

Algorithms for a Hand-held Miniature X-ray Fluorescence Analytical Instrument

A Report to the Department of Energy

By W. T. Elam
Naval Research Laboratory

Dan Newman
SFA, Inc.

Frank Ziemba, Adrew Cheng, and Erol Yesin
Quantrad Sensor, Inc.

and Gordon A. Anderson
Pacific Northwest Laboratory

Under Interagency Agreement DE-AI01-97EW57001
PR Number 01-97EW57001.000

Delivered to:

U. S. Department of Energy
Office of Environmental Restoration and Waste Management
Attn: Eric Lightner, EM-531
Washington, DC 20585

U. S. Department of Energy
Headquarters Procurement Operations
Attn: Calvin Lee
Washington, DC 20585

U. S. Department of Energy
Office of Scientific and Technical Information
Attn: Special Assistant for Repro. and Process.
P. O. Box 62
Oak Ridge, TN 37830

INTRODUCTION:

The purpose of this joint program was to provide technical assistance with the development of a Miniature X-ray Fluorescence (XRF) Analytical Instrument. This new XRF instrument is designed to overcome the weaknesses of spectrometers commercially available at the present time.

Currently available XRF spectrometers (for a complete list see reference 1) convert spectral information to sample composition using the influence coefficients technique or the fundamental parameters method. They require either a standard sample with composition relatively close to the unknown or a detailed knowledge of the sample matrix. They also require a highly-trained operator and the results often depend on the capabilities of the operator. In addition, almost all existing field-portable, hand-held instruments use radioactive sources for excitation. Regulatory limits on such sources restrict them such that they can only provide relatively weak excitation. This limits all current hand-held XRF instruments to poor detection limits and/or long data collection times, in addition to the licensing requirements and disposal problems for radioactive sources.

The new XRF instrument was developed jointly by Quantrad Sensor, Inc., the Naval Research Laboratory (NRL), and the Department of Energy (DOE). This report describes the analysis algorithms developed by NRL for the new instrument and the software which embodies them.

OBJECTIVE:

The following tasks were performed during this program in FY97:

1. Improve fundamental parameters calculations
 - 1.a Survey literature for best values of fundamental physical parameters needed to calculate x-ray yields
 - 1.b Incorporate new parameter values in fundamental parameters XRF calculations
 - 1.c Test accuracy of fundamental parameters calculations for a wide range of sample compositions and geometries
2. Develop fully automated analysis method for field XRF data
 - 2.a Peak identification and assignment to elements
 - 2.b Evaluation of available standards from library by comparison to unknown

2.c Calculation of standards from fundamental parameters when necessary

2.d Select regression model for optimal use of available standards and calculations

APPROACH:

1. The principal limitation to the fundamental parameters method of XRF analysis has been the accuracy of the atomic parameters used to calculate the x-ray emission. NRL developed one of the first fundamental parameters computer programs in the late 1960s and early 1970s². The method has remained virtually unchanged since then³. During the intervening years improved values of these parameters have become available.

1a. A complete survey of the literature was undertaken to find the latest available values of the atomic parameters used in the fundamental parameters method. The search included both the traditional, published, archival literature and online resources available over the Internet.

1b. A portion of these newer values were incorporated into the fundamental parameters program from NRL (called NRLXRF)². A few tests of calculations with the newer values were performed and compared to the results using the older values.

1c. Calculations of the predicted XRF intensities for several alloys, similar to those found in the expected uses of the new instrument, were performed and compared to the measured XRF intensities for the same alloys.

2. To achieve an effective and fully automated instrument requires analytical methods which convert the XRF spectrum into sample composition without operator decisions and in an adaptive manner. Algorithms were chosen to provide the best analysis available for a completely unknown sample, since such situations are often encountered in the field. Pure elements and a built-in library of physical standards are used and automatically selected by an algorithm which heavily weights those standards which are closest to the unknown in x-ray intensity. In addition, fundamental parameters calculations augment actual standards to achieve complete coverage of possible sample compositions.

2a. A novel, reliable, and very rapid algorithm was developed under this program to break the spectrum down into the intensities from each constituent element. The algorithm provides the x-ray intensity, relative to the corresponding pure element, from the raw XRF spectrum in a single calculation step.

2b. A weighting scheme was developed to select the most appropriate standard from the built-in library for analysis of a given unknown spectrum. The weighting scheme is based on differences between the intensities of the various constituent elements in the standard and unknown. The normalization and weighting of the differences was crucial to insure selection of an appropriate standard for a wide variety of unknown samples.

2c. Fundamental parameters calculations were performed using the algorithms from the NRLXRF computer program². These calculations were tested for accuracy in task 1c and the exact codes used in the tests were also used to perform the calculations for the database of coefficients used in the instrument.

2d. The regression model chosen to convert the x-ray intensities to sample composition was the method outlined by DeJongh⁴. This method takes advantage of both spectral measurements on physical standards and calculation via fundamental parameters in a natural and versatile way. It yields the best possible results when unknowns are analyzed which have compositions near the available standards but gives reasonable values for almost any unknown composition. The fundamental parameters calculations are used in a differential manner, which dramatically reduces the errors inherent in their use.

ACCOMPLISHMENTS:

The results of the literature survey for updated values of the atomic parameters are given in References 5-20. These include new values for the elemental x-ray absorption coefficients⁷, fluorescence yields¹¹, cross sections¹⁵, Coster-Kronig transition rates¹², and a variety of scattering intensities (Rayleigh/elastic, anomalous, and relativistic)^{16,17,18, 19, 20}. The principal benefit of these new values is the extension of reliable measurements of x-ray absorption cross sections to lower photon energies⁵⁻⁹. Substantial improvements in the calculation of the spectra for x-ray tubes has also been made (by the same group at NRL which did the original calculation for NRLXRF)¹³. There is, however, somewhat less new information than might be expected at first glance. In the range of x-ray emissions by most transition metals (1 to 30 keV), the values of the x-ray absorption coefficients are simply the values from the McMaster tables²¹ of 1969. The extension to lower energies (10-1000 eV) can be expected to improve the fundamental parameters calculation, but only secondarily. Several other important parameter values are changed relatively little in the new references.

The ultimate test of the new values is their effect on the results of the fundamental parameters calculations of interest for use in the new instrument. The new values for x-ray absorption were included in the NRLXRF codes, since they were deemed to be the greatest improvement over the old values and should make a definite improvement. It was rapidly discovered that there were discrepancies between the old and new values for some parameters. Updating one set of parameters without providing accurate values for the remainder actually made the results worse. The most glaring was tiny differences in the absorption edge energies between the old and new absorption tables. Since the jump in absorption just below and just above the absorption edge in a constituent element is a crucial factor in the x-ray fluorescence yield, this proved disastrous. The absorption is calculated by the program one eV below and one eV above the edge according to a table of edge energies. The new absorption coefficient tables had their edge jump values at energies different by 1 to 5 eV from the values in the old tables. An attempt was made to extract the actual edge jump energies from the new table, but no reliable method was

found during this project. It thus became impossible to get usable results with the new absorption tables.

The improvements in calculation of spectra from x-ray tubes was more fruitful. The values from the new calculation code described in reference 13 were used to calculate the expected yield from the x-ray tube used in the new instrument with excellent agreement in overall spectral shape. The calculations were also compared to very precise measurements of actual tube output in the literature²² and agreement was found to within a few percent in all cases. Again, however, incorporating the results into the fundamental parameters calculation done by NRLXRF made little noticeable difference.

Table II in the Appendix compares the x-ray intensities calculated via fundamental parameters to the measured x-ray intensities for 72 alloys. The fundamental parameters calculations use only the alloy composition and the experimental measurement conditions (the x-ray tube target and voltage plus the incident and detected beam angles). The measured values were obtained with the new XRF Analytical Instrument. Both intensities are presented as relative x-ray intensities (RXI), which is the ratio of the intensity of the x-ray emission line from a given constituent element of the alloy to the intensity from a pure sample of the same element. This ratio reduces the effect of systematic errors in some of the fundamental parameters and in the measured intensities.

The good news is that the fundamental parameters calculations performed by NRLXRF were more accurate than expected on the basis of the atomic parameters which were available at the time. The fundamental parameters calculations compare very well to the measured values, usually agreeing to within 10%. This is true even for the difficult case of chromium and iron in stainless steels. The calculations are almost universally about 10% higher than the measured values. Thus, if the calculated values are used in a differential mode, where they are corrected to measured values from a physical standard, their useability should be excellent. Work on improving the fundamental parameters calculations, including both improvements to the algorithms as well as updated values of the atomic parameters, will continue at NRL.

A fully automatic spectrum analysis method must accomplish the tasks listed above: convert the spectrum from the hardware into elemental intensities, select a standard from the built-in library, calculate the coefficients necessary to relate the standard intensities and composition to the unknown intensities and composition, and use this information to convert the spectral intensities from the unknown to its elemental composition.

