Development of Quantification Software using Multi-analytical Methods for an Instrumental Neutron Activation Analysis: KAERI-NAA

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1. Introduction

Instrumental neutron activation analysis (INAA) has been used for the quantification of various elements in a matter by neutron capture reaction. In this study, a new software for the quantification of concentrations and various quantities on the INAA data was developed using a multi-analytical methods and named KAERI-NAA. Quantifications were validated by comparing with those certificated values of NIST SRMs. This software adopted a HYPERMET routine for the peak analysis of the measured INAA gamma-ray spectrum and various analytical methods like absolute method, relative method and k_0-standardization method.

The gamma-ray spectrum is acquired and analyzed by using a commercial software GammaVision, which is compatible with ORTEC NIM modules. The peak information from a GammaVision is imported to old quantification software POWER NAA coded in LabView up to the present. Because these procedures are bothersome and cause human errors, it isn't easy for users to access more information included in a spectrum. Our aim for this new software is to obtain full familiarity for users by reducing effort and human errors in producing an analytical report.

2. Algorithm

A well-known equation for activation analysis is used in this software. This equation models the activation of a single element and radiation measurement for a single activation product [1].

$$W = \frac{CM\lambda e^{\lambda t_d}}{\varepsilon(E_\gamma, g)A_v \Im \sigma(E_a)\varphi(E_n)\Gamma(1-e^{-\lambda t_i})(1-e^{-\lambda t_c})}$$

(1)

, where W is weight of target element, C measured counts, t_i irradiation time, t_d decay time, t_c counting time, E_n energy of activating neutrons, A_v Avogadro's number, M atomic mass, $\Im$ natural abundance of target isotope, λ decay constant, G gamma-ray emission probability, E_g gamma-ray energy, $f(E_n)$ neutron flux, $s(E_n)$ reaction cross-section, g geometrical factor, $e(E_g,g)$ detection efficiency. Other geometrical factors such as thermal and epithermal neutron shield factors and neutron spectrum shape factor and so on were neglected because those factors can be considered as unit values in conventional experiments carried out in our laboratory. The software was coded using a MATLAB code and operated in a single and batch mode. In a single mode, the user can import and analyze a single spectrum. In a batch mode, the user can import a batch file where all experimental information like sample names, irradiation hole numbers, neutron flux, detector numbers, slot numbers, irradiation dates and times and methods of analysis are registered. More than one hundred spectra can be analyzed at a time in a batch mode without user's additional efforts.

The spectrum is analyzed by a peak analysis routine (HYPERMET routine) and the quantification for the identified elements are performed in due order. If the analysis condition is settled before analysis, the users don't need to concern themselves about peak analysis and generate a resultant report. Figure 1 shows a main frame of the KAERI-NAA software and figure 2 shows an example of peak analysis undertaken in this software by using HYPERMET automatic peak analysis routine, which was originally coded in FORTRAN language [2] and later converted into C language by Applied Nuclear Physics Group of Seoul National University [3].
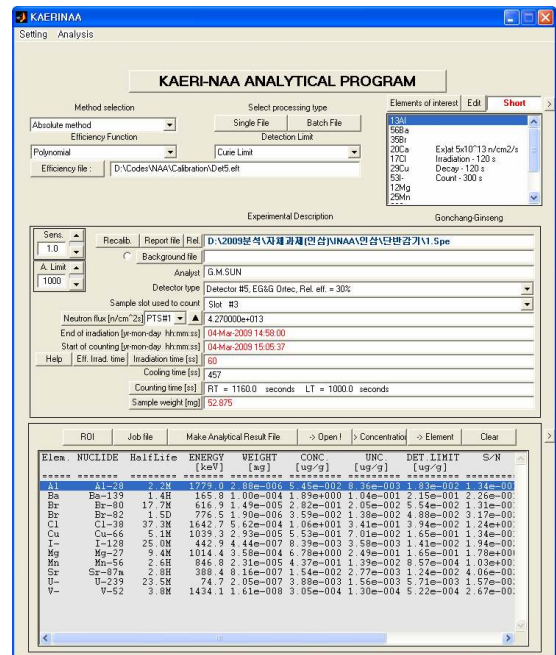

Fig. 1. KAERI-NAA software.

