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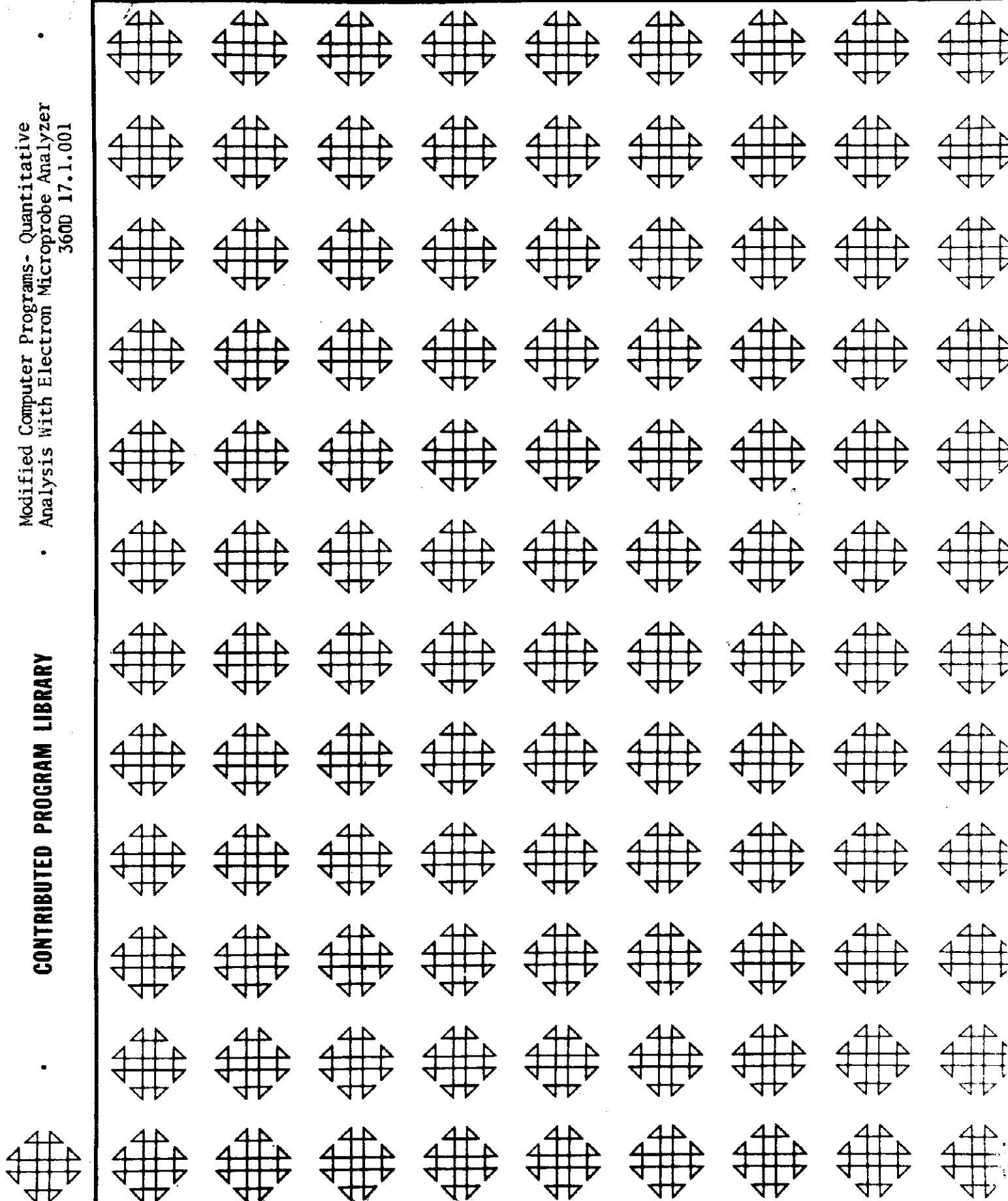
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Modified Computer Programs- Quantitative
Analysis With Electron Microprobe Analyzer
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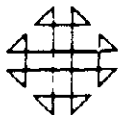
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- ① Program Order Number (to be filled in by PID) 360D-17.1.001
- ② System Type (machine) 3 6 0
- ③ Search Key ELECTRON MICROPROBE ANALYSIS WEIGHT FRACTION COMPOSITION
- ④ Programming Language FORTRAN 4
- ⑤ Author's Name and Address Dr. Samuel S. So
IBM Corporation
5600 Cottle Road
San Jose, CA 95193
- ⑥ Direct Inquiries to Name and Address (if different than Author) Same as above
- ⑦ Title of Program Quantitative Analysis With Electron Microprobe Analyzer
- ⑧ Submitter's User Group Affiliation Code and Installation Code S E L
- ⑨ Submitter's Own Program Identification and Suffix (optional) E P M P
- ⑩ Primary Subject Code 1 7 . 1
- ⑪ Secondary Subject Codes
- ⑫ Operating or Monitor System Required O S
- ⑬ New or Revision Code (if revision, show prior Program Order Number in item 1) N
- ⑭ Year Completed 6 8
- ⑮ Date of Submittal 0 8 2 6 6 8
- ⑯ Documentation (number of original pages submitted) 7 2
- ⑰ Abstract (should contain sufficient information for a reader to determine the value of the program). Listed on the reverse side of this form are subjects which may serve as a guide for a descriptive abstract.

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ABSTRACT

A DESCRIPTION OF TWO FORTRAN IV COMPUTER PROGRAMS IS PRESENTED TO SIMPLIFY QUANTITATIVE AND SEMIQUANTITATIVE ANALYSIS WITH THE ELECTRON MICROPROBE ANALYZER. THE FIRST PROGRAM, EPMP1, DETERMINES THE WEIGHT FRACTION OF EACH ELEMENT IN A SPECIMEN FROM THE CHARACTERISTIC X-RAY INTENSITY MEASUREMENTS OF THE SPECIMEN AND THE STANDARDS. THE SECOND PROGRAM, EPMP2, CALCULATES THE RELATIVE CHARACTERISTIC X-RAY INTENSITIES OF ALL THE ELEMENTS IN A SPECIMEN BY ASSUMING THE COMPOSITION OF THE SPECIMEN TO BE KNOWN. THE CORRECTION PROCEDURE INCLUDES DEAD TIME CORRECTION, ONE OF TWO BACKGROUND CORRECTIONS (EITHER CONSTANT BACKGROUND OR BACKGROUND DEPENDING ON COMPOSITION), PHILIBERT'S ABSORPTION CORRECTION MODIFIED BY DUNCUMB AND SHIELDS, ONE OF THREE FLUORESCENCE CORRECTIONS (EITHER BIRKS', CASTAING'S, OR REED'S), AND A COMPOUND STANDARD CORRECTION. THE EFFECTS OF THE ABSORPTION AND THE FLUORESCENCE OF EACH ELEMENT IN THE SPECIMEN ARE EASILY SEEN FROM THE OUTPUT RESULTS. VERSATILITY, EFFICIENCY, AND EASE OF OPERATION ARE EMPHASIZED IN THE PROGRAMS. PROGRAM LISTINGS, INPUT DATA FORMAT, AND VARIOUS EXAMPLES

(Please attach additional pages if necessary) Total pages attached 1

Signature of Submitter Samuel S. So Date 7/1/68
 Signature of Installation Addressee Alice U. Jones 7/3/68

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SHOWING THE USAGE OF THE PROGRAMS HAVE BEEN INCLUDED IN THE
APPENDICES. THE PROGRAMS OPERATE UNDER IBM S/360 OPERATING
SYSTEM WITH FORTRAN (LEVEL H) COMPILER AND REQUIRE A
MINIMUM CORE STORAGE OF 36K BYTES.

CARD DECK KEY

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Deck #1:	FORTAN IV Source Deck: Main Program
	Identification: E1 in cc 73-74
	Sequence 001 through 381 in cc 78-80
	FORTAN IV Source Deck: Subroutine
	Identification: CB in cc 73-74
	Sequence 001 through 197 in cc 78-80
	Total Cards: 488 Cards.
Deck #2:	Input Data for the three given examples
	Total Cards: 34 Cards
Deck #3:	FORTAN IV Source Deck: Main Program
	Identification: E2 in cc 73-74
	Sequence 001 through 223 in cc 78-80
	Total Cards: 223 Cards.
Deck #4:	Input data for the four given examples
	Total Cards: 40 Cards.
Job Control Cards Required:	
// JOB	
// EXEC FORTHCLG	
//FORT,SYSIN DD *	
Deck #1	
/*	
//GO,SYSIN DD *	
Deck #2	
/*	

ABSTRACT

A description of two FORTRAN IV computer programs is presented to simplify quantitative and semi-quantitative analysis with the electron microprobe analyzer. The first program, EPMP1, determines the weight fraction of each element in a specimen from the characteristic x-ray intensity measurements of the specimen and the standards. The second program, EPMP2, calculates the relative characteristic x-ray intensities of all the elements in a specimen by assuming the composition of the specimen to be known. The correction procedure includes dead time correction, one of two background corrections (either constant background or background depending on composition), Philibert's absorption correction modified by Duncumb and Shields, one of three fluorescence corrections (either Birks', Castaing's, or Reed's), and a compound standard correction. The effects of the absorption and the fluorescence of each element in the specimen are easily seen from the output results. Versatility, efficiency, and ease of operation are emphasized in the programs. Program listings, input data format, and various examples showing the usage of the programs have been included in the Appendices. The programs operate under IBM S/360 Operating System with fortran (level II) compiler and require a minimum core storage of 36K Bytes.

1. INTRODUCTION

Two FORTRAN IV computer programs have been written to facilitate quantitative and semi-quantitative analysis with the electron microprobe analyzer. The first program, EPMP1, calculates the weight fraction of each element in the specimen from the characteristic x-ray intensity measurements of the specimen and standards. The second program, EPMP2, which is essentially the inverse of the first program, calculates the relative characteristic x-ray intensities of all the elements in the specimen by assuming the composition of the specimen to be known.

Many correction procedures for electron microprobe analysis are available in literature (1-13). Each procedure has its merits and deficiencies, depending on the system being analyzed. Because of the complex, tedious, and time-consuming process of these correction procedures, computer techniques have been used to make proper correction for a more accurate quantitative analysis (14-18). The present programs include the following corrections: (a) dead time correction, (b) background correction (either constant background or background dependent on composition), (c) Philibert's absorption correction modified by Duncumb and Shields, (d) Birks', Castaing's, or Reed's fluorescence correction, and (e) compound standard correction. However,

there is no correction provided in the programs for the errors contributed by the following: (a) atomic number effect, (b) fluorescence excitation by the continuum, or (c) contamination of the specimen and the standards.

The programs emphasize versatility and ease of operation. The large combinations of input data indicate the flexibility of the programs; this flexibility allows use of experimental data from various commercial electron microprobes. Codes for the various corrections are provided to eliminate unnecessary input data and computations; these codes thus enhance the efficiency of the programs. Seven examples are included to illustrate these points.