Peak assignment methods in wide use fall into three types: region of interest, peak search, and peak stripping. The region-of-interest method assumes that a fixed region of the spectrum can be integrated, perhaps with subtraction of some background, to yield the integrated intensity for a particular element. This method does not handle overlapped peaks nor does it account for multiple peaks per element. The peak search method uses a smoothed second difference to locate peaks in the spectrum and select the region of interest for peak integration. Most methods also incorporate a nonlinear least squares

fitting procedure to fit overlapping peaks to an assumed shape. This procedure is the most sophisticated and requires the most computing time, but it still suffers from variations in the selection of the region of interest, which skews the fitting results, and does not incorporate multiple peaks per element. Peak stripping involves finding the largest peak in the spectrum, then subtraction of this peak from the spectrum. The process then proceeds with the second largest peak (the largest remaining peak) and so forth until all peaks are removed. This is less computationally intensive than peak searching with nonlinear fitting, but suffers badly if the assumed shape of the peaks is even slightly inaccurate.

For this project, NRL developed a new algorithm based on linear least squares fitting of the spectrum with the measured spectra of each constituent element. Using the measured spectra of the individual elements both insured that the peak shapes are correct and fits all of the peaks from a given element simultaneously. The algorithm works for overlapped peaks and treats measured backgrounds on the same basis as the peaks. It is very fast (the individual element spectra can be processed in advance) and, since it uses only linear least squares techniques, is stable, reproducible, and reliable. The algorithm is described in detail in the Appendix.

An additional feature of the algorithm is the ability to reduce the spectrum into "baskets", each of which is the sum of an arbitrary number and range of spectral channels. Using these baskets dramatically reduces the computational time and power required and makes the algorithm less sensitive to peak shape.

The algorithm has been tested with generated data including noise and easily reproduces the original spectral composition within better than one percent even with distorted peak widths and considerable noise. The algorithm is sensitive to the energy calibration, so input from the most recent calibration is used to sum the unknown spectrum into the baskets. The output of the algorithm is fractional intensities of each element, taking into account both alpha and beta lines and normalized to pure element intensities. These results are already calibrated and give a good first approximation to the unknown sample composition, uncorrected for matrix effects (absorption or enhancement). The computation time required to decompose an unknown spectrum via Gauss-Jordan elimination, using about 30 baskets, is only a few hundred milliseconds on an 80486 processor.

The results of tests on this algorithm are shown in Figure 1 below.

Once the spectrum has been reduced to elemental x-ray intensities, an appropriate standard must be chosen from the library of available standards. Since the actual composition of the unknown is not yet available, the selection must be made on the basis of a match in raw intensities. The comparison is made by calculating a weighting factor for each standard according to:

$$W_j = \sum_i [f (YS_{i,j} - YU_i) / YM_j]^2 / N_j$$

where

- W_j is the inverse weight for standard j
- j is the index of available standards
- i is the index of constituent elements
- f is a factor which multiplies the differences
- $YS_{i,j}$ is the intensity of element i in standard j
- YU_i is the intensity of element i in the unknown
- YM_j is the maximum intensity for standard j
- N_j is the number elements in standard j.

The standard with the smallest value of W_j is used. The factor f is chosen to magnify small fractional differences to near unity. Differences smaller than $1/f$ will be reduced by the squaring operation while differences larger than $1/f$ will be amplified. A judicious choice of f together with normalization by the largest elemental intensity in the standard are crucial to the proper operation of this algorithm. A value of 10 for f yields the best performance. The evaluation of this weighting scheme was based on the results produced by the overall process. That is, the scheme and values described above yielded the best agreement between measured and actual values of a list of alloys (see Table III in the Appendix).

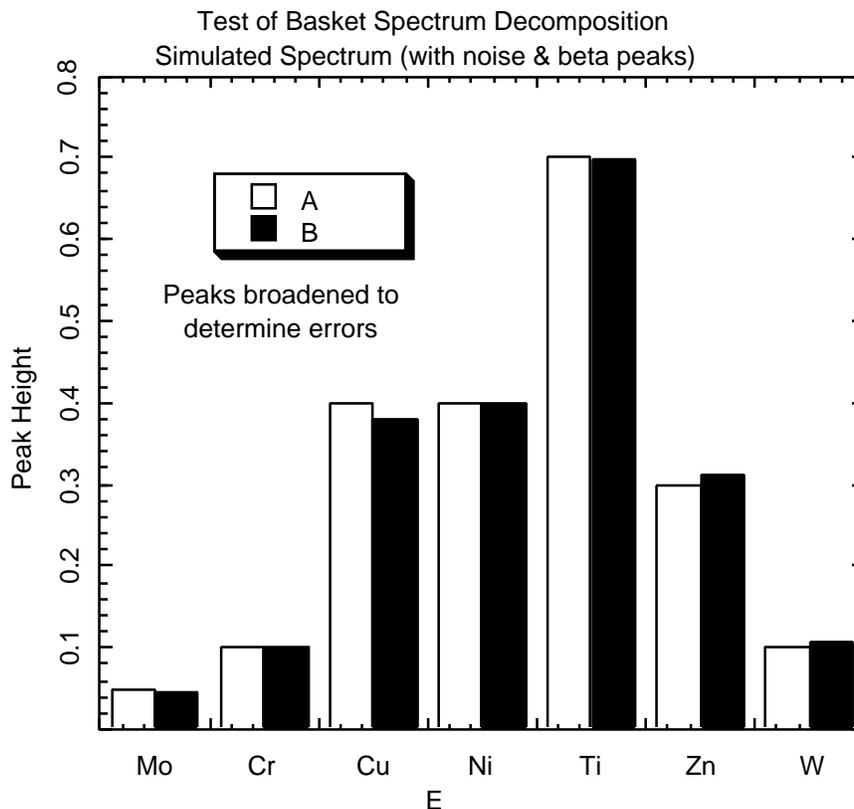


Figure 1. Results of application of the spectral decomposition algorithm to simulated XRF spectra including noise and peak broadening. The filled bars show the intensities from the decomposition algorithm applied to a simulated spectrum where noise has been added and the peaks broadened. The open bars are the actual intensities which were included in the simulated spectrum.

The fundamental parameters calculations used to augment the physical standards were based on the computer program NRLXRF, which is described in reference 2. The program is in the public domain, but the version used in this project has had improvements incorporated for this project, including changes to run on personal computers and the incorporation of updated atomic parameters as described above. The details of the fundamental parameters method are beyond the scope of this report, but are covered in reference 3 and in reference 23. The information relevant to this project has been covered in the discussion of atomic parameters above.

Conversion of the elemental intensities into composition of the unknown followed the method outlined by DeJongh⁴. This method is described in detail in reference 24. The conversion of intensities into composition must take into account the effects of the

matrix, such as absorption of the characteristic x-rays for each element and enhancement effects. The latter occur when the x-rays emitted by one element preferentially excite another element. Both of these effects depend on the actual composition, making the problem a set of interacting equations which must be solved via linear algebra. In general the problem is nonlinear, but all current methods assume a linear approximation is adequate. The DeJongh method is one of several "standard compensation" methods which use the differences in intensity between an unknown and a selected standard to determine the composition of the unknown relative to the composition of the standard. These methods do not attempt to determine a general calibration curve over all compositions. DeJongh's method takes advantage of the fundamental parameters method to calculate the coefficients which relate the differences in intensity to differences in composition. The method has two very strong advantages. It does not require a large number of standards to evaluate the coefficients or to generate a calibration curve over a wide range of compositions. However, it uses the fundamental parameters calculations only in a differential mode, greatly reducing its sensitivity to errors in the calculations. This method provides the best of both the accuracy of calibration standards and the wide composition range of fundamental parameters calculations. The results will be best where the unknown is close in composition to one of the available standards but will provide reasonable results over a very wide range of possible compositions. The actual algorithm and a few refinements included in the new instrument are given in the Appendix.

The results of applying the algorithms developed here to 72 alloys are given in Table III in the Appendix. The name and grade for each alloy are listed along with the measured intensities, the results of the calculated composition based on the measured intensities, and the known composition from the manufacturer for seven major elements. The agreement between the measured and given compositions are almost always within a few percent. The most difficult correction is the effect of iron on chromium (and vice versa) in stainless steels. The x-ray intensity from chromium is as dependent on the amount of iron as it is on the amount of chromium.

The 72 alloys in the table are the same alloys which make up the library of physical standards for the algorithm. Each alloy was excluded from the library when it was being analyzed, forcing the choice of the closest remaining alloy (as defined by the weighting scheme described above) to be used as the reference standard.

This algorithm has been incorporated in a hand-held device for alloy analysis. The unit is about 8 by 8 inches square and 20 inches long. It weighs less than 20 pounds and can be easily operated by a single individual. The results presented here were obtained with data taken by this device. A picture of the device is shown in Figure 2 below.



Figure 2. A photo of the hand-held Miniature Analytical X-ray Fluorescence Instrument.

