A Computer Program for the Quantitative Interpretation of Mass Spectrographic Photoplates

Paul P. Eby and James G. Allard
Optical Materials Branch
Optical Physics Division

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NAVAL RESEARCH LABORATORY
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CONTENTS

Abstract  ii
Problem Status  ii
Authorization  ii

INTRODUCTION  1

MATHEMATICAL FORMULATION  2

NUMERICAL CALCULATIONS  3

GENERAL DESCRIPTION OF THE PROGRAM

ACKNOWLEDGMENT  5

REFERENCES  5

APPENDIX A — Program Listing  6
APPENDIX B — Sample Program Output  9
APPENDIX C — Data Coding Form  11
ABSTRACT

To determine impurity concentrations in solids using mass spectrographs, ion-sensitive emulsions are used. The principal problem is obtaining quantitative results from a mass spectrum recorded on a photographic plate is determining the characteristic response curve. Calculations required to determine the parameters in an empirical function which accurately represents the response curve of Ilford QC emulsions are programmed in FORTRAN language. The program input data consists of the impurity-ion mass, line density, and exposure; the impurity-ion concentration and the detection limit are calculated and printed as output.

PROBLEM STATUS

This is a final report on the computer program for determining impurity concentrations in solids.

AUTHORIZATION

NRL Problem P03-07A
Project ARPA Order Number 418

A COMPUTER PROGRAM FOR THE QUANTITATIVE INTERPRETATION
OF MASS SPECTROGRAPHIC PHOTOPATES

INTRODUCTION

Solid-state mass spectrographs normally use ion-sensitive photographic plates as the output detector, due to the wide variation in ion intensity of the rf vacuum spark source. In addition, the photoplate is an excellent ion integrator and has the ability to detect and to record a wide range of masses simultaneously.

There are two principal procedures used for the analytical interpretation of photographic plates: (a) visual inspection (1), where an experienced analyst visually compares line densities and calculates concentrations from relative exposures, and (b) the photometric method (1-3), where a microdensitometer is used to determine line densities and the data are processed by manual calculations. The first method produces semiquantitative results; the latter method, by eliminating errors arising from visually matching densities, line width, emulsion background, etc., can produce quantitative results.

This report is not intended to argue in favor of one method over the other. Both methods are useful. However, if the densitometric method is used, the manual labor required to process the data is so great that the routine computation can be done best by a digital computer.

The primary problem in obtaining a quantitative analysis of a mass spectrum recorded on a photoplate is determining the characteristic response curve of the emulsion. There are several "functionless" methods (4) for obtaining the characteristic response curve, but the method most widely associated with mass spectrography is the modification by Duke (2), based on the "two-line technique" described by Churchill (5) for use in optical spectrography. The characteristic response curve may also be obtained by a "functional" method. An empirical function given by Hull (6) accurately represents the entire response range of Ilford Q2 emulsions, thus permitting all analytical data to be evaluated.

Both the functionless and the functional method have individual merit. The Churchill two-line method is applicable only for elements possessing an appropriate isotopic distribution, and it requires many pairs of measurements of two lines having a known intensity ratio (such as isotopes whose abundance ratio falls within the requisite range). In addition, only information from a single element is used to construct the characteristic curve. However, oven and Giardino (7) have demonstrated that emulsion response exhibits ion-mass dependence, ion-energy dependence, and, possibly, chemical dependence. However, Kennicott (8) has described a computer program using this method.

The functional method, in which the data are fitted to an empirical curve, is easier to program. However, it tends to force the data into a predetermined formula, and any errors of the ion-beam integrator are not corrected. Woolston (9) has described a computer program written in assembly-system language, using the functional method.

The program described below is modeled after Woolston's program, but it is written in FORTRAN IV, because NRL's CDC 3800 computer is more receptive to FORTRAN language. Generally the mathematical functions and symbols of both Woolston's program and our program are the same; there are slight additions or deletions that suited our
personal approach. However, the parameters calculated from the same data are essentially the same.

