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The deformation response of polycrystalline AA2024-T4 to cyclic loading has been determined by conventional and double-crystal diffractometry. These studies show a preferential work-hardening near the surface compared to the bulk. The defect distribution as a function of depth was also investigated as a function of the fraction of fatigue life. From these studies, it was determined that the remaining fatigue life could be predicted.
by determining the average ratio $\beta/\beta^*$ where $\beta$ is the linewidth at any number of fatigue cycles and $\beta^*$ is the critical linewidth at fracture. Current studies have shown these predictions to be valid for tests where the stress amplitude is held constant for the entire test. A few tests have also been performed where the loading sequence is more complicated. In these tests, the X-ray predictive method was found to be far more accurate than conventional methods.
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1 - Line Broadening Analysis by Conventional Diffractometer.
ABSTRACT

The deformation response of polycrystalline AA2024-T4 to cyclic loading has been determined by conventional and double-crystal diffractometry. These studies show a preferential work-hardening near the surface compared to the bulk. The defect distribution as a function of depth was also investigated as a function of the fraction of fatigue life. From these studies, it was determined that the remaining fatigue life could be predicted by determining the average ratio $\beta/\beta^*$ where $\beta$ is the linewidth at any number of fatigue cycles and $\beta^*$ is the critical linewidth at fracture. Current studies have shown these predictions to be valid for tests where the stress amplitude is held constant for the entire test. A few tests have also been performed where the loading sequence is more complicated. In these tests, the X-ray predictive method was found to be far more accurate than conventional methods.

ADMINISTRATIVE INFORMATION

This investigation is part of an in-house research program at the David W. Taylor Naval Ship Research and Development Center (DTNSRDC). It was conducted under Program Element 61152N, Task Area ZR 022-0101, Work Unit 2082-004.

INTRODUCTION

Early investigations of fatigue failure in metals provided substantial evidence of the surface sensitivity of mechanical behavior. Surface studies revealed the formation of slip bands and their topological development into intrusions and extrusions associated with subsequent crack initiation and eventual failure.1-4 Other fatigue investigations focused on the microstructural developments in metals during repeated stressing.5-9 During the 1960s, many studies were performed to relate the fatigue-induced defect structure with the slip morphology exhibited on the surface.10-14

*A complete listing of references is given on page 29.
While surface effects were recognized as a controlling factor in fatigue performance, early X-ray methods were incapable of predicting the impending onset of fatigue failure or even the span of the fatigue life.\textsuperscript{15,16} Line broadening was observed after cycling over a small fraction of the total fatigue life, but then it remained virtually unaltered both in extent and intensity throughout the remainder of the life.

A recent application of a special X-ray method\textsuperscript{17,18} to cyclically stressed 2024 Al enabled the prediction of both the fatigue life and failure of the aluminum with a considerable degree of accuracy. This nondestructive method for analysis of the fatigue-induced defect structure is based on the principle of X-ray double-crystal diffractometry and employs X-ray topography to afford a visualization of the defect configuration. The polycrystalline specimen is irradiated with a crystal-monochromated beam; and each reflecting grain is considered to function independently as the test crystal of a double-crystal diffractometer. Depending on the perfection of the grains, the specimen is rotated in intervals of seconds or minutes of arc; and the spot reflections, recorded along the Debye arcs of a cylindrical film for each discrete specimen rotation, are separated by film shifts. This multiple-exposure technique gives rise to an array of spots for each reflecting grain. These arrays of spots, with their intensity dependent on specimen rotation, represent X-ray rocking curves of the reflecting grains. Thus, if the grains contain a substructure, the intensity distribution of the arrays of diffraction spots will be multi-peaked not only along the horizontal, but also along the azimuthal elevation. From the angle subtending successive peaks of the rocking curve, the excess dislocation density between subgrains can be determined; while the excess dislocation density within the subgrain can be obtained from the spread of the subpeak curve. From the width $\beta$, at half the maximum intensity, the excess dislocation density of the entire grain is determined.\textsuperscript{17,18}

By analyzing various $(hkl)$ reflections, a representative statistical parameter $\overline{\beta}$ of the defect structure of the grain population is obtained. Furthermore, by taking Berg-Barrett reflection topographs and performing
a spatial tracing at the reflections to the spot reflections of the rocking curve, the analyzed rocking curve can be correlated to the grain topography on the specimen.\textsuperscript{18}

The double-crystal diffractometer arrangement has been successfully employed to study single crystals, pure polycrystalline metals, and multiphase alloys with ease. The method offers good resolution of the local effects in individual grains, but also provides information from a sufficient number of grains to permit accurate statistical analysis of an average or mean microstructural response. The film-recorded reflections represent an imaging of the subdomain structure which can also be interpreted quantitatively in terms of the excess dislocation density, which is known to be a factor in the accumulation of fatigue damage and the ultimate initiation of fracture. The purpose of the present study is to exploit these aspects of the X-ray method to isolate a suitable microstructural indicator of progressive fatigue damage, and thereby contribute to the capability for accurate determination of the fatigue life and failure prediction. In accomplishing this objective, the double-crystal diffractometer is particularly useful for the microstructural analysis of both the surface and the bulk. Analysis of these regions can be carried out independently, in a stepwise manner, by incremental removal of surface layers. In addition, nondestructive in-depth analysis is made possible by altering the depth of penetration of the incident radiation. This potential may be very important in technological applications when service components are to be examined.