CONCLUSION

A set of algorithms, including a novel linear-least-squares method of spectral decomposition, has been developed for a Miniature X-ray Fluorescence (XRF) Analytical Instrument. The algorithms have been tested to determine the performance, both as individual parts and collectively. The spectral decomposition algorithm uses minimal computing power and is insensitive to peak shape distortions and to noise. The conversion of x-ray spectral intensities to elemental composition follows the method of DeJongh, which uses differential coefficients to relate the differences in x-ray intensity between the unknown and a physical reference standard to differences in composition. The accuracy of the fundamental parameters method used to calculate the differential coefficients is within 10% for the 72 alloys used as the library of reference standards. A careful choice of the weighting scheme used to select the standard to be used in the DeJongh method was crucial. A weighting scheme based on summing the squares of normalized differences in x-ray intensities was developed and optimized based on performance. The complete algorithm was tested by treating each of the 72 physical standards as unknowns (and removing the respective standard from the library during its own analysis). The results confirm that the algorithms yield results within a few percent in almost all cases and are computationally very efficient. The algorithms have been incorporated into the hand-held alloy analyzer shown in Figure 2.

REFERENCES

1. "X-ray Spectrometry Source List", *Spectroscopy* 10(6), 1995
2. "Versatile X-ray Analysis Program Combining Fundamental Parameters and Empirical Coefficients", J. W. Criss, L. S. Birks, and J. V. Gilfrich, *Analytical Chemistry* **50**, 33-37 (1978).
3. *Principles of Quantitative X-ray Fluorescence Analysis*, R. Tertian and F. Claisse (Heyden, London, 1982), ISBN 0-85501-709-0, pp122-129.
4. "X-ray Fluorescence Analysis Applying Theoretical Matrix Corrections. Stainless Steel", Willy K. DeJongh, *X-ray Spectrometry* **2**, 151-158 (1973).
5. "A Temperature Dependent ENDF/B-VI, Release 4, Cross Section Library", D. E. Cullen, Lawrence Livermore National Laboratory Report UCRL-ID-127776, July 4, 1997.
6. "Tart 96, A coupled neutron-photon 3-D, combinatorial geometry Monte Carlo transport code", D. E. Cullen, Lawrence Livermore National Laboratory Report UCRL-ID-126455, November 22, 1996.
7. "Tables and Graphs of Photon Interaction Cross Sections from 0.1 keV to 100 MeV Derived from the LLL Evaluated Nuclear Data Library," Plechaty, E. F., Cullen, D. E., and Howerton, R. J., Report UCRL-50400, Vol. 6, Rev. 2, Lawrence Livermore National Laboratory, Livermore, CA. (1978).
8. "Tables and Graphs of Photon-Interaction Cross Sections from 0.1 keV to 100 MeV Derived from the LLL Evaluated-Nuclear-Data Library", Plechaty, E. F., Cullen, D. E., and Howerton, R. J., NTIS Report DE82004819 (UCRL-50400, Vol. 6, Rev. 3), November 11, 1981 (Lawrence Livermore National Laboratory, Livermore, CA).
9. "EPDL97 The Evaluated Data Library, '97 Version", D. E. Cullen, J. H. Hubbel, and L. Kissel, UCRL-50400, Vol. 6, Rev. 5, September 19, 1997 (Lawrence Livermore National Laboratory, Livermore, CA).
10. "A Suite of Programs for Calculating X-ray Absorption, Reflection and Diffraction Performance for a Variety of Materials at Arbitrary Wavelengths", S. Brennan and P. L. Cowan, *Rev. Sci. Instrum.*, **63**, 850 (1992).
11. "Atomic Radiative and Radiationless Yields for K and L Shells", M. O. Krause, *J. Phys. Chem. Ref. Data* **8**, 307-327 (1979). Also "Natural Widths of Atomic K and L

Levels, $K\alpha$ X-ray Lines and Several KLL Auger Lines", M. O. Krause and J. H. Oliver, J. Phys. Chem. Ref. Data 8, 329-338 (1979)

12. "Atomic L-Shell Coster-Kronig, Auger, and Radiative Rates and Fluorescence Yields for Na-Th", E. J. McGuire, Phys. Rev. A3, 587-593 (1971).

13. "Calculation of Spectra from Electron-Impact X-ray Sources", D. B. Brown and D. J. Nagel, in Low Energy X-ray Diagnostics - 1981 Ed. D. T. Atwood (AIP, New York, 1981).

14. A. P. Hitchcock and D. C. Mancini, in Journal of Electron Spectroscopy and Related Phenomena, Vol. 67, No. 1 (1994).

15. "Low-Energy X-ray Interaction Coefficients: Photoabsorption, Scattering, and Reflection $E = 30-30,000$ eV, $Z = 1-92$ ", B. L. Henke, E. M. Gullikson, and J. C. Davis, in Atomic Data and Nuclear Data Tables **54**, No. 2 (1993).

16. "Elastic Photon-Atom Scattering", Lynn Kissel and Paul M. Bergstrom, Jr., http://www-phys.llnl.gov/V_Div/scattering/elastic.html

17. "Validity of Form-Factor, Modified-Form-Factor and Anomalous-Scattering-Factor Approximations in Elastic Scattering Calculations," by Lynn Kissel, B. Zhou, S. C. Roy, S. K. Sen Gupta and R. H. Pratt, Acta Crystallographica **A51**, 271-288 (1995).

18. "New Relativistic S-Matrix Results for Scattering - Beyond the Usual Anomalous Factors/Beyond Impulse Approximation," R. H. Pratt, Lynn Kissel and P. M. Bergstrom, Jr., in *Resonant Anomalous X-Ray Scattering*, ed. G. Materlik, C. J. Sparks and K. Fischer (North-Holland: Amsterdam, 1994).

19. "Elastic Scattering of Gamma-Rays and X-Rays by Atoms," P. P. Kane, Lynn Kissel, R. H. Pratt and S. C. Roy, Physics Reports **140**, 75-159 (1986).

20. "Rayleigh Scattering - Elastic Photon Scattering by Bound Electrons," Lynn Kissel and R. H. Pratt, in *Atomic Inner-Shell Physics*, ed. Bernd Crasemann (Plenum Publishing: New York, 1985).

21. "Compilation of X-ray Cross Sections", W. H. McMaster, N. Kerr Del Grande, J. H. Mallett, and J. H. Hubbell, UCRL-50174, Sec. II, Rev. 1 Lawrence Livermore National Laboratory, Livermore, CA (1969).

22. "Spectral Distribution of X-ray Tubes for Quantitative X-ray Fluorescence Analysis", J. V. Gilfrich and L. S. Birks, Analytical Chemistry **40**, 1077-1080 (1968).

23. "Calculation Methods for Fluorescent X-ray Spectrometry, Empirical Coefficients vs. Fundamental Parameters", J. W. Criss and L. S. Birks, *Analytical Chemistry* **40**, 1080-1086 (1968).

24. Reference 3, pp164-167.

APPENDIX I.

Algorithm for Spectral Decomposition.

The XRF spectrum from the instrument is viewed as a superposition of one or more pure element spectra, which are known, plus a background with known profile and some amount of noise and other distortion. The elemental intensities in this spectrum can be obtained from the coefficients of superposition of the pure element spectra. Since the instrument spectrum contains noise and distortion, we must apply a least squares technique to the data to extract the elemental intensities.

The background is treated the same as the component spectra. If the background can be approximated as a polynomial, then each term of the polynomial can be calculated as a separate component and the algorithm will adjust the coefficients as necessary.

This algorithm assumes that each pure element spectrum profile is somewhat linearly independent. That is for any pair of pure element spectra (or background profiles) M(j) and N(j) consisting of n sampled data points:

$$\text{Sum}(|M(j) - a * N(j)|, j=1,2,\dots,n) \gg 0 \text{ for all values of } a.$$

Let L(i,j) be the spectrum of the i'th pure element (or background) with j the index for the j'th sample as a function of energy. There are m different pure element or background profiles. These spectra are assumed known a priori and are sampled with the same energy grid as the unknown spectrum. The unknown spectrum is approximately equal to the weighted sum of the L's with coefficients c(i) plus noise or other distortion. Let S(j) be the unknown spectrum.

$$S(j) \sim \text{Sum}(c(i) * L(i,j), i=1,\dots,m)$$

We wish to minimize the sum of the squares of the differences, d(j) (defined below), with respect to the coefficients, c(i).

$$d(j) = S(j) - \text{Sum}(c(i) * L(i,j), i=1,\dots,m).$$

To cast the problem as a least squares minimization, we want to minimize

$G = \text{Sum}(d(j)^2, j=1, \dots, n)$ with respect to each $c(i)$.

To do this, we set the partial derivatives of G wrt the $c(i)$ equal to zero and solve for the $c(i)$. This gives:

$$\frac{\partial G}{\partial c_i} = 2 \sum_j d_j \frac{\partial d_j}{\partial c_i}$$

Solving for the partial derivative in terms of the unknown and pure element spectra gives:

$$\frac{\partial G}{\partial c_i} = 2 \sum_j (L_{i,j}) [S_j - \sum_k c_k L_{k,j}]$$

This can be reformulated as a matrix eqn as follows:

Let $T(i,j) = \text{Sum}(L(i,k) * L(j,k), k=0,1,2, \dots, n-1)$
and $U(i) = \text{Sum}(S(j) * L(i,j), j=0,1, \dots, n-1)$ then

$$\sum_j T_{i,j} c_j = U_i$$

Since the matrix contains values that can be calculated purely from the already known spectral profiles, it need only be calculated once and inverted, or it can be used repeatedly in a Gauss-Jordan elimination on an augmented matrix.

