[Supplement](#HadjiSupplFirstCite).. Source of the programme used to analyse the here considered experimental data.

!! The following programme source is in Fortran 90. !!

! Absolute Atom concentration etc. determinations.

! The PROGRAMME uses the "Dichotomy" Method.

! - The effective mass must be provided to get the absolute atom concentration etc.

! - This programme source copy belongs to Noureddine HADJI and is "given" free of charge

! to whoever want(s) to use it as it is or to modify it before use.

module Some\_Const\_Params0

! Module containing definitions of parameters needed to compute the Atom Concentration

real(8) , parameter :: Ar0=5.292d-11 ! Bohr radius in m

real(8) , parameter :: ECHARGe=1.602d-19 ! electron charge in C

real(8) , parameter :: MASS0=9.110d-31 ! electron rest mass in kg

real(8) , parameter :: HPlckConst=6.626d-34 ! Planck's constant in Js

real(8) , parameter :: HBAR=1.055d-34 ! Planck's constant over two pi in Js

real(8) , parameter :: SpeedC=2.998d8 ! speed of light in ms-1

real(8) , parameter :: EPSILO=8.854D-12 ! permitivity of space in Fm-1

double precision, parameter :: Pi = 3.14159265358979323845

end module Some\_Const\_Params0

module For\_Concentrations\_etc0

! Module containing definitions of variables needed to compute the Atom Concentration

real(8) X,Var1,Y ,Q,STAR,XLAST,Var2, Var3

integer IL

end module For\_Concentrations\_etc0

!

module Incident\_electron\_Dta0

real(8) V0,D,WaveLengt,K0,ElecSpeed,Gama

end module Incident\_electron\_Dta0

!

module Get\_interval\_A1\_3\_0

real(8) , parameter :: P0InitVal = 1.D-15

integer SubType

real(8) A1,A2,A3,Y1,Y2,Y3,Alow,Aup,AplausMin

real(8) VA1,VA3, DeltaA,Var1LT,Ysmallest,Var1Ysmallest,P0

real(8) Yf, Yg

character\*52 OutCome

end module Get\_interval\_A1\_3\_0

!

module Calculated\_Factors0

real(8) PlPeaP, LambdaP, ElectConc, FEnerg,EFoverEp

real(8) LOGKF, LOGElectConc,Lambda,ElectConcToThird

real(8) Thetac,ThetaE, ElecEfMas,KF,Alfa,ThetaF,Nk1

real(8) ThetaFto3over2, KC

character(1) RPAorExCor

logical errKc, errThetaC

end module Calculated\_Factors0

!

subroutine If\_SubType13

use Get\_interval\_A1\_3\_0

implicit none

if (SubType.eq.13) then

call Elect\_Conc\_Dispersion\_etc\_Eff\_M\_Known\_FULL\_Kc13

end if

return

end subroutine If\_SubType13

!

subroutine Dichotoming !! Dichotomy Method for solving nonlinear equations.

use Get\_interval\_A1\_3\_0

use For\_Concentrations\_etc0

implicit none

integer i

i=0

if (A1.eq.A3) then

A2=A1

goto 1200

end if

! A2=(A1+A3)/2.

A2=(1.+A3/A1)/2.\*A1

Var1=A1

call If\_SubType13

Y1=Y

Var1=A2

call If\_SubType13

Y2=Y

Var1=A3

call If\_SubType13

Y3=Y

do

if (Y1\*Y2.lt.0.0) then

A3=A2

Y3=Y2

else

A1=A2

Y1=Y2

end if

A2=(1.+A3/A1)/2.\*A1

if (abs(Y).le.P0) then

write(\*,\*)' Condition abs(Y)<=P0 satisfied (in 1) after ',i,' small loops'

! A2 Returned value

A1=A2

A3=A1

goto 1200

end if

Var1=A2

call If\_SubType13

Y2=Y

i=i+1

end do

1200 continue

return

end subroutine Dichotoming

!

subroutine Get\_Incident\_electron\_Dta\_Final0

use Some\_Const\_Params0

use Incident\_electron\_Dta0

implicit none

760 write (\*,\*) 'Enter accelerating voltage, in kilovolts'

write (\*,\*) 'E.g. 100.'

write (\*,\*) ''

read(\*,\*,err=760) V0

V0=V0\*1000.0\_8

! Get k0=2pi/lambda

D=SQRT(V0+0.97845e-6\*V0\*V0)/1.22639\*1.e9

! Get wave length

WaveLengt=1.0\_8/D

K0=2.\_8\*Pi\*D

! Get incident electron velocity.

! First work out D.

D=D\*(HPlckConst/MASS0)

! Incident electron velocity is: ElecSpeed

ElecSpeed=D/SQRT(1.\_8+(D/SpeedC)\*(D/SpeedC))

! Get Gamma

Gama=1./SQRT(1.\_8-(ElecSpeed/SpeedC)\*(ElecSpeed/SpeedC))

print \*, '!------------------------------------------------------&

----------------------!'

print \*, ' '

print \*, ' Have obtained the following "incident-electron" data:'

print \*, ' '

print \*, '!------------------------------------------------------&

----------------------!'

write(\*,2510)' Incident electron wave length: ',WaveLengt\*1.e10,'&

angs'

print \*, '!------------------------------------------------------&

----------------------!'

write(\*,2520)' Incident electron wave vector: ',K0,' in m-1'

print \*, '!------------------------------------------------------&

----------------------!'

write(\*,2520)' Incident electron velocity: ',ElecSpeed,' m/s'

print \*, '!------------------------------------------------------&

----------------------!'

write(\*,2510)' Gamma : ',Gama

print \*, '!------------------------------------------------------&

----------------------!'

!

2510 format(A,F14.5,A)

2520 format(A,ES15.5,A)

return

end subroutine Get\_Incident\_electron\_Dta\_Final0

!

