An application of a simple computer program for neutron activation analysis

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Abstract: A simple computer program is designed for estimation of elemental concentration values in complex samples by neutron activation analysis technique. The program is applied for an Egyptian cement sample which irradiated at the Egyptian Research Reactor-1(ET-RR-1). The data obtained is compared with the reported values. The time consumed for such calculations has a remarkable reduction in comparison with the routine work.

Key words: neutron activation analysis; cement sample; Egypt

Introduction

Nowadays the neutron activation analysis technique is applied extensively for elemental analysis of complex samples. A rapid determination of estimating the concentration of each element in such materials is needed. Computer programmes applied for this purpose in many different places (Rubinson, 1949; Lewis, 1954; Friendlander, 1949; Seelman, 1981; Edgardo, 1978; Reus, 1985; Eissa, 1995).

In Egypt we have to apply such technique for our materials, and in this work a simple computer program is proposed and successfully applied for a cement sample.

1   Principles

The neutron activation analysis technique (NAAT) is based mainly on the formation of radioactive nuclides as a net result of neutron interaction with matter. The gamma-rays are emitted due to formation of the new nuclides during their decay. Such gamma-rays give a lot of information about the original element, it is used extensively in decay schemes construction(Edgardo, 1978) and in the mean time it characterises the element itself.

In NAA the gamma-rays obtained are used for qualitative and quantitative analysis of complex samples. This depends mainly on the properties of the gamma-rays such as the intensity of each line, and its energy. So, if the energy and the intensity of gamma-ray lines emitted due to thermal neutron capture in the nuclide of the elemental constituents of any material are identified, one can nominate each element and its concentration value could be estimated.

Many other parameters should be used and an empirical formula(Tsoulfanidis, 1983) include all of these parameters is applied as follows:

$$m = MA\lambda / \phi \sigma_e \varepsilon F I_\gamma N (1 - e^{-\lambda t_1})(1 - e^{-\lambda t_2})(e^{-\lambda t_3}), \tag{1}$$

where, m is the mass(in gram) of the trace element in one gram of the sample; M the atomic weight of the trace element(g/g atom); A the net peak area of the gamma-ray line; λ the decay constant of the nuclide(s^{-1}); ϕ the thermal neutron flux($n/(cm^2 . s)$); σ_e the thermal neutron capture cross-section(cm^2) of the element (e); ε the detector efficiency; F the fractional isotopic abundance of the target nuclide; I_γ the absolute intensity characterizing the trace radio nuclide; N the Avogadro's number(atom/(g. atom)); t_1 the irradiation time; t_2 the measuring time of the γ-ray spectrum; t_3 the time elapsed in transporting the sample to the detector.

It was very clear from this equation that lot of efforts should be done to have accurate results which needs long time.

In this work a simple computer program is designed especially to facilitate such complicated calculations and to minimize the calculation time.