A method which can be used in conjunction with the double-crystal technique described above is the Warren-Averbach (WA) method of Fourier analysis of X-ray line broadening. This technique is unique in that the sizes of coherently reflecting domains and the internal microstrains can be determined simultaneously. Alternate theories of line broadening assume that broadening of Bragg peaks is due predominately to either size or strain, but not both. The WA method is unique in that multiple sources of line broadening may be operating simultaneously.
Two peaks are selected for the WA analysis, usually the 200 and 400 Bragg reflections. A counter is used to record the intensity distribution, and the intensity peaks at 0.005-degree increments are fed into a PDP 11-34 computer. The Rachinger graphical separation of the $\text{Ka}_1$ and $\text{Ka}_2$ double profile is employed (see Appendix A); and the $\text{Ka}_1$ corrected profile of both annealed and worked samples is used in the analysis. The Stokes method is used for the correction of the instrumental broadening.

A FORTRAN computer program was written (see Appendix B) for calculating the Stokes-corrected Fourier coefficients of a broadened profile. According to the WA analysis, the corrected Fourier coefficients are related to the particle size and the root-mean-square microstrains as follows:

$$\ln A_L(h_0) = \ln A_L^S - \frac{2\pi^2 L^2}{a^2} < \varepsilon_L^2 > h_0^2$$

where $A_L$ = the corrected Fourier coefficients

$A_L^S$ = the corrected Fourier coefficients of particle size

$L$ = the distance normal to the reflecting planes

$h_0^2 = h^2 + k^2 + \ell^2$

$a$ = the lattice parameter

By plotting $\ln A_L(h_0)$ versus $h_0^2$ (usually for two reflections) the size effect and microstrains can be separated. The intercepts of these plots provide the particle size coefficients $A_L^S$ for various $L$ and from the slopes the microstrains can be calculated.

PREVIOUS WORK

Several reports covering previous work under this program have been published recently.19-21 These elucidate the preferential work hardening occurring at the surface of fatigued AA2024-T4 samples and the associated excess dislocation densities for grains near the surface. It was found
that an initial rapid increase in $\bar{\rho}$ comprised the first 20 to 25 percent of the life followed by a long intermediate period featuring very little structural change and a final rapid enhancement during the last 5 to 10 percent of the life, coinciding with crack initiation and growth. It was found that a critical excess dislocation density exists which is associated with fatigue fracture. This critical value was independent of the stress amplitude and varied according to a Petch-type relationship for different grain sizes of the same alloy. An in-depth analysis, carried out by stepwise removal of the surface layers of cycled specimens, disclosed a plastic response for the grains located in the bulk after about 5 percent of the fatigue life. The defect structure in the specimen core developed gradually during the cycling. The excess dislocation density for the bulk increased almost linearly as a function of the fatigue life, with a terminal value at failure identical to the critical excess dislocation density for surface grains. The fatigue process was interpreted as a rapid work hardening of the surface to form a barrier to dislocation egression and rearrangement. The dynamic interplay between the surface barrier and the eventual plastic response activated in the bulk leads to a critical defect accumulation at the surface and incipient cracking.

When the fatigue process was interrupted prior to failure and the surface layer was removed, a striking recovery phenomenon was observed throughout the specimen cross section during subsequent cycling. The bulk defect structure was thus shown to be extremely unstable in the absence of the restraining influence imposed by the work-hardened surface layer. The extension of the fatigue life of metals by judicious surface removal was ascribed primarily to the elimination of the surface barrier, rather than to the removal of microcracks.

The fatigue response at various depths from the surface was also investigated nondestructively by employing X-ray radiation with differing penetration capabilities. The excess dislocation density of grains located up to 300 micrometers in depth was examined using molybdenum radiation and was found to vary linearly with the fatigue life. This steep, linear dependence, in conjunction with the early life saturation
behavior of surface-grain densities measured with copper radiation, provided a new criterion for predicting accurately the fatigue life and failure.

PRESENT WORK

The striking feature of the previous work is that a linear relationship exists between the statistical average \( \overline{B} \) and the remaining fatigue life. This enabled accurate prediction of the useful remaining life by a simple nondestructive determination of \( \overline{B} \) using Mo radiation. However, these results were strictly applicable only to samples tested at a constant stress amplitude. Although tests indicated that \( \overline{B} \) was stress amplitude independent, it was not clear how a single sample would behave under more complex loading histories. Accordingly, the present tests were undertaken to determine the applicability of the X-ray double-crystal diffractometry technique for predicting fatigue failure in samples with a random stress loading sequence.