SUBROUTINE Elect\_Conc\_Dispersion\_etc\_Eff\_M\_Known\_FULL\_Kc13

use Some\_Const\_Params0

use Incident\_electron\_Dta0

use For\_Concentrations\_etc0

use Get\_interval\_A1\_3\_0

use Calculated\_Factors0

! NOTE: This routine is not based on the equations given in the paper

! by N. Hadji: Two Analytical Techniques for the Determination

! of the Absolute Atom Concentration Using Electron Energy

! Loss Spectroscopy (EELS). Int. J. Mod. Phys. B, 16, 4775 (2002).

! The equations given in the above text are used. That is in the text

! More Accurate Formulas for Determination of Absolute Atom Concentration Using Electron

! Energy-Loss Spectroscopy.

implicit none

! Q=PlSctCSec(1) is PSCA per atom of the first element entered.

! Var1=ElectConc

! Work out the plasmon peak energy

PlPeaP=(HBAR\*(Var1)\*\*(1./2.)/ElecEfMas\*\*(1./2.)/EPSILO\*\*(1./2.))\*ECHARGe

! Work out the Fermi vector

KF=(3.\*Pi\*Pi\*Var1)\*\*(1./3.)

! Work out the Fermi energy

FEnerg=(HBAR\*KF)/MASS0\*(HBAR\*KF)/2.

! Work out the ratio of the Fermi energy to the first plasmon peak position energy

EFoverEp=FEnerg/PlPeaP

if (RPAorExCor .eq. 'k' .or. RPAorExCor .eq. 'K') then

!! Value for alfa was provided

else

!! Either RPA or ExCor considered.

Alfa=3./5.\*(EFoverEp)

if ( RPAorExCor .eq. 'E' .or. RPAorExCor .eq. 'e') then

!! ExCor considered.

Alfa=Alfa\*(1.-(1./EFoverEp)\*(1./EFoverEp)/16.)

else

!! RPA considered.

end if

end if

if (Alfa .eq. 0.5) then

KC = KF/2.\*(PlPeaP/FEnerg)

else

if (1.-(2\*Alfa-1.)\*PlPeaP/FEnerg .le. 0) then

errKc = .true.

write(\*,\*) ' There is error !!:'

write(\*,\*) '(1.-(2\*Alfa-1.)\*PlPeaP/FEnerg) is negative'

return

end if

KC = KF/(2.\*Alfa-1.)\*(1.-DSQRT(1.-(2\*Alfa-1.)\*PlPeaP/FEnerg))

end if

ThetaE=PlPeaP/(Gama\*MASS0\*ElecSpeed\*ElecSpeed)

if ((KC/K0 - ThetaE)\*(KC/K0 + ThetaE) .le. 0) then

errThetaC = .true.

write(\*,\*) ' There is error !! I cannot calculate Thetac:'

write(\*,\*) '(KC/K0 - ThetaE)\*(KC/K0 + ThetaE) is negative'

return

end if

Thetac = DSQRT((KC/K0 - ThetaE)\*(KC/K0 + ThetaE))

!! The following next instruction is the equation to solve.

!! Var1 is the unknown to be determined.

!! The solution is obtained when Y=0.

Y=1.-Gama\*STAR\*ThetaE/(Q\*Var1)/Ar0\*DLOG(KC/K0/ThetaE)

Var1LT = (Var1LT-Var1)/Var1

IF (Y.eq.0.0.OR.ABS(Var1LT).le.P0) IL=1

Var1LT=Var1

if (Ysmallest.gt.abs(Y)) then

Ysmallest=abs(Y)

Var1Ysmallest=Var1

endif

return

END SUBROUTINE Elect\_Conc\_Dispersion\_etc\_Eff\_M\_Known\_FULL\_Kc13

!

subroutine get\_interval\_A1\_A3\_Lt

! This routine gets the interval [A1, A3] enclosing the solution Var1

! for a non-linear equation defined in another subroutine that this

! subroutine calls. This is for PHYSICAL QUANTITIES ONLY, and therefore

! for strictly positive quantities. To get it working for other quantities,

! e.g. including negative values for Var1, one needs to change

! the local variables Alow and Aup accordingly.

use Some\_Const\_Params0

use For\_Concentrations\_etc0

use Get\_interval\_A1\_3\_0

use Incident\_electron\_Dta0

use Calculated\_Factors0

implicit none

integer L, k

real(8) Mas0

!---------------------Get interval containing solution ------------------

Var1LT=1.e-38

errKc = .false.

errThetaC = .false.

write(\*,\*) ' Started Working, please wait for the results !!!!'

write(\*,\*) ' '

940 Mas0=MASS0

Alow=0.0

k=0

970 Aup=AplausMin\*100.

if (SubType.eq.6) Aup=AplausMin\*500.

Var1=1.e38

Ysmallest=1.e38

980 DeltaA=A2/100.

985 continue

if (SubType.eq.5) DeltaA=A2/3.

990 A1=A2

A3=A2

L=0

Var1LT=3.\*Var1

Var1=A2

995 continue

call If\_SubType13

if (errKc) return

if (errThetaC) return

Y2=Y

if (abs(Y).le.P0.or.DeltaA/Var1.le.P0InitVal) then

A2=Var1 ! Returned value

A1=A2

A3=A1

return

end if

Y1=Y2

Y3=Y2

1020 if (Y1\*Y3>0.0) then

A1=A1-DeltaA

if (A1<=Alow) then

if (A3>=Aup) then

L=1

goto 1120

end if

A1=A1+DeltaA-DeltaA/10.

else if (A3>=Aup) then

if (A1<=Alow) then

L=1

goto 1120

end if

A3=A3-DeltaA+DeltaA/10.

