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A Computer Program for the Quantitative Interpretation of Mass Spectrographic Photoplates

PAUL P. ERY AND JAMES C. ALLARD

Optical Materials Branch
Optical Physics Division

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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 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.

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

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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 Huli (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

$$K_x a_{x,i} E_x = \left(\frac{100 - T_L}{T_L - T_{SAT}}\right)_{x,i}^{1/R_x}, \tag{1}$$

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

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

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 $M^{0.6}$, where M is the mass of the ion. When this factor is included the equation for calculating the impurity-ion concentration C_i in ppma is determined from Eq. (1) and becomes

$$C_i = \frac{10^6 (MF_x)^{0.6} S_r K_x C_r}{(MF_r)^{0.6} S_x K_r}. \tag{3}$$

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 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

$$T_{Lw} = \frac{100 + T_{SAT}\left[\frac{1}{2}\left(\frac{100 - T_{LB}}{T_{LB} - T_{SAT}}\right)^{1/R_x} + \frac{1}{2}\left(\frac{100 - T_B}{T_B - T_{SAT}}\right)^{1/R_x}\right]^{R_x}}{1 + \left[\frac{1}{2}\left(\frac{100 - T_{LB}}{T_{LB} - T_{SAT}}\right)^{1/R_x} + \frac{1}{2}\left(\frac{100 - T_B}{T_B - T_{SAT}}\right)^{1/R_x}\right]^{R_x}} . \tag{4}$$

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

$$R_x = \frac{\log\left[\left(\frac{100 - T_{L1}}{T_{L1} - T_{SAT}}\right)\left(\frac{T_{L2} - T_{SAT}}{100 - T_{L2}}\right)\right]}{\log\left(\frac{a_1 E_1}{a_2 E_2}\right)} , \tag{5}$$

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_{AV}. If R_x is either greater than 1.25 or less than 1, R_{AV} is set equal to 1.0. Upon substituting R_{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_{AV}, is substituted 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 measurements, and the factor $w_{x,i}/w_{r,i}$ can be applied to Eq. (3).

The detection limit is determined by using R_{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