A modification of this algorithm uses variable sized bins, referred to here as baskets. Each spectrum from the multichannel analyzer is summed over a range of channels to form a basket. In areas where any spectral profile has a major feature, small baskets can be used. In regions where no features are expected, a basket can span many channels. This can be used to reduce the amount of data processing and increase the insensitivity to distortion of lines, etc. It is particularly important to chose the baskets such that a resolution is high where lines may overlap. The list of basket boundaries is given in Table I below.

Since the measured pure element spectra contain noise, generated spectra are used in computing the matrices. The generated pure element spectra are comprised of Gaussian lineshapes fit and summed to match the measured pure element spectra. This process was semi-automated with final comparison and adjustment by hand to insure that the generated spectra matched the measured pure element spectra. The background profiles were computed by repeatedly smoothing the measured background spectrum.

Table I. Basket definitions used to sum spectra:

Basket number	Start Energy	End Energy
1	1.000	2.519
2	2.569	3.779
3	3.829	4.681
4	4.731	5.136
5	5.186	5.626
6	5.676	6.121
7	6.171	6.641
8	6.691	7.183
9	7.233	7.740
10	7.790	8.234
11	8.284	8.388
12	8.438	8.600
13	8.650	8.860
14	8.910	9.095
15	9.145	9.360
16	9.410	9.540
17	9.590	10.050
18	10.100	10.346
19	10.396	11.050
20	11.100	12.016
21	12.066	15.720
22	15.770	17.014
23	17.064	18.078
24	18.128	19.137
25	19.187	20.041
26	20.091	21.441
27	21.491	22.697
28	22.747	24.467
29	24.517	25.367

Table II. Table of results for fundamental parameters calculation of x-ray fluorescence intensity compared to measured intensity for selected elements in 72 alloys. The alloy name and composition are given, followed by the calculated and measured x-ray intensities. Calculations were performed by the NRLXRF computer code. XG is the known composition, YC the calculated intensity, and YM the measured intensity.

Elements	Cr	Mn	Fe	Co	Ni	Cu	Zn
:							
BS44	C-	.5Mo	4419				
XG:	0.1	0.6	97.9	0.0	0.1	0.2	0.0
YC:	0.0021	0.0060	0.9772	0.0000	0.0005	0.0007	0.0000
YM:	0.0116	0.0180	0.9946	0.0000	0.0028	0.0000	0.0000
BS45A	1.25Cr-	.5Mo	F-1				
XG:	1.2	0.5	96.6	0.0	0.2	0.2	0.0
YC:	0.0223	0.0046	0.9411	0.0001	0.0005	0.0007	0.0000
YM:	0.0255	0.0166	0.9115	0.0058	0.0000	0.0000	0.0000
BS46A	2.25Cr-	1Mo	F-22				
XG:	2.4	0.6	95.4	0.0	0.2	0.1	0.0
YC:	0.0434	0.0054	0.8931	0.0001	0.0007	0.0005	0.0000
YM:	0.0651	0.0314	0.8920	0.0027	0.0057	0.0000	0.0001
BS47A	5Cr-	.5Mo	F-5				
XG:	4.2	0.4	94.1	0.0	0.1	0.1	0.0
YC:	0.0755	0.0044	0.8477	0.0001	0.0004	0.0004	0.0000
YM:	0.0896	0.0232	0.8830	0.0000	0.0007	-.0005	0.0000
BS48A	9Cr-1Mo		F-9				
XG:	8.8	0.4	88.5	0.0	0.3	0.1	0.0
YC:	0.1413	0.0042	0.7221	0.0002	0.0011	0.0005	0.0000
YM:	0.1551	0.0205	0.6849	0.0000	0.0052	0.0000	0.0000
BS150	182FM						
XG:	18.6	1.7	76.5	0.0	0.2	0.0	0.0
YC:	0.2520	0.0162	0.5180	0.0002	0.0007	0.0002	0.0000
YM:	0.2706	0.0129	0.4591	0.0000	-.0002	-.0002	0.0000
BS151	416	Se					
XG:	13.2	0.4	85.1	0.0	0.2	0.1	0.0
YC:	0.2033	0.0040	0.6401	0.0002	0.0009	0.0004	0.0000
YM:	0.2140	0.0143	0.6033	0.0033	0.0000	-.0004	0.0000
BS410A	410						
XG:	13.2	0.5	85.3	0.0	0.2	0.0	0.0
YC:	0.2022	0.0045	0.6406	0.0000	0.0009	0.0001	0.0000
YM:	0.2223	0.0077	0.5690	0.0084	0.0007	0.0000	0.0000
BS90F	416						
XG:	13.0	0.5	84.7	0.0	0.3	0.1	0.0
YC:	0.2007	0.0052	0.6401	0.0002	0.0011	0.0005	0.0000
YM:	0.2193	0.0234	0.5944	0.0000	0.0005	0.0000	0.0000
BS95A	450						

XG:	14.7	0.6	74.8	0.1	6.4	1.5	0.0
YC:	0.2036	0.0056	0.5516	0.0007	0.0252	0.0063	0.0000
YM:	0.2327	0.0117	0.5078	0.0000	0.0183	0.0027	0.0000
BS97	422						
XG:	11.8	0.7	83.7	0.0	0.8	0.1	0.0
YC:	0.1737	0.0067	0.6344	0.0003	0.0029	0.0003	0.0000
YM:	0.1777	0.0204	0.6076	0.0050	0.0036	0.0000	0.0000
BS98	420						
XG:	13.3	0.5	84.6	0.0	0.2	0.1	0.0
YC:	0.2060	0.0047	0.6362	0.0002	0.0008	0.0004	0.0000
YM:	0.2254	0.0121	0.5637	0.0033	0.0000	0.0000	0.0000
BS152	420F						
XG:	13.4	0.4	84.8	0.0	0.1	0.1	0.0
YC:	0.2070	0.0035	0.6368	0.0001	0.0005	0.0002	0.0000
YM:	0.2089	0.0129	0.5511	0.0009	0.0000	0.0000	0.0000
BS91E	430						
XG:	16.6	0.4	82.0	0.0	0.2	0.1	0.0
YC:	0.2439	0.0041	0.5796	0.0002	0.0006	0.0002	0.0000
YM:	0.2424	0.0114	0.5208	0.0024	0.0000	-0.0003	0.0000
BS153	430F						
XG:	17.4	0.4	80.8	0.0	0.1	0.1	0.0
YC:	0.2518	0.0040	0.5636	0.0001	0.0005	0.0002	0.0000
YM:	0.2403	0.0151	0.5050	0.0000	0.0000	-0.0003	0.0000
BS92B	431						
XG:	15.9	0.4	80.4	0.0	2.1	0.1	0.0
YC:	0.2322	0.0041	0.5774	0.0003	0.0080	0.0005	0.0000
YM:	0.2292	0.0142	0.4925	0.0033	0.0067	0.0000	0.0000
BS93E	440C						
XG:	17.3	0.5	78.8	0.0	0.4	0.1	0.0
YC:	0.2499	0.0051	0.5521	0.0004	0.0013	0.0005	0.0000
YM:	0.2578	0.0079	0.5006	0.0000	0.0009	0.0000	0.0000
BS155	440F						
XG:	16.6	0.4	80.7	0.0	0.1	0.0	0.0
YC:	0.2436	0.0034	0.5718	0.0002	0.0005	0.0001	0.0000
YM:	0.2399	0.0122	0.5168	0.0000	0.0000	0.0000	0.0000
BS156	440F	Se					
XG:	16.9	1.1	79.1	0.0	0.4	0.1	0.0
YC:	0.2437	0.0112	0.5587	0.0004	0.0013	0.0004	0.0000
YM:	0.2575	0.0256	0.5292	0.0000	0.0000	0.0001	0.0000
BS94C	446						
XG:	25.9	0.4	72.0	0.0	0.4	0.1	0.0
YC:	0.3410	0.0044	0.4395	0.0003	0.0016	0.0002	0.0000
YM:	0.3645	0.0027	0.3891	0.0000	0.0017	0.0000	0.0000
BS825A	Incoloy	825					
XG:	21.4	0.6	30.2	0.2	39.8	2.3	0.0