else

end if

Var1=A1

if (Var1<=0.0) then

goto 1060

end if

call If\_SubType13

if (errKc) return

if (errThetaC) return

Y1=Y

if (abs(Y).le.P0.or.DeltaA/Var1.le.P0InitVal) then

A2=Var1 ! Returned value

A1=A2

A3=A1

return

end if

1060 A3=A3+DeltaA

Var1=A3

call If\_SubType13

if (errKc) return

if (errThetaC) return

Y3=Y

if (abs(Y).le.P0.or.DeltaA/Var1.le.P0InitVal) then

A2=Var1 ! Returned value

A1=A2

A3=A1

return

end if

goto 1020

else

if (Y1\*Y2>0.0) then

A1=A3-DeltaA

Var1=A1

call If\_SubType13

if (errKc) return

if (errThetaC) return

Y1=Y

else if (Y3\*Y2>0.0) then

A3=A1+DeltaA

Var1=A3

call If\_SubType13

if (errKc) return

if (errThetaC) return

Y3=Y

else if (Y1.eq.0.0) then

A3=A1

A2=A1

VA1=A1

VA3=A3

return

else if (Y3.eq.0.0) then

A1=A3

A2=A3

VA1=A1

VA3=A3

return

end if

VA1=A1

VA3=A3

end if

1120 if (L.eq.1) then

write(\*,\*) ' '

write(\*,\*) '!------------------------------------------------------&

----------------------!'

write(\*,\*) ' Enter a number you expect is much larger than the'

write(\*,\*) ' '

write(\*,\*) ' solution you are looking for. Use MKSA units.'

write(\*,\*) '!------------------------------------------------------&

----------------------!'

write(\*,\*) ' '

1140 write(\*,\*) ' If you do not know what to enter, try', Aup\*5.

write(\*,\*) ' '

write(\*,\*) ' To return to the Menu enter 0.0'

1150 write(\*, '(A)', ADVANCE = "NO")' => '

read (\*,\*,err=1140)Aup

if (Aup.eq.0.0) return

if (Aup.lt.AplausMin) then

write(\*,\*) '!------------------------------------------------------&

----------------------!'

write(\*,\*) ' PLEASE try a larger number.'

goto 1140

end if

L=0

A2=AplausMin\*2.

goto 980

else if (L.eq.0) then

end if

return

end subroutine get\_interval\_A1\_A3\_Lt

!

program Absol\_Atom\_Concent\_Determ\_Need\_Eff\_Mass\_FULL

! NOTE: This programme is built on the basis of the equations given in the text

! " More Accurate Formulas for Determination of Absolute Atom Concentration Using Electron

! Energy-Loss Spectroscopy."

! These equations are for obtaining results more precise

! than those obtained using the equations given in the article "Two Analytical

! Techniques for the Determination of the Absolute Atom Concentration

! Using Electron Energy Loss Spectroscopy (EELS)". See International Journal

! of Modern Physics B, Vol. 16, No 31, pp 4775-4781 (2002)' N. Hadji.

! The electron concentration is the parameter varied to get the function Y zeroed.

use Some\_Const\_Params0

use Incident\_electron\_Dta0

use For\_Concentrations\_etc0

use Get\_interval\_A1\_3\_0

use Calculated\_Factors0

implicit none

character\*2, dimension(:), allocatable :: ElemNames

character\*1 choix,Choice, ChoiceP, RPAorExCorP

character(255) file

INTEGER(KIND=4)Ierr

integer n

integer i, ILLa,ILLb

integer AllocateStatus,DeAllocateStatus

real(8) X0

real(8) Alfa1

real(8), dimension(:), allocatable :: Nk

real(8), dimension(:), allocatable :: Pelect,PlSctCSec

print \*, ' This programme uses equations more precise than those'

print \*, ' considered in the article "Two Analytical Techniques for'

print \*, ' the Determination of the Absolute Atom Concentration'

print \*, ' Using Electron Energy Loss Spectroscopy (EELS)".'

print \*, ' [See International Journal of Modern Physics B,'

print \*, ' Vol. 16, No 31, pp 4775-4781 (2002)'

print \*, ' by N. Hadji.]'

print \*, ' '

print \*, ' The ELECTRON EFFECTIVE MASS is required.'

print \*, ' '

write(\*,\*) '/////////////////////////////////////////////////////////'

print \*, '/ This programme is entirely free of charge. /'

print \*, "/ So please don't pay for it. /"

write(\*,\*) '/////////////////////////////////////////////////////////'

! Write equation to solve in subroutine Elect\_Conc\_Dispersion\_etc\_Eff\_M\_Known\_FULL\_Kc13

print \*, ' '

100 do

RPAorExCor = 't'

write(\*,\*) '-------------------------- Menu -------------------- &

------------!'

write(\*,\*) ' '

write(\*,\*) ' Q to quit'

write(\*,\*) ' A for Technique no 1'

write(\*,\*) ' B for Technique no 2'

if (ILLa.eq.1) then

write(\*,\*) ' D to get thickness (Technique no 1)'

write(\*,\*) ' P to print results as Resutlts\_AAC\_etc.txt file.'

else if (ILLb.eq.1) then

write(\*,\*) ' E to get thickness (Technique no 2)'

write(\*,\*) ' P to print results as Resutlts\_AAC\_etc.txt file.'

end if

read (\*,\*) Choice

P0=P0InitVal

if (Choice=='Q'.or.Choice=='q') then

stop

else if (Choice=='A'.or.Choice=='a') then

IF (ILLb.eq.1.or.ILLa.eq.1) THEN

deallocate (ElemNames, STAT = DeAllocateStatus)

deallocate ( Nk, STAT = DeAllocateStatus )

deallocate ( Pelect, STAT = DeAllocateStatus )

deallocate ( PlSctCSec, STAT = DeAllocateStatus )

END IF

ILLa=0.

IL=0

ChoiceP = 'A'

Alfa = 0.0

Alfa1 = 0.0

goto 700

else if (Choice=='B'.or.Choice=='b') then

IF (ILLb.eq.1.or.ILLa.eq.1) THEN

deallocate (ElemNames, STAT = DeAllocateStatus)

deallocate ( Nk, STAT = DeAllocateStatus )

deallocate ( Pelect, STAT = DeAllocateStatus )

deallocate ( PlSctCSec, STAT = DeAllocateStatus )

END IF

580 write(\*,\*) 'Enter first plasmon peak position in electron volts.'

read(\*,\*,err=580) PlPeaP

PlPeaP=PlPeaP\*ECHARGe

ILLb=0.