II. Corrections to Experimental Data

The theory of electron microprobe analysis is based on relating the weight fraction of an element in a specimen to a ratio. This ratio is defined as the characteristic x-ray intensity generated in the specimen to that generated by a pure standard of the same element under the same experimental conditions. The characteristic x-ray intensity measured by the electron microprobe analyzer is affected by the following: finite resolving time of the detector, background x-ray spectrum, absorption of the emerging characteristic radiation in the specimen, and the fluorescence excitation by the characteristic radiations of other elements in the specimen. The program considers the previous effects in order to have an accurate quantitative analysis.

A. Dead Time Correction

Due to the finite resolving time of the detector, the measured x-ray intensity, I_M , is less than true intensity, I_T . If the dead time, DT , is known, the program will make a dead time correction for all measured x-ray intensities as given by:

$$I_T = \frac{I_M}{1 - I_M \cdot DT} \quad [1]$$

where DT is in microseconds. If no dead time correction is necessary, set $DT = 0$, and the program will bypass above calculation.

B. Background Intensity Correction

Two types of background intensity corrections are provided in the program, the constant background and the background depending on the composition. If the continuum x-ray intensity, I_B , is small compared with the measured characteristic intensity,

I_T (corrected for dead time), a constant background may be used. The corrected x-ray intensity for the i th element in a matrix or the i th standard element is simply given by

$$\begin{aligned} I_i &= I_T - I_B \\ I_{std} &= I_{T, std} - I_{B, std} \end{aligned} \quad [2]$$

However, for very small weight fractions (where the characteristic intensity approaches that of the continuum) the background intensity must be measured for each characteristic radiation and for each element in the specimen. Then the background intensity for the i th element is given by

$$(I_B)_i = \sum_j W_j I_{ji} \quad [3]$$

where W_j is the weight fraction of the j th element and I_{ji} is the background intensity of the i th element due to the j th element. The summation is carried over all the elements in the specimen.

C. Absorption Correction

The characteristic radiation is generated beneath the surface of the target and undergoes absorption when it emerges from the target before being detected by the spectrometer. Philibert's absorption correction (4), modified by Duncumb and Shields (11), is used in the program. The true weight fraction of the i th element in the specimen, with absorption correction, is given by

$$W_i = I_{rel} \left[\frac{F_{std}(x)}{F_i(x)} \right] \quad [4]$$

where the relative x-ray intensity, I_{rel} , is defined as the ratio of measured characteristic x-ray intensity from the

specimen to that of the standard (corrected for dead time and background)

$$I_{rel} = \frac{I_i}{I_{std}} \quad [5]$$

and $F_{std}(x)$ and $F_i(x)$ are the absorption correction factors for the standard and the specimen, respectively. The absorption correction parameter is given by

$$F(x) = \frac{1}{(1 + \frac{x}{\sigma}) \left[1 + h \left(1 + \frac{x}{\sigma} \right) \right]} \quad [6]$$

where

$$\chi = \cos \psi \cos \theta \sum_j \mu_{ij} W_j \quad [7]$$

$$h = 1.2 \frac{\sum_j A_j W_j}{\left[\sum_j Z_j W_j \right]^2} \quad [8]$$

$$\sigma = \frac{2.39 \times 10^5}{V^{1.5} - V_c} \quad [9]$$

with μ_{ij} as the mass absorption coefficient for characteristic radiation generated from the j th element absorbed by the i th element, ψ as x-ray emerging angle with respect to the surface of the target, θ as incident electron beam angle with respect to the normal of the target, A as the atomic weight, Z as the atomic number, V as the incident electron beam potential and V_c as the critical excitation potential. Note that the parameter χ has been modified to account for the inclination of the target to the electron beam.

D. Fluorescence Correction

When the characteristic radiation of the j th element is shorter in wavelength than the absorption edge of the i th

element, it is able to enhance the characteristic radiation of the i th element. The true weight fraction of the i th element in a specimen, with both absorption and fluorescence corrections, is then given by

$$W_i \cdot I_{rel} \left[\frac{F_{fd}(\lambda)}{F_i(\lambda)} \right] \left[\frac{1}{1+K_{fi}} \right] \quad [10]$$

where K_f is the fluorescence correction factor. Three methods are available in the program to calculate the fluorescence correction parameter, K_f .

Birks' equation (7) is given by

$$K_{fi} = 0.6 \sum_j E_{ij} W_j \left(\frac{\mu_{ij}}{\mu_j} \right) \left(\frac{V - V_{ci}}{V - V_{cj}} \right)^{1.65} \quad [11]$$

where E_{ij} is the excitation efficiency of the i th element by the characteristic radiation of the j th element, and μ_j is the mass absorption coefficient of the specimen for characteristic radiation generated from j th element.

Castaing's equation (1) is given by

$$K_{fi} = 0.5 \left(\frac{r_i - 1}{r_i} \right) \sum_{j \neq i} W_j \omega_j(\kappa) \left(\frac{\lambda_j}{\lambda_i} \right) \left(\frac{\mu_{ij}}{\mu_j} \right) \left(\frac{A_j}{A_i} \right) \cdot \left[\frac{1n(1+u)}{u} + \frac{1n(1+v)}{v} \right] \quad [12]$$

where

$$u = \left(\frac{\mu_i}{\mu_j} \right) \cos \psi \quad [13]$$

$$v = \left(\frac{\sigma}{\mu_j} \right) \sec \theta \quad [14]$$

with r_i as the absorption edge jump ratio (12), $\omega(\kappa)$ as the K-shell fluorescence yield (19), and λ as the characteristic wavelength.

Reed's equation (9) is a modified form of Castaing's equation; it considers all cases involving K and L characteristic radiations and may be written as

$$K_{fi} = 0.5 P_{mn} \left(\frac{r_i - 1}{r_i} \right) \sum_{j \neq i} W_j \omega_j(\kappa) \left(\frac{U_j - 1}{U_j - 1} \right)^{1.67} \cdot \left(\frac{\mu_{ij}}{\mu_j} \right) \left(\frac{A_j}{A_i} \right) \left[\frac{1n(1+u)}{u} + \frac{1n(1+v)}{v} \right] \quad [15]$$

where $P_{KK} = P_{LL} = 1$, $P_{KL} = 0.24$, $P_{LK} = 4.2$, and

$$U_i = \frac{V}{V_{ci}} \quad [16]$$

E. Compound Standard Correction

If a compound of known composition is used as a standard for the i th element instead of a pure standard, then the measured x-ray intensity of that element from the compound standard (I_{cs}) must be adjusted to be equivalent to the pure standard form (I_{std}). Namely,

$$I_{std} = \frac{I_{cs}}{\xi_i} \quad [17]$$

where the compound standard correction factor is calculated

$$\text{from } \xi_i = W_i \left[\frac{F_{fd}(\lambda)}{F_{cs}(\lambda)} \right] (1 + K_{fcs}) \quad [18]$$

to include both absorption and fluorescence effects of the compound standard.

III. BASIC OPERATIONS

A. Quantitative Analysis

The first program, EPIP1, calculates the weight fraction of each element in the specimen from the characteristic x-ray intensity measurements of the specimen and the standards. Figure 1 outlines the basic operation of EPIP1. Many features are built into the program to handle various situations in data compilation. Any number of problems can be analyzed in the same run of the program by simply stacking each set of input data one after another (see Appendix II). The program treats each set of input data as a separate analysis. However, in the analysis of system of specimens consisting of the same elements but different compositions, the standard intensity measurements may change from one specimen measurement to another because of the stability of the electron microprobe. In this case, the input data for the successive problems may be simplified by the continuation code. Other codes are provided for dead time, background, fluorescence, and compound standard corrections to enhance the efficiency of the program. If any of these correction are not necessary, then input data is not required for the correction and the program will bypass the execution of that correction.

The incident electron beam of variable energy may be inclined at any angle with respect to the target. The x-ray emerging angle may be varied from element to element in the

specimen. Each element in the specimen has its own compound standard code, so that any number of compound standards may be used as the standard of the specimen. The elements in the specimen may be analyzed in any order. Furthermore, if there is an uncertainty in any of the specimen x-ray intensity measurements, that intensity may be set to zero in the input data (see Appendix IIIA, example 1). The program will calculate the weight fractions of all other elements in the specimen and will set the remaining weight fraction in the specimen equal to the weight fraction of the uncertain element. This is the only case where the quantitative analysis will yield normalized weight fractions.

Note that the background (dependent on composition), absorption, fluorescence, and compound standard corrections are all dependent on the weight fractions of each element in the specimen. However, these weight fractions are the unknowns of the quantitative analysis. Therefore, the normalized relative x-ray intensities are taken as a first approximation for the weight fractions in calculating the correction terms. This is the only place where any normalization occurs in the iterative approximation. After having made the proper correction, the unnormalized weight fractions obtained from the previous approximation are then used to recalculate the correction terms for the successive approximations. This sets up the iterative procedure which is satisfied by either: (1) the successive approximations of the weight fractions do not change by more

than a specified error, ϵ , or (2) the specified number of iterations has been reached. In the latter case, a warning message will be printed out to indicate the slow convergence or the divergence of the iterative steps.

All input data are printed out for easy reference, and they also serve as a record of the problem analyzed. In the output data, the measured relative x-ray intensity and the unnormalized weight fractions (with absorption correction or with both absorption and fluorescence corrections) are printed out. From these values, the effect of the absorption and the fluorescence of each element in the analyzed system is clearly seen. The value of the total unnormalized weight fractions gives an indication of the accuracy of the experimental data.

B. Semiquantitative Analysis

The second program, EPMP2, is particularly useful in a quick semiquantitative analysis, especially for binary alloys. By assuming various combinations of the weight fractions of a specimen, this program calculates the relative x-ray intensity of each element in the specimen. Figure 2 outlines the basic operation of EPMP2. The correction procedure is the same as the first program, EPMP1, except no iterative approximation is necessary since the weight fractions of the specimen are assumed to be known. The calculated results may be plotted on a graph. Then, from the measured relative x-ray

intensity (taken with the electron microprobe analyzer), the graph directly gives the weight fraction of that element (See Figure 3). Furthermore, it gives an indication of the degree of accuracy of the x-ray intensity measurements by noting: (1) how near the measured relative intensities approximate a vertical line, or (2) how close the total measured relative x-ray intensity compared with the total calculated relative x-ray intensity.

Examples

Table I and Figure 3 are included to illustrate quantitative and semiquantitative analysis with the electron microprobe analyzer on a system of FeNi alloys over a wide range of compositions. The data used in each alloy correspond to the averaged values of three different locations on the alloy, with ten consecutive measurements over each location. The measured relative intensities (in percent) of Table I are calculated by Equation [5].

