K=1,20
      READ(12,32)YINT(I,K)
      IF(YINT(I,K).GT.FIX3) FIX3=YINT(I,K)
   32 FORMAT(E12.4)
   56 CONTINUE
      CALL FIXAXS(XVAL(1),XVAL(20),0.0,FIX3)
      IF(KK.EQ.1)GOTO 703
      DO 37 I=1,NF
      DO 36 K=1,20
      YVAL(K)=YINT(I,K)
   36 CONTINUE
      JG=0
      IF(I.NE.1)JG=1
C
C   PLOTS DISTRIBUTION FUNCTIONS ON ONE GRAPH ON VDU.
C   AFTER EACH CURVE,SOUNDS BUZZER AND WAITS FOR
C   CARRIAGE RETURN
C
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      CALL FGPLT(XVAL,YVAL,20,3,I,1,JG,IT3,5)
      CALL CHAMOD
      CALL T1OU(7)
      CALL ZREALD(A)
   37 CONTINUE
C
C   CLOSE DISTRIBUTION DATA FILE
C
      CALL SEARCH(4,0,8)
      GOTO 888
C
C   RESTARTS MONTE CARLO CALCULATION.
C
  883 CALL RESUME('*CARLO')
C
C         END PROGRAM HARD COPY GRAPHICAL OUTPUT STARTS AT THIS POINT
C
  884 CALL DEVFIN
      STOP
      END
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MONTE CARLO PROGRAM

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C
C     A MONTE CARLO CALCULATION OF THE DRIFT VELOCITY,MEAN ENERGY
C     AND DISTRIBUTION FUNCTION OF HOT ELECTRONS IN A ONE OR TWO
C     VALLEY SEMICONDUCTOR.SCATTERING PROCESSES INCLUDE ACOUSTIC
C     ,POLAR OPTICAL AND INTERVALLEY PHONON SCATTERING.
C
      REAL KB,KRHO,KZF,KZTOT,KZI,KT,L,KZ,NPR1,NPR2,MNE,M
     1 ,NO,NE,NI,KMESH,KKI,KKZF,KKZI,KM,KR
      INTEGER NF,VV,VR,TT,V,SR,SS,K,GMAX,NRC
      DIMENSION KR(20),F(10),GAMMA(2),L(10),VTIM(2),EF(10)
     1 ,SCATT(10),VEL(10)
     1 ,ET(2),KZ(2),V1(10),V2(10),U1(10),U2(10),NPR1(10)
     2 ,NPR2(10),DK(2),KMESH(2,21,21)
      DATA Y/4HNEW /
C
C     OPEN DATA STORAGE FILES
C
      CALL SEARCH(2,'MONTEF',5)
      CALL SEARCH(2,'MDATA1',6)
      CALL SEARCH(2,'MDATA2',7)
      CALL SEARCH(2,'MDATA3',8)
      CALL SEARCH(2,'MDATA4',9)
      CALL SEARCH(3,'MDATA5',10)
C
C     FUNDAMENTAL CONSTANTS
C
      H=1.05459
      E=1.60219
      C=4.803213
      KB=1.38062
      M=9.109136
C
C     DATA RECALL OPTION OR NEW DATA INPUT
C
      CALL PAGE
      WRITE(1,47)
47    FORMAT(//,10X,43HMONTE CARLO CALCULATION OF DRIFT VELOCITIES,/
     1 ,10X,43H-------------------------------------------,//
     1 ,48HFOR SAME MATERIAL DATA TYPE OLD,FOR NEW TYPE NEW)
      READ(1,303)X
303   FORMAT(A3)
      IF(X.EQ.Y) GOTO 49
      READ(14,789)RHE
      READ(14,789)S
      READ(14,789)R1
      READ(14,789)R2
      READ(14,789)WO
      READ(14,789)WE
      READ(14,789)WI
      READ(14,789)THA
      READ(14,789)THE
      READ(14,789)THI
      READ(14,789)D
      READ(14,789)EM1
      READ(14,789)EM2
789   FORMAT(E10.4)