ChoiceP = 'B'

Alfa = 0.0

Alfa1 = 0.0

goto 700

else if (Choice=='P'.or.Choice=='p') then

goto 40000

else if (Choice=='D'.or.Choice=='d'.or. &

Choice=='E'.or.Choice=='e') then

if (ILLa.eq.0.and.ILLb.eq.0) goto 100

610 print \*, 'Enter thickness to plasmon mean free path ratio'

print \*, ' enter the number of atoms per unit are &

of element ',ElemNames(1)

read (\*,\*,err=610) X0

if (X0.lt.5.0.and.X0.gt.0.001) then

print \*, ' '

print \*, ' Thickness = ',X0\*LambdaP,' m'

else if (X0>1.e20) then

print \*, ' '

print \*, ' Thickness = ',X0/Nk(1),' m'

else

print \*, ' '

print \*,' Error !!!, thickness = ',X0\*LambdaP,' m'

end if

print \*, ' '

pause 'Press return to go back to menu'

else

end if

end do

700 write(\*,\*) ' Enter R for RPA, E for ExCor or K for '

write(\*,\*) ' known volume plasmon dispersion coefficient.'

write(\*,\*) ' (NOTE: to use approximate cutoff vector'

write(\*,\*) ' enter k and type in 0.5 for Alfa).'

read(\*,\*, err=700) RPAorExCor

RPAorExCorP = RPAorExCor

if (RPAorExCor .ne. 'R' .and. RPAorExCor .ne. 'r' &

& .and. RPAorExCor .ne. 'E' .and. RPAorExCor .ne. 'e' &

& .and. RPAorExCor .ne. 'k' .and. RPAorExCor .ne. 'K') goto 700

if (RPAorExCor .eq. 'k' .or. RPAorExCor .eq. 'K') then

710 write(\*,\*) 'Enter value for plasmon dispersion coefficient'

read(\*,\*, err=710) Alfa

end if

730 print \*, ' Enter electron effective mass in MKSA units '

read (\*,\*,err=730) ElecEfMas

if (ElecEfMas .ge. 1.e-25) then

740 write(\*,\*) ' The entered electron effective mass is ',ElecEfMas

write(\*,\*) " Isn't it too large ? If it is not then enter N."

write(\*,\*) 'Otherwise, enter any character to continue or m to Menu.'

read(\*,\*, err= 740) choix

if (choix .ne. 'n' .and. choix .ne.'N') goto 730

if (choix .eq. 'm' .or. choix .eq.'M') goto 100

end if

760 write (\*,\*) 'Enter the number of chemical elements in specimen'

read(\*,\*, err=760) n

if (Choice=='B'.or.Choice=='b') then

if (n.lt.2) then

print \*, 'Technique No 2 cannot be used, the &

& numbers of elements in specimen less than 2'

goto 100

end if

else

end if

allocate (ElemNames(n))

IF (AllocateStatus /= 0) STOP "\*\*\* ElemNames(:) Not enough &

& memory \*\*\*"

allocate ( Nk(n), STAT = AllocateStatus )

IF (AllocateStatus /= 0) STOP "\*\*\* Nk(:) Not enough memory \*\*\*"

allocate ( Pelect(n), STAT = AllocateStatus )

IF (AllocateStatus /= 0) STOP "\*\*\* Pelect(:) Not enough &

& memory \*\*\*"

allocate ( PlSctCSec(n), STAT = AllocateStatus )

IF (AllocateStatus /= 0) STOP "\*\*\* PlSctCSec(:) Not enough &

& memory \*\*\*"

print \*, ' '

print \*, ' '

if (Choice.eq.'A'.or.Choice.eq.'a') print \*, ' &

& We are using Technique No 1'

if (Choice.eq.'B'.or.Choice.eq.'b') print \*, ' &

& We are using Technique No 2'

print \*, ' '

print \*, ' '

write (\*,\*) ' Data PPROVISION (in MKSA units).'

print \*, ' '

print \*, ' '

write (\*,\*) ' Enter data for the DETECTABLE chemical'

print \*, ' elements in the following order:'

print \*, ' '

write (\*,\*) "element's name; valency; plasmon scattering cross&

& section per element."

print \*, ' '

if (Choice.eq.'A'.or.Choice.eq.'a') then

write (\*,\*) 'E.g.: name: Si, valency: 4., Plasm Scat Cros Sect&

& per Si at = 1.77e-22 to get:'

write(\*,\*) 'Si,4.,1.77e-22'

else if (Choice.eq.'B'.or.Choice.eq.'b') then

write (\*,\*) 'E.g.: name: Si, valency: 4., Plasm Scat Cros Sect&

& per Si at = 1.93e-22 to get:'

write(\*,\*) 'Si,4.,1.93e-22'

end if

print \*, ' '

do i=1,n

write (\*,\*) 'Element No ',i

print \*, ' '

if (i.eq.n) then

if (Choice.eq.'B'.or.Choice.eq.'b') then

800 print \*, ' NOW: enter just the name and the valency for &

the element'

print \*, ' which is NOT EASY TO DETECT.'

print \*, ' For example: H,1.0'

read(\*,\*,err=800) ElemNames(i),Pelect(i)

goto 900

end if

end if

840 read(\*,\*,err=840) ElemNames(i),Pelect(i),PlSctCSec(i)