By assuming various combinations of weight fractions of Fe and Ni, the relative characteristic x-ray intensities are calculated by EPMP2. These results are plotted on a graph as shown in Figure 3. Using the values of measured, relative, characteristic x-ray intensities from Table I (column 3), Figure 3 directly yields the weight fractions which are shown in column 4 of Table I. This gives a quick semiquantitative analysis of FeNi alloys. If more accurate results are required, the raw data from the electron microprobe analyzer measurements can be fed into EPMP1. Since three methods of fluorescence correction are available in the program, the differences between Birks', Castaing's, and Reed's equations are easily detected by comparing their results as shown in columns 5, 6, and 7 of Table I. The weight fractions of the FeNi alloys were determined by chemical analysis, and listed in column 8 of Table I.

By comparing column 4 of Table I with columns 5, 6, and 7, one can see that the results of EPMP2 are a good approximation to the quantitative analysis. Furthermore, by comparing columns 5, 6, and 7, one should note that the fluorescence corrections by Birks', Castaing's, and Reed's equations differ more significantly for small weight fraction of Fe but tend to agree for larger weight fraction of Fe.

One way to check the accuracy of the iterative approximation of EPMP1 is to use the output from EPMP2 as the input of EPMP1. Then by comparing the output from EPMP1 with the original input to EPMP2, the difference gives a direct indication of the accuracy of the iterative approximation used in EPMP1. Table II illustrates this check with a system of PCu alloys. Nine sets of weight fractions of P and Cu are assumed and used in the input data to EPMP2. The relative characteristic x-ray intensities calculated by EPMP2 are then used as the input data to EPMP1. The weight fractions calculated by EPMP1 may be compared with the original assumed weight fractions. The difference, less than $\pm 0.03\%$, is the error of the iterative approximation of the EPMP1.

Similarly, the uncertainty in any parameter of the correction procedure may be detected by varying that parameter. By comparing the output results, one gets an indication of the resultant effect on the quantitative analysis due to that particular parameter.

Examples 1 to 3 in Appendix II illustrate the usage of the EPMP1 program, while examples 4 to 7 illustrate that of the EPMP2 program. Example 1 shows the normal run of FeNi binary alloys. The output data are slightly different from those of Table I, since different value of k has been imposed. Data set numbers 2 and 4 show that the

results obtained by the uncertainty of one element (Fe in this case) agree closely with those of data set numbers 1 and 3, respectively, where intensity measurements on both elements have been used.

Examples 2 and 3 illustrate the usage of the continuation code for different number of sets of specimen intensities and different fluorescence correction methods. Results from these three examples can be compared to see the variation of the fluorescence correction methods.

Similarly, examples 4, 5, and 6 illustrate the different input data required. Example 7 is the same as example 4, except that the order of input element cards have been reversed. User should compare the differences in the input data format, even though the output results from these two examples are obviously the same.

All computations for this work were performed on the IBM S/360 Model 65 with the Operating System Fortran (Level H) Compiler. The first three examples were under the same run of EPMP1 program. The total compiling and execution time is 1.16 minutes. Similarly, the last four examples of EPMP2 program took only 0.75 minute.

TABLE I. QUANTITATIVE ANALYSIS OF FeNi ALLOYS

SET		Measured Relative Intensity %	EPMP2 Weight Fraction	EPMP1 Weight Fraction ^a	EPMP1 Weight Fraction ^b	EPMP1 Weight Fraction ^c	Chemical Analysis*
							Weight Fraction
I	Fe	14.06	0.105	0.09810	0.10005	0.10607	0.106
	Ni	86.28	0.895	0.88945	0.88988	0.89125	0.888
	Total	100.34	1.000	0.98755	0.98993	0.99732	0.994
II	Fe	43.42	0.375	0.37907	0.36623	0.37804	0.370
	Ni	54.32	0.610	0.60810	0.60635	0.60799	0.628
	Total	97.74	0.985	0.98717	0.97258	0.98603	0.998
III	Fe	49.42	0.435	0.44155	0.42675	0.43862	0.437
	Ni	48.92	0.555	0.55706	0.55525	0.55674	0.564
	Total	98.34	0.990	0.99861	0.98200	0.99536	1.001
IV	Fe	95.00	0.940	0.94693	0.94484	0.94590	0.939
	Ni	2.51	0.030	0.03278	0.03278	0.03278	0.051
	Total	97.51	0.970	0.97971	0.97762	0.97868	0.990

^aBirks' fluorescence correction.

^bCastaing's fluorescence correction.

^cReed's fluorescence correction.

*G. Fisher, INCO.

TABLE II.

Correlation of Relative Intensities Calculated From Weight Fractions
by EPMP2 and Weight fractions Calculated From These Intensities by EPMP1

SET	Input to EPMP2 Weight Fractions		Output from EPMP2 = Input to EPMP1		Output From EPMP1	
			Relative Intensity (%) *		Weight Fractions*	
	P	Cu	P	Cu	P	Cu
1	0.1	0.9	3.71182	89.45734	0.10001	0.90000
2	0.2	0.8	7.99170	79.00667	0.20002	0.79999
3	0.3	0.7	12.97807	68.65514	0.30005	0.69999
4	0.4	0.6	18.85751	58.41150	0.40008	0.59999
5	0.5	0.5	25.88731	48.28600	0.50011	0.49999
6	0.6	0.4	34.43199	38.29140	0.59999	0.40000
7	0.7	0.3	45.02460	28.44341	0.70012	0.29999
8	0.8	0.2	58.47522	18.76149	0.80007	0.20000
9	0.9	0.1	76.07399	9.27002	0.89999	0.10000

*Modified Philibert's absorption correction and Reed's fluorescence correction.

V. Conclusions

Two FORTRAN IV computer programs have been used to facilitate quantitative and semi-quantitative analysis with the electron microprobe analyzer. These programs emphasize versatility, efficiency, and ease of operation. A primary advantage of these programs is the freedom of the user to utilize many alternative forms of correction to coincide with the data available.

The efficiency of the programs is enhanced by the codes provided, so that unnecessary input data and computations are eliminated. All input data are printed out for easy reference, and they also serve as a record of the problem analyzed. From the output results, the effect of the absorption and the fluorescence of each element in the analyzed system is clearly indicated.

The over-all accuracy of the quantitative and the semiquantitative analysis with the electron microprobe analyzer is still limited by many factors. It not only depends on the system of elements being analyzed, but also depends on the correction procedures, the uncertainty in their parameter values, and the over-all experimental error. As better theories for the electron microprobe analysis are developed, the present programs can be easily modified to give more accurate results.

VI. ACKNOWLEDGMENTS

The authors wish to thank Mr. H. R. MacQueen for experimental data measurements; Metropolitan New York Section of the Electron Probe Analysis Society of America for supplying the FeNi specimens and the wet chemistry data on them.

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APPENDIX I

PROGRAM LISTINGS
(with data)


```

153 FORMAT (140,10X,20H LEARNED COEFFICIENTS //)
DO 155 I = 1,NC
WRITE (6,123) SYMBO(I),SIGMA(I)
155 CONTINUE
C ***** COMPOUND STANDARD CORRECTION *****
C *****
16 DO 24 I = 1,NC
NCTO(I) = CTGO(I)
IF (NCTO(I) 23,23,17
17 CALL COMPOST (I,CSC,SIGMA,FSTD,PSI,ARC,THETA,V,STOCC)
22 PSI(I) = PSI(I) / STOCC(I)
PS2(I) = PS2(I) / STOCC(I)
PO1(I) = PSI(I) - PS2(I)
23 CONTINUE
C *****
C ***** INITIALIZATION FOR THE ITERATIVE APPROXIMATION *****
C *****
N = 0
ANC = NC
ANS = NS
25 N = N + 1
AN = N
NTTN = 0
KR = 0
SRINT = 0.0
C ***** CALCULATE THE RELATIVE INTENSITY *****
C *****
DO 26 I = 1,NC
AT = 1
FAC = (AN+ANC-AT) / (ANC+ANS)
RINT(I) = (SINT(N,I)-SR(I))*MDI(I)*FAC)/(PS1(I)-PO1(I)*FAC)
IF (RINT(I) 26,26,255
255 SRINT = SRINT + RINT(I)
26 CONTINUE
DO 31 I = 1,NC
IF (PRINT(I) 29,29,31
29 RINT(I) = 1.0 - SRINT
KR = 1
DO 30 J = 1,NC
CONC(J) = RINT(J)
GO TO 325
31 CONTINUE
32 FAC = 1.0 / SRINT
DO 33 I = 1,NC
CONC(I) = RINT(I) * FAC
33 CONTINUE
335 IF (INTI 58,58,34
C *****
C ***** BACKGROUND DEPENDS ON COMPOSITION *****
C *****
34 IF (NRKCD) 43,43,35
39 SR3(I) = 0.0
SR4(I) = 0.0
DO 40 J = 1,NC
SR3(I) = SR3(I) + CONC(J)*BK1(I,J,I)

```

29

```

GO TO (136,131,134,134), NCTO
131 WRITE (6,132) (SYMBO(I),I=1,NC)
132 FORMAT (140,10X,20H EXCITATION EFFICIENCY FAB // 8X,4(18X,A2))
DO 133 I = 1,NC
133 WRITE (6,123) SYMBO(I),(EAR(I,J),J=1,NC)
GO TO 136
134 WRITE (6,135) (SYMBO(I),ML(I),RK(I),WK(I),I=1,NC)
135 FORMAT (140,4X,A2,10X,20H CHARACTERISTIC WAVELENGTH = F6.2, 10X,
1 18H ABS. JUMP RATIO = F8.4,10X,21H FLUORESCENCE YIELD =
2 F7.3 )
1352 WRITE (6,1354)
1354 FORMAT (140,10X,13H ALPHA MATRIX //)
DO 1358 I = 1,NC
1356 WRITE (6,1356) (ALPHA(I,J),J=1,NC)
1358 CONTINUE
136 IF (NRKCD) 140,140,137
137 DO 138 I = 1,NC
138 WRITE (6,130) (RK1(I,J),J=1,NC)
138 WRITE (6,130) (RK2(I,J),J=1,NC)
C *****
C ***** DEAD TIME CORRECTION *****
C *****
DO 145 I = 1,NC
140 IF (DT(I)) 145,145,141
141 SPI(I) = SPI(I)/(1.0-(SPI(I)*DT(I))/L.E6))
SPF(I) = SPF(I)/(1.0-(SPF(I)*DT(I))/L.E6))
SRI(I) = SRI(I)/(1.0-(SRI(I)*DT(I))/L.E6))
SRF(I) = SRF(I)/(1.0-(SRF(I)*DT(I))/L.E6))
DO 142 J = 1,NS
SINT(I,J) = SINT(I,J)/(1.0-(SINT(I,J)*DT(I))/L.E6))
142 CONTINUE
143 IF (NRKCD) 145,145,143
DO 144 J = 1,NC
RK1(I,J) = RK1(I,J)/(1.0-(RK1(I,J)*DT(I))/L.E6))
RK2(I,J) = RK2(I,J)/(1.0-(RK2(I,J)*DT(I))/L.E6))
144 CONTINUE
145 CONTINUE
C *****
C ***** STANDARD INTENSITY WITH BACKGROUND CORRECTION *****
C *****
NCC = NC - 1
DO 15 I = 1,NC
PS1(I) = SPI(I) - SRI(I)
PS2(I) = SPF(I) - SRF(I)
PO1(I) = PSI(I) - PS2(I)
PO2(I) = PSI(I) - SRI(I)
15 DO1(I) = SRI(I) - SRF(I)
C *****
C ***** CALCULATE FICHI OF EACH STANDARD ELEMENT *****
C *****
DO 151 I = 1,NC
CSC(I) = COS(THETA/57.2958) / SIN(PSI(I)/57.2958)
CHI = ARC(I,I) * CSC(I)
H = 1.2 * ATMT(I) / (ATNO(I)**2)
SIGMA(I) = 2.39E5 / (V**1.5 - VC(I)**1.5)
FSTD(I) = 1.0/(1.0+CHI/SIGMA(I))*1.0+H*(1.0+CHI/SIGMA(I)))
151 CONTINUE
WRITE (6,153)