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      GOTO 46
49    WRITE(1,41)
41    FORMAT(1H ,30HTYPE MATERIAL DENSITY(GM.CM-3))
      CALL ZREALD(RHE)
      IF(RHE.EQ.0.0)RHE=1.0
      WRITE(1,42)
42    FORMAT(1H ,34HTYPE VELOCITY OF SOUND IN MATERIAL,
     1  23H(UNITS OF 10**5 CM.S-1))
      CALL ZREALD(S)
      IF(S.EQ.0.0)S=1.0
      WRITE(1,43)
43    FORMAT(1H ,39HTYPE HIGH FREQUENCY DIELECTRIC CONSTANT)
      CALL ZREALD(R1)
      WRITE(1,44)
44    FORMAT(1H ,38HTYPE LOW FREQUENCY DIELECTRIC CONSTANT)
      CALL ZREALD(R2)
      WRITE(1,1)
1     FORMAT(1H ,29HTYPE OPTICAL PHONON FREQUENCY,
     1  25H(UNITS 10**13 RAD.SEC.-1))
      CALL ZREALD(WO)
      WRITE(1,2)
2     FORMAT(1H ,44HTYPE EQUIVALENT INTERVALLEY PHONON FREQUENCY,
     1  28H(UNITS OF 10**13 RAD.SEC.-1))
      CALL ZREALD(WE)
      IF(WE.EQ.0.0)WE=1.0
      WRITE(1,3)
3     FORMAT(1H ,33HTYPE INTERVALLEY PHONON FREQUENCY,
     1  28H(UNITS OF 10**13 RAD.SEC.-1))
      CALL ZREALD(WI)
      IF(WI.EQ.0.0)WI=1.0
      WRITE(1,4)
4     FORMAT(1H ,39HTYPE ACOUSTIC DEFORMATION POTENTIAL(EV))
      CALL ZREALD(THA)
      WRITE(1,5)
5     FORMAT(1H ,45HTYPE EQUIV. INTERVALLEY DEFORMATION POTENTIAL,
     1  24H(UNITS OF 10**9 EV.CM-1))
      CALL ZREALD(THE)
      WRITE(1,6)
6     FORMAT(1H ,38HTYPE INTERVALLEY DEFORMATION POTENTIAL,
     1  24H(UNITS OF 10**9 EV.CM-1))
      CALL ZREALD(THI)
      WRITE(1,7)
7     FORMAT(1H ,26HTYPE VALLEY SEPARATION(EV))
      CALL ZREALD(D)
      WRITE(1,8)
8     FORMAT(1H ,34HTYPE CENTRAL VALLEY EFFECTIVE MASS)
      CALL ZREALD(EM1)
      WRITE(1,9)
9     FORMAT(1H ,36HTYPE SATELLITE VALLEY EFFECTIVE MASS)
      CALL ZREALD(EM2)
      WRITE(14,689)RHE
      WRITE(14,689)S
      WRITE(14,689)R1
      WRITE(14,689)R2
      WRITE(14,689)WO
      WRITE(14,689)WE
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MONTE CARLO PROGRAM

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      WRITE(14,689)WI
      WRITE(14,689)THA
      WRITE(14,689)THE
      WRITE(14,689)THI
      WRITE(14,689)D
      WRITE(14,689)EM1
      WRITE(14,689)EM2
689   FORMAT(E10.4)
C
C     FINAL DATA INPUT
C
46    CALL PAGE
      WRITE(1,10)
10    FORMAT(1H ,32HTYPE TEMPERATURE(DEGREES KELVIN))
      CALL ZREALD(T)
      WRITE(1,21)
21    FORMAT(1H ,23HTYPE MAXIMUM ENERGY(EV))
      CALL ZREALD(EMAX)
      WRITE(1,11)
11    FORMAT(1H ,30HTYPE NUMBER OF REAL COLLISIONS)
18     CALL ZINTRD(NRC)
      IF(THI.NE.0.0) GOTO 750
      IF(NRC.LE.3000) GOTO 16
      WRITE(1,710)
710   FORMAT(1H ,45HMAXIMUM COLLISIONS IN ONE VALLEY =3000:RETYPE)
      GOTO 18
750   IF(NRC.LE.2000) GOTO 16