900 continue

end do

call Get\_Incident\_electron\_Dta\_Final0

print \*, '-----------------------------------------------'

print \*, ' Entered data: '

print \*, '-----------------------------------------------'

print \*, ' '

print \*, 'Electron effective mass ',ElecEfMas,' kg'

print \*, ' '

print \*, 'Element ; Valency ; plasmon scatt. &

cr-section'

do i=1,n

print\*, ' '

if (i.eq.n) then

if (Choice.eq.'B'.or.Choice.eq.'b') then

print \*, ElemNames(i),' ',Pelect(i)

print \*, ' '

print \*, 'Plasmon energy ', PlPeaP/ECHARGe,' eV'

print \*, ' '

goto 920

end if

end if

print \*, ElemNames(i),' ',Pelect(i),PlSctCSec(i),' m2 &

& per ',ElemNames(i),' atom'

920 continue

end do

print \*, ' '

940 print\*, ' Is this OK ? Enter yes or no.'

read(\*,\*) choix

945 if (choix.ne.'y'.or.choix.ne.'Y') then

if (choix.eq.'N'.or.choix.eq.'n') then

deallocate (ElemNames, STAT = DeAllocateStatus)

deallocate ( Nk, STAT = DeAllocateStatus )

deallocate ( Pelect, STAT = DeAllocateStatus )

deallocate ( PlSctCSec, STAT = DeAllocateStatus )

if (Aup.eq.0.0) goto 100

goto 700

end if

else

print \*, ' '

print \*, ' Please enter yes or no.'

goto 940

end if

If (Choice=='A'.or.Choice=='a') Then

!! USING Tehnique 1.

! Get STAR, STAR is equal to the electron concentration

! divided by the atom concentration of the first element entered.

STAR=0.0

do i=1,n

STAR=STAR+Pelect(i)\*(PlSctCSec(1)/PlSctCSec(i))

end do

Q=PlSctCSec(1)

!---------------------Get interval containing solution -----------------------!

A2=2.e31 !!

i=0

SubType=13 !! For calling Elect\_Conc\_Dispers\_etc\_Eff\_M\_Known\_FULL\_Kc13

AplausMin=5.e29 !! AplausMin\*10. is the initial value starting

!! with when looking for the appropriate upper

!! limit of the interval containing the

!! actual electron concentration.

call get\_interval\_A1\_A3\_Lt

if (errKc) then

write(\*,\*) 'Interruption, entered data cannot be analyzed'

write(\*,\*) 'Cutoff vector cannot be calculated'

write(\*,\*) ' OK ? Enter any character to continue'

read(\*,\*) RPAorExCor

goto 100

else if (errThetaC) then

write(\*,\*) 'Interruption, entered data cannot be analyzed'

write(\*,\*) 'Cutoff angle cannot be calculated'

write(\*,\*) ' OK ? Enter any character to continue'

read(\*,\*) RPAorExCor

goto 100

end if

if (Aup.eq.0.0) then

choix='n'

goto 945

end if

call Dichotoming

1200 continue

! The electron concentration has been obtained

ElectConc=A2

! Work out the first plasmon peak position.

PlPeaP=(HBAR\*(ElectConc)\*\*(1./2.)/ElecEfMas\*\*(1./2.)/EPSILO\*\*(1./2.))\*ECHARGe

IF (RPAorExCor == 'k' .or. RPAorExCor == 'K') THEN

!! Alfa = Entered Alfa

ELSE

Alfa1 = 3./5.\*FEnerg/PlPeaP

! Work out Alfa.

Alfa=Alfa1

if (RPAorExCor == 'E' .or. RPAorExCor == 'e') then

!! ExCor considered

Alfa=Alfa\*(1.-(1./EFoverEp)\*(1./EFoverEp)/16.)

else

!! RPA considered

end if

END IF

! Work out the various absolute atom concentrations

Nk(1)=ElectConc/STAR

do i=2,n

Nk(i)=Nk(1)\*PlSctCSec(1)/PlSctCSec(i)

end do

! Get plasmon mean free path

LambdaP=1.0/Nk(1)/PlSctCSec(1)

if (Alfa .eq. 0.5) then

KC = KF/2.\*(PlPeaP/FEnerg)

else

KC = KF/(2.\*Alfa-1.)\*(1.-DSQRT(1.-(2\*Alfa-1.)\*PlPeaP/FEnerg))

end if

ILLa=1 ! Now we can get the specimen thickness via Technique 1

ILLb=0

Else If (Choice=='B'.or.Choice=='b') Then

!! USING Technique 2.

! Effective mass known, first plasmon peak position known and PlSctCSec(n) not known

! Work out the electron concentration

ElectConc=(ElecEfMas/HBAR)\*(PlPeaP/ECHARGe)\*\*2.\*(EPSILO/HBAR)

! Work out the Fermi vector

KF=(3.\*Pi\*Pi\*ElectConc)\*\*(1./3.)

! Get the Fermi energy

FEnerg=(HBAR\*KF)/MASS0\*(HBAR\*KF)/2.

! Get EFoverEp

EFoverEp=FEnerg/PlPeaP

! Get Alfa1

IF (RPAorExCor == 'k' .or. RPAorExCor == 'K') THEN

! Value entered for alfa

ELSE

Alfa1 = 3./5.\*EFoverEp

! Get Alfa

if (RPAorExCor == 'E' .or. RPAorExCor == 'e') then ! ExCor considered

Alfa = Alfa1\*(1.-(1./(Alfa1/3.\*5.)/4.)\*\*2.)

else ! RPA considered

Alfa = Alfa1

end if

END IF

if (Alfa .eq. 0.5) then

KC = KF/2.\*(PlPeaP/FEnerg)

else

if (1.-(2\*Alfa-1.)\*PlPeaP/FEnerg .le. 0) then

errKc = .true.

write(\*,\*) ' There is error !!:'

write(\*,\*) '(1.-(2\*Alfa-1.)\*PlPeaP/FEnerg) is negative'

write(\*,\*) ' OK ? Enter any character to continue.'

read(\*,\*) RPAorExCor

goto 100

end if

KC = KF/(2.\*Alfa-1.)\*(1.-DSQRT(1.-(2\*Alfa-1.)\*PlPeaP/FEnerg))

end if

! And third get Thetac:

if ((KC/K0 - ThetaE)\*(KC/K0 + ThetaE) .le. 0) then

errThetaC = .true.

write(\*,\*) ' There is error !! I cannot calculate Thetac:'

write(\*,\*) '(KC/K0 - ThetaE)\*(KC/K0 + ThetaE) is negative'

write(\*,\*) ' OK ? Enter any character to continue.'

read(\*,\*) RPAorExCor

goto 100

end if

Thetac = DSQRT((KC/K0 - ThetaE)\*(KC/K0 + ThetaE))

! Get Theta E

ThetaE=PlPeaP/(Gama\*MASS0\*ElecSpeed\*ElecSpeed)

! Get plasmon men free path

LambdaP=Ar0/(Gama\*ThetaE)/DLOG(1.+(Thetac/ThetaE)\*(Thetac/ThetaE))\*2.