```

28

```

40 SR4(I) = SR4(I) + CONC(J)*RK2(J,I)
   RD2(I) = SR3(I) - SR4(I)
   AT = T
   FAC = (AN+ANC-AI) / (ANC+ANS)
41 RINT(I) = (SINT(N,I)-SR3(I)+RD2(I)*FAC)/(PSI(I)-PCI(I)*FAC)
   DO 422 I = 1,NC
   IF (RINT(I)) 42,42,422
42 SR = 0.0
   RK = T
   DO 421 J = 1,NC
   IF (KK - J) 420,421,420
420 SR = SR + RINT(I)
421 CONTINUE
   RINT(I) = 1.0 - SR
422 CONTINUE
43 ***** WEIGHT FRACTIONS (ABSORPTION CORRECTION ONLY) *****
   *****
   NITN = NITN + 1
   DO 44 J = 1,NC
   ABSAM(J) = 0.0
   DO 44 K = 1,NC
   ABSAM(J) = ABSAM(J) + CONC(K) * ABC(K,J)
44 CONTINUE
   ATNS = 0.0
   ATMS = 0.0
   DO 45 K = 1,NC
   ATNS = ATNS + ATND(K) * CONC(K)
   ATMS = ATMS + ATWT(K) * CONC(K)
   H = 1.2 * ATMS / (ATNS**2)
   DO 45 I = 1,NC
   CHIS = ABSAM(I) * CSC(I)
   FSAM(I) = 1.0/(1.0+CHIS/SIGMA(I))+1.0+H*(1.0+CHIS/SIGMA(I))
   CON(I) = RINT(I) * FSTD(I) / FSAM(I)
455 CONTINUE
   *****
   ***** FLUORESCENCE CORRECTION *****
   *****
   GO TO (51,46,48,49), NPLCD
   *****
   ***** RIRKS* FLUORESCENCE CORRECTION *****
   *****
   DO 47 I = 1,NC
   FCT(I) = 0.0
   DO 47 J = 1,NC
   FCT(I) = FCT(I) + 0.6*EAB(I,J)*CONC(J)*(ARC(I,J)/ABSAM(J))
   1 * (V-VC(J))*1.65/(IV-VC(I))*1.65)
47 CONTINUE
   GO TO 50
   *****
   ***** CASTAING'S FLUORESCENCE CORRECTION *****
   *****
   DO 48 I = 1,NC
   FCT(I) = 0.0
   DO 48 J = 1,NC
   IF (I - J) 482,485,482
   UU = ABSAM(I) / (ABSAM(J)*SIN(PSI(I)/57.2958))
   FCT(I) = FCT(I) + 0.5* CONC(J) * (ARC(I,J)*WK(J)*WL(J)
   1 / (UU+ALOG(1.0+VV)/VV) * ALPHA(I,J)
   *****
   ***** DEFIN'S FLUORESCENCE CORRECTION *****
   *****
   GO TO 50
   *****
   DO 49 I = 1,NC
   FCT(I) = 0.0
   DO 49 J = 1,NC
   UU = ABSAM(I) / (ABSAM(J)*SIN(PSI(I)/57.2958))
   VV = SIGMA(I) / (ABSAM(J)*COS(THETA/57.2958))
   FCT(I) = FCT(I) + 0.5* CONC(J) * ((RK(I)-1.0)/RK(I))*WK(J)
   1 * ((V/VV(I)-1.0)/(V/VV(I)-1.0))*ALOG(1.0+UU)/UU+ALCC(1.0+VV)/VV)
   2 * ((ATWT(I)/ATWT(J))*ALOG(1.0+LU)/LU+ALCC(1.0+VV)/VV)
   3 * ALPHA(I,J)
495 CONTINUE
   *****
   ***** WEIGHT FRACTIONS (ABSORPTION AND FLUORESCENCE CORRECTIONS) *****
   *****
   DO 50 I = 1,NC
   CON2(I) = CON(I) * FSTD(I) / (1.0 + FCT(I)) * FSAM(I)
50 CONTINUE
   SI SUMC1 = 0.0
   SUMC2 = 0.0
   DO 51 I = 1,NC
   IF (KK - I) 516,513,516
513 SCNA4 = 0.0
   SCNA5 = 0.0
   DO 515 J = 1,NC
   IF (KK - J) 514,515,514
514 SCNA4 = SCNA4 + CON2(J)
   SCNA5 = SCNA5 + CON2(J)
515 CONTINUE
   CON(I) = 1.0 - SCNA4
   CON2(I) = 1.0 - SCNA5
516 SUMC1 = SUMC1 + CON1(I)
   SUMC2 = SUMC2 + CON2(I)
517 CONTINUE
   GO TO 62
   *****
   ***** OUTPUT DATA *****
   *****
   58 IF (N - 1) 592,591,593
591 WRITE (A,592)
592 FORMAT (I4,4X,2X) ***** OUTPUT DATA ***** / / / /
593 WRITE (A,60) N,(SYMBOL(I),I=1,NC)
60 FORMAT (I40, 20H***** DATA SET NUMBER,13,5H ***** ,36X,
   1 4H SUM,4(13X,A2))
   SUMIN = 0.0
   DO 605 J = 1,NC
   RFLINT(J) = RINT(J) * 100.0
   SUMIN = SUMIN + RFLINT(J)
605 WRITE (A,61) SUMIN,RFLINT(J),J=1,NC)
61 FORMAT (I40, 24H MEASURED REL. INTENSITIES,29X,5F15.5 //)
   GO TO 34

```



```

30 CONTINUE
H = 1.2 * AATWT / (AATNO**2)
CHIS = AABSC(NPOST) * CSC(I)
CSFCHI = 1.0 / ((1.0 + CHIS / SIGMA(I)))
STDCHI = CSFCHI / F100A(I)

C **** FLUORESCENCE CORRECTION ****
C ****
IF (NCSFCD) 50,5C,40
DO 44 J = 1,NELT
CSECT(J) = 0.
DO 44 K = 1,NELT
CSUV = AABSC(J) / (AABSC(K)*SIN(PSI(I)/57.2958))
CSVV = SIGMA(I) / (AABSC(K)*COS(THETA / 57.2958))
CSECT(J) = CSFCHI * (0.5 * CSUV * ((CSRK(J)-1.1) / CSVK(J)) * CSWK(K) *
1 ((V/CSVK(K)-1.1) / (V/CSVK(J)-1.1)) * 1.67 * (CSAPS(J,K) /
2 AABSC(K)) * (CSATWT(J) / CSATWT(K)) * (ALOG(1.0 + CSUV) / CSUV
3 + ALOG(1.0 + CSVV) / CSVV) * BETAJ,K)

44 CONTINUE
STDCHI = STDCHI * (1.0 + CSECT(NPOST))

C ****
C **** OUTPUT DATA ****
C ****
50 WRITE (6,52)
52 FORMAT (1H1,45X,28H **** COMPOUND STANDARD **** //)
WRITE (6,54) NELT,NPOST,NCSFCD,(CSATND(J),CSATWT(J),CSVC(J),
1 J = 1,NELT)
54 FORMAT (11X,18H NO. OF ELEMENTS =,13//11X,31H POSITION OF STANDARD
1 ELEMENT =,13 //11X,58H CODE FOR COMPOUND STANDARD WITH FLUORESCEN
2CE CORRECTION =,13 // 13F20.5))
WRITE (6,56)
56 FORMAT (1H0,10X,29H MASS ABSORPTION COEFFICIENTS //)
DO 60 J = 1,NELT
WRITE (6,58) (CSAPS(J,K),K=1,NELT)
58 FORMAT (5F15.3)
60 CONTINUE
IF (NCSFCD) 72,72,62
62 WRITE (6,64) (CSHL(J),CSRK(J),CSWK(J),J=1,NELT)
64 FORMAT (1H0,10X,13H WAVELENGTH =,F8.3,10X,29H ABSORPTION EDGE JUMP
1 RATIO =,F8.4,10X,21H FLUORESCENCE YIELD =,F8.4)
WRITE (6,66)
66 FORMAT (1H0,10X,12H BETA MATRIX //)
DO 70 J = 1,NELT
WRITE (6,68) (BETA(J,K),K=1,NELT)
68 FORMAT (8F15.3)
70 CONTINUE
72 WRITE (6,74) 1,STDCHI
74 FORMAT (1H0,10X,15H ELEMENT NUMBER,13,10X,38H COMPOUND STANDARD CO
1RRECTION FACTOR =,F10.5 //)
RETURN
END

```

```

INPUT1 NCONT=0, NPROB=1, NC=2, NS=6, NFLCD=4, NBKCD=0, V=30.0, THETA=27.5,
EPSLN=0.05, ITERAN=20 END

PE 26.0 55.85 7.1 35.0 0.0 0.0
NI 28.0 58.71 8.3 35.0 0.0 0.0
71.4 379.6
90.0 58.9
100.0 0.0 100.0 0.0
100.0 0.0 100.0 0.0
14.06 86.28
0.0 86.28
43.42 54.32
0.0 54.32
49.42 48.92
95.0 2.51
1.93 8.09976 0.28
1.66 7.7521 0.37
0.0 1.0
0.0 0.0

INPUT1 NCONT=1, NPROB=2, NC=2, NS=4, NFLCD=3, NBKCD=0, V=30.0, THETA=27.5,
EPSLN=0.05, ITERAN=20 END

100.0 0.0 100.0 0.0
100.0 0.0 100.0 0.0
14.06 86.28
43.42 54.32
49.42 48.92