2   Program description

The chart of their program is shown in Fig. 1. The program depends mainly on the calculation of the mass of each element and its concentration percentage value in complex sample.
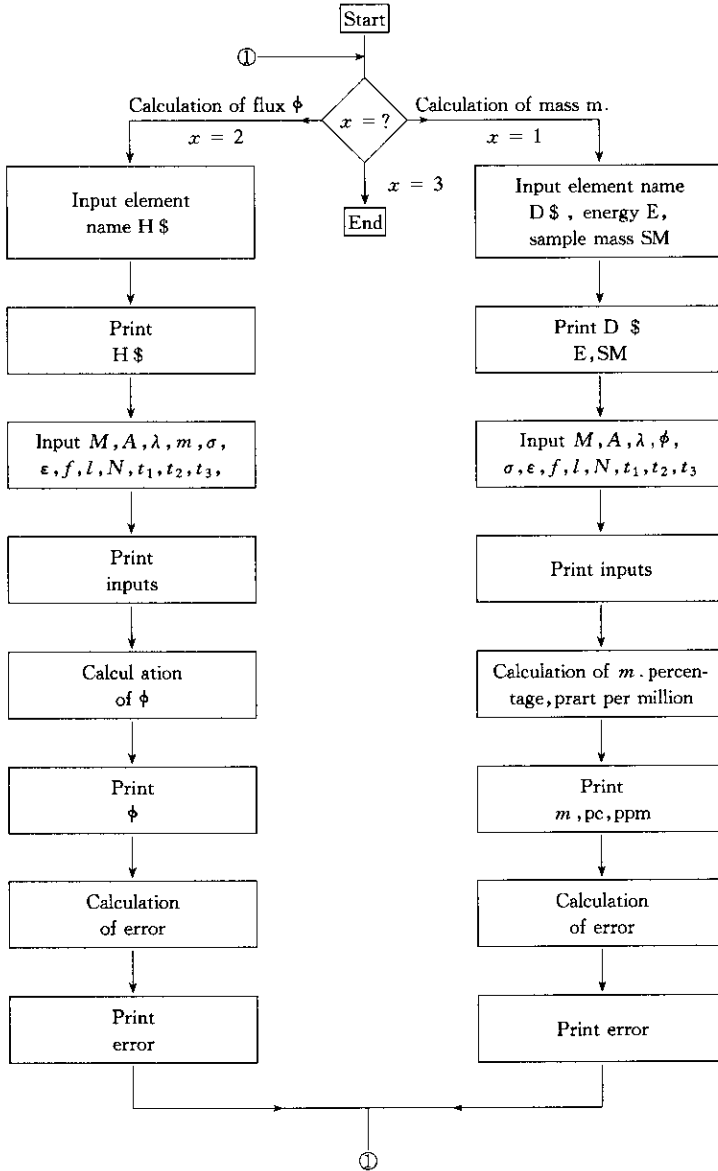

Fig. 1 Programme flow chart

The error in the value of m depends on the error of the quantities that comprise Eq. (1) such as A, λ, ε, I_γ, σ and ϕ. In the most general case, the standard error m is:

$$\sigma_m = (\partial m/\partial A)^2(\sigma_A)^2 + (\partial m/\partial \phi)^2(\sigma_\phi)^2 + (\partial m/\partial t)^2(\sigma_t)^2 + \cdots\cdots. \tag{2}$$

In practice, certain error are always negligible when compared to others. The quantities A, λ, I_γ and σ are known very accurately for most isotopes. Also, ϕ and ε can be determined with a known but small error. The error in the times can be negligible. Thus the major contribution to the error of m comes from the error of A, i.e., the error of the area under the peak. Assuming that σ_A is the only important error, the standard error of m is

$$\sigma_m = (\partial m/\partial A)\sigma_A, \tag{3}$$

or the relative error(Tsoulfanidis, 1983; Eq. (1)) is

$$\sigma_m/m = \sigma_A/A. \tag{4}$$

Thus, the relative error of m is equal to the relative error of A, in this case as included in our program.

3 Applications

In order to check the validity of this program a sample of cement was irradiated in a thermal neutron flux of (ET-RR-1) and the concentration of some major elements were obtained and compared with the reported values as follows:

(Mn) gamma-ray photo peaks have been collected by means of the HPGe detection system after irradiating 30 mg of a cement sample for 48h duration in a thermal neutron flux of 1.65×10^{11} n/(cm^2.s).

The above equation is applied manually and by using the suggested program using the same characteristic gamma-ray line shown in Table 1.

Table 1   The nuclear data of manganese used in this work

Element	Product isotope	Abundance, % F	Cross-section, cm^2	γ-line, keV	I_γ, %
Manganese	^{56}Mn	100	13.3×10^{-24}	847.6	98.9

Table 2 shows a comparison between the results obtained once manually and again by computer program and the reported values for manganese in cement sample, using the gamma-ray line at 847.6 keV.

Table 2 A comparison between the results obtained manually, by computer program
and the reported values for manganese in cement sample

Element	Manually conc. value, ppm	Conc. value by computer, ppm	Reported value, ppm(Eissa, 1995)
Manganese	288 ± 5	306 ± 5	305 ± 15

4 Conclusion

It is obvious that the program applied in this work can give in a very short time the concentration value which was in good agreement with that obtained manually and also to the reported values.

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