! Work out the various absolute atom concentrations relative to the detectable species.

do i=1,n-1

Nk(i)=1./LambdaP/PlSctCSec(i)

end do

! Work out the contribution to the electron concentration due to the detectable

! elements: use X0 for that.

X0=0.0

do i=1,n-1

X0=X0+Pelect(i)\*Nk(i)

end do

! Work out the absolute atom concentration for the non-easily detectable species by

! subtracting the contributions of the detectable elements from the total electron

! concentration and dividing by the valency of the non-easily detectable element..

Nk(n)=(ElectConc-X0)/Pelect(n)

! Work out the plasmon scattering cross section per nth atom species (i.e. that of the

! non-easily detectable element).

PlSctCSec(n)=PlSctCSec(1)\*Nk(1)/Nk(n)

ILLb=1 ! Now we can get the specimen thickness via Technique 2.

ILLa=0

Else

End If

print \*,' '

print \*,' '

if (ILLa.eq.1) print \*,' / Technique No 1 &

was used /'

if (ILLb.eq.1) print \*,' / Technique No 2 &

was used /'

print \*,' '; print \*,' '

!--------------------------- Results are given hereafter. -----------------

print \*, '!------------------------------------------------------&

----------------------!'

if (RPAorExCor == 'r' .or. RPAorExCor == 'R') then

write(\*,\*) '////////// Random Phase Approximation considered.&

//////////////////////.'

print \*, "!-------------------------------------------------------&

----------------------!"

else if (RPAorExCor == 'e' .or. RPAorExCor == 'E') then

write(\*,\*) '////////// Exchange plus Correlation considered.&

//////////////////////.'

print \*, ' '

print \*, '!-------------------------------------------------------&

---------------------!'

else if (RPAorExCor == 'k' .or. RPAorExCor == 'K') then

write(\*,\*) '////////// Known dispersion coefficient considered.&

///////////////////.'

print \*, '!--------------------------------------------------&

----------------------!'

end if

print \*, ' '

print \*, ' Calculated physical quantities.'

print \*, ' '

print \*, '!-------------------------------------------------------&

---------------------!'

print \*, ' '

write(\*,2530)' Plasmon mean free path is: ',LambdaP\*1.e10,' &

angs-1'

print \*, '!------------------------------------------------------&

----------------------!'

print \*, ' '

write(\*,2520) ' Electron concentration is: ',ElectConc,' electron/m3'

print \*, '!------------------------------------------------------&

----------------------!'

print \*, ' '

write(\*,2520) ' The Fermi vector is: ',KF,' 1/m'

print \*, '!------------------------------------------------------&

----------------------!'

print \*, ' '

write(\*,2510) ' The Fermi energy is: ',FEnerg/1.602e-19,' eV'

print \*, '!------------------------------------------------------&

----------------------!'

print \*, ' '

write(\*,2510) ' Theta E is: ',ThetaE\*1000.,' mrad'

print \*, '!------------------------------------------------------&

----------------------!'

print \*, ' '

write(\*,2520) ' Plasmon cutoff vector (kc) ',KC,' 1/m'

print \*, '!------------------------------------------------------&

----------------------!'

print \*, ' '

write(\*,2510) ' Plasmon cutoff angle (Theta c) ',Thetac\*1000.,' mrad'

print \*, '!------------------------------------------------------&

----------------------!'

if (Choice.eq.'A'.or.Choice.eq.'a') then

print \*, '!------------------------------------------------------&

----------------------!'

print \*, ' '

write(\*,2510) ' First plasmon peak position is: ',PlPeaP/1.602D-19,' eV'

print \*, '!------------------------------------------------------&

----------------------!'

print \*, ' '

else if (Choice.eq.'B'.or.Choice.eq.'b') then

print \*, '!------------------------------------------------------&

----------------------!'

print \*, ' '

write(\*,2540) ' Plasmon Scatt. Cros Sect for ',ElemNames(n),'is: '&

,PlSctCSec(n),' m2 per ',ElemNames(n),'atom'

print \*, '!------------------------------------------------------&

----------------------!'

print \*, ' '

else if (Choice.eq.'C'.or.Choice.eq.'c') then

print \*, '!------------------------------------------------------&

----------------------!'

print \*, ' '

end if

print \*, ' Element Absolute atom concentration &

(in at/m3).'

print \*, '!------------------------------------------------------&

----------------------!'

do i=1,n

print \*,' '

write(\*,2550) ' ', ElemNames(i),' ',Nk(i)

if (Nk(i).lt.0.0) print \*,' This is negative, maybe this should be zero?'

end do

if (n>=2) then

print \*, '!------------------------------------------------------&

----------------------!'

print \*, ' '

print \*, ' The relative content ratios are:'

print \*, ''

do i=2,n

write(\*,2560)' ',ElemNames(i),'/',&

ElemNames(1),': ',Nk(i)/Nk(1)

end do

end if

print \*, ' '

print \*, ' '

print \*, '!-------------------------------------------------------&

----------------------!'