The spectral loading sequence chosen is shown in Figure 1. Four stress levels were selected between 25 ksi and 41 ksi, corresponding approximately to the fatigue limit and the proportional limit, respectively. The number of cycles at each stress level was determined by setting each loading step to 20 percent of the fatigue life at each stress level. The stress versus number of cycles (S-N) curve for such a determination is shown in Figure 2 and was obtained for a constant stress amplitude (\( R = -1 \)).

After each loading step, the sample was analyzed using the double-crystal diffractometer with Mo radiation to determine the rocking curve halfwidth. The value of \( \overline{B} \) obtained after each step was then compared to the calibration curve shown in Figure 3. This curve was determined in the previous studies on constant amplitude fatigue cycling. At the end of the fourth loading cycle (41 ksi), \( \overline{B} \) was determined and located on the calibration curve. As shown in Figure 4, the predicted remaining life was 39 percent based on the X-ray method. Figure 4 also shows the predicted remaining fatigue life of 20 percent based on the conventional technique using the S-N curve. The actual remaining fatigue life was
found to be 42.5 percent. Therefore, the error in estimating the remaining life on the basis of the usual techniques was over 100 percent; while the error of the X-ray technique was less than 10 percent.

Analyses using line broadening techniques and conventional diffractometry have also been performed. After each stage of cycling, a conventional diffractometer trace is run to determine the peak halfwidths for the 111, 200, 222, and 400 peaks; and corrections are made to take into account variations in the initial halfwidths. If a Cauchy line profile is assumed, it can be shown\(^2\) that the line broadening is related to the coherently reflecting domain size \(\ell\) and the strain \(e\) through the equation

\[
dS_\theta = \frac{1}{\ell} + 2eS
\]

where \(S = 2\sin\theta/\lambda\)
\(dS = 2\cos\theta d\theta/\lambda\)
\(\theta =\) Bragg angle for \(hkl\) reflection
\(\lambda =\) X-ray wavelength

The quantity \(2d\theta\) is equivalent to \(\bar{b}\), the peak halfwidth; and, by a simple substitution, Equation (2) becomes

\[
\bar{b}\cos\theta = \frac{\lambda}{\ell} + 4esin\theta
\]

By a linear regression analysis, the quantities \(\ell\) and \(e\) can be readily determined from the experimentally measured \(\bar{b}\). As shown in Figure 5, the relationship between \(\bar{b}\cos\theta\) and \(\sin\theta\) is indeed linear for the four fractions of life investigated \((N/N_F = 0.22, 0.28, 0.42,\) and 0.57). The slope of each line is equal to \(4e\) and the intercept is \(\lambda/\ell\).

Once the values of \(e\) and \(\ell\) are determined, the individual contributions to the dislocation density \(\rho_e\) and \(\rho_\ell\) can be determined through the equations
\[ \rho_e = \frac{12}{b^2} < e^2 > = \frac{7.68}{b^2} e^2 \]  

(4a)

\[ \rho_g = \frac{1}{\bar{\rho}^2} \]  

(4b)

\[ \bar{\rho} = (\rho_e \rho_g)^{1/2} \]  

(4c)

The quantities \( \rho_e, \rho_g, \) and \( \bar{\rho} \) derived from Figure 5 are summarized in Table 1 along with the quantities \( e \) and \( \ell \). Note that the coherently diffracting domain size remains nearly constant over the life interval 0.22 to 0.57, while the strain steadily increases.