      WRITE(1,17)
17    FORMAT(1H ,46HMAXIMUM COLLISIONS IN TWO VALLEYS =2000:RETYPE)
      GOTO 18
16    WRITE(1,12)
12    FORMAT(1H ,30HTYPE NUMBER OF ELECTRIC FIELDS)
      CALL ZINTRD(NF)
      WRITE(10,801)NF
801   FORMAT(I2)
      DO 30 I=1,NF
      WRITE(1,13)I
13    FORMAT(1H ,10HTYPE FIELD,I2,10H (KV.CM-1))
      CALL ZREALD(F(I))
30    CONTINUE
      WRITE(1,23)
23    FORMAT(1H ,44HTYPE VALLEY FOR DISTRIBUTION FUNCTION:1 OR 2)
      CALL ZINTRD(VV)
      WRITE(1,22)
22    FORMAT(1H ,49HTYPE DISTANCE FROM KZ AXIS OF DSTRIBUTION:1 TO 21)
      CALL ZINTRD(VR)
      CA_L PAGE
C
C     CALCULATE PHONON FREQUENCIES AND OCCUPATION RATIOS
C
      HWO=H*WO/(E*100.0)
      HWI=H*WI/(E*100.0)
      HWE=H*WE/(E*100.0)
      IF(WO.NE.0.0) GOTO 909
      NO=0.0
      GOTO 908
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909   NO=1/(EXP(WO*H/(KB*T)*100.0)-1)
908   NI=1/(EXP(WI*H/(KB*T)*100.0)-1)
      NE=1/(EXP(WE*H/(KB*T)*100.0)-1)
C
C     CONSTANTS FOR SCATTERING RATES
C
      C1=1.0E+12*C*C*SQRT(M)*WO*(1/R1-1/R2)*(NO+1)/(1.4142*H*SQRT(E))
      C2=C1*NO/(NO+1)
      C3=1.0E+10*(2*M)**1.5*KB*T*THA*THA*E*E*SQRT(E)/(4.0*3.142*RHE
     1  *S*S*H*H*H*H)
      C4=2.0E+14*M**1.5*THE*THE*E*E*(NE+1)*SQRT(E) (1.4142*3.142
     2  *RHE*WE*H*H*H)
      C5=C4*NE/(NE+1)
      C6=1.0E+14*(EM1*M)**1.5*THI*THI*E*E*(NI+1)*SQRT(E)/(1.4142*3.142
     3  *RHE*WI*H*H*H)
      C7=3.0E+14*(EM2*M)**1.5*THI*THI*E*E*(NI+1)*SQRT(E)/(1.4142
     4  *3.142*RHE*WI*H*H*H)
      C8=C7*NI/(NI+1)
      C9=C6*NI/(NI+1)
C
C     CALCULATE K SPACE MESH ELEMENT FOR BOTH VALLEYS
C
      DK(1)=1.0E+7*SQRT(2*EM1*M*EMAX*E)/(H*20.0)
      DK(2)=1.0E+7*SQRT(2*EM2*M*EMAX*E)/(H*20.0)
C
C     CALCULATE VALUES OF KZ AT CENTRE OF EACH MESH ELEMENT
C     IN CHOSEN VALLEY AND WRITE TO FILE
C
      KZI=-DK(VV)*9.5
      DO 805 LL=1,20
      WRITE(13,807)KZI
807   FORMAT(E12.4)
      KZI=KZI+DK(VV)
805   CONTINUE
C
C     SET PARAMETERS FOR CENTRAL VALLEY,THEN CALCULATE THE
C     TOTAL SCATTERING RATE FOR REAL PROCESSES (R) FOR A NUMBER
C     OF ENERGIES UP TO THE MESH SIZE.STORE MAXIMUM VALUE OF R
C     IN GAMMA(1) TO CALCULATE PSEUDO (SELF) SCATTERING RATE.
C     TT=1 ENABLES PROGRAM TO RETURN TO LABEL 40
C
      TT=1
      EM=EM1
      V=1
31    GAMMA(V)=0.0
      EI=0.0
      J=1
35    EI=EI+EMAX/20.0
      GOTO 100
40    R=0.0
      DO 50 I=1,10
      R=R+L(I)
50    CONTINUE
      IF(R.GT.GAMMA(V)) GAMMA(V)=R
      J=J+1
      IF(J.NE.21) GOTO 35
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C
C     SET PARAMETERS FOR SATELLITE VALLEY AND REPEAT PROCESS TO
C     OBTAIN GAMMA(2).