print \*, ' '

if (RPAorExCor == 'r' .or. RPAorExCor == 'R') then

write(\*,2570) ' Alfa (RPA) = (3/5)EF/Ep = ',Alfa1

print \*, '!-------------------------------------------------------&

----------------------!'

else if (RPAorExCor == 'e' .or. RPAorExCor == 'E') then

print \*, ' '

write(\*,2570) ' Alfa1 = (3/5)EF/Ep = ',Alfa1

print \*, '!-------------------------------------------------------&

----------------------!'

print \*, ' '

write(\*,2570) ' Alfa = Alfa1(1-Ep/4EF)\*\*2) = ',Alfa

print \*, '!-------------------------------------------------------&

----------------------!'

else if (RPAorExCor == 'k' .or. RPAorExCor == 'K') then

print \*, ' '

write(\*,2570) ' Entered Alfa = ',Alfa

print \*, '!-------------------------------------------------------&

----------------------!'

end if

2570 format(A,f15.5)

print \*, ' '; print \*, ' '

if (Choice.eq.'C'.or.Choice.eq.'c') ILLa=1

1400 print \*, '!------------------------------------------------------&

----------------------!'

print \*, ' !-------------------------------------&

--------------!'

print \*, ' // The entered data is the following&

: //'

if (Choice.eq.'B'.or.Choice.eq.'b'.or.&

Choice.eq.'C'.or.Choice.eq.'c') then

print \*, '!------------------------------------------------------&

----------------------!'

print \*, ' '

write(\*,2100)'First plasmon peak energy: ',PlPeaP/1.602E-19,' eV'

end if

print \*, ' !-------------------------------------&

--------------!'

print \*, '!------------------------------------------------------&

----------------------!'

print \*, ' '

write(\*,2520)' Electron effective mass is: ',ElecEfMas,' kg'

print \*, ' '

print \*, '!------------------------------------------------------&

----------------------!'

print \*, ' '

write(\*,2200) 'Accelarating voltage: ',V0/1000.,' kV'

print \*, '!------------------------------------------------------&

----------------------!'

print \*, ' '

print \*, 'Element; Valency; plasmon scatt. &

cross-section'

do i=1,n

print \*, '!------------------------------------------------------&

----------------------!'

print\*, ' '

if (i.eq.n) then

if (Choice.eq.'B'.or.Choice.eq.'b') then

write(\*,2400) ElemNames(i),' ',Pelect(i)

print \*, ' '

print \*, '!------------------------------------------------------&

----------------------!'

print \*, 'Plasmon enargy ',PlPeaP/ECHARGe,' eV'

print \*, ' '

goto 1240

end if

end if

write(\*,2300) ElemNames(i),' ',Pelect(i),' ',&

PlSctCSec(i),' m2 per ',ElemNames(i),' atom'

1240 continue

end do

print\*, ' ' ; print\*, ' '

print\*, ' ' ; print\*, ' '

do

print \*, ' Enter Q to quit or'

print \*,' any other key to return to the menu'

write(\*, '(A)', ADVANCE = "NO")' => '

read (\*,\*,err=100) choix

if (choix=='Q'.or.choix=='q') stop

Choice='~'

goto 100

end do

2100 format(1x, A,F8.3,A)

2200 format(1x, A,ES12.3,A)

2300 format(3x,A2,A,F10.1,A,ES12.3,A,A2,A)

2400 format(3x,A2,A,F10.1)

2510 format(A,F14.5,A)

2520 format(A,ES15.5,A)

2530 format(A,F10.2,A)

2540 format(A,A2,A,ES14.5,A,A2,A)

2550 format(A,A2,A,ES14.5)

2560 format(A,A2,A,A2,A,F10.5)

print \*, ' '

40000 continue

if (ChoiceP.eq.'B'.or.ChoiceP.eq.'b') then

file = 'Resutlts\_AAC\_etc\_tec\_2.txt'

else if (ChoiceP.eq.'A'.or.ChoiceP.eq.'a') then

file = 'Resutlts\_AAC\_etc\_tec\_1.txt'

end if

OPEN (7,STATUS='new',File=file,IOSTAT = Ierr)

IF(Ierr .ne. 0)THEN

40010 if (ChoiceP.eq.'B'.or.ChoiceP.eq.'b') then

write(\*,\*) ' File: Resutlts\_AAC\_etc\_2.txt exists, filing as Resutlts\_AAC\_etc\_04.txt.'

file = 'Resutlts\_AAC\_etc\_tec\_4.txt'

else if (ChoiceP.eq.'A'.or.ChoiceP.eq.'a') then

write(\*,\*) ' File: Resutlts\_AAC\_etc\_1.txt exists, filing as Resutlts\_AAC\_etc\_03.txt.'

file = 'Resutlts\_AAC\_etc\_tec\_3.txt'

end if

write(\*,\*) ' OK ? Yes/No.'

read(\*,\*) RPAorExCor

if (RPAorExCor == 'n' .or. RPAorExCor == 'N') then

write(\*,\*) ' Enter a file name.'

read(\*,\*) file

file = trim(file)//'.txt'

else if (RPAorExCor == 'y' .or. RPAorExCor == 'Y') then

else

goto 40010

end if

OPEN(7, STATUS = 'unknown', FILE = file, IOSTAT = Ierr)

REWIND(7)

ENDIF

write(7,\*)' '

write(7,\*) ' !-------------------------------------------&

&--------------!'

write(7,\*) ' // The entered data is the following&

& : //'

write(7,\*) ' !-------------------------------------------&

&--------------!'

write(7,\*) ' '

write(7,\*) '!------------------------------------------------------&

&----------------------!'

write(7,\*) ' '

if (RPAorExCorP == 'r' .or. RPAorExCorP == 'R') then

write(7,2570) ' Random phase approximation used.'

write(7,\*)' '

write(7,\*) ' !-------------------------------------------&

&--------------!'

else if (RPAorExCorP == 'e' .or. RPAorExCorP == 'E') then

write(7,\*)' '

write(7,2570) ' Exchange and electron correlation used.'