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

*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

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

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

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Appendix A

PROGRAM LISTING

```
      PROGRAM SPECTRA
      DIMENSION TLB(3),TB(3),TSAT(3),TLW(3),TL(3),R(3),KX(3),ID2(3),
     CID(3),AB(287),IDEN(287),MASS(287),MI(3),EI(3),AI(3),Q(2)
      TYPE REAL MFACTOR,KAV,KX,MI,KDL,KAVR
  201 FORMAT(7F10.5)
  202 FORMAT(9A8)
  203 FORMAT(19I4)
  204 FORMAT(2(O16))
      READ201,AB
      READ202,IDEN
      READ203,MASS
      READ204,MSK1,MSK2
      LINES=47
      READ 206
      PRINT 205
      PRINT 206
      CALL HEADING
      READ30 ,NO RUNS,REF CONC,EIMAX
      DO 26 I=1,NO RUNS
      READ 31,CHG,AT WT,N,Q,S
      MFACTOR=(AT WT/(30.0*CHG))**0.6
      DO 4 J=1,N
      READ 32,ID(J),TLB(J),TB(J),TSAT(J),EI(J)
      TLB(J)=10.0**(-TLB(J))*100.0
      TB(J)=10.0**(-TB(J))*100.0
        TSAT(J)=10.0**(-TSAT(J))*100.0
      ID2(J)=MSK2.AND.ID(J)
      L=0
    1 L=L+1
      IF(L.GT.287)33,2
    2 IF(ID(J).EQ.IDEN(L))3,1
    3 AI(J)=AB(L)/100.0
      MI(J)=MASS(L)
      CALL CALC TL(TLB(J),TB(J),TSAT(J),TL(J))
    4 CONTINUE
      ID1=MSK1.AND.ID
      IF(N.EQ.1)5,6
    5 R=1.0
      R(2)=1.0
      RAV=1.0
      CALL CALC K(R,TL,TSAT,EI,AI,KX)
      CALL CALC TLW(R,TLB,TB,TSAT,TLW)
      KAV=MFACTOR*KX
      GO TO 11
    6 IF(N.EQ.2)7,9
    7 CALL CALC R(TL,TL(2),AI*EI,AI(2)*EI(2),TSAT,TSAT(2),R)
      R(2)=R
      RAV=R
      DO 8 M=1,2
      CALL CALC K(R,TL(M),TSAT(M),EI(M),AI(M),KX(M))
    8 CALL CALC TLW(R,TLB(M),TB(M),TSAT(M),TLW(M))
      KAV= SQRTF(KX*KX(2))*MFACTOR
      GO TO 11
    9 DO 10 M=2,3
```

```
 10 CALL CALC R(TL,TL(M),AI*EI,AI(M)*EI(M),TSAT,TSAT(M),R(M-1))
    CALL CALC R(TL(2),TL(3),AI(2)*EI(2),AI(3)*EI(3),TSAT(2),TSAT(3),
   CR(3))
    EX=1.0/3.0
    RAV=(R*R(2)*R(3))**EX
    DO101 M=1,3
    CALL CALC K(RAV,TL(M),TSAT(M),EI(M),AI(M),KX(M))
101 CALL CALC TLW(RAV,TLB(M),TB(M),TSAT(M),TLW(M))
    KAV=(KX*KX(2)*KX(3))**EX*MFACTOR
 11 IF(I.EQ.1)12,13
 12 CI=REF CONC
    SR=S
    KAVR=KAV
    GO TO 131
 13 CI= SR*KAV/(S*KAVR)* REF CONC
131 IF(N.EQ.1)14,15
 14 M1=1
    GO TO 20
 15 N1=N-1
    DO 18 M=1,N1
    IF(AI(M).LT.AI(M+1))16,17
 16 M1=M+1
    GO TO 18
 17 M1=M
 18 CONTINUE
    IF(N.EQ.3)19,20
 19 RX=RAV
    GO TO 21
 20 RX=R
 21 CALL CALC K(RX,98.0,0.0,EIMAX,AI(M1),KDL)
    DET LIM=SR*KDL/(KAVR*S)* REF CONC* MFACTOR
    PRINT 27,ID1,CI,DET LIM,Q(1),Q(2),ID2(1),TLB(1),TB(1),TSAT(1),
   CTL(1),TLW(1),R(1),KX(1),MFACTOR,S,EI(1)
    IF(N.EQ.1)24,23
 23 DO 231 LN=2,N
    PRINT 28,ID2(LN),TLB(LN),TB(LN),TSAT(LN),TL(LN),TLW(LN),R(LN),
   CKX(LN),EI(LN)
231 CONTINUE
 24 PRINT 29,RAV,KAV
    LINES=LINES-N-3
    IF(LINES.LT.0)25,26
 25 LINES=47
    PRINT 205
    PRINT 206
    CALL HEADING
 26 CONTINUE
    GO TO 35
 33 PRINT 34
 34 FORMAT(19H ISOTOPE NOT LISTED)
    IF(I.EQ.NO RUNS)35,36
 27 FORMAT(3X,A2,4X,E10.3,2X,F8.4,3X,A9,A1,2X,R3,5(2X,F5.1),5X,F6.3,
   C6X,E10.3,2X,F6.3,2X,F5.2,2X,E8.1)
 28 FORMAT(43X,R3,5(2X,F5.1),5X,F6.3,6X,E10.3,17X,E8.1)
 29 FORMAT(82X,4HRAV=,F6.3,2X,4HKAV=,E10.3,//)
205 FORMAT(1H1)
206 FORMAT(55H                                                        )
 30 FORMAT(1X,I4,10X,E11.4,2X,F10.4)
 31 FORMAT(1X,F4.1,9X,F7.2,10X,I2,10X,A8,A1,7X,F5.2)
 32 FOPMAT(A8,1X,F8.4,2(2X,F8.4),3X,E10.3)
 36 IF(J.EQ.N)26,37
 37 JE1=J+1
    DO 38 JE=JE1,N
    READ 32,ID(JE),TLB(JE),TB(JE),TSAT(JE),EI(JE)
```

```
 38 CONTINUE
    GO TO 6
 35 CONTINUE
    END
    SUBROUTINE HEADING
    PRINT 1
  1 FORMAT(/1X,6HSYMBOL,6X,3HPPM,5X,9HDET LIMIT,3X,8HCOMMENTS,2X,
   C4HMASS,3X,3HTLB,4X,2HTB,5X,4HTSAT,4X,2HTL,4X,3HTLW,8X,1HR,13X,
   C1HK,9X,2HMF,6X,1HS,8X,2HEI/)
    END
    SUBROUTINE CALC K(R,TL,TSAT,EI,AI,KX)
    TYPE REAL KX
    IF(R.GT.1.25)1,2
  1 RX1=1.0/1.25
    GO TO 5
  2 IF(R.LT.1.0)3,4
  3 RX1=1.0
    GO TO 5
  4 RX1=1.0/R
  5 KX=((100.0-TL)/(TL-TSAT))**RX1/(AI*EI)
    END
    SUBROUTINE CALC TLW(R,TLB,TB,TSAT,TLW)
    IF(R.GT.1.25)1,2
  1 RX=1.25
    RX1=1/1.25
    GO TO 3
  2 RX=R
    RX1=1.0/R
  3 TS1=((100.0-TLB)/(TLB-TSAT))**RX1/2.0
    TS2=((100.0-TB)/(TB-TSAT))**RX1/2.0
    TS3=(TS1+TS2)**RX
    TLW=(100.0+TSAT*TS3)/(1.0+TS3)
    END
    SUBROUTINE CALC TL(TLB,TB,TSAT,TL)
    TS=(100.0-TLB)/(TLB-TSAT)-(100.0-TB)/(TB-TSAT)
    TL=(100.0+TSAT*TS)/(1.0+TS)
    END
    SUBROUTINE CALC R(TL1,TL2,AE1,AE2,TSAT1,TSAT2,R)
    R=LOGF((100.0-TL1)/(TL1-TSAT1)*(TL2-TSAT2)/(100.0-TL2))/
   CLOGF(AE1/AE2)
    END
```