C
      IF(V.EQ.2) GOTO 71
      EM=EM2
       V=2
      GOTO 31
71    WRITE( 1,75)GAMMA(1),GAMMA(2)
      WRITE(9,75)GAMMA(1),GAMMA(2)
75    FORMAT(1H ,8HGAMMA1= ,E10.4,10H  GAMMA2= ,E10.4)
      WRITE(1,72)T,NRC,EMAX
      WRITE(9,72)T,NRC,EMAX
72    FORMAT(1H ,5HTEMP=,E10.4,12H REALCOLSNS=,I6,15H MAXENERGY(EV)=
     3  ,F4.2)
      WRITE(1,333)
      WRITE(9,333)
333   FORMAT(2X,5HFIELD,4X,8HVELOCITY,1X,9HTIME IN 1,1X
     2  ,9HTIME IN 2,1X,9HMN.ENERGY,4X,4HSELF,4X,4HMESH)
C
C     SET MESH REGISTERS TO ZERO. AND PLACE ELECTRON AT
C     STARTING POINT IN MESH.TT=0 FOR ITERATIVE PROCESS.
C
      TT=0
      J=1
80    V=1
      EM=EM1
      PSI=0.0
      KRHO=0.0
      KZF=1.0E+6
      SR=0
      SS=0
      GMAX=0
      EFIN=H*H*KZF*KZF*1.0E-14/(E*2*EM*M)
      ETOT=0.0
      KZTOT=0.0
      VTIM(1)=0.0
      VTIM(2)=0.0
      KZ(1)=0.0
      KZ(2)=0.0
      ET(1)=0.0
      ET(2)=0.0
      DO 999 K=1,20
      KMESH(VV,VR,K)=0.0
999   CONTINUE
C
C     IF NO. OF REAL PROCESSES EQUALS CHOSEN VALUE,END ITERATION
C     AND GOTO FINAL CALCULATION.
C
90    IF(SR.EQ.NRC) GOTO 470
C
C     CALL RANDOM NUMBER(NOT=0) AND CALCULATE TIME OF FLIGHT UNDER
C     ELECTRIC FIELD AND NEW POSITION OF ELECTRON IN K SPACE
C
      R=RND(B)
      IF(R.EQ.0.0) R=1.0E-20
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      TIME=ALOG(1/R)/GAMMA(V)
      KZI=KZF+(TIME*E*F(J)*1.0E+18)/H
      KT=SQRT(KRHO*KRHO+KZI*KZI)
      EI=H*H*KT*KT*1.0E-14/(E*2*EM*M)
C
C     IF ELECTRON LEAVES MESH PLACE IT ON EDGE OF MESH AND
C     REGISTER OCCURRENCE IN COUNTER GMAX.
C
      IF(EI.LE.EMAX) GOTO 95
      GMAX=GMAX+1
      EI=EMAX
      KT=1.0E+7*SQRT(2*EM*M*EMAX*E)/H
      IF(KZI.GT.0.0)GOTO 94
      KZI=-SQRT(ABS(KT*KT-KRHO*KRHO))
      GOTO 95
   94 KZI=SQRT(ABS(KT*KT-KRHO*KRHO))
C
C     STORE FLIGHT TIME IN TOTAL TIME REGISTER FOR APPROPRIATE
C     VALLEY,THEN REGISTER PASSAGE OF ELECTRON THROUGH ELEMENTS
C     OF K SPACE MESH.
C
   95 VTIM(V)=VTIM(V)+TIME
      KKRHO=KRHO/DK(V)+1
      IF(KKRHO.NE.VR) GOTO 890
      KKZI=KZI/DK(V)+10
      KKZF=KZF/DK(V)+10
      KF=KKZF
      KI=KKZI
      KF1=KF+1
      KI1=KI+1
      IF(KI.EQ.KF) GOTO 880
      DO 870 LL=KF1,KI1
      KMESH(V,KKRHO,LL)=KMESH(V,KKRHO,LL)+1.0
870   CONTINUE
      KMESH(V,KKRHO,KF1)=KMESH(V,KKRHO,KF1)+KF-KKZF
      KMESH(V,KKRHO,KI1)=KMESH(V,KKRHO,KI1)+KKZI-KI1
      GOTO 890
880   KMESH(V,KKRHO,KF1)=KMESH(V,KKRHO,KF1)+KKZI-KKZF
C
C     SUM TOTAL CHANGES IN K SPACE POSITION AND ENERGY SPACE POSITION
C     AND STORE IN KZTOT AND ETOT.SUM MEAN ENERGY CHANGE IN MNE.
