A Computer Program for the Quantitative Interpretation of Mass Spectrographic Photoplates

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ABSTRACT

To determine impurity concentrations in solids using mass spectrographs, 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 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 PHOTOPLATES

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, but Owens 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

$$K_x a_{x,i} E_x = \frac{(100 - T_l)}{(T_l - T_{SAT})} \frac{1}{R_x}, \tag{1}$$

where, for a sample component $x$,

- $K_x$ is directly proportional to the component concentration in the total ion beam striking the plate and to the photoplate sensitivity,
- $a_{x,i}$ is the abundance of isotope $i$ of the sample component,
- $E_x$ 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

$$T_L = \frac{100 + T_{SAT} \left[ \left( \frac{100 - T_{LB}}{T_{LB} - T_{SAT}} \right)^{1/R} - \left( \frac{100 - T_{LB}}{T_{LB} - T_{SAT}} \right)^{1/N} \right]}{1 + \left[ \left( \frac{100 - T_{LB}}{T_{LB} - T_{SAT}} \right)^{1/R} - \left( \frac{100 - T_{LB}}{T_{LB} - T_{SAT}} \right)^{1/N} \right]} \tag{2},$$

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 $N_{0.6}^0$, where $N$ 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

$$C_i = \frac{10^4 (\Psi F)^{0.6} s_x K_x C_r}{(MF_{r})^{0.6} s_x N_{r}}, \tag{3}$$

where $\Psi F$ is a factor proportional to the mass in atomic mass units, $C_r$ is the fractional concentration of the reference ion, and $s$ is the relative sensitivity coefficient (unless both $s_x$ 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 $w_{x,i} w_{r,j}$, 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

\[
T_{Lw} = \frac{100 + T_{SAT} \left( \frac{1}{2} \left( \frac{100 - T_{LB}}{T_{LB} - T_{SAT}} \right)^{1/R_S} + \frac{1}{2} \left( \frac{100 - T_{B}}{T_{B} - T_{SAT}} \right)^{1/R_S} \right) R_S}{1 + \left( \frac{1}{2} \left( \frac{100 - T_{LB}}{T_{LB} - T_{SAT}} \right)^{1/R_S} + \frac{1}{2} \left( \frac{100 - T_{B}}{T_{B} - T_{SAT}} \right)^{1/R_S} \right) R_S}
\]  

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

\[
R_x = \frac{\log \left( \left( \frac{100 - T_{L1}}{T_{L1} - T_{SAT}} \right) \left( \frac{T_{L1} - T_{SAT}}{100 - T_{L1}} \right) \right)}{\log \left( \frac{\sigma_1 \sigma_2 \sigma_3}{\sigma_2 \sigma_3} \right)}
\]  

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 calcu-
lated and is designated as \( R_{AVx} \). If \( R_x \) is either greater than 1.25 or less than 1, \( R_{AVx} \) is set
equal to 1.0. Upon substituting \( R_{AVx} \) into Eq. (1), numerical values of \( K_x \) are calculated
for each data point, and the root mean square of this result, denoted by \( \sqrt{K_{AVx}} \), is substi-
tuted into Eq. (3) to determine the ion concentration.

Numerical values of \( T_{Lw} \) are calculated from Eq. (4) for each data point; an average
value of the correction for line width can be determined by the densitometric measure-
ments, and the factor \( w_{x, i} \) can be applied to Eq. (3).

The detection limit is determined by using \( K_{AVx} \) 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, E1M^-*</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</td>
<td>(A8 1x, F8.4, 2 (2x, F8.4), 3x, E10.3)</td>
<td>ID, TLB, TB, TSAT, EI</td>
</tr>
<tr>
<td>4+(N-1)</td>
<td></td>
<td></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


PROGRAM SPECTRA

DIMENSION LEJ(3), TB(3), TSAT(3)

CID(3), AL(287), IDEN(287), MASS(287), MI(3), EI(3), AL(3), Q(2)

TYPE REAL $\alpha$, $\beta$, $\gamma$, $\delta$, $\epsilon$, $\zeta$

2 FORMAT(7F1.5)

2w Format($\times 10^n$)