MATHEMATICAL FORMULATION

The equation for the photographic calibration curve given by Hull (6) may be expressed by

\[ K_{z,i} E_z = \left( \frac{100 - T_L}{T_L - T_{SAT}} \right)^{1/R_x} \]

where, for a sample component \( z \),

- \( K_{z,i} \) is directly proportional to the component concentration in the total ion beam striking the plate and to the photoplate sensitivity,
- \( a_{z,i} \) is the abundance of isotope \( i \) of the sample component,
- \( E_z \) is the exposure, indicated by the beam-monitor integrator, in nanocoulombs,
- \( T_L \) is the percent line transmission (corrected for background) of the spectral line \( i \),
- \( T_{SAT} \) is the percent transmission of the spectral line \( i \) for an infinite (saturation) exposure, and
- \( R_x \) is proportional to the maximum slope of the photographic response curve.

The corrected line transmission \( T_L \) in Eq. (1) is given by

\[ T_L = \frac{100 + T_{SAT} \left[ \left( \frac{100 - T_{LB}}{T_{LB} - T_{SAT}} \right)^{1/R_x} - \left( \frac{100 - T_B}{T_B - T_{SAT}} \right)^{1/R_x} \right]}{1 + \left[ \left( \frac{100 - T_{LB}}{T_{LB} - T_{SAT}} \right)^{1/R_x} - \left( \frac{100 - T_B}{T_B - T_{SAT}} \right)^{1/R_x} \right]} \]

where \( T_{LB} \) is the measured line transmission and \( T_B \) is the measured background transmission, both in percent transmission.

The sensitivity of the emulsion is proportional to \( M^{0.4} \), where \( M \) is the mass of the ion. When this factor is included the equation for calculating the impurity-ion concentration \( C_i \) in ppm is determined from Eq. (1) and becomes

\[ C_i = \frac{10^{4}(MF) 0.65 S_z K_x C_r}{(MF) 0.65 S_z K_r} \]

where \( MF \) is a factor proportional to the mass in atomic mass units, \( C_r \) is the fractional concentration of the reference ion, and \( S_z \) is the relative sensitivity coefficient (unless both \( S_z \) and \( S_r \) are known, they are taken to be unity).

When the lines have finite width the concentrations are corrected by a factor equal to the line width. Thus, Eq. (3) must be multiplied by \( w_{z,i} w_{r,i} \), where \( w \) is the width of
the line as determined at the points of half-maximum on the intensity profile. When the background is considered, these points correspond to the transmission

\[ T_{L_{\text{W}}} = \frac{100 + T_{\text{SAT}} \left( \frac{1}{2} \left( \frac{100 - T_{L_{\text{B}}}}{T_{L_{\text{B}}} - T_{\text{SAT}}} \right)^{1/R_x} + \frac{1}{2} \left( \frac{100 - T_{B}}{T_{B} - T_{\text{SAT}}} \right)^{1/R_x} \right)^{R_x}}{1 + \left( \frac{1}{2} \left( \frac{100 - T_{L_{\text{B}}}}{T_{L_{\text{B}}} - T_{\text{SAT}}} \right)^{1/R_x} + \frac{1}{2} \left( \frac{100 - T_{B}}{T_{B} - T_{\text{SAT}}} \right)^{1/R_x} \right)^{R_x}}. \]  

(4)

NUMERICAL CALCULATIONS

When only one data point is available, \( R_x \) is taken to be 1. For two data points (1 and 2) \( R_x \) is determined from the relationship

\[ \log \left( \frac{100 - T_{L_{\text{1}}}}{100 - T_{L_{\text{2}}}} \right) = \log \left( \frac{R_x^{1/R_x}}{R_x^{1/R_x}} \right), \]

(5)

which may be derived from Eq. (1). Only three data points are allowed in the program. When three points are used, an average value of \( R_x \) (equal to the root-mean-square of \( R_x \) obtained from the calculation for the three combinations of pairs of data points) is calculated and is designated as \( R_{x_{\text{AV}}} \). If \( R_x \) is either greater than 1.25 or less than 1, \( R_{x_{\text{AV}}} \) is set equal to 1.0. Upon substituting \( R_{x_{\text{AV}}} \) into Eq. (1), numerical values of \( K_x \) are calculated for each data point, and the root mean square of this result, denoted by \( K_{x_{\text{AV}}} \), is substituted into Eq. (3) to determine the ion concentration.