C     SUM INDIVIDUAL VALUES FOR EACH VALLEY IN KZ(V) AND ET(V).
C
890   KZTOT=KZTOT+ABS(KZI-KZF)
      ETOT=ETOT+(KZI*KZI-KZF*KZF)*10.0*H/(2*EM*M)
      MNE=MNE+(KZI*KZI*KZI-KZF*KZF*KZF)*1.0E-14*H*H/(2*EM*M*E)
      KZ(V)=KZ(V)+ABS(KZI-KZF)
      ET(V)=ET(V)+(KZI*KZI-KZF**2)*10.0*H/(2*EM*M)
C
C     CHECK FOR ROUNDING ERRORS LEADING TO NEGATIVE ENERGY VALUES.
C     IF THIS OCCURS,PLACE ELECTRON AT STARTING POSITION.
C
      IF(EI.GT.0.0) GOTO 100
      KRHO=0.0
      PSI=0.0
      KZF=1.0E+6
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ONTE CA<LO PROGRAM

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      EM=EM1
      V=1
      GOTO 90
C
C     CALCULATE FINAL ENERGY VALUE FOR EACH SCATTERING PROCESS.
C
 100  EF(1)=EI-HWO
      EF(2)=EI+HWO
      EF(3)=EI
      EF(4)=EI
       EF(5)=EI HWE
      EF(6)=EI+HWE
      EF(7)=EI-HWI+D
      EF(8)=EI-HWI-D
      EF(9)=EI-HWI-D
      EF(10)=EI+HWI+D
C
C     SCATTERING RATES FOR REAL PROCESSES
C
      IF(EF(1).GT.0.0) GOTO 110
      L(1)=0.0
      GOTO 120
110   L(1)=C1*SQRT(EM)*ALOG(ABS((SQRT(EI)+SQRT(EF(1)))/(SQRT(EI)-
     4  SQRT(EF(1)))))/SQRT(EI)
C
C     EMISSION OF OPTICAL PHONON
C
120   IF(EF(2).GT.0.0) GOTO 125
      L(2)=0.0
      GOTO 130
125   L(2)=C2*SQRT(EM)*ALOG(ABS((SQRT(EI)+SQRT(EF(2)))/(SQRT(EI)-
     5  SQRT(EF(2)))))/SQRT(EI)
C
C     ABSORPTION OF OPTICAL PHONON
C
130   IF(EF(3).GT.0.0) GOTO 135
      L(3)=0.0
      GOTO 140
135   L(3)=C3*EM**1.5*SQRT(EF(3))
C
C     EMISSION OF ACOUSIC PHONON
C
140   IF(EF(4).GT.0.0) GOTO 145
      L(4)=0.0
      GOTO 150
145   L(4)=L(3)
C
C     ABSORPTION OF ACOUSTIC PHONON
C
150   IF(EF(5).GT.0.0) GOTO 155
      L(5)=0.0
      GOTO 170
155   IF(V.EQ.2) GOTO 160
      L(5)=0.0
      GOTO 170
160   L(5)=C4*EM**1.5*SQRT(EF(5))
```

MONTE CARLO PROGRAM

```
C
C     EMISSION OF EQUIVALENT INTERVALLEY PHONON
C
170   IF(EF(6 .GT.0.0) GOTO 175
      L(6)=0.0
      GOTO 190
175   IF(V.EQ.2) GOTO 180
      L(6)=0.0
      GOTO 190
180   L(6)=C5*EM**1.5*SQRT(EF(6))
C
C     ABSORPTION OF EQUIVALENT INTERVALLEY PHONON
C
190   IF(EF(7).GT.0.0) GOTO 195
      L(7)=0.0
      GOTO 210
195   IF(V.EQ.2) GOTO 200
      L(7)=0.0
      GOTO 210
200   L(7)=C6*SQRT(EF(7))
C
C     EMISSION OF INTERVALLEY PHONON(SATELLITE TO CENTRAL)
C
210   IF(EF(8).GT.0.0) GOTO 215
      L(8)=0.0
      GOTO 230
215   IF(V.EQ.1) GOTO 220
      L(8)=0.0
      GOTO 230
220   L(8)=C7*SQRT(EF(8))
C
C     EMISSION OF INTERVALLEY PHONON(CENTRAL TO SATELLITE)
C
230   IF(EF(9).GT.0.0) GOTO 235
      L(9)=0.0
      GOTO 250
235   IF(V.EQ.1) GOTO 240
      L(9)=0.0
      GOTO 250
240   L(9)=C8*SQRT(EF(9))
C
C     ABSORPTION OF INTERVALLEY PHONON(CENTRAL TO SATELLITE)
C
250   IF(EF(10).GT.0.0) GOTO 255
      L(10)=0.0
      GOTO 270
255   IF(V.EQ.2) GOTO 260
      L(10)=0.0
      GOTO 270
260   L(10)=C9*SQRT(EF(10))
C
C     ABSORPTION OF INTERVALLEY PHONON(SATELLITE TO CENTRAL)
C
270   IF(TT.EQ.1) GOTO 40
C
C     CALCULATE SUM OF REAL PROCESS SCATTERING RATES
```

```
MONTE CARLO PPJGRAM
C
280    SCATT(1)=L(1)/GAMMA(V)
       DO 290 K=2,10
       SCATT(K)=SCATT(K-1)+L(K)/GAMMA(V)
290    CONTINUE
C
C       CALL RANDOM NUMBER.SELECT SCATTERING CHANNEL.
