Software for the Quantitative Determination of Elements Mass Fractions in Samples by the Absolute Method of Neutron Activation Analysis

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Basic facilities of the Frank Laboratory of Neutron Physics (FLNP), Joint Institute for Nuclear Research (JINR), the IBR-2 reactor and the IREN facility, are actively used for carrying out of neutron activation analysis (NAA). The determination of elements content is performed by the comparative method of NAA using the software previously created at FLNP JINR. Sometimes, there is a necessity to check or complement the obtained results, for example, in the case of absence of the required element in the used SRMs or in the case of determining of the elements mass fractions with a large uncertainty, etc. To solve such problems, software was created that allows calculating the elements content in the samples by the absolute method of NAA.

A text file with nuclear constants was created. The file contains cross sections, resonance integrals, isotopic abundances, and half-lives of the isotopes to be determined.

The software uses report files with the results of the spectra of induced activity processing. These are report files for flux monitors, SRMs and investigated samples created by the Genie-2000 program.

At the first stage, thermal and resonance neutron fluxes are calculated. The created software calculates fluxes in two ways – by the cadmium difference method and by two zirconium isotopes – ^{95}Zr and ^{97}Zr.

Further, the elements mass fractions of the samples are calculated by the absolute method using isotopes activities from the report files. Calculations are performed by two significant energy lines for each isotope and by maximum of four spectra measurements for each sample. The results of calculations for each sample are saved in text files. A summary table of results for whole sample set is created using these files. It is possible to save the created summary table to a file with MS Excel format for further work.

The developed software allowed to get rid of routine long-term manual calculations, to increase productivity, significantly reduced the possibility of errors due to the human factor.