AN EXPERT SYSTEM FOR NEUTRON ACTIVATION ANALYSIS*

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ABSTRACT

An expert system for neutron activation analysis has been designed on personal computer. It is mainly structured by means of the MDBS GURU, and composed of three subsystems: spectrum analysis, experiment design and data management. The gamma spectra from multiple channel analyzer can be treated conveniently with conventional methods and/or intellectualized isotope identification based on expert experiences. Fuzzy variable and its algebra are employed for inferring and expression of some conclusions. A procedure for quality control has been created to check the analytical quality. Suggestion of planning an experiment for a certain material can be obtained, and a gamma spectrum can be predicted or simulated. There is a data bank for saving the element concentrations.

Keywords: Expert system Neutron activation analysis

Ⅰ. INTRODUCTION

As an elemental analysis technique, the neutron activation analysis (NAA) method has been developed quite well. The automatic processing for a vast sum of data, however, is still unsatisfactory. We have to spend a great deal of time on the spectrum analysis, especially on the isotopic identification for some nuclides, quality check for the analytical results and selection of the element concentrations from two or more characteristic peaks of each nuclide or from the results of two or more measurements.

To simplify the data processing, improve the analytical quality, optimize the experimental conditions and accumulate the experimental data. We have been building an Expert system for the neutron activation analysis (ESNAA) on personal computer.

Ⅱ. AN EXPERT SYSTEM FOR NAA

1. Frame of the ESNAA system

This system was built by means of the Micro Data Base Systems GURU[1]. It is composed of three subsystems: the spectrum analyses, the experiment design and the data management. Structure frame of the system is shown in Fig.1. Their major functions are listed in Table 1. The abilities of GURU provide much convenience to make use of the experts' experiences in our system. The fuzzy variable in GURU with its certainty factor makes it possible to express our results more precisely.

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A series of menus have been made as user's interface. Fig.2 shows a part of the menus' tree. A program written in Turbo C is used as the interface to the spectrum data files.

Table 1

Objects and main functions of the three subsystems

Subsystem 1	Subsystem 2	Subsystem 3
Object:	Object:	Object:
gamma spectrum analysis	experiment design and prediction	data management
Functions:	Functions:	Functions:
1. regular analyses	1. Giving suggestions	1.Data accumulation
2. Intellectualized	for the NAA experiment of	2. Common mathematical
isotope identification	a sample and/or	process
3. Various corrections	some elements.	3. Data mangement
4. Quantity analysis for	2. Optimizing the experiment	
element contents	parameters.	
5. Checking results for	3. Simulating the experiment and	
quality control	predicting results.	