20 FORMAT(2(16))

READ201, AB
READ202, IDEN
READ203, MASS
READ204, MSK1, MSK2

LINES = 1
READ 2-6
PRINT 205
PRINT 206
CALL HEADIN

RA0201, AB
READ201, IDEN
READ202, IDEN
READ203, MASS
READ204, MSK1, MSK2

LINES = 1
READ 2-6
PRINT 205
PRINT 206
CALL HEADIN

RFAD30, NO RUNS, REF, CONC, EIMAX

DO 26 L = 1, NO RUNS

READ 31, CHG, AT, WT, N, O, S
MFAC = AT/WT/(10^0 * CHG) ** C + 6

DO 4 J = 1, N

READ 32, TLb(J), TB(J), TSAT(J), EJ(J)

LJ = C

IF (L .LE. 287) THEN

IF (L .EQ. 287) THEN

IF (ID(J) .NE. IDEN(L)) THEN

CALL CALC TLb(J), TB(J), TSAT(J), TL(J)

CONTINUE

IF (ID(J) .EQ. 1 AND L .NE. 0)

IF (N .EQ. 115) THEN

IF (L .EQ. 1) THEN

R(1) = 1

R(2) = 1

RAV = 1

CALL CALC K1 * TLb(J), TSAT(J), EJ(J), AL(J)

CALL CALC TLW(R, TLb(J), TB(J), TSAT(J))

KAV = MFAC * KX

GO TO 11

DO 8 M = 1, 2

CALL CALC K(R, TLb(M), TSAT(M), EJ(M), AL(M), KX(M))

CALL CALC TLW(R, TLb(M), TB(M), TSAT(M))

KAV = SORTF(KX * KX(M)) ** MFAC

GO TO 11

DO 5 M = 2, 3

KAV = KAV

GO TO 11

6 IF (N .EQ. 2) THEN

CALL CALC R(TLb(2), AL, EJ, AL(2), TSAT, TSAT(2), R)

R(2) = R

RAV = R

DO 8 M = 1, 2

CALL CALC K(R, TLb(M), TSAT(M), EJ(M), AL(M), KX(M))

CALL CALC TLW(R, TLb(M), TB(M), TSAT(M))

KAV = SORTF(KX * KX(M)) ** MFAC

GO TO 11

DO 5 M = 2, 3

KAV = KAV

GO TO 11

7 IF (N .NE. 0) THEN

CALL CALC R(TLb(2), AL, EJ, AL(2), TSAT, TSAT(2))
CALL CALC R(TL,TL(M),AI,1M),TSAT,TSAT(M),R(N-1)  
CALL CALC K(R(K),1M,TSAT,TSAT(M),R(N-1)  
CALL CALC K(RAV,1M,1M)  
CALL CALC K(RX,1M,1M)  
CLE  = RFF CONC  
KAVR=KAV  
GO TO 20  
DO 1 N=1,N  
IF(AI(M),LT.AI(M+1),16,17)  
M=M+1  
GO TO 18  
CONTINUE  
IF(N.EQ.1),20,21  
RX=RAV  
GO TO 21  
DO 21 RX=RAV,20  
CALL CALC K(RX,98,0)  
DO 21 RX=RAV  
PRINT 29,RAV,1M  
LINE=S-LINE-N-3  
IF(LINES,LT.0),26,25  
LINES=47  
PRINT 24  
CALL HEADING  
GO TO 36  
PRINT 34  
FORMAT(19H ISOTOPE NOT LISTED)  
FORMAT(55H)  
FORMAT(1X,I4,10X,E2.2X,F10,4)  
FORMAT(A8,2X-.F8,4,2(2X.F8,4,"3X.E10.3)  
IF(J,EO.N),37,36  
DO 38 J=JE1,N  
READ 32,1D(JE1),TL(JE1),TL(JE1),TSAT(JE1),E11(JE1)  
READ 32,1D(JE1),TL(JE1),TL(JE1),TSAT(JE1),E11(JE1)  
60  
61  
62  
63  
64  
65  
66  
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112  
113  
114
SUBROUTINE HEADING
PRINT 1
1 FORMAT(/1X.6HSYMBO,.6).3HPPM»5X.9HDET,.3X.9HCOMMENTS,.2X,
       5HMMAS,3X.3HILG.4X.2HILB.5Y.4HTS1,4X.2HTL.4X.3HTLW.8X.1HR.13X,
       5X,.9X.2HMF,.6X.9X.2ME1,1)
END