C
       R=RND(B)
       IF(R.LT.SCATT(1)) GOTO 300
       IF(R.LT.SCATT(2)) GOTO 310
       IF(R.LT.SCATT(3)) GOTO 320
       IF(R.LT.SCATT(4)) GOTO 330
       IF(P.LT.SCATT(5)) GOTO 340
       IF(P.LT.SCATT(6)) GOTO 350
       IF(P.LT.SCATT(7)) GOTO 360
       IF(P.LT.SCATT(8)) GOTO 370
       IF(R.LT.SCATT(9 ) GOTO 380
       IF(R.LT.SCATT(10)) GOTO 390
       GOTO 400
C
C      SET ENERGY AFTER SCATTERING PROCESS.
C
300    EFIN=EF(1)
       GOTO 420
310    EFIN=EF(2)
       GOTO 420
320    EFIN=EF(3)
       GOTO 410
330    EFIN=EF(4)
       GOTO 410
340    EFIN=EF(5)
       GOTO 410
350    EFIN=EF(6)
       GOTO 410
360    EFIN=EF(7)
       GOTO 430
370    EFIN=EF(8)
       GOTO 430
380    EFIN=EF(9)
       GOTO 430
390    EFIN=EF(10)
       GOTO 430
400    EFIN=EI
       GOTO 450
410    SR=SR+1
C
C      REGISTER REAL COLLISION.CALCULATE K SPACE POSITION AFTER
C      ACOUSTIC, INTERVALLEY OR EQUIVALENT INTERVALLEY PHONON SCATTERING.
C
       R=RND(B)
       KT=1.0E+7*SQRT(2*EM*M*EFIN*E)/H
       KZF=KT*(1-2*R)
       KRHO=KT*SQRT(4*R*(1-R))
       GOTO 460
420    SR=SR+1
```

MONTE CARLO PROGRAM

```
C
C      REGISTER REAL COLLISION.CALCULATE K SPACE POSITION AFTER
C      OPTICAL PHONON SCATTERING.
C
       R=RND(B)
       U=RND(B)
       PHI=2*3.142*R
       EX=2*SQRT(EFIN*EI)/((SQRT(EI)-SQRT(EFIN))**2)
       BETA=(((1+EX)-(1+2*EX)**U)/EX)
       RHO=(BETA*KZI/KT-SQRT(ABS(1-BETA*BETA))*KRHO/KT*COS(PHI))
       KT=1.0E17*SQRT(2*EM*M*EFIN*E)/H
       KZF=KT*RHO
       KRHO=KT*SQRT(ABS(1-RHO*RHO))
       GOTO 460
C
C      CHANGE VALLEY PARAMETERS FOR INTERVALLEY PROCESSES.
C
430    IF(V.EQ.1) GOTO 440
       V=1
       EM=EM1
       GOTO 410
440    V=2
       EM=EM2
       GOTO 410
450    SS=SS+1
C
C      REGISTER SELF SCATTERING PROCESS.K SPACE POSITION UNCHANGED.