Numerical values of \( T_{L_{\text{W}}} \) are calculated from Eq. (4) for each data point; an average value of the correction for line width can be determined by the densitometric measurements, and the factor \( w_{x_{\text{r}}, i} \) can be applied to Eq. (3).

The detection limit is determined by using \( R_{x_{\text{AV}}} \) to calculate \( K_x \) for the maximum component exposure, setting \( T_L = 100\% \) and \( T_B = 98\% \) in Eq. (1) and substituting these values of \( K_x \) in Eq. (3).

GENERAL DESCRIPTION OF THE PROGRAM

Expressions are programmed for the calculations described in the previous section for experimental data read in from punched cards. Tables of isotope abundances and identifications are punched on IBM cards and are read in preceding the experimental data cards. If an incorrect isotope identification is made on the corresponding data card, NO ISOTOPE LISTED is printed, and the calculation for that isotope is bypassed. Other errors are determined by the system error identifiers. Formats of the experimental data cards are given in Table 1.

The input data are punched on cards. A table of isotope abundances is read in with the measured data. Table 2 gives a definition of the symbols used in the program.

Cards 3 through 4 + (N - 1) are included, in order, for each isotope. Three cards (identified as 23-1, 23-2, and 23-3) may be inserted into the program between cards 23 and 24. The data are then punched in as optical density.
Table 1
Input Data Format

<table>
<thead>
<tr>
<th>Data Card Number</th>
<th>Format</th>
<th>Symbols</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(55H )</td>
<td>Run Identification</td>
</tr>
<tr>
<td>2</td>
<td>(1x, I4, 10x, E11.4, 2x, F10.4)</td>
<td>NO RUNS, REF CONC, EIM** X</td>
</tr>
<tr>
<td>3</td>
<td>(1x, F4.1, 9x, F7.2, 10x, I2, 10x, A8, A1, 7x, F5.2)</td>
<td>CHG, ATWT, N, Q, S*</td>
</tr>
<tr>
<td>4 through 4 + (N - 1)</td>
<td>(A8, 1x, F8.4, 2 (2x, F8.4), 3x, E10.3)</td>
<td>ID, TLB, TB, TSAT, EI</td>
</tr>
</tbody>
</table>

*The sequence of cards 3 through 4 + (N - 1) is repeated a number of times equal to the number of runs.

Table 2
Definition of Symbols

<table>
<thead>
<tr>
<th>Card Number</th>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>NO RUNS</td>
<td>The number of isotopes processed</td>
</tr>
<tr>
<td>2</td>
<td>Ref Conc</td>
<td>The concentration of the reference isotope</td>
</tr>
<tr>
<td>2</td>
<td>EIMAX</td>
<td>The maximum photoplate exposure in nanocoulombs</td>
</tr>
<tr>
<td>3</td>
<td>CHG</td>
<td>The isotopic charge</td>
</tr>
<tr>
<td>3</td>
<td>ATWT</td>
<td>The average atomic weight of the element</td>
</tr>
<tr>
<td>3</td>
<td>N</td>
<td>The number of data points used for the isotope processed</td>
</tr>
<tr>
<td>3</td>
<td>Q</td>
<td>The comments</td>
</tr>
<tr>
<td>3</td>
<td>S</td>
<td>(Defined in text)</td>
</tr>
<tr>
<td>4</td>
<td>ID</td>
<td>The atomic symbol and mass number</td>
</tr>
<tr>
<td>4</td>
<td>TLB, TB, TSAT, EI</td>
<td>(Defined in text)</td>
</tr>
</tbody>
</table>

The first 1-2 characters in the A8 specification of ID refers to the atomic symbol, and the last 1-3 characters correspond to the atomic mass.