YC:	0.2241	0.0062	0.2239	0.0017	0.2126	0.0132	0.0000
YM:	0.2296	0.0137	0.2077	0.0069	0.1605	0.0094	0.0000
BS96A	455						
XG:	11.6	0.0	76.2	0.0	8.4	2.1	0.0
YC:	0.1621	0.0004	0.5904	0.0003	0.0330	0.0087	0.0000
YM:	0.1699	0.0064	0.5433	0.0026	0.0237	0.0061	0.0000
BS203MN	203						
XG:	16.8	6.0	68.7	0.1	5.5	1.9	0.0
YC:	0.2286	0.0584	0.4958	0.0004	0.0217	0.0079	0.0000
YM:	0.2498	0.0659	0.4623	0.0000	0.0105	0.0053	0.0000
BS80F	303						
XG:	17.1	1.8	70.2	0.2	8.6	0.4	0.0
YC:	0.2325	0.0172	0.5033	0.0012	0.0342	0.0017	0.0000
YM:	0.2410	0.0157	0.4540	0.0000	0.0259	0.0013	0.0000
BSCA304	304						
XG:	18.3	1.1	70.1	0.2	8.6	0.3	0.0
YC:	0.2465	0.0104	0.4915	0.0015	0.0341	0.0014	0.0000
YM:	0.2601	0.0102	0.4544	0.0014	0.0182	0.0038	0.0000
BS81G	304L						
XG:	18.6	1.7	68.9	0.3	8.2	0.5	0.0
YC:	0.2473	0.0164	0.4791	0.0022	0.0326	0.0023	0.0000
YM:	0.2435	0.0212	0.4250	0.0049	0.0251	0.0022	0.0000
BS82D	309						
XG:	22.4	1.9	60.3	0.0	14.1	0.2	0.0
YC:	0.2813	0.0182	0.4032	0.0003	0.0586	0.0007	0.0000
YM:	0.3100	0.0252	0.3609	0.0054	0.0485	0.0002	0.0000
BS83H	310						
XG:	24.2	1.5	52.6	0.2	20.0	0.2	0.0
YC:	0.2924	0.0151	0.3498	0.0016	0.0874	0.0007	0.0000
YM:	0.3271	0.0130	0.2949	0.0042	0.0619	0.0000	0.0000
BS316B	316						
XG:	16.2	1.3	69.3	0.2	10.1	0.4	0.0
YC:	0.2115	0.0121	0.4985	0.0014	0.0406	0.0015	0.0000
YM:	0.2289	0.0217	0.4596	0.0000	0.0287	0.0010	0.0000
BS84J	316L						
XG:	17.1	1.5	67.4	0.2	10.3	0.5	0.0
YC:	0.2202	0.0139	0.4787	0.0017	0.0420	0.0020	0.0000
YM:	0.2307	0.0221	0.4460	0.0074	0.0329	0.0008	0.0000
BS317L	317L						
XG:	18.2	1.2	62.8	0.1	13.5	0.2	0.0
YC:	0.2222	0.0110	0.4394	0.0010	0.0565	0.0010	0.0000
YM:	0.2246	0.0218	0.3899	0.0000	0.0429	-0.0001	0.0000
BS321A	321						
XG:	17.2	1.2	70.3	0.2	9.4	0.3	0.0
YC:	0.2297	0.0118	0.4995	0.0011	0.0373	0.0012	0.0000

YM:	0.2184	0.0225	0.4415	0.0013	0.0237	0.0019	0.0000
BS86E	330						
XG:	18.5	1.4	42.7	0.1	35.3	0.2	0.0
YC:	0.2203	0.0149	0.3304	0.0008	0.1721	0.0011	0.0000
YM:	0.2204	0.0171	0.3011	0.0036	0.1263	0.0044	0.0000
BS347A	347						
XG:	17.4	1.5	69.6	0.1	9.2	0.3	0.0
YC:	0.2317	0.0145	0.4934	0.0004	0.0367	0.0013	0.0000
YM:	0.2471	0.0226	0.4574	0.0000	0.0268	-0.0007	0.0000
BS192	17-7PH						
XG:	16.4	0.8	72.6	0.1	7.1	0.4	0.0
YC:	0.2277	0.0082	0.5250	0.0008	0.0281	0.0017	0.0000
YM:	0.2301	0.0074	0.4545	0.0038	0.0172	0.0023	0.0000
BS318	2205						
XG:	22.3	1.4	66.4	0.1	5.6	0.2	0.0
YC:	0.2717	0.0130	0.4258	0.0007	0.0224	0.0007	0.0000
YM:	0.3032	0.0160	0.3989	0.0000	0.0221	0.0000	0.0000
BS88G	17-4PH						
XG:	15.7	0.4	74.4	0.1	4.3	4.0	0.0
YC:	0.2185	0.0042	0.5433	0.0005	0.0168	0.0166	0.0000
YM:	0.2204	0.0094	0.4927	0.0009	0.0130	0.0097	0.0000
BS185A	15-5PH						
XG:	14.5	0.5	76.0	0.0	4.4	3.4	0.0
YC:	0.2044	0.0048	0.5656	0.0002	0.0173	0.0142	0.0000
YM:	0.2235	0.0136	0.5305	0.0016	0.0090	0.0127	0.0000
BS263	Alloy	263					
XG:	19.8	0.4	0.5	20.0	50.3	0.0	0.0
YC:	0.2077	0.0045	0.0040	0.1357	0.3840	0.0002	0.0000
YM:	0.2130	0.0000	0.0079	0.1219	0.3441	0.0000	0.0000
BS189	N08367						
XG:	20.6	0.3	47.8	0.0	23.8	0.6	0.0
YC:	0.2195	0.0024	0.3275	0.0003	0.1100	0.0030	0.0000
YM:	0.2401	0.0061	0.2941	0.0040	0.0873	0.0024	0.0000
BS179A	Alloy	255					
XG:	25.5	1.0	61.1	0.6	5.8	1.9	0.0
YC:	0.2988	0.0098	0.3768	0.0039	0.0238	0.0084	0.0000
YM:	0.3132	0.0083	0.3337	0.0056	0.0166	0.0051	0.0000
BS184A	PH13-8	Mo					
XG:	12.7	0.1	75.4	0.0	8.3	0.0	0.0
YC:	0.1756	0.0006	0.5755	0.0003	0.0331	0.0002	0.0000
YM:	0.1700	0.0134	0.5000	0.0012	0.0232	0.0001	0.0000
BS183	Greek	Ascoloy					
XG:	12.8	0.4	81.0	0.0	2.0	0.1	0.0
YC:	0.1781	0.0040	0.5989	0.0002	0.0076	0.0003	0.0000
YM:	0.1751	0.0117	0.5210	0.0000	0.0021	0.0000	0.0000

BS186A	Invar	36					
XG:	0.2	0.7	63.0	0.0	35.9	0.0	0.0
YC:	0.0024	0.0074	0.6885	0.0003	0.1651	0.0001	0.0000
YM:	0.0103	0.0169	0.7479	0.0047	0.1346	0.0009	0.0000
BS187A	Carp.	20Cb3					
XG:	19.8	0.5	40.2	0.3	33.1	3.1	0.0
YC:	0.2196	0.0052	0.2984	0.0023	0.1637	0.0163	0.0000
YM:	0.2632	0.0051	0.2762	0.0093	0.1374	0.0122	0.0000
BS188A	A-286						
XG:	14.0	0.1	56.9	0.2	24.6	0.1	0.0
YC:	0.1654	0.0013	0.4326	0.0014	0.1094	0.0005	0.0000
YM:	0.1746	0.0037	0.3953	0.0025	0.0842	0.0008	0.0000
BS190	Nitronic	40					
XG:	19.6	9.7	62.8	0.0	6.7	0.1	0.0
YC:	0.2559	0.0945	0.4331	0.0003	0.0266	0.0003	0.0000
YM:	0.2785	0.1006	0.3876	0.0000	0.0196	0.0000	0.0000
BS180A	Nitronic	50					
XG:	21.1	5.1	57.4	0.0	13.2	0.1	0.0
YC:	0.2528	0.0479	0.3861	0.0003	0.0551	0.0003	0.0000
YM:	0.2684	0.0486	0.3317	0.0000	0.0410	0.0000	0.0000
BS181A	Nitronic	60					
XG:	16.5	8.2	62.3	0.1	8.2	0.2	0.0
YC:	0.2280	0.0822	0.4647	0.0005	0.0336	0.0008	0.0000
YM:	0.2386	0.0729	0.3977	0.0000	0.0253	0.0000	0.0000
BS193	18Cr-12Mn						
XG:	18.5	12.1	66.0	0.0	1.8	0.1	0.0
YC:	0.2501	0.1175	0.4599	0.0002	0.0070	0.0004	0.0000
YM:	0.2795	0.1197	0.3965	0.0000	0.0043	0.0000	0.0000
BS182	17Cr-15Mn						
XG:	16.7	15.1	65.0	0.0	1.1	0.6	0.0
YC:	0.2223	0.1437	0.4639	0.0002	0.0043	0.0023	0.0000
YM:	0.2149	0.1524	0.4243	0.0000	0.0017	0.0005	0.0000
BS200A	Nickel	200					
XG:	0.0	0.2	0.1	0.1	99.5	0.0	0.0
YC:	0.0000	0.0027	0.0016	0.0006	0.9921	0.0000	0.0000
YM:	0.0073	0.0073	0.0071	0.0149	0.9942	0.0000	0.0012
BS400C	Monel	400					
XG:	0.5	1.0	1.6	0.1	64.6	31.7	0.0
YC:	0.0071	0.0174	0.0307	0.0007	0.6225	0.3105	0.0000
YM:	0.0130	0.0359	0.0462	0.0115	0.6209	0.2947	0.0000
BS500D	Monel	K500					
XG:	0.2	0.7	0.7	0.0	64.9	29.7	0.0
YC:	0.0032	0.0120	0.0147	0.0005	0.6579	0.3064	0.0000
YM:	0.0089	0.0282	0.0211	0.0145	0.6565	0.2843	0.0000
BS600C	Inconel	600					