<table>
<thead>
<tr>
<th>Fraction of Life (-(N/N_F))</th>
<th>Strain (-e)</th>
<th>Domain Size (-\ell)</th>
<th>Dislocation Density (\rho_e)</th>
<th>Dislocation Density (\rho_g)</th>
<th>Root Mean Dislocation Density ((\rho_e \rho_g)^{1/2})</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.22</td>
<td>0.00157</td>
<td>319</td>
<td>(2.33 \times 10^{10})</td>
<td>(9.83 \times 10^{10})</td>
<td>(4.79 \times 10^{10})</td>
</tr>
<tr>
<td>0.28</td>
<td>0.00322</td>
<td>462</td>
<td>(9.77 \times 10^{10})</td>
<td>(4.69 \times 10^{10})</td>
<td>(6.77 \times 10^{10})</td>
</tr>
<tr>
<td>0.42</td>
<td>0.00406</td>
<td>344</td>
<td>(15.50 \times 10^{10})</td>
<td>(8.45 \times 10^{10})</td>
<td>(11.44 \times 10^{10})</td>
</tr>
<tr>
<td>0.57</td>
<td>0.00436</td>
<td>305</td>
<td>(17.86 \times 10^{10})</td>
<td>(10.80 \times 10^{10})</td>
<td>(13.89 \times 10^{10})</td>
</tr>
</tbody>
</table>
Both quantities $p_e$ and $\bar{p}$ are linearly related to the fraction of life $N/N_F$, as shown in Figures 6 and 7. The best fit is obtained by utilizing $\bar{p}$, which includes variations in both $p_e$ and $p_f$. The error between the experimental value of $\bar{p}$ and the value obtained from the linear regression is in no case worse than 10 percent. Thus, these types of measurements should be capable of being used to accurately predict the remaining life. Subsequent experiments are being initiated to verify this assumption.
Figure 1 - Spectral Loading Sequence for AA2024-T4 Samples
Figure 2 - Fatigue Curve Determined from Constant Stress Amplitude Tests
Figure 3 - Experimentally Determined Calibration Curve of Corrected Average Halfwidth as a Function of Fatigue Life
Figure 5 - Results of Conventional Diffractometer Study for Various Fractions of Fatigue Life, N/N_f
Figure 6 - Correlation Between Strain Dislocation Density \( \rho_d \) and Fraction of Fatigue Life.
Figure 7 - Correlation Between Mean Dislocation Density and Fraction of Fatigue Life
APPENDIX A

FORTRAN PROGRAM FOR RACHINGER SEPARATION
OF $K_{\alpha_1}$ AND $K_{\alpha_2}$ PEAKS
THERE EXISTS DIFFERENCES BETWEEN THE UPDATED HARD COPY AND THIS VERSION OF THE PROGRAM.

PROGRAM RACHC
IMPLICIT INTEGER (A-Z)
INTEGER TLU, NP, IDEL2
REAL CPS(500), DEL, IDEL, YINC, SUM, A, B, C, FRA
REAL*8 FSPEC
REAL*4 DEV
LOGICAL*1 DSN(10), TEM(3)
DATA DEV/3RDXI/
DO 40 I=1,10
40 DSN(I)=''
GO TO 16
15 WRITE(5,20)
DO 43 I=1,10
43 DSN(I)=''
FORMAT(/' FILENAME MUST BE 6 CHARACTERS WITH 3 CHARACTER
* EXTENSION; '/)
* EX: 'FILNAM.DAT' (OMIT QUOTES); '/ RE-/)
16 WRITE (5,1)
1 FORMAT(' ENTER THE FILE NAME!';$)
READ(5,2)(DSN(I), I=1,10)
2 FORMAT(10A1)
I=1
3 IF (DSN(I).EQ.','') GO TO 12
I=I+1
IF (I.EQ.10) GO TO 11
GO TO 3
12 IF (I. GT.7) GO TO 15
TEM(1)=DSN(I+1)
TEM(2)=DSN(I+2)
TEM(3)=DSN(I+3)
DSN(7)=TEM(1)
DSN(8)=TEM(2)
DSN(9)=TEM(3)
IF (I. EQ.7) GO TO 11
DO 99 K=IP6
99 DSN(K)=''
11 DSN(10)=''
J = IARADS(9, DSN, FSPEC)
I = IASIGN(9, DEV, FSPEC)
TLU=5
17 FORMAT(/' ENTER THE 2 THETA SEPERATION BETWEEN THE
* ALPHAS 1 AND 2';$)
37 FORMAT(/' ENTER THE RATIO BETWEEN THE ALPHA 1 AND ALPHA 2';$)
41 FORMAT(/' INTEGRATED AREA CORRECTED FOR ALPHA 1, ALPHAS 2 =';$)
97 FORMAT(I3)
READ(9,97)NP
97 FORMAT(I3)
DO30 I=1, NP
READ(9,96)CPS(I)
96 FORMAT(F12.6)
30 CONTINUE
A=0.
B=0.
D0421=1,10
A=A+ CPS(I)/10.
B=B+ CPS(NP+1-I)/10.
DO38 I=1, NP
38 CPS(I)= CPS(I) - ((A-B)*((I-1)/(NP-1)))
WRITE(TLU,17)
READ(TLU,6)
17 FORMAT(/F12.6)
6 WRITE(F12.6)
7 FORMAT(/' ENTER YINC';$)
READ(5,8) YINC
FORMAT(F12.6)
IDEL=DEL/YINC
DEL=DEL/YINC
C=DEL-IDEL
SUM=0.0
IDEL2=INT(IDEL)
DO100I=1, IDEL2
100 SUM=SUM+CPS(I)
WRITE(TLU,37)
READ(TLU,9)FRA
 FORMAT(F12.6)
 DD1101=IDEL+1,NP
 CPS(I)=CPS(I)-(CPS(I-IDEL+1)-(CPS(I-IDEL+1)-CPS(I-IDEL))*C)*FRA
 SUM=SUM+CPS(I)
 WRITE(S,99)
98 FORMAT(/' THE PRINTED DATA SET WILL BE ALLOWED TO BE STORED ON',
       ' DISC AFTER THE RESULTS HAVE BEEN VERIFIED.')
 DO350I=1,NP
 WRITE(6,95)CPS(I)
350 CONTINUE
95 FORMAT(F12.6)
 WRITE(TLU,41)SUM
END
APPENDIX B