```



```

      FCT(I) = FCT(I) + 0.5*WTFN(L,J)*(RK(I)-1.0)/RK(I)*WK(J)*IWL(J)
      /W(L,I))*(ABSC(I,J)/SABSC(I,J))*(ATW(I)/ATW(J))*(ALOG(I.0+
      (UJ)/UU+ALOG(1.0+VV)/VV) + ALPHA(I,J)
100 CONTINUE
      GO TO 18
C ***** REFLECTANCE CORRECTION *****
C *****
17 DO 175 I = 1,NCOMP
   FCT(I) = 0.0
   DO 175 J = 1,NCOMP
     IF (I - J) 172,175, 172
     UU = SABSC(I) / (SABSC(J)*SIN(PSI(I)/57.2958))
     VV = SIGMA(I) / (SABSC(J)*COS(THETA/57.2958))
     FCT(I) = FCT(I) + 0.5*WTFN(L,J)*(IRK(I)-1.0)/RK(I)*WK(J)
172 * (VV/VV(J))-1.0)/(V/V(J))-1.0)*1.67*1ARSCC(I,J)/SABSC(J)
175 * (ATW(I)/ATW(J))*(ALOG(1.0+UU)/UU+ALOG(1.0+VV)/VV)
      * ALPHA(I,J)
175 CONTINUE
C ***** CALCULATE MEASURED RELATIVE X-RAY INTENSITIES *****
C *****
18 SRIN1 = 0.0
   SRIN2 = 0.0
   SWTET = 0.0
   DO 24 I = 1,NCOMP
     RINT1(I) = WTFN(L,I) * FA(I) * 100.0 / FLOODA(I)
     RINT2(I) = WTFN(L,I) * (1.0+FCT(I)) * FA(I) * 100.0 / FLOODA(I)
23 SRIN1 = SRIN1 + RINT1(I)
   SRIN2 = SRIN2 + RINT2(I)
   SWTET = SWTET + WTFN(L,I)
24 CONTINUE
C ***** OUTPUT *****
C *****
      IF (I - 1) 25,25,38
25 WRITE (6,26) NPROB,NCOMP,NSPOT,THETA,V,NELCO
26 FORMAT (I1,4X,I5H PROBLEM NUMBER,16//45X,21H ***** INPUT DATA *****
      // 10X,23H NUMBER OF COMPONENTS = 14 // 10X,
27 37H NUMBER OF SETS OF WEIGHT FRACTIONS = 14 // 10X,
28 31H INCIDENT ELECTRON BEAM ANGLE = F6.2 //
29 10X,24H ELECTRON BEAM VOLTAGE = F6.2 // 10X,
30 31H FLUORESCENCE CORRECTION CODE = 13 // 1
      WRITE (6,27)
27 FORMAT (1H0,17X,9H AT. NO. ,11X,9H AT. WT. , 9X,18H Y.O. ANGLE,
      9X,11H CR.EX.PNT.,11X,6H SIGMA)
1 WRITE (6,28) (SYMBOL(I),ATW(I),ATW(J),PSI(I),VC(I),SIGMA(I),
      I=1,NCOMP)
28 FORMAT (2X,A2,5F20.3)
29 WRITE (6,29) (SYMBOL(I),I=1,NCOMP)
30 FORMAT (1H0,10X,20H MASS ABSORPTION COEFFICIENTS // 3X,
      6(18X,A2) //)
      DO 31 I = 1,NCOMP
31 WRITE (6,30) SYMBOL(I),1ARSCC(I,J),J=1,NCOMP)
32 FORMAT (3X,A2,5F20.3)
32 CONTINUE
32 WRITE (6,32) (SYMBOL(I),I=1,NCOMP)
32 FORMAT (1H0,10X,23H WEIGHT FRACTION OF EACH ELEMENT // 2X,6(18X,

```

```

1      A2) //)
DO 33 I = 1, NSPOT
  WRITE (6,333) I, (WRITEIN(I,J), J=1, NCOMP)
  FORMAT (15, 6F20.5)
333  CONTINUE
34  WRITE (6,342) (SYMBOL(I), I=1, NCOMP)
  FORMAT (1H0, 10X, 37H CRITICAL EXCITATION POTENTIALS IN KV //
    (3X, A2, F20.5 //))
342  GO TO (36, 343, 35, 35), NFLCD
343  WRITE (6,344) (SYMBOL(I), I=1, NCOMP)
  FORMAT (1H0, 10X, 22H EXCITATION EFFICIENCY // 3X, 6(18X, A2) //)
344  DO 346 I = 1, NCOMP
  WRITE (6,30) SYMBOL(I), (EAR(I,J), J=1, NCOMP)
346  CONTINUE
  GO TO 36
35  WRITE (6,351) (SYMBOL(I), I=1, NCOMP)
  FORMAT (1H0, 2X, A2, 6X, 13H WAVELENGTH = F8.3, 10X,
    18H ABS. JUMP RATIO = F8.3, 10X, 15H FLUOR. YIELD = F8.5 //)
351  GO TO 36
352  WRITE (6,352)
  FORMAT (1H0, 10X, 13H ALPHA MATRIX //)
353  DO 354 I = 1, NCOMP
  WRITE (6,353) (ALPHA(I,J), J=1, NCOMP)
  FORMAT (8F15.3)
354  CONTINUE
355  WRITE (6,37)
  FORMAT (1H1, 44X, 22H *** OUTPUT DATA *** //)
356  WRITE (6,39) I, (SYMBOL(I), I=1, NCOMP)
  FORMAT (1H0, 44X, 21H *** DATA SET NUMBER, I3, 5H *** // 63X,
    4H SUM, 4(13X, A2) // 37X, 6(13X, A2) //)
357  WRITE (6,46) SWFT, (WFTIN(I), I=1, NCOMP)
  FORMAT (1H0, 17H WEIGHT FRACTIONS, 38X, 5F15.5 // 40X, 6F15.5 //)
358  WRITE (6,47) SRIN1, (RINT1(I), I=1, NCOMP)
  FORMAT (1H0, 27H REL. INT. (ABS. COR. ONLY), 28X, 5F15.5 // 40X,
    6F15.5 //)
359  GO TO (60, 50, 52, 54), NFLCD
360  WRITE (6,51) SRIN2, (RINT2(I), I=1, NCOMP)
  FORMAT (1H0, 45H REL. INT. (ABS. COR. AND BIRKS' FLUOR. COR.), 10X,
    5F15.5 // 40X, 6F15.5 //)
361  GO TO 60
362  WRITE (6,53) SRIN2, (RINT2(I), I=1, NCOMP)
  FORMAT (1H0, 49H REL. INT. (ABS. COR. AND CASTAING'S FLUOR. COR.),
    6X, 5F15.5 // 40X, 6F15.5 //)
363  GO TO 60
364  WRITE (6,55) SRIN2, (RINT2(I), I=1, NCOMP)
  FORMAT (1H0, 45H REL. INT. (ABS. COR. AND REED'S FLUOR. COR.), 10X,
    5F15.5 // 40X, 6F15.5 //)
365  CONTINUE
  GO TO 1
END

```

40

41

```

&INPUT1 NCONT=0, NPROB=4, NCOMP=2, NSPOT=5, NFLCD=4, V=30.0, THETA=27.5  &END

PE      26.0      55.85      7.1      35.0
NI      28.0      58.71      8.3      35.0
71.4    379.6
90.0     58.9
0.1      0.9
0.3      0.7
0.5      0.5
0.7      0.3
0.9      0.1
1.93     8.09976  0.28
1.66     7.7521  0.37
0.0      1.0
0.0      0.0

&INPUT1 NCONT=1, NPROB=5, NCOMP=2, NSPOT=4, NFLCD=3, V=30.0, THETA=27.5  &END

0.2      0.8
0.4      0.6
0.6      0.4
0.8      0.2
1.93     8.09976  0.28
1.66     7.7521  0.37
0.0      1.0
0.0      0.0

&INPUT1 NCONT=-1, NPROB=6, NCOMP=2, NSPOT=4, NFLCD=2, V=30.0, THETA=27.5  &END

0.0      0.215

```

```

0.0      0.0
$INPUT1 NCONT=0, NPROB=7, NCOMP=2, NSPOT=5, NFLCD=4, V=30.0, THETA=27.5 $END
NI      28.0      58.71      8.3      35.0
PE      26.0      55.85      7.1      35.0
58.9
379.6
0.9      0.1
0.7      0.3
0.5      0.5
0.3      0.7
0.1      0.9
1.66     7.7521     0.37
1.93     8.09976    0.28
0.0
1.0

```

APPENDIX II

INPUT DATA FORMAT

A. EMP1

B. EMP2

APPENDIX IIA

EPMPI INPUT DATA FORMAT

A. Control Card: 1 card. Format: Namelist

```

2      8 10
&INPUT1 NCONT=0,NPROB=1,NC=2,NS=4,NFLCD=4,NBKCD=0,V=30.0,THETA=27.5,
&PSILN=0.005,ITERAN=20  &END

```

NCONT = continuation code: - 0 - start a new problem

- 1 - continue with new sets of x-ray intensities

- -1 - continue with new fluorescence correction

NPROB = problem number

NC = number of components or elements in the specimen

NS = number of sets of specimen intensities

NFLCD = fluorescence correction code:

- 1 - no fluorescence correction

- 2 - Birks' method

- 3 - Castaing's method

- 4 - Reed's method

NBKCD = background correction code:

- 0 - constant background

- 1 - background depends on composition

V = electron beam potential in kv

THETA = electron beam incidence angle

PSILN = maximum allowable difference between successive approximation

ITERAN = maximum number of iterations

B. Element Cards: NC cards. Format (2X,A2,6X,6F10.3)

CARDS	SYMBOL	ATNO	ATWT	VC	PSI	CTCD	DT
i=1	Fe	26.0	55.85	7.1	35.0	0.0	0.0
i=2	Ni	28.0	58.71	8.3	35.0	0.0	0.0

i = 1, NC

SYMBOL = One or two characters, symbol of the element

ATNO = atomic number

ATWT = atomic weight

CTCD = compound standard code: - 0 - pure standard

- 1 - compound standard

DT = dead time in microseconds

PSI = x-ray emerging angle with respect to surface of the target

VC = critical excitation potential in kv

NOTE: The order in which the element cards are read in is very important. Although these cards may be arranged in any order in this section (such as that of the intensity measurements) the order for the rest of the input data must follow the same order as that of the element cards in the form of a matrix. All symbols beginning with V or T have fixed-point format and must be right justified in their fields. Other symbols are in the floating-point format.

C. Mass Absorption Coefficients matrix: NC cards. Format (7F10.3)

	j=1		j=2	
Cards	1	10	11	20
i=1	71.4		379.6	
i=2	90.0		58.9	

Absorber: i=1,NC
Emitter: j=1,NC

D. Standard Intensities: NC cards. Format (4F10.3)

	SPI	SBI	SPF	SBF
Cards	1	10	11	20
i=1	100.0	0.0	100.0	0.0
i=2	100.0	0.0	100.0	0.0

SPI = standard initial peak intensity

SBI = standard initial background intensity

SPP = standard final peak intensity

SBF = standard final background intensity

NOTE: If drift correction is not required, the final standard intensities must be set equal to the initial standard intensities. If all the input intensities have been corrected for background, then set the background intensities (initial and final) to be zero.