XG:	15.6	0.5	9.3	0.0	73.6	0.1	0.0
YC:	0.1880	0.0064	0.0972	0.0003	0.5207	0.0004	0.0000
YM:	0.1926	0.0084	0.1047	0.0069	0.4756	0.0000	0.0005
BS625A	Inconel	625					
XG:	21.7	0.1	3.1	0.1	61.4	0.1	0.0
YC:	0.2026	0.0007	0.0251	0.0005	0.4351	0.0005	0.0000
YM:	0.2061	0.0034	0.0305	0.0060	0.3870	0.0004	0.0000
BS690	Inconel	690					
XG:	30.1	0.2	9.5	0.1	58.5	0.3	0.0
YC:	0.3293	0.0023	0.0708	0.0005	0.3644	0.0019	0.0000
YM:	0.3422	0.0000	0.0639	0.0088	0.3118	0.0046	0.0006
BS800	Incoloy	800					
XG:	19.9	0.8	45.8	0.1	31.4	0.3	0.0
YC:	0.2344	0.0080	0.3372	0.0004	0.1480	0.0016	0.0000
YM:	0.2605	0.0065	0.3263	0.0078	0.1196	0.0016	0.0000
BS718A	Inconel	718					
XG:	18.2	0.1	19.2	0.3	52.0	0.1	0.0
YC:	0.1777	0.0008	0.1555	0.0023	0.3172	0.0004	0.0000
YM:	0.1832	0.0015	0.1419	0.0060	0.2529	-.0001	0.0000
BS750A	Inconel	x750					
XG:	15.7	0.1	7.1	0.3	71.9	0.0	0.0
YC:	0.1750	0.0011	0.0711	0.0022	0.5188	0.0003	0.0000
YM:	0.1767	0.0086	0.0785	0.0110	0.4539	0.0007	0.0000
BSH-1B	Hastelloy	B					
XG:	0.0	0.8	1.0	0.0	71.4	0.0	0.0
YC:	0.0000	0.0081	0.0119	0.0000	0.6224	0.0000	0.0000
YM:	0.0033	0.0124	0.0153	0.0095	0.5734	-.0003	0.0005
BSH-2B	Hastelloy	C-276					
XG:	15.4	0.6	6.5	0.4	56.8	0.1	0.0
YC:	0.1297	0.0053	0.0537	0.0027	0.3964	0.0007	0.0000
YM:	0.1284	0.0124	0.0514	0.0103	0.3605	0.0022	0.0000
BSH-3B	Hastelloy	X					
XG:	22.2	0.1	19.9	2.0	44.9	0.3	0.0
YC:	0.2121	0.0011	0.1460	0.0132	0.2637	0.0017	0.0000
YM:	0.2351	0.0000	0.1572	0.0137	0.2229	0.0042	0.0000
BSH-6A	Hastelloy	C-22					
XG:	21.4	0.3	4.3	1.1	55.8	0.1	0.0
YC:	0.1855	0.0030	0.0334	0.0072	0.3843	0.0005	0.0000
YM:	0.1901	0.0000	0.0357	0.0073	0.3231	-.0006	0.0000
BSH-8	Hastelloy	G-30					
XG:	29.4	1.1	14.6	2.6	41.8	1.7	0.0
YC:	0.2762	0.0109	0.0967	0.0159	0.2434	0.0099	0.0000
YM:	0.2940	0.0125	0.0837	0.0176	0.2121	0.0091	0.0009
BS197A	RA	333					
XG:	25.1	1.6	18.1	3.1	44.4	0.1	0.0

YC:	0.2515	0.0161	0.1298	0.0198	0.2593	0.0007	0.0000
YM:	0.2638	0.0170	0.1139	0.0199	0.2087	-0.0004	0.0000
BS199A	Waspaloy						
XG:	19.2	0.0	1.0	13.5	57.8	0.0	0.0
YC:	0.2038	0.0002	0.0093	0.0932	0.4393	0.0001	0.0000
YM:	0.1883	0.0059	0.0175	0.0885	0.3751	0.0000	0.0007
BS191	16Cr-6Mn-4Si						
XG:	16.3	5.7	67.7	0.1	5.3	0.3	0.0
YC:	0.2305	0.0571	0.5006	0.0008	0.0215	0.0014	0.0000
YM:	0.2199	0.0662	0.4223	0.0000	0.0152	0.0012	0.0000
MANGANIN	Cu86/Mn12/Ni2						
XG:	0.0	12.0	0.0	0.0	2.0	86.0	0.0
YC:	0.0000	0.1756	0.0000	0.0000	0.0192	0.7300	0.0000
YM:	0.0101	0.1735	0.0183	0.0037	0.0370	0.6680	0.0000
NIAG	Cu62/Ni18/Zn20						
XG:	0.0	0.0	0.0	0.0	18.0	62.0	20.0
YC:	0.0000	0.0000	0.0000	0.0000	0.2292	0.6183	0.1598
YM:	0.0119	0.0065	0.0169	0.0021	0.2496	0.6339	0.1045
CONSTANT	Cu55/Ni45						
XG:	0.0	0.0	0.0	0.0	45.0	55.0	0.0
YC:	0.0000	0.0000	0.0000	0.0000	0.4705	0.5617	0.0000
YM:	0.0069	0.0349	0.0216	0.0057	0.4382	0.5460	0.0000
CU63ZN37	Brass						
XG:	0.0	0.0	0.0	0.0	0.0	63.0	37.0
YC:	0.0000	0.0000	0.0000	0.0000	0.0000	0.6206	0.4006
YM:	0.0045	0.0039	0.0118	0.0052	0.0141	0.6228	0.3660

Table III. Table of results for the analysis algorithm described in this report applied to the 72 alloys used as the standard library. Each alloy was excluded from the library during its analysis. Only the major constituents are shown. The alloy name and grade are given followed by the measured intensity, the composition from the algorithm, and the known composition from the manufacturer. YU is the measured intensity, XU the measured composition, and XG the known composition.

	Cr	Mn	Fe	Co	Ni	Cu	Zn
BS44	C-	.5Mo	4419				
YU:	0.0116	0.0180	0.9946	0.0000	0.0028	0.0000	0.0000
XU:	0.5	0.5	96.2	0.0	0.5	0.0	0.0
XG:	0.1	0.6	97.9	0.0	0.1	0.2	0.0
BS45A	1.25Cr-	.5Mo	F-1				
YU:	0.0255	0.0166	0.9115	0.0058	0.0000	0.0000	0.0000
XU:	1.3	0.3	94.2	0.2	0.0	0.0	0.0
XG:	1.2	0.5	96.6	0.0	0.2	0.2	0.0
BS46A	2.25Cr-1Mo	F-22					
YU:	0.0651	0.0314	0.8920	0.0027	0.0057	0.0000	0.0001
XU:	3.5	0.6	87.0	0.1	0.8	0.0	0.0
XG:	2.4	0.6	95.4	0.0	0.2	0.1	0.0
BS47A	5Cr-	.5Mo	F-5				
YU:	0.0896	0.0232	0.8830	0.0000	0.0007	-.0005	0.0000
XU:	4.2	0.6	92.6	0.0	0.1	0.0	0.0
XG:	4.2	0.4	94.1	0.0	0.1	0.1	0.0
BS48A	9Cr-1Mo	F-9					
YU:	0.1551	0.0205	0.6849	0.0000	0.0052	0.0000	0.0000
XU:	9.5	0.7	86.3	0.0	1.1	0.0	0.0
XG:	8.8	0.4	88.5	0.0	0.3	0.1	0.0
BS150	182FM						
YU:	0.2706	0.0129	0.4591	0.0000	-.0002	-.0002	0.0000
XU:	19.5	1.5	77.2	0.0	0.0	0.0	0.0
XG:	18.6	1.7	76.5	0.0	0.2	0.0	0.0
BS151	416	Se					
YU:	0.2140	0.0143	0.6033	0.0033	0.0000	-.0004	0.0000
XU:	12.8	0.3	85.9	0.2	0.0	0.0	0.0
XG:	13.2	0.4	85.1	0.0	0.2	0.1	0.0
BS410A	410						
YU:	0.2223	0.0077	0.5690	0.0084	0.0007	0.0000	0.0000
XU:	13.3	0.3	86.2	0.1	0.1	0.0	0.0
XG:	13.2	0.5	85.3	0.0	0.2	0.0	0.0
BS90F	416						
YU:	0.2193	0.0234	0.5944	0.0000	0.0005	0.0000	0.0000
XU:	14.1	0.7	81.7	0.0	0.1	0.0	0.0
XG:	13.0	0.5	84.7	0.0	0.3	0.1	0.0
BS95A	450						