FORTRAN PROGRAM FOR CALCULATING THE STOKES-CORRECTED FOURIER COEFFICIENTS
REAL*4 DEV
REAL*4 DEV2
REAL*4 FILE(2)
REAL*4 FILE2(2)
DATA DEV/3RDX1/
DATA DEV2/3RDX1/
DATA FILE/6RWORKED,3RDAT/
I=IASIGN(9,DEV,FILE)
I=IASIGN(8,DEV2,FILE2)
DEFINE FILE 9(500,4,UNREC)
DEFINE FILE 8(500,4,UNREC2)
REAL XINTA(500)
REAL FRW(60)
REAL FIA(60)
REAL FCCR(60)
SAVE(60)
REAL LACAPLACWPKVPMA
INTEGER*4 FLAGS(60)
INTEGER YES/NO,HANS
INTEGER ILU/IPRAM(5),TOF,R1W(128),R1A(128),TLEW32,
D:ATA YES/3HYES/
DATA NO/3HNI/
DATA PPDAIA/2H-PPr,2HDA,2H*TA/

KV=0.0
DO 6668 I=1,6
   FLAGS(I)='
   FORMAT(' THE FOLLOWING REQUESTS ARE FOR THE ANNEALED SAMPLE.
   FORMAT(' WHAT IS THE WAVELENGTH USED
   FORMAT(' ENTER THE MAXIMUM AND MINIMUM TWO THETA VALUES
   FORMAT(' HARMONIC R.C.F.C. = REAL CORRECTED FOURIER COEF.
   FORMAT(' I.C.F.C. = IMAGINARY CORRECTED FOURIER COEF.
   FORMAT(' L.F.C.C. = LOG OF THE REAL CORRECTED FOURIER COEF.
   FORMAT(' DISP. = DISPLACEMENT BETWEEN SAMPLED CELLS
   FORMAT(' R.U.F.C. = REAL UNCORRECTED FOURIER COEF.
   FORMAT(' I.U.F.C. = IMAGINARY UNCORRECTED FOURIER COEF.
   FORMAT(' R.F.C.A. = REAL FOURIER COEF. OF ANNEALED SAMPLE
   FORMAT(' L.U.F.C.R. = LOG OF UN-NORMALIZED REAL FOURIER COEF.
   FORMAT(2XF5.2,2XFB.3,2XFB.3,6XF6,3,6XF7.2,2X,F8.3,
   FORMAT(1X)
   FORMAT(, ENTER THE MINIMUM TWO THETA VALUE WHICH WILL EVER BE
   FORMAT(, ENTER THE BRAGG ANGLE FOR THE PEAK
   FORMAT(AAAM=F12.7)
   FORMAT( DO YOU WISH TO ENTER DATA FOR ANOTHER WORKED PEAK
   FORMAT( DO YOU WISH TO CHANGE THE HARMONIC FACTOR FROM 5
   FORMAT( THE FOLLOWING DATA REQUESTS ARE FOR THE WORKED SAMPLE
   FORMAT(' DO YOU WISH TO CHANGE THE HARMONIC FACTOR FROM 5