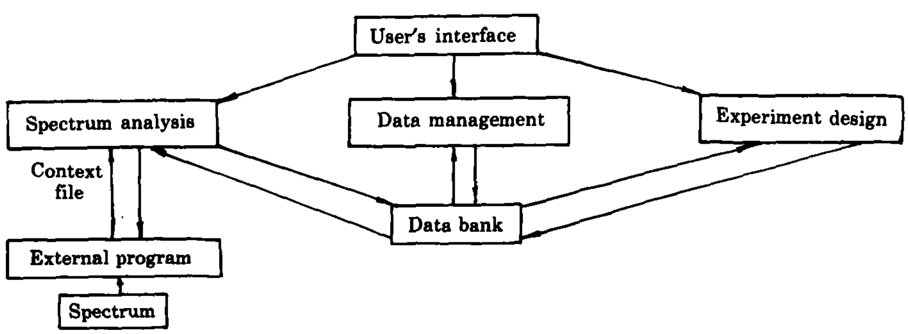

Fig.1 Frame of the ESNAA

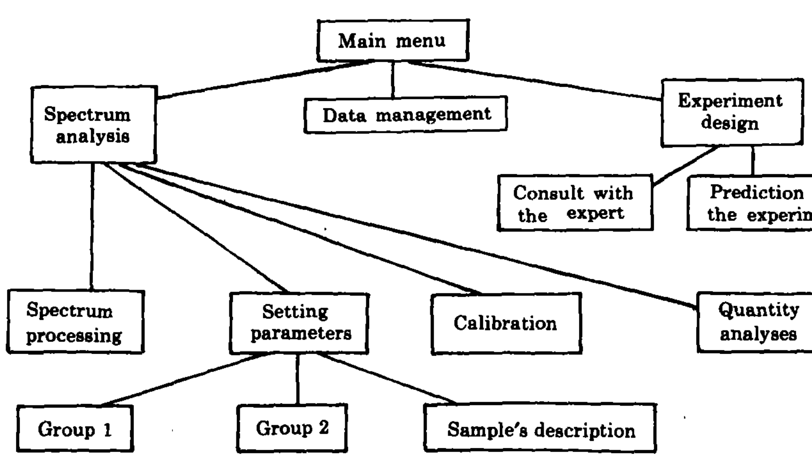

Fig.2 A part of the menu's tree in the ESNAA

2. Spectrum analysis

As many programs do, the data handling of gamma- ray spectra includes peak search, energy determination, calculation of the peak area and its statistical deviation, isotopic identification, quantity calculation for elemental concentration, as well as various corrections. The principles involved have been established before[2], only those points unique in our system are to be dealt with in this paper.

1) External spectrum data interface An external program written in Turbo C is used for pretreating the spectrum data files obtained from MCA, producing a context file holding the information of the positions, areas, statistical deviations and the energies of the peaks. The context file can be accepted by the GURU system. This program is automatically executed when we make a spectrum analysis by the ESNAA.

2) Isotopic identification There are three groups of rules built for the isotopic identification. They are the general rules, special isotopes' rules and the sample- type's rules. Fig.3 shows the logical diagram of the general rules.

The general rules are based on the characteristic gamma rays of radioisotopes and certainties of identification. In our isotope library, each gamma ray of a nuclide is followed by a certainty factor value. The variable ISOTOPE holding possible nuclide names for a particular energy is designed as a fuzzy variable in which more than one values can be stored with their certainty factors. When a nuclide matching a peak is recognized, its name with its certainty factor is then assigned to the ISOTOPE using the additive assignment calculator "+ =", or else using the subtractive assignment calculator "- =". If the name has already existed in the ISOTOPE before the operation, then its certainty factor will be changed in the probability sum style for the additive assignment or in the product style for the subtractive assignment. For example, if the peak of 1173.1 keV is found in a spectrum, the matching isotope is ^{60}Co with a certainty value of 90 for this peak, which is assigned to the ISOTOPE. Then another characteristic peak of 1332.5 keV will be sought. If it is found in the spectrum, the ^{60}Co will be additionally assigned to the ISOTOPE again with a certainty value of 90. The value of ^{60}Co in the fuzzy variable ISOTOPE is then of a new certainty: $90+90-90\times 90/100=99$. If the peak of 1332.5 keV does not exist in the spectrum, the ^{60}Co will be subtractively assigned to the ISOTOPE and the new certainty value will be calculated to be: $(100-90)\times 90/100=9$. The more the characteristic peaks are found in the spectrum, the higher the certainty of the isotope will be.

For the identification of some isotopes which are often interfered by other radionuclides, a special nuclide rule set was built. For example, the rule for the ^{198}Au checks the presence of the peak at 1408.03 keV and calculates the fraction of the ^{152}Eu at 411.2 keV. By removing the fraction, and the remaining area is more than 3 times the square root of the peak- area, the ^{198}Au exists with a certainty value around 90, otherwise with a certainty of zero.

For a nuclide whose identification can only be done by certain knowledge of the sample itself, the rules involved are stored in another set.

3) *Quality control* The reliability of the results is essential to an analysis. We have built a set of rules for quality control of an analysis in which standards of the multi- groups and multi- elements are used. A reference material has to be employed for this purpose. The logical diagram of the quality check is shown in Fig.4.