write(7,\*) ' !-------------------------------------------&

&--------------!'

else if (RPAorExCorP == 'k' .or. RPAorExCorP == 'K') then

write(7,\*)' '

write(7,2570) ' Constant value for Alfa entered.'

write(7,\*) ' !-------------------------------------------&

&--------------!'

write(7,\*)' '

end if

write(7,2520)' Electron effective mass is: ',ElecEfMas,' kg'

if (ChoiceP.eq.'B'.or.ChoiceP.eq.'b'.or. &

& Choice.eq.'C'.or.Choice.eq.'c') then

write(7,\*) '!------------------------------------------------------&

&----------------------!'

write(7,\*) ' '

write(7,2100)' First plasmon peak energy: ',PlPeaP/1.602E-19,' eV'

end if

write(7,\*) '!------------------------------------------------------&

&----------------------!'

write(7,\*) ' '

write(7,2200) 'Accelarating voltage: ',V0/1000.,' kV'

write(7,\*) '!------------------------------------------------------&

&----------------------!'

write(7,\*) ' '

write(7,\*) 'Element; Valency; plasmon scatt.cross-&

&section'

do i=1,n

write(7,\*) '!------------------------------------------------------&

&----------------------!'

write(7,\*) ' '

if (i.eq.n) then

if (ChoiceP.eq.'B'.or.ChoiceP.eq.'b') then

write(7,2400) ElemNames(i),' ',Pelect(i)

goto 1340

end if

end if

write(7,2300) ElemNames(i),' ',Pelect(i),' ', &

& PlSctCSec(i),' m2 per ',ElemNames(i),' atom'

1340 continue

end do

write(7,\*) ' '

write(7,\*) ' Calculated physical quantities.'

write(7,\*) ' '

write(7,\*) '!-------------------------------------------------------&

&---------------------!'

write(7,\*) ' '

write(7,2530)' Plasmon mean free path is: ',LambdaP\*1.e10,' &

& angs-1'

write(7,\*) '!------------------------------------------------------&

& ----------------------!'

write(7,\*) ' '

write(7,2520)' Electron concentration is: ',ElectConc,' electron/m3'

write(7,\*) '!------------------------------------------------------&

&----------------------!'

write(7,\*) ' '

write(7,2520) ' The Fermi vector is: ',KF,' radians/m'

write(7,\*) '!------------------------------------------------------&

&----------------------!'

write(7,\*) ' '

write(7,2510) ' The Fermi energy is: ',FEnerg/1.602e-19,' eV'

write(7,\*) '!------------------------------------------------------&

&----------------------!'

write(7,\*) ' '

write(7,2510) ' Theta E is: ',ThetaE\*1000.,' mrad'

write(7,\*) '!------------------------------------------------------&

&----------------------!'

write(7,\*) ' '

write(7,2510) ' Plasmon cutoff angle (Theta c) ',Thetac\*1000.,' mrad'

write(7,\*) ' '

write(7,\*) '!------------------------------------------------------&

&----------------------!'

write(7,\*) ' '

write(7,2520) ' Critical wavevector (kc) ',KC,' radians/m'

if (ChoiceP.eq.'A'.or.ChoiceP.eq.'a') then

write(7,\*) '!------------------------------------------------------&

&----------------------!'

write(7,\*) ' '

write(7,2510) ' First plasmon peak position : ',PlPeaP/1.602E-19,' eV'

write(7,\*) '!------------------------------------------------------&

&----------------------!'

write(7,\*) ' '

else if (ChoiceP.eq.'B'.or.ChoiceP.eq.'b') then

write(7,\*) '!------------------------------------------------------&

&----------------------!'

write(7,\*) ' '

write(7,2540) ' Plasmon Scatt. Cros Sect for ',ElemNames(n),'is:'&

&,PlSctCSec(n),' m2 per ',ElemNames(n),'atom'

write(7,\*) '!------------------------------------------------------&

&----------------------!'

write(7,\*) ' '

else if (ChoiceP.eq.'C'.or.ChoiceP.eq.'c') then

write(7,\*) '!------------------------------------------------------&

&----------------------!'

write(7,\*) ' '

end if

write(7,\*) ' Element Absolute atom concentration &

& (in at/m3).'

write(7,\*) '!------------------------------------------------------&

&----------------------!'

do i=1,n

write(7,\*)' '

write(7,2550) ' ', ElemNames(i),' ',Nk(i)

if (Nk(i).lt.0.0) write(7,\*)' This is negative, maybe this should be zero?'

end do

if (n>=2) then

write(7,\*) '!------------------------------------------------------&

&----------------------!'

write(7,\*) ' '

write(7,\*) ' The relative content ratios are:'

write(7,\*) ''

do i=2,n

write(7,2560)' ',ElemNames(i),'/', &

&ElemNames(1),': ',Nk(i)/Nk(1)

end do

end if

write(7,\*) ' '

if (RPAorExCorP == 'r' .or. RPAorExCorP == 'R') then

write(7,2570) ' Alfa (RPA) = (3/5)EF/Ep = ',Alfa1

write(7,\*) ' !-------------------------------------------&

&--------------!'

else if (RPAorExCorP == 'e' .or. RPAorExCorP == 'E') then

write(7,\*)' '

write(7,2570) ' Alfa1 = (3/5)EF/Ep = ',Alfa1

write(7,\*) ' !-------------------------------------------&

&--------------!'

write(7,\*)' '

write(7,2570) ' Alfa = Alfa1(1-Ep/4EF)\*\*2) = ',Alfa

write(7,\*) ' !-------------------------------------------&

&--------------!'

else if (RPAorExCorP == 'k' .or. RPAorExCorP == 'K') then

write(7,\*)' '

write(7,2570) ' Entered Alfa value = ',Alfa

write(7,\*) ' !-------------------------------------------&

&--------------!'

end if

close(7)

goto 100

end program Absol\_Atom\_Concent\_Determ\_Need\_Eff\_Mass\_FULL