   IF UF=3
   IF UF=1
38 FORMAT(' HARMONIC FACTOR= ') 
40 FORMAT(' ENTER THE SAMPLES IDENTIFICATION') 
41 FORMAT(32A2) 
47 FORMAT(//F' PAGE 'PI3,/932A'v/.' DATA WAS TAKEN 'tAY,5XiA5) 
48 FORMAT(35XP" INITIAL 'P1IX,' THICKNESS',19X,' RADIATION',11X, 
'2 THETA',13X,' IN CH.,',19X,'ABS. COEF.,19X,F4.1x17X, 
'F4.12X,F7.2,///15X,' KV',12X,'POINTS',18X,F4.1x15X, 
'2-THE',15X,'MONOCHROMETER',7X,'AAA',17X,'HARMONIC',15X, 
' T THETA',30X,'FACTOR',18XF6.2,SXF12.6,14XF6.3,//) 
49 FORMAT(' IS THERE ANOTHER ANNEALED PEAK YOU WISH TO USE') 
50 FOR A STANDARD ?') 
59 LACA=0. 
5A PAGE=1 
7 FORMAT(' ENTER THE DATE:',$) 
8 FORMAT(A9) 
9 WRITE(5,3) 
10  
1111 FORMAT(F12.6) 
11 TLOW=TLOW#3.1416/360. 
12 WRITE(5,20) 
13 READ(5,1111)BRAGG 
14 BRAGG=BRAGG#3.1416/180 
15 WRITE(5,11) 
16 READ(5,40) 
17 READ(Sp1111)TLEA(I),I=1,32) 
18 WRITE(5,2) 
19 READ(5,1111)WAVE 
20 PAUSE 'MOUNT THE DISC CONTAINING THE ANNEALED SAMPLE' 
21 READ(B'1)NPA 
22 CONTINUE 
23 WRITE(5,5) 
24 READ(5,1111)TTHA2 
25 WRITE(5,6) 
26 READ(5,1111)TTHA1 
27 YAINC=(TTHA2-TTHA1)/(NPA-1) 
28 XMINA=0.00 
29 WRITE(5,9) 
30 READ(5,1111)HF 
31 WRITE(5,1111)HF 
32 FORMAT(' WHAT RADIATION WAS USED# 
33 ENTER 2-LETTER CODE FOR TARGET ELEMENT.') 
34 FORMAT(' HARMONIC FACTOR= ') 
35 WRITE(5,34) 
36 READ(5,32)IANS 
37 IF(IANS.EQ.0)GOTO1092 
38 IF(IANS.NE.YES)GOTO090 
39 WRITE(5,38) 
40 READ(5,1111)HF 
41 WRITE(5,451) 
42 FORMAT(' WHAT RADIATION WAS USED# 
43 ENTER 2-LETTER CODE FOR TARGET ELEMENT.') 
44 READ(5,34) 
45 WRITE(5,451) 
46 FORMAT(' WHAT RADIATION WAS USED# 
47 ENTER 2-LETTER CODE FOR TARGET ELEMENT.') 
48 READ(5,34) 
49 WRITE(5,451)
452  READ(5,452) RADW
   FORMAT(A2)
   CALL BKGD(XINTA,NPA)
   CALL LRNTZ(WAVE,THH1,NPA,XINTA,YAINC,TLU,TAM,AC+ALPHA)
   CALL FRCOF(INH+XINTA,NPA,FRA,FIA,AA+YAINC,THH1,THH2,
   #WAVE,TLU, HF)
   WRITE(5,33)
370  LACW=0.0
   TM=0.0
   WRITE(5,40)
   READ(5,41)(TLE&JCK), K=1,32)
   WRITE(5,2)
   READ(5,1111)WAVE
   D036 I=1,500
36   XINTW(I)=0.0
   PAUSE 'MOUNT THE DISC CONTAINING THE WORKED SAMPLE'
   READ(9' 1)NPW
   DO251=2,NPW+1
   READ(9'2)XINTW(I-1)
   25   CONTINUE
   WRITE(5,5)
   READ(5,1111)THH2
   WRITE(5,6)
   READ(5,1111)THH1
   YINCW=(THH2-THH1)/(NPW-1)
   XMIXW=0.0
   D0105 J=1,NPW-2
   DINT=XINTW(I)+XINTW(I+1)+XINTW(I+2)
   IF(XMXW.GT.DINT)G0T0105
   XMIXW=DINT
   XMK=I+1
   105   CONTINUE
   CALL BKGD(XINTW,NPW)
   CALL LRNTZ(WAVE,THH1,NPW,XINTW,YINCW,TLU,TM,AC+ALPHA)
   CALL FRCOF(INH+XINTW,NPW,FRA,FIA,AA+YINCW+THH1,THH2,
   #WAVE,TLU, HF)
   WRITE(6,47)PAGE,TLEW,DATEN,TIME
   WRITE(6,48)RADW,TTLOW,TL&HMA,YINCW,AC+LAM+LACW. AAAA14F
   BAG=BRAGG*180./3.1416
   60   WRITE(6,9)
   WRITE(6,10)
   SLPMX=0.
   D0170 I=1,60
   IF(FRA(I)*EQ.0. AND FIA(I)*EQ.0.)G0T0150
   FCCR(I)=(FRA(I)*FRA(I)+FIA(I)*FIA(I))/(FRA(I)**2+FIA(I)
   **2)
   FCCI(I)=(FRA(I)*FIA(I)+FIA(I)*FRA(I))/(FRA(I)**2+FIA(I)
   **2)
   G0T0155
150   FCCR(I)=0.
   FCCI(I)=0.
   155   IF(I.LT.7) N=2*(I-1)
   IF(I.GT.6.AND. I.LT.12) N=5*(I-4)
   IF(I.GT.11) N=10*(I-9)
   ZZ=N/((AA+HF)
   DIS=AA*ZZ
   IF(I.EQ.1)G0T0170
   DDIS=DIS-DIS0
   SLF=(FCCR(I)-FCCR(1))/DDIS
   IF(SLP+SLF/SLPMX*G0T0170
   SLPMX=SLP
   AO=FCCR(I)*DIS*SLPMX
   170   DISO=DIS
   D0666 I=1,60
   IF (FCCR(I), LE.0.) SAVF(I)=FCCR(I)
   IF (FCCR(I), LE.0.) FLAGS(I)=' '
IF (FCCR(I) .LE. 0.) GO TO 6669
SAVE(I)=ALOG(FCCR(I))
CONTINUE
DO1751=1,60
FCCR(I)=FCCR(I)/AO
FCCI(I)=FCCI(I)/AO
LNFCR(I)=-11.51293
 IF(FCCR(I),GT,0.00001)LNFCR(I)=ALOG(FCCR(I))
172 IF(I.LT.7)N=2*(I-1)
 IF(I.GT.6.AND.I.LT.12)N=5*(I-4)
 IF(I.GT.11)N=10*(I-8)
ZZ=N/(AAA#HF)
DIS=AAA#ZZ
 WRITE(6,16)ZZ,FCCR(I),FCCI(I),LNFCR(I),DIS,FRM(I),
16*FWM(I),FRA(I),FIA(I),SAVE(I),FLAGS(I)
 IF((I-25)/45*45.EO. I) WRITE(6,1S)
 IF((I1-25)/45*45.NE.:I-25)G0T0175
PAGE=PAGE+1
 WRITE(6,47)PAGE,TIME
175 CONTINUE
210 WRITE(5,31)
 READ(5,32)IANS
 IF(IANS.EQ.YES)G0T0370
 IF(IANS.NE.NO)G0T0210
215 WRITE(5,49)
 READ(5,32)IANS
 IF(IANS.EQ.YES)G0T059
 IF(IANS.NE.NO)G0T0215
220 STOP
END
*
SUBROUTINEFRCOF(IMAX,XINT,NF,FI,AAA,YINC,TTH1,
* TTH2,WAVE,TLU,HH)
WRITE(5,4444)
4444 FORMAT(/' #FRCOF#',
 REAL XSYM(251),XASYM(251),XINT(500),FR(60),FI(60)
1 FORMAT('+/**+',YNORM='PF1O.6)
5 FORMAT(' THE NUMBER OF POINTS IN RECIPROCAL SPACE',15,'*/F' HAS EXCEEDED THE PERMITTED VALUE OF 251. AN ERROR WILL
#/* RESULT. CHANGE THE DIMENSIONS OF XSYM AND XASYM)
8 FORMAT(' THE MAXIMUM VALUE OF THE CALCULATED RECIPROCAL
*SPACE COORDINATE',F8.3,'/ HAS EXCEEDED 0.5. THE FOURIER
* COEF.S WHICH FOLLOW CONTAIN THIS ERROR.',
 RINC=YINC*3.1416/(2.*180.,)
 TMX=((TTH1+YINC*(IMAX-1))/2.)*3.1416/180.,
 DELS=2.*AAA#(SIN(TMX)+RINC)-SIN(TMX))/WAVE
 S1=2.*AAA#SIN(TM1)/WAVE
 S2=S1
do 91=1,251
 XASYM(1)=0.0
9 XSYM(I)=0.0
 XSYM(I)=2.*XINT(I)
 XASYM(1)=0.0
 MM=2.*AAA#(SIN(TMX)-SIN(TTH1*3.1416/(2.*180.)))/DELS#WAVE+1
10 IF(MM.GT.MM)MM=MM
 N=1
15 IF(MM.LE.251)G0T015
 WRITE(5,5)MM
51-51-DELS
 52xS2+DELS
 T3=WAVE/(2.*AAA)
 N=S1+DELS
25