ACKNOWLEDGMENT

Mr. Kenneth Moran of the NRL Computer Center is gratefully acknowledged for his programming assistance.
REFERENCES


Appendix A

PROGRAM LISTING

PROGRAM SPECTRA
DIMENSION LEJ(3), TB(3), TSAT(3), ID2(3)
CID(3), AT(287), IDEN(287), MASS(287), MI(3), E1(3), AI(3), IQ2(2)

TYPE REAL /FACTOR, KAV, XX, MI, KD, KAVR

2.1 FORMAT(7FU..5)
2.2 FORMAT(9A1)
2.3 FORMAT(19U)
2.4 FORMAT(2016)
RFA201, AB
READ2C2.IDEN...
READ20'MASS...
LINE5=*7
READ 2V6...
PRINT 205
PRINT 2C6...
CALL HEADIN...
RFA30 .NO RUNS, REF, CONC, FIMAX...
DO 26 I=1, NO RUNS
READ 31*CHG*AT * W.T.N.*, G5
MFATOR=(AT WT/(3*0*CHG1)***C.6
DO 4 J=1,N
READ 32*ID(J), TL(J), Tu(J), TSAT(J), EJ(J)
TLB(J)*100.0*(TLB(J))**3.0
TB(J)*100.0*(TB(J))**100.0
TSAT(J)*100.0*(TSAT(J))**100.0
ID2(J)*MSK2*AND*ID(I)
L=0
1 L=L+1
IF(L>GT.287)33,2
2 IF(IDC(J), EU*1DEN(L))3,1
3 AI(J)*AB(L)/100.0
W(J)*MASS(L)
CALL CALC TL'TLRIJ, TB(J), TSAT(J), TL(J)
4 CONTINUE
ID1*MSK1*AND*ID
IF(N*EQ.115)3
5 R=1.0
R(2)=1.0
RAV=1.0
CALL CALC KIR*TL*TSAT*EI.AI*KX
CALL CALC TLW(R, TL, TB, TSAT, TLX)
KAV=MFATOR*KX
GO TO 11
6 IF(N*EQ.2)7,9
7 CALL CALC R1, T1, A1*EI(A1), E1(2), TSAT, TSAT(2), R
R(2)=R
RAV=R
10 DO 8 M=1,2
CALL CALC KIR, TL(M), TSAT(M), EI(M), A! (M), KX(M)
8 CALL CALC TLW(R, TL(M), TB(M), TSAT(M), TLW(M))
KAV=SORTF(KK*XX(2))**MFATOR
GO TO 11
9 DO 10 M=2,3
10 10
CALL CALC R(M); A1[M]; E1[M]; A1(M); E1(M); TSAT(M); TSAT(R(N-1));
CALL CALC R(J); A1(J); E1(J); A1(M); E1(M); TSAT(J); TSAT(R(N-1));

CALL CALC R(TL); A1[TL]; E1(TL); A1(M); E1(M); TSAT(TL); TSAT(M);

KAV=KAV*(KX12;KK13)*EX*MACTUR

IF(I=EQ1;112J;13)

CONTINUE

R(1)=RFF CONC

SR=S

KAV=KAV

GO TO 22

DO 18 M1=M M1=M+1

CONTINUE

IF(N.EQ1;112J;20)

RX=R

GO TO 21

DO 21 RX=RAV

CONTINUE

PR INJ 27;DL(U);R(U);=;IK);TSAT(U);TL(U);TLW(U); R(U)

CONTINUE

CALL HEADING

CONTINUE

IF(J.EQ1;20)

READ 32(TL(J);R(J);=;IK);TSAT(J);TL(J);TLW(J); R(J)

CONTINUE

FORMAT(19H ISOTOPE NOT LISTED)

FORMAT(55H)

FORMAT(1X;F4;1;9X;F7;2;1X;I2;10X;A8;A1;7X;F5;2)

FORMAT(82X;4HRAV=F4;3;2X;4HKAV=,t=0.5;/

CONTINUE

GO TO 39

PRINT 34

CONTINUE

FORMAT(19H ISOTOPE NOT LISTED)

FORMAT(55H)