Appendix B

SAMPLE PROGRAM OUTPUT

SAMPLE PROGRAM 5-50B KBR:KCL 8-10-67

SYMBOL	PPM	DET LIMIT	COMMENTS	MASS	TLB	TB	TSAT	TL	TLM	R	K	MF	S	EI
K	5.000+005	0.0705	REFERENCE	41	56.5	94.8	2.6	58.2	72.1	1.115	3.781+003	1.172	1.00	3.0-003
				41	27.1	91.2	2.6	27.7	43.1	1.171	3.569+003			1.0-002
				41	10.5	83.8	2.6	10.6	18.3	1.232	3.775+003			3.0-002
										RAV= 1.172	4.346+003			
CL	5.042+003	0.0052		35	53.5	97.3	2.6	54.2	70.1	1.120	3.965+001	1.105	1.00	3.0-002
				35	24.5	96.4	2.6	24.7	39.8	1.120	3.965+001			1.0-001
										RAV= 1.120	KAV= 4.383+001			
S	1.644-001	0.0148		10	94.8	96.6	2.6	98.1	95.7	1.388	2.321-003	0.542	1.00	1.0+002
				10	56.5	76.2	2.6	68.2	65.3	1.388	2.994-003			1.0+003
										RAV= 1.388	KAV= 1.429-003			
NA	5.912+001	0.0020		23	78.7	99.3	2.6	79.1	84.6	0.577	9.094-001	0.852	1.00	3.0-001
				23	65.3	99.3	2.6	65.6	73.6	0.577	5.463-001			1.0+000
										RAV= 0.577	KAV= 6.008-001			
B	6.084-002	0.0034		11	94.2	96.8	2.6	97.2	95.5	1.550	7.399-004	0.542	1.00	1.0+002
				11	43.9	77.3	2.6	50.0	56.8	1.550	1.386-003			1.0+003
										RAV= 1.550	KAV= 9.288-004			
FE	1.189+000	0.0081		56	58.3	81.3	2.6	67.1	68.5	1.372	6.362-003	1.452	1.00	1.0+002
				56	9.1	35.0	2.6	10.1	14.1	1.372	7.960-003			1.0+003
										RAV= 1.372	KAV= 1.033-002			
CU	8.097-001	0.0116		63	75.9	90.8	2.6	82.1	83.0	1.273	4.390-003	1.569	1.00	1.0+002
				63	17.9	47.5	2.6	21.3	26.2	1.273	4.582-003			1.0+003
										RAV= 1.273	KAV= 7.038-003			
SI	3.328+000	0.1041		29	34.3	72.4	2.6	38.9	47.5	1.659	3.219-002	0.961	1.00	1.0+003
				30	45.2	70.3	2.6	55.3	55.5	1.659	2.813-002			1.0+003
										RAV= 1.659	KAV= 2.892-002			
MN	2.925-001	0.0034		55	23.3	35.8	2.6	37.8	28.1	1.000	1.768-003	1.438	1.00	1.0+003
										RAV= 1.000	KAV= 2.542-003			
RB	2.166+000	0.0061	F ASSUMED	85	50.5	76.9	2.6	59.1	60.8	1.000	1.004-002	1.874	1.00	1.0+002
										RAV= 1.000	KAV= 1.083-002			