E. Specimen Intensities: NS cards. Format (7F10.3)

	i=1		i=2	
Cards	1	10	11	20
j=1	14.06		86.28	
j=2	43.42		54.32	
j=3	49.42		48.92	
j=4	95.0		2.51	

i=1,NS
j=1,NS

NOTE: If the x-ray intensity measurement of any one element is questionable, but those of other elements are considered to be reliable, then the intensity of the uncertain element may be set to zero to get approximate results.

F. Fluorescence Correction:

No input data in this section are required if NFICD = 1 in the control card.

1. Birks' method (NFLCD=2): Excitation efficiency coefficients

	j=1		j=2	
Cards	1	10	11	20
i=1	0.0		0.215	
i=2	0.0		0.0	

Element being excited: i=1,NC

Element doing the exciting: j=1,NC

2. Castaing's or Reed's method (NFLCD=3 or 4):

	WL	BK	WK
Cards	1	10	11
i=1	1.93	8.0999	0.28
i=2	1.66	7.7521	0.37

WL = characteristic wavelength

RK = absorption edge jump ratio

WK = fluorescence yield

Alpha matrix:

	j=1		j=2	
Cards	1	10	11	20
i=1	0.0		1.0	
i=2	0.0		0.0	

i=1, NC Element being excited

j=1, NC Element doing the exciting

0 for i=j

1.0 for K excites K and L excites L

ALPHA = 0.24 for K excites L

4.2 for L excites K

G. Background Depends on Composition: 2*NC cards: Format (7F10.3)

NOTE: The input data in this section are required, if NBKCD=1 in

the control card. If there is no drift, then set BK1(i,j) =

BK2(i,j).

	j=1		j=2	
Cards	1	10	11	20
i=1	BK1(1,1)		BK1(1,2)	
i=1	BK2(1,1)		BK2(1,2)	
i=2	BK1(2,1)		BK1(2,2)	
i=2	BK2(2,1)		BK2(2,2)	

BK1(i,j) = the initial background intensity of the ith element measured on the jth element.

BK2(i,j) = the final background intensity of the ith element measured on the jth element.

H. Compound Standard: (2*NFLT+2) cards

The input data in this section are required only if any of the element cards in (H) has a 1.0 in compound standard code column.

1. Control Card: 1 card Format (3I5)

	NFLT		NPOST		NCSPCD	
Cards	1	10	11	20	21	30
1						

NFLT = number of elements in the compound standard

NPOST = position of the standard as it appears in (2).

NCSPCD = standard fluorescence correction code:

- 0 - no fluorescence correction

- 1 - correction with Reed's method

2. Element Cards: NFLT cards Format (4F10.3)

	CSATNO		CSATWT		CSVC	
Cards	1	10	11	20	21	30
i=1						

i=1, NFLT

CSATNO = compound standard atomic number

CSATWT = compound standard atomic weight

CSVC = compound standard critical excitation potential in kV

3. Mass Absorption Coefficient matrix: Format (7F10.3)

	j=1		j=2	
Cards	1	10	11	20
i=1				
i=2				

Absorber: i=1, NFELT

Emitter : j=1, NFELT

4. Fluorescence correction (Read's method): Format (3F10.3)

The input data in this section are required if NSPCD=1 in part 1.

	CSWL	CSRK	CSWK
Cards	1	10	11
i=1			
i=2			

i=1, NFELT

Beta Matrix: Same as Alpha matrix in section F.2.

APPENDIX IIB

EPMP2 INPUT DATA FORMATA. Control Card:1 card. Format (Name1ist)

2	10
\$INPUT1 NCONT=0, NPROB=1, NCOMP=2, NSPOT=5, NFLCD=4, V=30.0, THETA=27.5 \$END	

NCONT = continuation code: - 0 - start a new problem

- 1 - continue with new sets of weight fractions

- -1 - continue with new fluorescence correction

NPROB = problem number

NCOMP = number of components or elements in the specimen

NSPOT = number of spots or sets of data

THETA = incident electron beam angle (w.r.t. normal)

V = electron beam accelerating voltage in kv

NFLCD = fluorescence correction code:

- 1 - no fluorescence correction

- 2 - Birks' method

- 3 - Castaing's method

- 4 - Reed's method

B. Element Cards: NCOMP cards. Format (5F10.3)

Cards	1	10	11	20	21	30	31	40	41	50
i=1		Fe		26.0		55.85		7.1		35.0
i=2		Ni		28.0		58.71		8.3		35.0

i=1, NCOMP

SYMBOL = one or two characters for the symbol of the element

ATNO = atomic number

ATWT = atomic weight

PSI = x-ray emerging angle

VC = critical excitation potential in keV

C. Mass Absorption Coefficient matrix: NCOMP cards.

Format (7F10.3)

	j=1		j=2	
Cards	1	10	11	20
i=1	71.4		379.6	
i=2	90.0		58.9	

Absorber: i=1,NCOMP

Emitter: j=1,NCOMP

D. Weight Fractions: NSPOT cards Format (7F10.3)

	i=1		i=2	
Cards	1	10	11	20
j=1	0.1		0.9	
j=2	0.3		0.7	
...	
j=5	0.9		0.1	

i=1,NCOMP

j=1,NSPOT

E. Fluorescence Correction:

The input data in this section is required only if NFLCD=1 in the control card.

1. Birks's Method: Excitation Efficiency Coefficients

	j=1		j=2	
Cards	1	10	11	20
i=1	0.0		0.215	
i=2	0.0		0.0	

Element being excited: i=1,NCOMP

Element doing the exciting: j=1,NCOMP

2. Castaing's or Reed's Method: (NFLCD=3 or 4)

	WL		RK		WK	
Cards	1	10	11	20	21	30
i=1	1.93		8.0999		0.28	
i=2	1.66		7.7521		0.37	

i=1,NCOMP

WL = characteristic wavelength

RK = absorption edge jump ratio

WK = fluorescence yield

Alpha Matrix:

	j=1		j=2	
Cards	1	10	11	20
i=1	0.0		1.0	
i=2	0.0		0.0	

Element being excited: i=1,NCOMP

Element doing exciting: j=1,NCOMP

$$\text{Alpha} = \begin{cases} 0.0 & \text{for } i=j \\ 1.0 & \text{for K excites K and L excites L} \\ 0.24 & \text{for K excites L} \\ 4.2 & \text{for L excites K} \end{cases}$$

APPENDIX III
OUTPUT LISTING OF EXAMPLE RESULTS

PROBLEM NUMBER 1

**** INPUT DATA ****

NO. OF ELEMENTS = 2
 NO. OF DATA SETS = 6
 FLUORESCENCE CODE = 4
 BACKGROUND CODE = 0
 INCIDENT ELECTRON BEAM ENERGY IN eV = 30.00
 INCIDENT ELECTRON BEAM ANGLE = 27.50
 EPSILON = 0.05000000
 MAXIMUM NUMBER OF ITERATIONS = 20

FE	AT. NO.	AT. WT.	VC	COMP. ST. CODE	DEAD TIME	T.C. ANGLE
NI	28.000	58.710	7.100	0.0	C.C	35.000
			8.300	0.0	C.C	35.000

MASS ABSORPTION COEFFICIENTS

FE	FE	NI
NI	71.400	379.600
	90.000	58.900

STANDARD INTENSITIES, INITIAL AND FINAL

FE	100.00	0.0	100.00	0.0
NI	100.00	0.0	100.00	0.0

SETS OF SPECIMEN INTENSITIES

FE	NI
14.060	86.280
0.0	86.280
43.420	54.320
0.0	54.320
49.420	48.920
45.000	2.510

FE CHARACTERISTIC WAVELENGTH = 1.93

ABS. JUMP RATIO = 8.0998

FLUORESCENCE YIELD = C.28C

NI CHARACTERISTIC WAVELENGTH = 1.66

ABS. JUMP RATIO = 7.7521

FLUORESCENCE YIELD = C.37C

ALPHA MATRIX

0.0	1.000
0.0	0.0

LENARD COEFFICIENTS

FE	1643.761
NI	1702.222

55

**** OUTPUT DATA ****

**** DATA SET NUMBER 1 ****

MEASURED REL. INTENSITIES

WEIGHT FRACTIONS (ABSORPTION COR. ONLY)

WEIGHT FRACTIONS (ABS. COR. AND REED'S FLUOR. COR.)

**** DATA SET NUMBER 2 ****

MEASURED REL. INTENSITIES

WEIGHT FRACTIONS (ABSORPTION COR. ONLY)

WEIGHT FRACTIONS (ABS. COR. AND REED'S FLUOR. COR.)

**** DATA SET NUMBER 3 ****

MEASURED REL. INTENSITIES

WEIGHT FRACTIONS (ABSORPTION COR. ONLY)

WEIGHT FRACTIONS (ABS. COR. AND REED'S FLUOR. COR.)

**** DATA SET NUMBER 4 ****

MEASURED REL. INTENSITIES

WEIGHT FRACTIONS (ABSORPTION COR. ONLY)

WEIGHT FRACTIONS (ABS. COR. AND REED'S FLUOR. COR.)

**** DATA SET NUMBER 5 ****

MEASURED REL. INTENSITIES

WEIGHT FRACTIONS (ABSORPTION COR. ONLY)

WEIGHT FRACTIONS (ABS. COR. AND REED'S FLUOR. COR.)

**** DATA SET NUMBER 6 ****

MEASURED REL. INTENSITIES

WEIGHT FRACTIONS (ABSORPTION COR. ONLY)

WEIGHT FRACTIONS (ABS. COR. AND REED'S FLUOR. COR.)