FORMAT(1X;F4;1;9X;F7;2;1X;I2;10X;A8;A1;7X;F5;2)
SUBROUTINE HEADING
PRINT 1
1 FORMAT (/1X.6HSYMBOL,.6)' .3HPPM.' .9HDET I. .8HCOMMENTS.' .2X. END
SUBROUTINE CAUC IC(R,TL,TSAT,E1,A1,KX)
TYPE REAL KX
IF (R.GT.1.25) 128
1 RX1=1.0/R
GO TO 5
2 IF (R.LT.0.134)
3 RX1=1.0
GO TO 5
4 RX1=1.0/R
5 RX1=(1.0R-TL)/(TL-TSAT)1*RX1/(A1*E1)
END
SUBROUTINE CALCI TLW(R,TLB,TG,TSAT,TLW)
RX1=1/1.25
GO TO 3
2 RX=R
RX1=R/R
3 TS1=(1.0R-TLB)/(TLB-TSAT)1*RX1/2.0
TS2=(1.0R-TB)/(TB-TSAT)1*RX1/2.0
TS3=(TS1+TS2)*RX
TLW=(1.0R+TSAT*TS3)/(1.0+TS3)
END
SUBROUTINE CALC TL(TLB,TSAT,TL)
TS=(1.0R-TLB)/(TLB-TSAT)-(1.0R-TB)/(TB-TSAT)
TL=(1.0R+TSAT*TS)/(1.0+TS)
END
SUBROUTINE CALC R(TL2,TL2,AE1,AE2,TSAT1,TSAT2,R)
R=LOGF((1.0R-TL2)/(TL1-TSAT1)*(TL2-TSAT2)/(1.0R-TL2))/CLOGF(AE1/AE2)
END
Appendix B

SAMPLE PROGRAM OUTPUT
<table>
<thead>
<tr>
<th>SYMBOL</th>
<th>PPM</th>
<th>DET LIMIT</th>
<th>COMMENTS</th>
<th>MASS</th>
<th>TLR</th>
<th>TB</th>
<th>TSAT</th>
<th>TL</th>
<th>TLW</th>
<th>R</th>
<th>K</th>
<th>KF</th>
<th>S</th>
<th>E1</th>
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<td>K</td>
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<td>0.0705</td>
<td>REFERENCE</td>
<td>41</td>
<td>56.5</td>
<td>94.8</td>
<td>2.6</td>
<td>98.2</td>
<td>72.1</td>
<td>1.115</td>
<td>3.781E+03</td>
<td>1.172</td>
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<td>3.0E-03</td>
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<td>41</td>
<td>27.1</td>
<td>91.2</td>
<td>2.6</td>
<td>27.7</td>
<td>43.1</td>
<td>1.171</td>
<td>3.569E+03</td>
<td>1.000</td>
<td>3.0E-02</td>
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<td>1.00</td>
<td>1.0E+03</td>
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<td>1.00</td>
<td>1.0E+02</td>
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<td>47.3</td>
<td>2.6</td>
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<td>4.582E-03</td>
<td>1.0E+03</td>
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Appendix C

DATA CODING FORM
### Document Control Data - R & D

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### Report Title

A COMPUTER PROGRAM FOR THE QUANTITATIVE INTERPRETATION OF MASS SPECTROGRAPHIC PHOTOPLATES

### Descriptive Notes (Type of report and inclusive dates)

This is a final report on the computer program for determining impurity concentration in solids.

### Authors (First name, middle initial, last name)

Paul P. Bey and James G. Allard

### Report Date

April 8, 1968

### Total No. of Pages

16

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NRL Problem P03-07A

### Project No.

ARPA Order Number 418

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Any other numbers that may be assigned this report

### Distribution Statement

This document has been approved for public release and sale; its distribution is unlimited.

### Abstract

To determine impurity concentrations in solids using mass spectographs, ion-sensitive emulsions are used. The principal problem in obtaining quantitative results from a mass spectrum recorded on a photographic plate is determining the characteristic response curve. Calculations required to determine the parameters in an empirical function which accurately represents the response curve of Ilford Q2 emulsions are programmed in FORTRAN language. The program input data consists of the impurity-ion mass, line density, and exposure; the impurity-ion concentration and the detection limit are calculated and printed as output.
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