YU:	0.2327	0.0117	0.5078	0.0000	0.0183	0.0027	0.0000
XU:	16.3	0.5	74.2	0.0	5.8	1.1	0.0
XG:	14.7	0.6	74.8	0.1	6.4	1.5	0.0
BS97	422						
YU:	0.1777	0.0204	0.6076	0.0050	0.0036	0.0000	0.0000
XU:	11.2	0.5	82.4	0.2	2.0	0.0	0.0
XG:	11.8	0.7	83.7	0.0	0.8	0.1	0.0
BS98	420						
YU:	0.2254	0.0121	0.5637	0.0033	0.0000	0.0000	0.0000
XU:	13.7	0.7	83.5	0.3	0.0	0.0	0.0
XG:	13.3	0.5	84.6	0.0	0.2	0.1	0.0
BS152	420F						
YU:	0.2089	0.0129	0.5511	0.0009	0.0000	0.0000	0.0000
XU:	12.9	0.5	86.5	0.0	0.0	0.0	0.0
XG:	13.4	0.4	84.8	0.0	0.1	0.1	0.0
BS91E	430						
YU:	0.2424	0.0114	0.5208	0.0024	0.0000	-0.0003	0.0000
XU:	17.4	0.3	79.3	0.1	0.0	0.0	0.0
XG:	16.6	0.4	82.0	0.0	0.2	0.1	0.0
BS153	430F						
YU:	0.2403	0.0151	0.5050	0.0000	0.0000	-0.0003	0.0000
XU:	17.5	0.6	79.2	0.0	0.0	0.0	0.0
XG:	17.4	0.4	80.8	0.0	0.1	0.1	0.0
BS92B	431						
YU:	0.2292	0.0142	0.4925	0.0033	0.0067	0.0000	0.0000
XU:	16.4	0.7	79.2	0.2	2.4	0.0	0.0
XG:	15.9	0.4	80.4	0.0	2.1	0.1	0.0
BS93E	440C						
YU:	0.2578	0.0079	0.5006	0.0000	0.0009	0.0000	0.0000
XU:	18.9	0.2	78.9	0.0	0.1	0.0	0.0
XG:	17.3	0.5	78.8	0.0	0.4	0.1	0.0
BS155	440F						
YU:	0.2399	0.0122	0.5168	0.0000	0.0000	0.0000	0.0000
XU:	17.0	0.5	80.6	0.0	0.0	0.0	0.0
XG:	16.6	0.4	80.7	0.0	0.1	0.0	0.0
BS156	440F	Se					
YU:	0.2575	0.0256	0.5292	0.0000	0.0000	0.0001	0.0000
XU:	17.7	0.9	79.2	0.0	0.0	0.0	0.0
XG:	16.9	1.1	79.1	0.0	0.4	0.1	0.0
BS94C	446						
YU:	0.3645	0.0027	0.3891	0.0000	0.0017	0.0000	0.0000
XU:	26.7	0.2	69.8	0.0	0.5	0.0	0.0
XG:	25.9	0.4	72.0	0.0	0.4	0.1	0.0
BS825A	Incoloy	825					
YU:	0.2296	0.0137	0.2077	0.0069	0.1605	0.0094	0.0000

XU:	20.2	1.5	32.4	0.3	37.8	2.3	0.0
XG:	21.4	0.6	30.2	0.2	39.8	2.3	0.0
BS96A	455						
YU:	0.1699	0.0064	0.5433	0.0026	0.0237	0.0061	0.0000
XU:	11.3	0.2	69.3	0.1	17.7	0.6	0.0
XG:	11.6	0.0	76.2	0.0	8.4	2.1	0.0
BS203MN	203						
YU:	0.2498	0.0659	0.4623	0.0000	0.0105	0.0053	0.0000
XU:	17.5	7.3	67.7	0.0	3.3	1.6	0.0
XG:	16.8	6.0	68.7	0.1	5.5	1.9	0.0
BS80F	303						
YU:	0.2410	0.0157	0.4540	0.0000	0.0259	0.0013	0.0000
XU:	17.1	1.7	69.3	0.0	9.9	0.2	0.0
XG:	17.1	1.8	70.2	0.2	8.6	0.4	0.0
BSCA304	304						
YU:	0.2601	0.0102	0.4544	0.0014	0.0182	0.0038	0.0000
XU:	18.9	1.1	69.3	0.1	5.7	1.1	0.0
XG:	18.3	1.1	70.1	0.2	8.6	0.3	0.0
BS81G	304L						
YU:	0.2435	0.0212	0.4250	0.0049	0.0251	0.0022	0.0000
XU:	18.2	2.4	68.3	0.4	8.2	0.7	0.0
XG:	18.6	1.7	68.9	0.3	8.2	0.5	0.0
BS82D	309						
YU:	0.3100	0.0252	0.3609	0.0054	0.0485	0.0002	0.0000
XU:	23.4	2.1	60.4	0.4	11.5	0.0	0.0
XG:	22.4	1.9	60.3	0.0	14.1	0.2	0.0
BS83H	310						
YU:	0.3271	0.0130	0.2949	0.0042	0.0619	0.0000	0.0000
XU:	26.2	1.0	55.0	0.0	17.7	0.0	0.0
XG:	24.2	1.5	52.6	0.2	20.0	0.2	0.0
BS316B	316						
YU:	0.2289	0.0217	0.4596	0.0000	0.0287	0.0010	0.0000
XU:	17.0	1.5	68.5	0.0	9.0	0.6	0.0
XG:	16.2	1.3	69.3	0.2	10.1	0.4	0.0
BS84J	316L						
YU:	0.2307	0.0221	0.4460	0.0074	0.0329	0.0008	0.0000
XU:	17.0	1.3	65.0	0.5	10.5	0.3	0.0
XG:	17.1	1.5	67.4	0.2	10.3	0.5	0.0
BS317L	317L						
YU:	0.2246	0.0218	0.3899	0.0000	0.0429	-.0001	0.0000
XU:	18.8	1.8	63.3	0.0	12.9	0.0	0.0
XG:	18.2	1.2	62.8	0.1	13.5	0.2	0.0
BS321A	321						
YU:	0.2184	0.0225	0.4415	0.0013	0.0237	0.0019	0.0000
XU:	15.9	2.6	71.1	0.0	9.8	0.3	0.0

XG:	17.2	1.2	70.3	0.2	9.4	0.3	0.0
BS86E	330						
YU:	0.2204	0.0171	0.3011	0.0036	0.1263	0.0044	0.0000
XU:	18.2	2.2	43.6	0.0	34.5	0.9	0.0
XG:	18.5	1.4	42.7	0.1	35.3	0.2	0.0
BS347A	347						
YU:	0.2471	0.0226	0.4574	0.0000	0.0268	-.0007	0.0000
XU:	17.4	2.5	70.9	0.0	9.0	0.0	0.0
XG:	17.4	1.5	69.6	0.1	9.2	0.3	0.0
BS192	17-7PH						
YU:	0.2301	0.0074	0.4545	0.0038	0.0172	0.0023	0.0000
XU:	17.2	0.9	72.8	0.3	5.9	0.8	0.0
XG:	16.4	0.8	72.6	0.1	7.1	0.4	0.0
BS318	2205						
YU:	0.3032	0.0160	0.3989	0.0000	0.0221	0.0000	0.0000
XU:	22.8	2.1	67.2	0.0	2.2	0.0	0.0
XG:	22.3	1.4	66.4	0.1	5.6	0.2	0.0
BS88G	17-4PH						
YU:	0.2204	0.0094	0.4927	0.0009	0.0130	0.0097	0.0000
XU:	15.7	0.3	76.9	0.0	3.8	1.1	0.0
XG:	15.7	0.4	74.4	0.1	4.3	4.0	0.0
BS185A	15-5PH						
YU:	0.2235	0.0136	0.5305	0.0016	0.0090	0.0127	0.0000
XU:	15.6	0.5	78.7	0.0	1.0	1.4	0.0
XG:	14.5	0.5	76.0	0.0	4.4	3.4	0.0
BS263	Alloy	263					
YU:	0.2130	0.0000	0.0079	0.1219	0.3441	0.0000	0.0000
XU:	21.5	0.0	0.5	18.4	51.1	0.0	0.0
XG:	19.8	0.4	0.5	20.0	50.3	0.0	0.0
BS189	N08367						
YU:	0.2401	0.0061	0.2941	0.0040	0.0873	0.0024	0.0000
XU:	21.0	0.9	48.3	0.0	25.9	0.5	0.0
XG:	20.6	0.3	47.8	0.0	23.8	0.6	0.0
BS179A	Alloy	255					
YU:	0.3132	0.0083	0.3337	0.0056	0.0166	0.0051	0.0000
XU:	26.1	0.8	63.4	0.5	4.3	0.6	0.0
XG:	25.5	1.0	61.1	0.6	5.8	1.9	0.0
BS184A	PH13-8	Mo					
YU:	0.1700	0.0134	0.5000	0.0012	0.0232	0.0001	0.0000
XU:	12.2	0.4	68.5	0.1	17.6	0.0	0.0
XG:	12.7	0.1	75.4	0.0	8.3	0.0	0.0
BS183	Greek	Ascoloy					
YU:	0.1751	0.0117	0.5210	0.0000	0.0021	0.0000	0.0000
XU:	12.9	0.1	82.5	0.0	0.8	0.0	0.0
XG:	12.8	0.4	81.0	0.0	2.0	0.1	0.0