SUBROUTINE CALC (R,T,L,TSAT,E1,A1,XX)
TYPE REAL XX
IF(R.GT.1.25)1,2,9

1 RX1=1.0/1.25
GO TO 5

2 IF(R.LT.0.134)
3 RX1=1.0
GO TO 5

4 RX1=1.0/R

5 RX=(1.0/R-TL)/(TL-TSAT)**RX/(A(A1))
END

SUBROUTINE CALC TLW(R,T,LB,TB,TSAT,TLW)
IF(R.GT.1.29)1,2,9

1 RX=1.25

2 RX=R

3 TLW=(100.0-TSAT)/(TL-TSAT)**RX/(1.0+TSAT)
END

SUBROUTINE CALC (T,R,T,L2,AE1,AE2,TSAT1,TSAT2,R)

R=LOGF ((100.0-TL)/(TL-TSAT1)**(TL2-TSAT2)/(100.0-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>TLM</th>
<th>R</th>
<th>K</th>
<th>NF</th>
<th>S</th>
<th>E1</th>
</tr>
</thead>
<tbody>
<tr>
<td>X</td>
<td>5.000×10⁵</td>
<td>0.0705</td>
<td>REFERENCE</td>
<td>41</td>
<td>96.5</td>
<td>94.8</td>
<td>2.6</td>
<td>98.2</td>
<td>72.1</td>
<td>1.115</td>
<td>3.761×10⁵</td>
<td>1.172</td>
<td>1.00</td>
<td>3.0×10³</td>
</tr>
<tr>
<td></td>
<td>41</td>
<td>27.1</td>
<td>91.2</td>
<td>2.6</td>
<td>92.7</td>
<td>43.1</td>
<td>1.171</td>
<td>3.569×10⁵</td>
<td>1.000</td>
<td>1.0×10⁻²</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>41</td>
<td>10.5</td>
<td>82.8</td>
<td>2.6</td>
<td>15.6</td>
<td>17.3</td>
<td>1.232</td>
<td>3.772×10⁻³</td>
<td>3.0×10⁻³</td>
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<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td></td>
<td>RAV=1.172</td>
<td>4.345×10⁵</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>CL</td>
<td>5.042×10⁻³</td>
<td>0.0052</td>
<td></td>
<td>35</td>
<td>53.5</td>
<td>97.3</td>
<td>2.6</td>
<td>91.2</td>
<td>70.1</td>
<td>1.120</td>
<td>3.965×10⁻¹</td>
<td>1.105</td>
<td>1.00</td>
<td>3.0×10⁻²</td>
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<tr>
<td></td>
<td>35</td>
<td>24.5</td>
<td>96.4</td>
<td>2.6</td>
<td>24.7</td>
<td>39.8</td>
<td>1.120</td>
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<td>1.001</td>
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<td></td>
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<tr>
<td></td>
<td>RAV=1.120</td>
<td>KAV=4.363×10⁻¹</td>
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<tr>
<td>S</td>
<td>1.644×10⁻¹</td>
<td>0.0148</td>
<td></td>
<td>10</td>
<td>94.8</td>
<td>96.6</td>
<td>2.6</td>
<td>98.1</td>
<td>95.7</td>
<td>1.388</td>
<td>2.321×10⁻³</td>
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<td>1.00</td>
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<td></td>
<td>10</td>
<td>56.5</td>
<td>76.2</td>
<td>2.4</td>
<td>66.2</td>
<td>63.5</td>
<td>1.388</td>
<td>2.094×10⁻³</td>
<td>1.0×10⁻³</td>
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<td>KAV=1.429×10⁻³</td>
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<tr>
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<td>23</td>
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<td>99.3</td>
<td>2.6</td>
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<td>1.00</td>
<td>3.0×10⁻¹</td>
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<td></td>
<td>23</td>
<td>65.3</td>
<td>99.3</td>
<td>2.6</td>
<td>65.6</td>
<td>73.8</td>
<td>0.577</td>
<td>9.443×10⁻¹</td>
<td>1.0×10⁻⁰</td>
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<td></td>
<td></td>
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<td>KAV=6.008×10⁻¹</td>
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<td></td>
</tr>
<tr>
<td>B</td>
<td>6.084×10⁻²</td>
<td>0.0034</td>
<td></td>
<td>11</td>
<td>94.2</td>
<td>96.8</td>
<td>2.6</td>
<td>97.2</td>
<td>95.9</td>
<td>1.550</td>
<td>7.399×10⁻⁴</td>
<td>0.542</td>
<td>1.00</td>
<td>1.0×10⁻²</td>
</tr>
<tr>
<td></td>
<td>11</td>
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Appendix C

DATA CODING FORM
A COMPUTER PROGRAM FOR THE QUANTITATIVE INTERPRETATION OF MASS SPECTROGRAPHIC PHOTOPlates

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

Paul P. Bey and James G. Allard

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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