SUM	FE	NI
100.33997	14.06000	86.27998
1.03376	0.14169	0.89208
1.00176	0.10968	0.89208
SUM	FE	NI
99.99998	13.72001	86.27998
1.00000	0.10825	0.89175
1.00000	0.10825	0.89175
SUM	FE	NI
97.73996	43.41998	54.31998
1.04538	0.43650	0.60687
0.99363	0.38476	0.60687
SUM	FE	NI
99.99998	45.68001	54.31998
1.00000	0.39034	0.60966
1.00000	0.39034	0.60966
SUM	FE	NI
98.33997	49.41998	48.91998
1.05404	0.49651	0.55753
1.00287	0.44534	0.55753
SUM	FE	NI
97.50998	94.99998	2.51000
0.98359	0.95080	0.03278
0.97928	0.94650	0.03278

PROBLEM NUMBER 2

**** INPUT DATA ****

NO. OF ELEMENTS = 2
 NO. OF DATA SETS = 4
 FLUORESCENCE CODE = 3
 BACKGROUND CODE = 0
 INCIDENT ELECTRON BEAM ENERGY IN KV = 30.00
 INCIDENT ELECTRON BEAM ANGLE = 27.50
 EPSILON = 0.09000000
 MAXIMUM NUMBER OF ITERATIONS = 20

	AT. NO.	AT. WT.	VE	COMP. ST. CODE	DEAD TIME	T.O. ANGLE
FE	26.000	55.850	7.100	0.0	0.0	35.000
NI	28.000	58.710	8.300	0.0	0.0	35.000

MASS ABSORPTION COEFFICIENTS

	FE	NI
FE	71.400	379.600
NI	90.000	58.900

STANDARD INTENSITIES, INITIAL AND FINAL

	100.00	0.0	100.00	0.0
FE	100.00	0.0	100.00	0.0
NI	100.00	0.0	100.00	0.0

SETS OF SPECIMEN INTENSITIES

FE	NI
14.060	86.280
43.420	54.320
49.420	48.920
99.000	2.510

	CHARACTERISTIC WAVELENGTH =	ABS. JUMP RATIO =	FLUORESCENCE YIELD =
FE	1.93	8.0998	0.280
NI	1.66	7.7921	0.370

ALPHA MATRIX

0.0	1.000
0.0	0.0

LENARD COEFFICIENTS

FE	1643.761
NI	1702.222

57

**** OUTPUT DATA ****

**** DATA SET NUMBER 1 ****	SUM	FE	NI
MEASURED REL. INTENSITIES	100.33997	14.06000	86.27998
WEIGHT FRACTIONS (ABSORPTION COR. ONLY)	1.03250	0.14170	0.89080
WEIGHT FRACTIONS (ABS. COR. AND CASTAING'S FLU. COR.)	0.99489	0.10409	0.89080
**** DATA SET NUMBER 2 ****	SUM	FE	NI
MEASURED REL. INTENSITIES	97.73996	43.41998	54.31998
WEIGHT FRACTIONS (ABSORPTION COR. ONLY)	1.04403	0.43660	0.60743
WEIGHT FRACTIONS (ABS. COR. AND CASTAING'S FLU. COR.)	0.98165	0.37422	0.60743
**** DATA SET NUMBER 3 ****	SUM	FE	NI
MEASURED REL. INTENSITIES	98.33997	49.41998	48.91998
WEIGHT FRACTIONS (ABSORPTION COR. ONLY)	1.05285	0.49662	0.55623
WEIGHT FRACTIONS (ABS. COR. AND CASTAING'S FLU. COR.)	0.99101	0.43478	0.55623
**** DATA SET NUMBER 4 ****	SUM	FE	NI
MEASURED REL. INTENSITIES	97.50998	94.99998	2.51000
WEIGHT FRACTIONS (ABSORPTION COR. ONLY)	0.98361	0.95083	0.03218
WEIGHT FRACTIONS (ABS. COR. AND CASTAING'S FLU. COR.)	0.97836	0.94558	0.03218

PROBLEM NUMBER 3

*** INPUT DATA ***

NO. OF ELEMENTS = 2
 NO. OF DATA SETS = 4
 FLUORESCENCE CODE = 2
 BACKGROUND CODE = 0
 INCIDENT ELECTRON BEAM ENERGY IN KV = 30.00
 INCIDENT ELECTRON BEAM ANGLE = 27.50
 EPSILON = 0.05000000
 MAXIMUM NUMBER OF ITERATIONS = 20

	AT. NO.	AT. WT.	VC	COMP. ST. CODE	DEAD TIME	T.O. ANGLE
FF	26.000	55.850	7.100	0.0	0.0	35.000
NI	28.000	58.710	8.300	0.0	0.0	35.000

MASS ABSORPTION COEFFICIENTS

	FE	NI
FF	71.400	379.600
NI	90.000	58.900

STANDARD INTENSITIES, INITIAL AND FINAL

	100.00	0.0	100.00	0.0
FF	100.00	0.0	100.00	0.0
NI	100.00	0.0	100.00	0.0

SETS OF SPECIMEN INTENSITIES

FE	NI
14.060	86.280
43.420	54.320
49.420	48.920
95.000	2.510

EXCITATION EFFICIENCY EAB

	FF	NI
FF	0.0	0.215
NI	0.0	0.0

LENARD COEFFICIENTS

FF	1643.761
NI	1702.272

59

*** OUTPUT DATA ***

*** DATA SET NUMBER 1 ***	SUM	FE	NI
MEASURED REL. INTENSITIES	100.33997	14.06000	86.27998
WEIGHT FRACTIONS (ABSORPTION COR. ONLY)	1.03114	0.14171	0.88943
WEIGHT FRACTIONS (ABS. COR. AND BIRKS' FLUOR. COR.)	0.98752	0.09809	0.88943
*** DATA SET NUMBER 2 ***	SUM	FE	NI
MEASURED REL. INTENSITIES	97.73996	43.41998	54.31998
WEIGHT FRACTIONS (ABSORPTION COR. ONLY)	1.04465	0.43656	0.60810
WEIGHT FRACTIONS (ABS. COR. AND BIRKS' FLUOR. COR.)	0.98717	0.37907	0.60810
*** DATA SET NUMBER 3 ***	SUM	FE	NI
MEASURED REL. INTENSITIES	98.33997	49.41998	48.91998
WEIGHT FRACTIONS (ABSORPTION COR. ONLY)	1.05361	0.49635	0.55706
WEIGHT FRACTIONS (ABS. COR. AND BIRKS' FLUOR. COR.)	0.99861	0.44155	0.55706
*** DATA SET NUMBER 4 ***	SUM	FE	NI
MEASURED REL. INTENSITIES	97.50998	94.99998	2.51000
WEIGHT FRACTIONS (ABSORPTION COR. ONLY)	0.98357	0.95079	0.03278
WEIGHT FRACTIONS (ABS. COR. AND BIRKS' FLUOR. COR.)	0.97973	0.94694	0.03278

60

**** INPUT DATA ****

NUMBER OF COMPONENTS = 2
 NUMBER OF SETS OF WEIGHT FRACTIONS = 5
 INCIDENT ELECTRON BEAM ANGLE = 27.50
 ELECTRON BEAM VOLTAGE = 30.00
 FLUORESCENCE CORRECTION CODE = 4

	AT. NO.	AT. WT.	T.O. ANGLE	CR. EX. POT.	SIGMA
FE	26.000	55.850	35.000	7.100	1643.761
NI	28.000	58.710	35.000	8.300	1702.222

MASS ABSORPTION COEFFICIENTS

	FE	NI
FE	71.400	379.600
NI	90.000	58.900

WEIGHT FRACTION OF EACH ELEMENT

	FE	NI
1	0.10000	0.90000
2	0.30000	0.70000
3	0.50000	0.50000
4	0.70000	0.30000
5	0.90000	0.10000

CRITICAL EXCITATION POTENTIALS IN KV

FE	7.100
NI	8.300

FE	WAVELENGTH = 1.930	ARS. JUMP RATIO = 6.100	FLUOR. YIELD = 0.28000
NI	WAVELENGTH = 1.660	ARS. JUMP RATIO = 7.752	FLUOR. YIELD = 0.37000

ALPHA MATRIX

0.0	1.000
0.0	0.0

61

**** OUTPUT DATA ****

**** DATA SET NUMBER 1 ****

	SUM	FE	NI
WEIGHT FRACTIONS	1.00000	0.10000	0.90000
RFL. INT. (ARS. COR. ONLY)	97.21705	9.92244	87.29543
RFL. INT. (ARS. COR. AND REED'S FLUOR. COR.)	100.10000	12.90154	87.29543

**** DATA SET NUMBER 2 ****

	SUM	FE	NI
WEIGHT FRACTIONS	1.00000	0.30000	0.70000
RFL. INT. (ARS. COR. ONLY)	93.82510	24.82103	64.00407
RFL. INT. (ARS. COR. AND REED'S FLUOR. COR.)	98.91716	34.91309	64.00407

**** DATA SET NUMBER 3 ****

	SUM	FE	NI
WEIGHT FRACTIONS	1.00000	0.50000	0.50000
RFL. INT. (ARS. COR. ONLY)	92.98963	49.78951	43.19992
RFL. INT. (ARS. COR. AND REED'S FLUOR. COR.)	97.85886	54.65894	43.19992

**** DATA SET NUMBER 4 ****

	SUM	FE	NI
WEIGHT FRACTIONS	1.00000	0.70000	0.30000
RFL. INT. (ARS. COR. ONLY)	94.37071	69.82539	24.54532
RFL. INT. (ARS. COR. AND REED'S FLUOR. COR.)	97.80765	73.26233	24.54532

**** DATA SET NUMBER 5 ****

	SUM	FE	NI
WEIGHT FRACTIONS	1.00000	0.90000	0.10000
RFL. INT. (ARS. COR. ONLY)	97.68889	89.92613	7.76277
RFL. INT. (ARS. COR. AND REED'S FLUOR. COR.)	98.96689	91.28613	7.76277

PROBLEM NUMBER 5

**** INPUT DATA ****

NUMBER OF COMPONENTS = 2
 NUMBER OF SETS OF WEIGHT FRACTIONS = 4
 INCIDENT ELECTRON BEAM ANGLE = 27.50
 ELECTRON BEAM VOLTAGE = 30.00
 FLUORESCENCE CORRECTION CODE = 3

	AT. NO.	AT. WT.	T.O. ANGLE	CR. EX. POT.	SIGMA
FE	26.000	55.850	35.000	7.100	1643.761
NI	28.000	58.710	35.000	8.300	1702.222

MASS ABSORPTION COEFFICIENTS

	FE	NI
FE	71.400	375.600
NI	90.000	58.900

WEIGHT FRACTION OF EACH ELEMENT

	FE	NI
1	0.20000	0.80000
2	0.40000	0.60000
3	0.60000	0.40000
4	0.80000	0.20000

CRITICAL EXCITATION POTENTIALS IN KV

FE	7.100
NI	8.300

FE	WAVELENGTH = 1.930	ABS. JUMP RATIO = 8.100	FLUOR. YIELD = 0.28000
NI	WAVELENGTH = 1.660	ABS. JUMP RATIO = 7.752	FLUOR. YIELD = 0.37000

ALPHA MATRIX

0.0	1.000
0.0	0.0

63

**** OUTPUT DATA ****

**** DATA SET NUMBER 1 ****

	SUM	FE	NI
WEIGHT FRACTIONS	1.00000	0.20000	0.80000
REL. INT. (ABS. COR. ONLY)	95.17786	19.86288	75.31497
REL. INT. (ABS. COR. AND CASTING'S FLUOR. COR.)	100.62610	25.31113	75.31497

**** DATA SET NUMBER 2 ****

	SUM	FE	NI
WEIGHT FRACTIONS	1.00000	0.40000	0.60000
REL. INT. (ABS. COR. ONLY)	93.11046	39.79669	53.31377
REL. INT. (ABS. COR. AND CASTING'S FLUOR. COR.)	99.42644	46.11267	53.31377