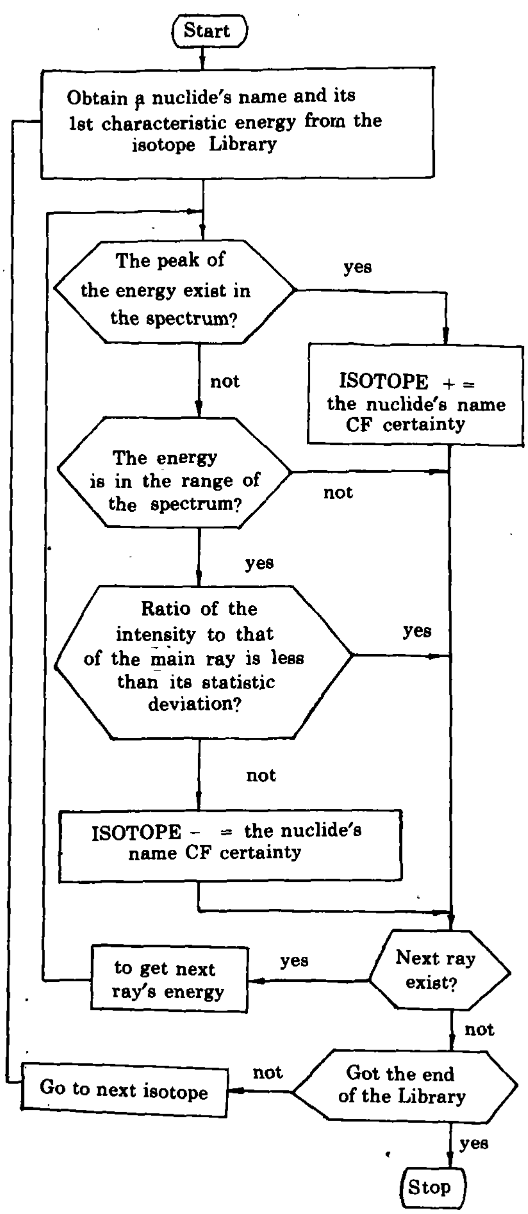

Fig.3 Logical diagram of the general rules

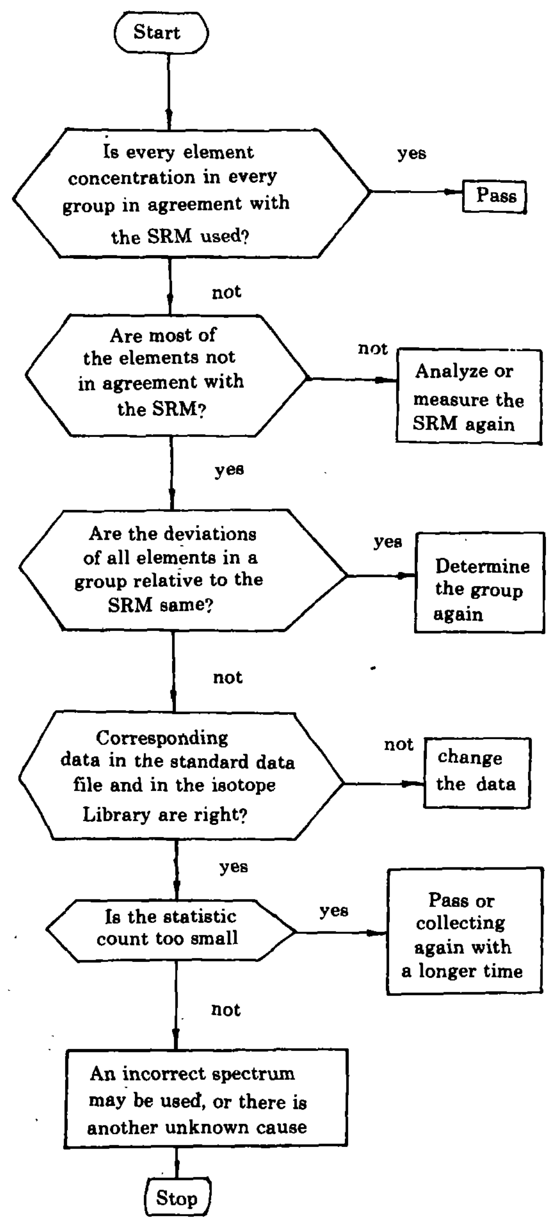

Fig.4 Logical diagram of the quality check

4) Choosing element concentration Before giving a formal report, we have to decide on the final result from multiple concentration data for each element. The general criteria are the highest certainty and the lowest deviation. That is, the element concentration from a characteristic peak with the highest certainty will be chosen.

3. Experiment design

This subsystem is composed of two independent procedures. One of them is based on expert experiences which are expressed in a set of parameters including type and weight of sample, system efficiency, neutron flux, irradiation time, decay time,collection time, detectable elements, radiochemical methods and if any, references. A rule set is employed for choosing the experiences, inferring, and answering inquiries from user. From the rule set, users will get suggestions of designing an experiment for a certain type of sample.

When the experiment condition, such as the neutron flux, is changed, other parameters will be calculated again by an optimization method. We set a target function as:

$$TF = c \cdot F1 + (1-c) \cdot F2 \tag{1}$$

$$F1 = \sum_{1}^{n} (r_i - R_i)^2 / R_i^2 \qquad i = 1,2,3,\ldots,n \tag{2}$$

$$R_i = f_e \cdot \varphi \cdot w \cdot [1 - \exp(-\Gamma_i T_{irra})] \cdot [1 - \exp(-\Gamma_i T_c)] \cdot \exp(\Gamma_i T_d)$$

$$r_i = f'_e \cdot \varphi' \cdot w' \cdot [1 - \exp(-\Gamma_i T'_{irra})] \cdot [1 - \exp(-\Gamma_i T'_c)] \cdot \exp(\Gamma_i T'_d)$$

where the f_e, φ , w, T_{irra}, T_c and T_d represent respectively system efficiency, neutron flux, weight of sample, irradiation time, collection time and decay time, which are obtained from expert experience and stored in a data file. The f'_e, φ', T'_{irra}, T'_c and T'_d represent the newly calculated values. When the function *F1* gets the least, the corresponding set of parameters is considered to be the optimal effect.