T1=ATAN(T3/T5)
T4=(S2*WAVE/(2.*AAA))
T6=SQRT(1-T4*T4)
T2=ATAN(T4/T6)
M=NP-IMAX
IF(IMAX.GT.N)M=IMAX-1
XHIGH=0.0
XLOW=0.0
DO100 J=N+1
TH1=TMX-J*RINC
TH2=TMX+J*RINC
IF((TH1.GT.T1.OR.FLG1.NE.0.)AND.0.5))GOTO50
JN=J
FLG1=1.0
IF(IMAX-J.GT.0.0)GOTO20
XX=0.0
GOTO25
XX=XINT(IMAX-J)
IF(XXI.LT.0.)XXI=0.
25 IF(IMAX+J.GT.0.0)GOTO30
XLOW=0.0
GOTO50
XX=XINT(IMAX-J+1)
IF(XX2.LT.0.)XX2=0.
XX=XXI+(XX2-XX1)*(T1-TH1)/RINC
50 IF(TH2.LT.T2.OR.FLG2.NE.0.0)GOTO90
JN=J
FLG2=1.0
IF(IMAX+J.LT.NP+1)GOTO60
YY=0.0
GOTO65
YY=XINT(IMAX-J)
IF(YY1.LT.0.)YY1=0.
65 IF(IMAX+J-1.GT.NP)GOTO70
XHIGH=0.0
GOTO90
70 YY=XINT(IMAX-J+1)
IF(YY2.LT.0.)YY2=0.
XHIGH=YY1+(YY2-YY1)*(T2-TH2)/RINC
90 IF(FLG1.NE.1.0.OR.FLG2.NE.1.)GOTO100
GOTO102
CONTINUE
102 XSYM(I+1)=XHIGH+XLOW
XASYM(I+1)=XHIGH-XLOW
P=1
RAT=XS0M(I+1)/COS(3.14159265*DELS*P*HAR/(0.5))
N=JM
IF(JM.LT.JN)N=JM
IF(I.EQ.1)GOTO110
K=I-1
110 CONTINUE
120 DO130=1,60
FR(I)=0.0
130 FI(I)=0.0
G=(K-1)*DELS
IF(G.GT.0.5)WRITE(5,5555)
WRITE(5,5555)
5555 FORMAT(//'A LENTHLY CALCULATION HAS STARTED,'//', PROGRESS IS DOCUMENTED','//', NOTE! EXECUTION TERMINATES AT 0'))
IEST=60
DO150=1,60
WRITE(5,5556)IEST
5556 FORMAT('(',I2,')')
IF(IEST.EQ.30)WRITE(5,5557)
5557 FORMAT('')
IF(I.LT.7)N=2*(I-1)
IF(I.GT.6.AND.I.LT.12)N=5*(I-1)
IF(I.GT.11)N=10*(I-8)
Z=N/(AAA*HF)