**** DATA SET NUMBER 3 ****

	SUM	FE	NI
WEIGHT FRACTIONS	1.00000	0.60000	0.40000
REL. INT. (ABS. COR. ONLY)	93.42169	59.79918	33.62251
REL. INT. (ABS. COR. AND CASTING'S FLUOR. COR.)	98.62688	65.00436	33.62251

**** DATA SET NUMBER 4 ****

	SUM	FE	NI
WEIGHT FRACTIONS	1.00000	0.80000	0.20000
REL. INT. (ABS. COR. ONLY)	95.80327	79.86786	15.93542
REL. INT. (ABS. COR. AND CASTING'S FLUOR. COR.)	98.77321	82.83780	15.93542

**** INPUT DATA ****

NUMBER OF COMPONENTS = 2
 NUMBER OF SETS OF WEIGHT FRACTIONS = 4
 INCIDENT ELECTRON BEAM ANGLE = 27.50
 ELECTRON BEAM VOLTAGE = 30.00
 FLUORESCENCE CORRECTION CODE = 2

	AT. NO.	AT. WT.	T.O. ANGLE	CR. EX. POT.	SIGMA
FE	26.000	55.850	35.000	7.100	1643.761
NI	28.000	58.710	35.000	8.300	1702.222

MASS ABSORPTION COEFFICIENTS

	FE	NI
FE	71.400	379.600
NI	90.000	58.900

WEIGHT FRACTION OF EACH ELEMENT

	FE	NI
1	0.20000	0.80000
2	0.40000	0.60000
3	0.60000	0.40000
4	0.80000	0.20000

CRITICAL EXCITATION POTENTIALS IN KV

FE	7.100
----	-------

NI	8.300
----	-------

EXCITATION EFFICIENCY

	FE	NI
FE	0.0	0.215
NI	0.0	0.0

85

**** OUTPUT DATA ****

**** DATA SET NUMBER 1 ****

	SUM	FE	NI
WEIGHT FRACTIONS	1.00000	0.20000	0.80000
REL. INT. (ARS. COR. ONLY)	95.17786	19.86288	75.31497
REL. INT. (ARS. COR. AND BIRKS' FLUOR. COR.)	100.96454	25.64957	75.31497

**** DATA SET NUMBER 2 ****

	SUM	FE	NI
WEIGHT FRACTIONS	1.00000	0.40000	0.60000
REL. INT. (ARS. COR. ONLY)	93.11046	39.79669	53.31377
REL. INT. (ARS. COR. AND BIRKS' FLUOR. COR.)	98.82634	45.51257	53.31377

**** DATA SET NUMBER 3 ****

	SUM	FE	NI
WEIGHT FRACTIONS	1.00000	0.60000	0.40000
REL. INT. (ARS. COR. ONLY)	93.42169	59.79918	33.62251
REL. INT. (ARS. COR. AND BIRKS' FLUOR. COR.)	97.68620	64.06369	33.62251

**** DATA SET NUMBER 4 ****

	SUM	FE	NI
WEIGHT FRACTIONS	1.00000	0.80000	0.20000
REL. INT. (ARS. COR. ONLY)	95.80327	79.86786	15.93542
REL. INT. (ARS. COR. AND BIRKS' FLUOR. COR.)	98.07208	82.13667	15.93542

PROBLEM NUMBER 7

**** INPUT DATA ****

NUMBER OF COMPONENTS = 2
 NUMBER OF SETS OF WEIGHT FRACTIONS = 5
 INCIDENT ELECTRON BEAM ANGLE = 27.50
 ELECTRON BEAM VOLTAGE = 30.00
 FLUORESCENCE CORRECTION CODE = 4

	AT. NO.	AT. WT.	T.O. ANGLE	CR. EX. POT.	SIGMA
NI	28.000	58.710	35.000	8.300	1702.222
FE	26.000	55.850	35.000	7.100	1643.761

MASS ABSORPTION COEFFICIENTS

	NI	FE
NI	58.900	90.000
FE	179.600	71.400

WEIGHT FRACTION OF EACH ELEMENT

	NI	FE
1	0.90000	0.10000
2	0.70000	0.30000
3	0.50000	0.50000
4	0.30000	0.70000
5	0.10000	0.90000

CRITICAL EXCITATION POTENTIALS IN KV

NI	8.300
FE	7.100

NI	WAVELENGTH = 1.660	ABS. JUMP RATIO = 7.752	FLUOR. YIELD = 0.37000
FE	WAVELENGTH = 1.930	ABS. JUMP RATIO = 8.100	FLUOR. YIELD = 0.28000

ALPHA MATRIX

0.0	0.0
1.000	0.0

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**** OUTPUT DATA ****

**** DATA SET NUMBER 1 ****

	SUM	NI	FE
WEIGHT FRACTIONS	1.00000	0.90000	0.10000
REL. INT. (ABS. COR. ONLY)	97.21705	87.29543	9.92244
REL. INT. (ABS. COR. AND REED'S FLUOR. COR.)	100.19600	87.29543	12.90156

**** DATA SET NUMBER 2 ****

	SUM	NI	FE
WEIGHT FRACTIONS	1.00000	0.70000	0.30000
REL. INT. (ABS. COR. ONLY)	93.82510	64.00407	29.82103
REL. INT. (ABS. COR. AND REED'S FLUOR. COR.)	98.91716	64.00407	34.91309

**** DATA SET NUMBER 3 ****

	SUM	NI	FE
WEIGHT FRACTIONS	1.00000	0.50000	0.50000
REL. INT. (ABS. COR. ONLY)	92.98943	43.19992	49.78951
REL. INT. (ABS. COR. AND REED'S FLUOR. COR.)	97.85086	43.19992	54.65094

**** DATA SET NUMBER 4 ****

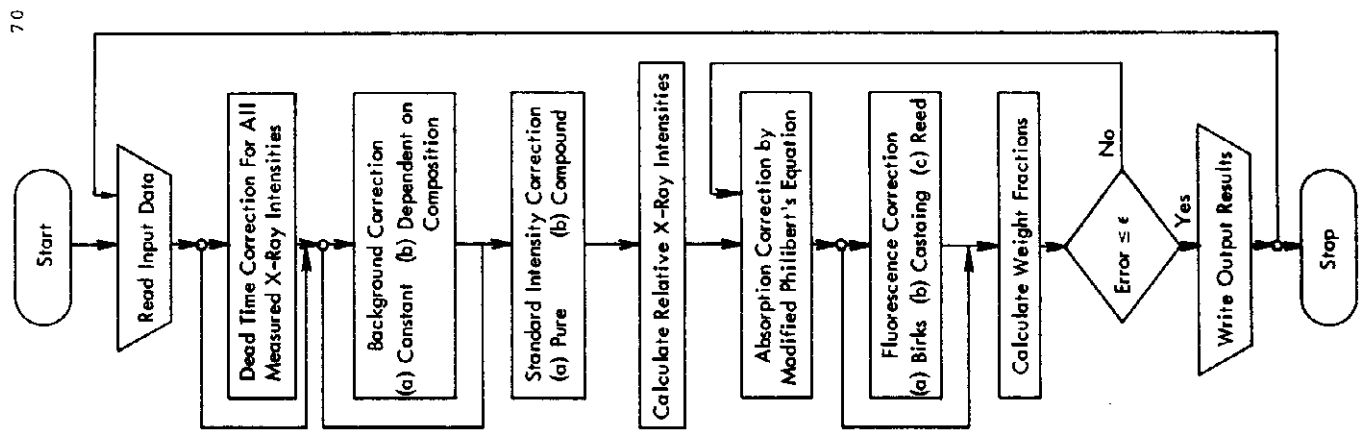
	SUM	NI	FE
WEIGHT FRACTIONS	1.00000	0.30000	0.70000
REL. INT. (ABS. COR. ONLY)	94.37871	24.54532	69.83339
REL. INT. (ABS. COR. AND REED'S FLUOR. COR.)	97.00765	24.54532	72.46233

**** DATA SET NUMBER 5 ****

	SUM	NI	FE
WEIGHT FRACTIONS	1.00000	0.10000	0.90000
REL. INT. (ABS. COR. ONLY)	97.60889	7.76277	89.84612
REL. INT. (ABS. COR. AND REED'S FLUOR. COR.)	98.86689	7.76277	91.10412

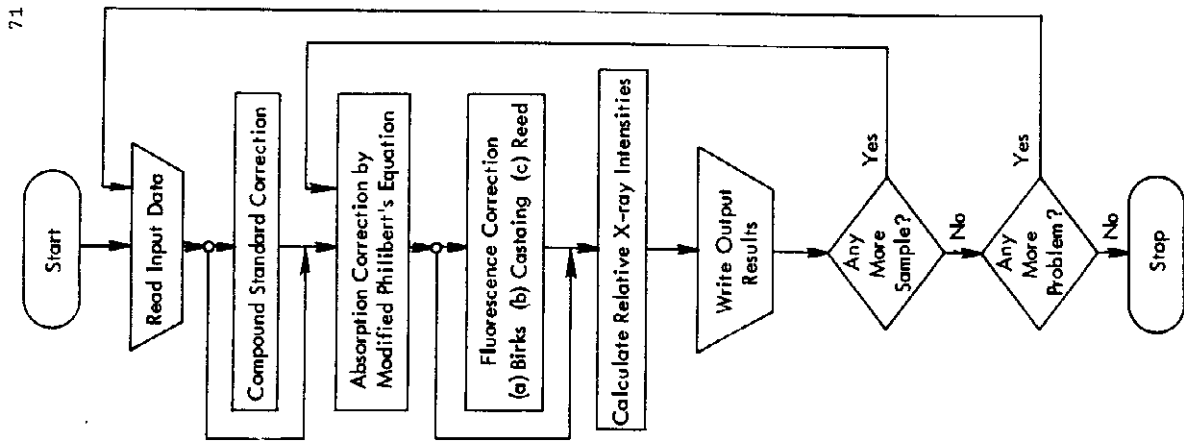
LIST OF FIGURES

- Figure 1: EPMP1 Flow Chart of Operations
 Figure 2: EPMP2 Flow Chart of Operations
 Figure 3: Relative X-ray intensity VS weight fractions plot of FeNi Binary Alloys.



List of Input Data

1. Codes for dead time correction, background correction, compound standard correction, and fluorescence correction.
2. Instrument parameters V , θ , ψ , DT .
3. Element parameters Z , A , V_c .
4. Intensity measurements I_M , I_B , I_{std} .
5. Mass absorption coefficient matrix, μ_{ij} .
6. (a) Excitation efficiency matrix, E_{AB}
 (b) Absorption edge jump ratio, r_k ,
 and fluorescence yield, u_k .



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List of Input Data

1. Codes for compound standard correction and fluorescence correction.
2. Instrument parameters V, θ, ψ .
3. Element parameters Z, A, V_c .
4. Weight fractions for each set of samples.
5. Mass absorption coefficient, μ_{ij} .
6. (a) Excitation efficiency, E_{AB}
 (b) $r_j, \omega_j (K)$

