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Analytical estimation of the emitted gamma ray spectrum in the PGNAA method for bauxite ore of Jajarm mine

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Extended Abstract

Summary

The prompt gamma neutron activation analysis (PGNAA) method is a rapid, non-destructive, and well-established technique for quantitative and qualitative elemental analysis, widely used in pharmaceuticals, industry, and mining. A critical part of PGNAA is the analysis of the resulting gamma ray spectrum, which can currently be obtained or analyzed using four approaches: direct experimental measurement, Monte Carlo simulation, neural networks, and analytical estimation. This research focuses on the analytical estimation method, which simulates the spectrum based on the physical principles governing the interaction of thermal neutrons with the nuclei of elements in the sample, and the interaction of prompt gamma photons emitted from the activated sample with the material inside the desired detector. Advantages of this method include accurate determination of elemental peak positions including main, single-escape, and double-escape peaks. identification of smaller peaks overlapping with larger ones and determination of the main components shaping the spectrum due to multiple overlapping peaks. Another goal of this study is to identify a suitable detector for gamma spectroscopy in PGNAA testing of a bauxite ore sample from the Jajarm mine, to determine Al_2O_3 and SiO_2 percentages. Analytical spectra for the sample were acquired using three detectors NaI, HPGe, and BGO. Examination and comparison of these spectra showed that the NaI detector is the most suitable for this application, providing reliable spectral information for elemental analysis of the bauxite sample. This paper focuses on presenting and explaining the analytical estimation method for generating and interpreting gamma-ray spectra via PGNAA and selecting a suitable detector to determine the percentage of Al_2O_3 and SiO_2 in bauxite ore samples from the Jajarm mine. In brief, the analytical estimation method involves applying the principles and foundations of the physical interaction of thermal neutrons with the nuclei present in the sample and applying the principles and foundations of the physical interaction of gamma photons emitted from the sample with the material inside the desired detector.

Introduction

The necessity of quantitative and qualitative determination of elements using the neutron activation method in samples whose atomic nuclei do not produce isotopes with a known half-life upon interaction with thermal neutrons has led to the complementary PGNAA method being proposed alongside the conventional NAA method. In this paper, for analyzing or simulating gamma-ray spectra in the PGNAA method, an analytical spectrum estimation method is introduced and explained. The three previously reported methods for this analysis include direct experimental testing, the Monte Carlo method using the MCNPX code, and the neural network method. The most important feature that distinguishes this method from previous ones is its ability to determine the area under the peaks and their heights with adequate accuracy by revealing the details of the overlap of smaller peaks with larger peaks, clarifying the entanglement of two or more element peaks, and identifying the locations and heights of single-escape and double-escape photopeaks. In summary, by applying this method, there will essentially be no hidden details in the resulting spectrum.

Methodology and Approaches

The details of the research are as follows:

a. Applying the principles and foundations of the physical interaction of thermal neutrons with the specific nuclei of elements in rock samples, using data and reports from the International Atomic Energy Agency regarding thermal neutron capture cross-sections and the list of photon emission energies from those nuclei. Photon attenuation coefficients were also used to calculate the reduction in photon intensity passing through the rock sample, using values obtained from the XCOM database.
b. Principles and foundations of the physical interaction of gamma photons emitted from the activated rock sample with the material inside the desired detectors were applied, using the calculation of absorption efficiency derived from photon attenuation coefficients in the detector material via XCOM reports. Fixed G.E.B. coefficients for the relevant detectors, presented in previous reports, were also applied to perform Folding to achieve the true spectral shape.
c. Initial calculations were performed using Excel software, and peak heights versus energy graphs were plotted using Origin software.

Results and Conclusions

By observing and comparing the analytical graphs of the bar spectrum with the convoluted graphs that are much more similar to the actual shape of the spectrum, the exact locations of the desired photopeaks can be obtained, and the overlaps and entanglements of the peaks are also clearly visible. For example, in the Al N1 peak, the overlap of the K N1 peak by the Al N1 peak can be seen and a correction must be made for the height of the Al N1 peak of the potassium element. Moreover, the entanglement of the Al N2 and ^{56}Fe peaks can be observed on the right side of the spectrum, and by subtracting the number of iron photons entangled through ^{54}Fe from this peak, the correct number of photons of the Al N2 peak can be obtained and the percentage of Al is obtained. Of course, this is almost not needed in the HPGe detector due to the proper separation of these two peaks, but it is necessary in the other two detectors, practical in the sodium iodide detector, and impractical or very difficult in the BGO detector.