DO145 J=1,KI
S=DELS*(J-1)
B=6.6666667
IF(J.EQ.2.EQ.J)B=1.3333333
IF(J.EQ.1)B=1.3333333
FR(I)=FR(I)+XSYM(J)*COS(3.1416*Z*S/0.5)*DELS*B
FI(I)=FI(I)+XASYM(J)*SIN(3.1416*Z*S/0.5)*DELS*B
IF(I.EQ.1)YNORM=FR(I)
IF(I.EQ.1)YNORM=FR(I)
FR(I)=FR(I)/YNORM
FI(I)=FI(I)/YNORM
WRITE(5,1)YNORM
RETURN
END
SUBROUTINEBKOND(XINT,NP)
WRITE(5,1)
1 FORMAT(' #BKOND')
REAL XINT(500)
BKGMN=0.0
BKGMX=0.0
DO120 I=1,NP
120 BKGMN=BKGMN+XINT(I)/9.0
BKGMX=BKGMX+XINT(NP+1-I)/9.0
BGSLP=(BKGMX-BKGMN)/(NP-10)
DO130 I=1,NP
130 XINT(I)=XINT(I)-(BKGMN+BGSLP*(1-5))
RETURN
END
SUBROUTINELRNTZ(WAVETTH1,NPXINT,YINCTLU,TALPHA)
WRITE(5,11)
11 FORMAT(' #LRNTZ')
REAL LAC,XINT(500)
INTEGER*4 YES,yNO. IANS
DATA YES/3HYES/
DATA NO/3HNO /
1 FORMAT(' IS THE DATA FROM A THIN FILM?')
2 FORMAT(' ENTER THE LINEAR ABSORPTION COEF.,''/''L.A.C.--')
3 FORMAT(' WHAT IS THE FILM THICKNESS IN CENTIMETERS')
4 FORMAT(' WAS A MONOCHROMETER USED?')
5 FORMAT(' ENTER THE BRAGG ANGLE OF THE MONOCHROMETER.')
6 FORMAT(' A')
7 FORMAT(A3)
8 FORMAT(A3)
9 FORMAT(A3)
10 WRITE(5,1)
11 READ(5,6)IANS
12 IF(IANS.EQ.NO)GOTO20
13 IF(IANS.EQ.YES)GOTO10
14 WRITE(5,1)
15 READ(5,1111)LAC
16 FORMAT(F12.6)
17 WRITE(5,3)
18 READ(5,1111)T
19 GOTO30
20 LAC=4
21 T=4
22 ALPHA=0.0
23 IANS=YES
24 WRITE(5,4)
25 READ(5,6)IANS
26 IF(IANS.EQ.NO)GOTO50
IF(IANS.NE.YES)GO TO 30
WRITE(5,5)
READ(5,1111)ALPHA
CSASQ=(COS(2*ALPHA*3.1416/180.0))**2
DO40 I=1,MP
N=I-1
TT=(TTH1+N*YINC)*3.1416/180.0
XZ=-2.0*LAC*T/SIN(TT/2.0)
T1=SIN(TT/2.)*SIN(TT/2.)
T2=COS(TT)
T3=T2*TS
T4=EXP(XZ)
XINT(I)=XINT(I)*SIN(TT)*SIN(TT/2.0)/COS(TT/2.0)*(1.0+COS(TT)**2.0)/(1.0-EXP(-2.0*LAC*T/SIN(TT/2.0)))/CSASQ*COS(TT)**2)
CONTINUE
RETURN
END
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