$$F2 = A \cdot w + B \cdot T_{irra} + C \cdot T_c \tag{3}$$

where A, B and C are constants. We can define A as the cost per mg for the sample weight, B as the cost per hour for irradiation, C as the cost per hour for collection. *F2* represents the total cost of an experiment under a set of parameters. In most cases, we have to balance the quality and the cost. A weight factor c was set to adjust the fraction of the *F1* and *F2*.

Another independent procedure similar to the APCP program is used in this subsystem for experiment prediction.

4. Data management

The core of the subsystem is a data bank for storing the element concentrations. Three fields are used to describe the sample in each record, which are also used as key words to search for records. Common data processing functions are provided with a set of menus for users, and some special procedures, such as graphics, will be gradually built.

Ⅲ. FUTURE

It is expected that the ESNAA is able to do as many things for us as possible. We intend to add another subsystem to control MCA for automatic measurement. A sample exchange system has been installed in our laboratory, which is controllable by a computer. After the ESNAA is completed, all we have to do on the data processing in a measurement is input sample descriptions, thll what we want to do, and pick up the reports from the system.

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REFERENCES

[1] C.W.Holsapple and A.B.Whinston, Manager's guide to expert systems using guru, Dow Jones- Irwin, 1986.
[2] J.Ma, Fast data processing programme for neutron activation analysis on personal computer system, ICR- Report- 204- 89- 21, 1989.