C
       KZF=KZI
C
C      CHECK IF ELECTRON IS SCATTERED OUT OF MESH.IF SO,REGISTER
C      PROCESS ON COUNTEP GMAX,AND PLACE ELECTRON ON EDGE OF MESH.
C      LABEL 90 REPEATS ITERATIVE PROCESS STARTING WITH FREE
C      ELECTRON FLIGHT UNDER ELECTRIC FIELD.
C
4 0    IF(EFIN.LE.1.0) GOTO 90
       GMAX=GMAX+1
       KT=1.0E+7*SQRT(2*EM*M*EMAX*E)/H
       IF(KRHO.GT.KT) KRHO=KT
       KZF=SQRT(ABS(KT*KT-KRHO*KRHO))
       GOTO 90
C
C      FINAL CALCULATION OF DRIFT VELOCITY-VEL,TIME SPENT IN EACH
C      VALLEY-VTIM(V),MEAN ENERGY-MNE.ALSO OUTPUT NO. OF SELF
C       SCATTERING PROCESSES AND NUMBER OF TIMES MESH EXCEEDED.
C
C      SECOND TABLE OF DATA CONTAINS MEAN VELOCITY IN EACH
C      VALLEY(V1 AND V2),MOBILITY(U1 AND U2) AND FRACTIONAL TIME
C      IN EACH VALLEY(NPR1 AND NPR2).
C
470    IF(KZTOT.EQ.0.0)KZTOT=1.0E-20
       VEL(J)=ETOT/KZTOT
       MNE=MNE/KZTOT
       IF(VTIM(1).EQ.0.0) VTIM(1)=1.0E-25
       IF(KZ(1).EQ.0.0) KZ(1)=1.0E-25
       IF(KZ(2).EQ.0.0) KZ(2)=1.0E-25
```

MONTE CARLO PROGRAM

```
      V1(J)=ET(1)/KZ(1)
      V2(J)=ET(2)/KZ(2)
      U1(J)=V1(J)/(F(J)*1000.0)
      U2(J)=V2(J)/(F(J)*1000.0)
      NPR1(J)=VTIM(1)/(VTIM(1)+VTIM(2))
      NPR2(J)=VTIM(2)/(VTIM(1)+VTIM(2))
      WRITE(1,480)F(J),VEL(J),VTIM(1),VTIM(2),MNE,SS,GMAX
      WRITE(9,480)F(J),VEL(J),VTIM(1),VTIM(2),MNE,SS,GMAX
480   FORMAT(5(E9.3,1X),I7,1X,I5)
      CALL T10U(7)
C
C     WRITE DATA TO FILES FOR GRAPHICAL DISPLAY.
C
      WRITE(10,800)F(J)
      WRITE(11,800)VEL(J)
      WRITE(12,800)MNE
800   FORMAT(E12.4)
      DO 810 LL=1,20
      WRITE(13,820)KMESH(VV,VR,LL)
820   FORMAT(E12.4)
810   CONTINUE
      J=J+1
      IF(J.NE.NF+1) GOTO 80
      WRITE(9,501)
      WRITE(1,501)
501   FORMAT(//,2X,5HFIELD,5X,4HVEL1,6X,4HVEL2,6X,4HMOB1,6X
     2   ,4HMOB2,8X,2HN1,8X,2HN2)
      DO 510 J=1,NF
      WRITE(9,500)F(J),U1(J),U2(J),U1(J),U2(J),NPR1(J),NPR2(J)
      WRITE(1,500)F(J),U1(J),J2(J),U1(J),U2(J),NPP1'J),NPR2(J)
500   FORMAT(7(E9.3,1X))
510   CONTINUE
C
C     TRUNCATE AND CLOSE ALL DATA FILES.