Appendix C

DATA CODING FORM

NOW-NRL-5230/6007 (5-66)

FORTRAN CODING FORM

PROGRAM | NAME

ROUTINE | DATE | PAGE OF

FORTRAN STATEMENT: 0 = ZERO, Ø = ALPHA O; 1 = ONE, I = ALPHA I; 2 = TWO, Z = ALPHA Z

TYPE	STATEMENT NO.	CONT.	FORTRAN STATEMENT	SEQUENCING NUMBER
			SAMPLE PROGRAM 5-50B KBr:KCl 8-10-67	1
	12		5.0000E+05 1000.0000	2
	1.0		39.10 3 REFERENCE 1.00	3
K		41	0.248 0.023 1.580 3.000E-03	4
K		41	0.567 0.040 1.580 1.000E-02	5
K		41	0.978 0.077 1.580 3.000E-02	6
	1.0		35.45 2 1.00	7
CL		25	0.272 0.012 1.580 3.000E-02	8
CL		25	0.611 0.016 1.580 1.000E-01	9
	1.0		10.81 2 1.00	10
B		10	0.023 0.015 1.580 1.000E+02	11
R		10	0.248 0.118 1.580 1.000E+03	12
	1.0		22.99 2 1.00	13
NA		23	0.104 0.003 1.580 3.000E+01	14
NA		23	0.185 0.003 1.580 1.000E+00	15
	1.0		10.81 2 1.00	16
B		11	0.026 0.014 1.580 1.000E+02	17
B		11	0.358 0.112 1.580 1.000E+03	18
	1.0		55.85 2 1.00	19
FE		56	0.234 0.090 1.580 1.000E+02	20
FE		56	1.040 0.465 1.580 1.000E+03	21
	1.0		63.54 2 1.00	22
CU		63	0.120 0.042 1.580 1.000E+02	23
CU		63	0.748 0.323 1.580 1.000E+03	24
	1.0		28.09 2 1.00	25
SI		29	0.465 0.140 1.580 1.000E+03	26
SI		30	0.354 0.153 1.580 1.000E+03	27
	1.0		54.94 1 1.00	28
MN		55	0.632 0.446 1.580 1.000E+03	29

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A COMPUTER PROGRAM FOR THE QUANTITATIVE INTERPRETATION OF MASS SPECTROGRAPHIC PHOTOPLATES

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5. AUTHOR(S) (First name, middle initial, last name)
Paul P. Bey and James G. Allard

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13. 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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