BS186A	Invar	36					
YU:	0.0103	0.0169	0.7479	0.0047	0.1346	0.0009	0.0000
XU:	0.6	0.5	78.2	0.0	19.5	0.1	0.0
XG:	0.2	0.7	63.0	0.0	35.9	0.0	0.0
BS187A	Carp.	20Cb3					
YU:	0.2632	0.0051	0.2762	0.0093	0.1374	0.0122	0.0000
XU:	21.6	0.6	39.6	0.1	33.6	2.2	0.0
XG:	19.8	0.5	40.2	0.3	33.1	3.1	0.0
BS188A	A-286						
YU:	0.1746	0.0037	0.3953	0.0025	0.0842	0.0008	0.0000
XU:	14.9	0.2	56.3	0.1	21.8	0.4	0.0
XG:	14.0	0.1	56.9	0.2	24.6	0.1	0.0
BS190	Nitronic	40					
YU:	0.2785	0.1006	0.3876	0.0000	0.0196	0.0000	0.0000
XU:	18.5	9.9	63.1	0.0	7.9	0.0	0.0
XG:	19.6	9.7	62.8	0.0	6.7	0.1	0.0
BS180A	Nitronic	50					
YU:	0.2684	0.0486	0.3317	0.0000	0.0410	0.0000	0.0000
XU:	21.6	3.9	60.6	0.0	13.0	0.0	0.0
XG:	21.1	5.1	57.4	0.0	13.2	0.1	0.0
BS181A	Nitronic	60					
YU:	0.2386	0.0729	0.3977	0.0000	0.0253	0.0000	0.0000
XU:	18.6	6.3	66.0	0.0	8.6	0.0	0.0
XG:	16.5	8.2	62.3	0.1	8.2	0.2	0.0
BS193	18Cr-12Mn						
YU:	0.2795	0.1197	0.3965	0.0000	0.0043	0.0000	0.0000
XU:	19.6	12.0	66.5	0.0	1.6	0.0	0.0
XG:	18.5	12.1	66.0	0.0	1.8	0.1	0.0
BS182	17Cr-15Mn						
YU:	0.2149	0.1524	0.4243	0.0000	0.0017	0.0005	0.0000
XU:	14.3	16.3	68.1	0.0	0.7	0.1	0.0
XG:	16.7	15.1	65.0	0.0	1.1	0.6	0.0
BS200A	Nickel	200					
YU:	0.0073	0.0073	0.0071	0.0149	0.9942	0.0000	0.0012
XU:	0.2	0.2	0.2	0.0	98.1	0.0	0.1
XG:	0.0	0.2	0.1	0.1	99.5	0.0	0.0
BS400C	Monel	400					
YU:	0.0130	0.0359	0.0462	0.0115	0.6209	0.2947	0.0000
XU:	0.3	0.9	1.7	0.0	62.8	31.6	0.0
XG:	0.5	1.0	1.6	0.1	64.6	31.7	0.0
BS500D	Monel	K500					
YU:	0.0089	0.0282	0.0211	0.0145	0.6565	0.2843	0.0000
XU:	0.3	0.8	0.7	0.1	66.1	29.6	0.0
XG:	0.2	0.7	0.7	0.0	64.9	29.7	0.0
BS600C	Inconel	600					

YU:	0.1926	0.0084	0.1047	0.0069	0.4756	0.0000	0.0005
XU:	15.8	0.1	8.7	0.2	73.1	0.0	0.1
XG:	15.6	0.5	9.3	0.0	73.6	0.1	0.0
BS625A	Inconel	625					
YU:	0.2061	0.0034	0.0305	0.0060	0.3870	0.0004	0.0000
XU:	20.2	0.2	3.2	0.9	63.6	0.0	0.0
XG:	21.7	0.1	3.1	0.1	61.4	0.1	0.0
BS690	Inconel	690					
YU:	0.3422	0.0000	0.0639	0.0088	0.3118	0.0046	0.0006
XU:	30.0	0.0	9.6	1.3	57.5	0.8	0.1
XG:	30.1	0.2	9.5	0.1	58.5	0.3	0.0
BS800	Incoloy	800					
YU:	0.2605	0.0065	0.3263	0.0078	0.1196	0.0016	0.0000
XU:	20.5	0.5	45.0	0.2	31.4	0.1	0.0
XG:	19.9	0.8	45.8	0.1	31.4	0.3	0.0
BS718A	Inconel	718					
YU:	0.1832	0.0015	0.1419	0.0060	0.2529	-0.0001	0.0000
XU:	18.8	0.1	17.8	0.9	53.9	0.0	0.0
XG:	18.2	0.1	19.2	0.3	52.0	0.1	0.0
BS750A	Inconel	x750					
YU:	0.1767	0.0086	0.0785	0.0110	0.4539	0.0007	0.0000
XU:	15.6	0.6	7.7	0.1	74.6	0.0	0.0
XG:	15.7	0.1	7.1	0.3	71.9	0.0	0.0
BSH-1B	Hastelloy	B					
YU:	0.0033	0.0124	0.0153	0.0095	0.5734	-0.0003	0.0005
XU:	0.3	0.5	0.3	0.1	69.8	0.0	0.0
XG:	0.0	0.8	1.0	0.0	71.4	0.0	0.0
BSH-2B	Hastelloy	C-276					
YU:	0.1284	0.0124	0.0514	0.0103	0.3605	0.0022	0.0000
XU:	14.4	1.0	5.2	1.4	55.0	0.2	0.0
XG:	15.4	0.6	6.5	0.4	56.8	0.1	0.0
BSH-3B	Hastelloy	X					
YU:	0.2351	0.0000	0.1572	0.0137	0.2229	0.0042	0.0000
XU:	22.1	0.0	22.9	1.7	43.0	0.7	0.0
XG:	22.2	0.1	19.9	2.0	44.9	0.3	0.0
BSH-6A	Hastelloy	C-22					
YU:	0.1901	0.0000	0.0357	0.0073	0.3231	-0.0006	0.0000
XU:	23.2	0.0	4.4	0.1	58.7	0.0	0.0
XG:	21.4	0.3	4.3	1.1	55.8	0.1	0.0
BSH-8	Hastelloy	G-30					
YU:	0.2940	0.0125	0.0837	0.0176	0.2121	0.0091	0.0009
XU:	29.1	1.2	14.1	2.8	43.3	0.8	0.1
XG:	29.4	1.1	14.6	2.6	41.8	1.7	0.0
BS197A	RA	333					
YU:	0.2638	0.0170	0.1139	0.0199	0.2087	-0.0004	0.0000

XU:	26.2	1.5	19.3	2.9	44.0	0.0	0.0
XG:	25.1	1.6	18.1	3.1	44.4	0.1	0.0
BS199A	Waspaloy						
YU:	0.1883	0.0059	0.0175	0.0885	0.3751	0.0000	0.0007
XU:	17.8	0.5	1.0	15.1	58.1	0.0	0.1
XG:	19.2	0.0	1.0	13.5	57.8	0.0	0.0
BS191	16Cr-6Mn-4Si						
YU:	0.2199	0.0662	0.4223	0.0000	0.0152	0.0012	0.0000
XU:	15.9	8.1	69.2	0.0	5.4	0.2	0.0
XG:	16.3	5.7	67.7	0.1	5.3	0.3	0.0
MANGANIN	Cu86/Mn12/Ni2						
YU:	0.0101	0.1735	0.0183	0.0037	0.0370	0.6680	0.0000
XU:	0.9	14.7	1.6	0.3	3.5	75.2	0.0
XG:	0.0	12.0	0.0	0.0	2.0	86.0	0.0
NIAG	Cu62/Ni18/Zn20						
YU:	0.0119	0.0065	0.0169	0.0021	0.2496	0.6339	0.1045
XU:	1.0	0.6	1.5	0.2	22.0	62.5	9.1
XG:	0.0	0.0	0.0	0.0	18.0	62.0	20.0
CONSTANT	Cu55/Ni45						
YU:	0.0069	0.0349	0.0216	0.0057	0.4382	0.5460	0.0000
XU:	0.5	2.7	1.7	0.4	41.0	48.2	0.0
XG:	0.0	0.0	0.0	0.0	45.0	55.0	0.0
CU63ZN37	Brass						
YU:	0.0045	0.0039	0.0118	0.0052	0.0141	0.6228	0.3660
XU:	0.4	0.3	1.0	0.4	0.6	55.7	39.7
XG:	0.0	0.0	0.0	0.0	0.0	63.0	37.0