This software adopted three analytical methods like absolute method, relative method and k_0-standardization method. An absolute method can theoretically determine the elemental concentrations using an eq. (1), where the user should determine the neutron flux and other parameters such as detection efficiency and geometrical effects exactly. A relative method determines the elemental contents of a sample by

comparing gamma-ray peak count rates of the element in the sample with that of standard samples. In a k_0-standardization method, a specific gamma-ray line from a nuclide of interest is used as an internal comparator and the elemental mass ratio can be obtained by the following equation:

$$\rho_{x:y} = \frac{C_x/\varepsilon_x}{C_y/\varepsilon_y} \cdot \frac{k_{0,c}(y)}{k_{0,c}(x)} \qquad (2)$$

, where $k_{0,c}$ is the k_0 factor determined for a comparator line c.
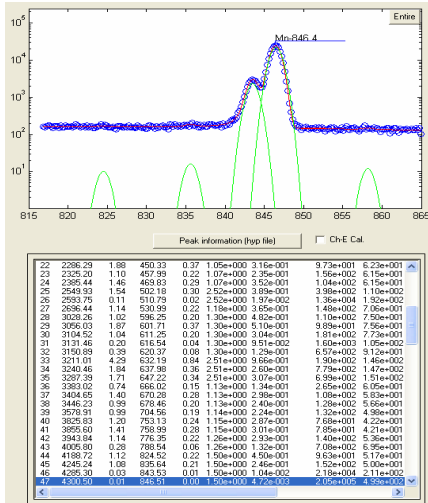

Fig. 2. An example of peak analysis.
Decomposition of multiplet gamma-ray peaks.

3. Analysis of NIST SRMs

For a validation of KAERI-NAA software, several NIST certified reference materials (CRMs) were used as shown in a Table 1~3. CRMs are apple leaves (NIST SRM 1515), San Joaquin soil (NIST SRM 2709) and bone ashes (NIST SRM 1400), respectively. The differences between measured and certified values are consistent within 5 %, which is mainly attributed to statistical error of the peak area and uncertainty of detection efficiency and so on.

Table 1. Comparison of determined and certified values for NIST SRM 1515 Apple leaves.

Element	Measured value [ug/g]		Certified value [ug/g]	
		NIST SRM 1515 Apple leaves		
Na	2.48E+01	1.25E+00	2.44E+01	1.20E+00
Mg	2.68E+03	1.30E+02	2.71E+03	8.00E+01
Al	2.89E+02	1.50E+01	2.86E+02	9.00E+00
K	1.58E+04	7.90E+02	1.61E+04	2.00E+02
Ca	1.50E+04	7.50E+02	1.53E+04	1.50E+02
Mn	5.24E+01	2.60E+00	5.40E+01	3.00E+00
Fe	8.61E+01	4.30E+00	8.30E+01	5.00E+00
Zn	1.18E+01	5.90E-01	1.25E+01	3.00E-01

Table 2. Comparison of determined and certified values for NIST SRM 1709 San Joaquin soil.

NIST SRM 1709 San Joaquin soil

Element	Measured value [ug/g]		Certified value [ug/g]	
Na	1.19E+04	6.20E+02	1.16E+04	3.00E+02
Mg	1.57E+04	8.10E+02	1.51E+04	4.00E+02
Al	7.31E+04	4.00E+03	7.50E+04	6.00E+02
K	2.04E+04	1.10E+03	2.03E+04	6.00E+02
Ca	1.80E+04	1.00E+03	1.89E+04	5.00E+02
Mn	4.60E+02	2.30E+01	4.38E+02	1.70E+01
Fe	3.61E+04	1.83E+03	3.50E+04	1.10E+03
Ti	3.32E+03	1.80E+02	3.42E+03	2.40E-02

Table 3. Comparison of determined and certified values for NIST SRM 1400 bone ashes.

Element	Measured value [ug/g]		Certified value [ug/g]	
		NIST SRM 1400 bone ashes		
Mg	6.78E+03	3.30E+02	6.84E+03	1.30E+02
K	1.83E+02	9.10E+00	1.86E+02	8.00E+00
Ca	3.98E+05	1.90E+03	3.82E+05	1.30E+03
Fe	6.39E+02	3.30E+01	6.60E+02	2.70E+01
Sr	2.62E+02	1.30E+00	2.49E+02	7.00E+00
Zn	1.77E+02	9.10E+00	1.81E+02	3.00E+00

4. Conclusions

A quantification software for an instrumental neutron activation analysis has been developed for the user's convenience and the automatic analysis of numerous measured spectra to reduce the efforts of the analyst and human errors. The software has been validated by measuring several NIST SRMs.

REFERENCES

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[3] C.S. Park, H.D. Choi, G.M. Sun, J.H. Whang, "Status of developing HPGe g-ray spectrum analysis code HYPERGAM", Progress in Nuclear Energy 50 (2008) 389-393.