C
      CALL SEARCH(8,0,5)
      CALL SEARCH(8,0,6)
      CALL SEARCH(8,0,7)
      CALL SEARCH(8,0,8)
      CALL SEARCH(8,0,9)
      CALL SEARCH(8,0,10
      CALL SEARCH(4,0,5)
      CALL SEARCH(4,0,6)
      CALL SEARCH(4,0,7)
      CALL SEARCH(4,0,8)
      CALL SEARCH(4,0,9)
      CALL SEARCH(4,0,10)
      CALL SEARCH(3,'GRAPHS',5)
      READ(9,951)Y
951   FORMAT(A3)
      CALL SEARCH(4,0,5)
      WRITE(1,952)
952   FORMAT(/,28HTO OBTAIN GRAPHS TYPE GRAPHS,//
     1 ,28HTO LEAVE PROGRAM TYPE FINISH)
      READ(1,951)X
      IF(X.NE.Y)GOTO 983
```

```
MONTE CARLO PROGRAM
C
C     START GRAPHICAL DISPLAY
C
      CALL RESUME('*GMONTE')

  983 STOP
      END
```

Physics Programs
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CHAPTER 12

Modelling of the Thermal Conductivity of Unidirectional Composite Materials

G. S. Keen and B. W. James

1. INTRODUCTION

Composite materials, made of a host (matrix) with a number of fibres inserted into it (inserts), are now widely used because of their special mechanical properties and high strength to weight ratio. In some applications it is necessary to know the heat flow along, or through, the composite material. This heat flow will depend upon the thermal conductivities of the constituent materials. If the composite material has an anisotropic structure, the heat flow will also be anisotropic, and cannot, in general, be calculated simply on the basis of the ratios of the constituent materials since it depends upon the geometrical arrangement of the composite in the heat flow direction. It is therefore convenient to characterize the composite material by a number of effective thermal conductivities which take account of these factors.

Obviously the effective thermal conductivity of the composite material can be measured experimentally with special apparatus. However, this approach can be very time consuming if a number of different composite materials have to be considered over a wide temperature range. Also, whilst experimental measurements of the thermal conductivity of the composite material and the matrix material used in the composite are readily made, it is not possible to measure the thermal conductivity of the fibre reinforcement, due to the small physical dimensions of the fibres, although the bulk value can be found for materials which exist (occur) in bulk form. (The anisotropic structure of some fibres is not repeated in the bulk form, e.g. carbon fibres.) In contrast, an investigation of the thermal properties of composite materials, over a wide range of temperature, and for various configurations of fibres inserted into the matrix material, can be carried out with a computer program which models the real material. The advantages of this approach include obtaining values of the effective thermal conductivities much more rapidly, and at a lower cost than that involved in experimental measurement. Another advantage of computer modelling to obtain the effective thermal conductivity is that, if the thermal conductivity of the insert material is not known, and cannot be measured in the bulk form, it may be found by iterative calculations from measured values of the matrix thermal conductivity and the effective thermal conductivity of the composite.

2. HEAT CONDUCTION IN COMPOSITES

2.1 Basic ideas

The general form of the heat flow equation is

$$\mathbf{Q} = \mathbf{K} \cdot \nabla T, \tag{1}$$

where $\mathbf{Q}$ is the thermal flux vector, whose dimensions are energy transmitted, per unit area, per unit time, $\mathbf{K}$ is the thermal conductivity tensor of the medium conducting the heat, and ∇T is the vector temperature gradient across it.

A unidirectional composite material may be idealized by a regular array of inserts, aligned in one direction in the matrix material. The basic rectangular prism, or cell, of such a composite, is a single insert, immersed in the matrix material with its axis parallel to the longest side of the prism. All cross-sections of this cell that are perpendicular to the insert axis are identical, therefore, and any sample of composite material can be simulated by using a large number of basic cells. In Figure 1 a cylindrical insert, or fibre, is shown, but any other shape is possible. If the insert is, in fact, a cylindrical fibre and is at the centre of a cell that has, in addition, a square cross-section then only a quarter of the basic cell needs to be considered because of its fourfold axis of symmetry. This has the advantage, as will be seen later, that the accuracy of the calculations improves if a fraction of the basic cell is used.

If a temperature difference is applied between any two opposite faces of a cell that is part of a large assembly then the edge effects arising from the other faces can be ignored as there will be no flow of heat across them. Since this is the case, the application of the temperature difference between faces 1 and 2, of Figure 1 causes the heat to flow in a direction parallel to the fibre axis. This is called longitudinal heat flow, whereas if the temperature difference is applied between either of the two other opposite pairs of faces, the direction of heat flow is in a direction transverse to the fibre axis and is called transverse heat flow.

In a unidirectional composite material there are three independent coefficients in the conductivity tensor, K_x, K_y, and K_z, if the insert axis is taken as the z-axis (Nye,[1] Boardman, O'Connor, and Young.[2]). Furthermore, if the