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PREDICTION OF NUCLEAR PROPERTIES OF ISOTOPES

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The creation of a software model for predicting the nuclear properties of isotopes based on a phenomenological parametric model of nuclear masses is considered. The model allows calculating the mass excess and estimating the binding energy. The main requirements for the software implementation of the model are formulated, the structure of the input and output data is determined, and the mathematical dependencies for calculating the mass excess and derived nuclear characteristics are described.

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INTRODUCTION

In nuclear physics, an important place is occupied by the task of determining the properties of isotopes and predicting possible nuclear transformations. Mass excess, binding energy, nuclear stability, decay energies and particle capture are used to assess the possibility of nuclear processes, analyze the stability region of nuclides and build transformation schemes. These quantities are especially important for isotopes for which experimental data are incomplete, have significant uncertainty or are absent altogether.

Traditionally, nuclear characteristics are determined experimentally or taken from reference databases. However, such sources primarily cover known or estimated nuclides and cannot always be used as a full-fledged predictive model for as yet unexplored isotopes. For such cases, computational approaches are needed that allow obtaining preliminary estimates of nuclear properties based on a minimum number of input parameters.

One possible approach is phenomenological parametric modeling of nuclear masses, in which the mass-energy characteristics of an isotope are considered as functions of the number of protons and neutrons in the nucleus. Such a model does not replace high-precision experimental tables or complex microscopic calculations, but can be useful for preliminary predictions, training analysis, and automated processing of large numbers of isotopes.

The aim of the work is to develop a software model for predicting the nuclear properties of isotopes to calculate the mass excess, binding energy, and energy characteristics of the main nuclear transformations based on the nucleon composition of the nucleus.

1. NUCLEAR TRANSFORMATIONS AND METHODS OF THEIR PREDICTION

Prediction of radioactive decay patterns is important for many applications [1]. The most common methods used to model and predict these processes include empirical, semi-empirical, and theoretical models.

Empirical methods for predicting decay schemes are based on statistical analysis of a large number of experimental data. This approach allows to obtain general patterns and correlations that determine the paths of nuclear transformations. The main advantage of empirical models is their relative simplicity and sufficiently high accuracy for most practical problems. However, these models have limited applicability for predicting reactions that go beyond the already studied isotopes [2–4].

Semi-empirical methods combine elements of empirical and theoretical approaches. They are based on theoretical equations, the parameters of which are selected using experimental data. A well-known example of a semi-empirical method is the Weizsäcker model, which takes into account the influence of various factors on the stability of nuclei, such as the Coulomb interaction, the asymmetry of the nuclear composition, the surface energy and the spin binding energy [5]. Such methods allow predicting the properties of nuclei and their decay patterns with sufficient accuracy even for poorly studied isotopes [5, 6].

Theoretical prediction methods are based on fundamental physical principles and equations of nuclear physics, in particular quantum mechanics and the nuclear shell model. These models include detailed calculations of the structure of nuclei, binding energy, nuclear states and probabilities of various types of decay. Theoretical models allow predicting the behavior of even those isotopes that have not yet been obtained experimentally [6, 7]. One of the most common theoretical models is the shell model of the nucleus, which takes into account the structure of the energy levels of nucleons in the nucleus. It is thanks to this model that it was possible to explain the existence of the so-called "magic numbers" of protons and neutrons, at which nuclei exhibit special stability.

For practical prediction of decay schemes, computer methods based on numerical calculations and simulation modeling are often used [8–11]. Computer models allow taking into account a large number of parameters and complex interactions between nuclei. They are able to effectively process large data sets and quickly predict the paths and products of nuclear reactions. A popular

approach is the use of the Monte Carlo method, which is used to simulate random processes of radioactive decay and allows obtaining statistical characteristics of predicted transformations with high accuracy [9].

To predict the nuclear properties of isotopes, it is necessary to predict those that determine the stability of the nucleus and the possibility of its transformations [2–4].

The first and main property is the mass of the nucleus, which determines the binding energy of the nucleus and the energy potential of nuclear reactions [2, 3].

The second key parameter is the nuclear transformation energy, or Q-value of the reaction [2, 3]. If the transformation is energetically disadvantageous, it will not occur spontaneously and further calculations become meaningless.

The third parameter is the stability of the isotope. An isotope can be stable, β-unstable, α-unstable, neutron-excessive, or proton-excessive [1, 4]. If the isotope is unstable, it is necessary to calculate a fourth parameter, the half-life, which determines how quickly the decay process occurs [1, 3].

Comparing different decay rates allows us to calculate the fifth parameter – the probable decay channels and daughter nuclei [8], i.e. to know what exactly the isotope will transform into.

To do this, it is necessary to know two basic parameters: the number of protons Z and the number of neutrons N [2, 3]. The ratio between N and Z is one of the main factors of nuclear stability. All other parameters can be obtained based on these parameters [12].

For preliminary prediction and research model, the accuracy is sufficient to correctly determine the general patterns: the stability region, the most probable decay channels, the approximate reaction energies and the order of magnitude of the half-life [12]. In this case, the mass defect error of the order of units of MeV can be acceptable if the model correctly reproduces the general form of the dependences and does not contradict the known decay series [6, 7].

For accurate nuclear physics, medical, or engineering calculations, reference experimental or estimated data from verified databases are required, which allows calculations to be made with an accuracy of up to 0.1 MeV [2–4].

2. MAIN MATHEMATICAL DEPENDENCES OF THE MODEL

The model is based on a computational kernel, the task of which is the mathematical relationship between the composition of an isotope and its mass. The user input is the number of protons and the number of neutrons Z, N, or for convenience, the number of protons and the total number of nucleons Z, A.

The main input quantity is the mass excess of the Me(Z,N) isotope in MeV, which allows us to calculate all other additional input data:

$M_a(Z,N)$ – the atomic mass of a neutral atom in atomic mass units u;

$M_n(Z,N)$ – mass of the nucleus without electrons;

$B(Z,N)$ – nuclear binding energy;

$\delta m(Z,N)$ – nuclear mass defect;

B/A – specific binding energy, i.e. binding energy per nucleon;

Q – nuclear transformation energy;

S_n, S_p – neutron and proton separation energies;

S_{2n}, S_{2p} – the energy of separation of two neutrons or two protons, if the corresponding functions are added.

This, in turn, allows us to assess the energy potential of the main nuclear processes:

$n-emission$ neutron radiation;

$n-capture$ neutron capture;

$p-emission$ proton radiation;

$p-capture$ proton capture;

$\alpha-emission$ alpha decay;

$\alpha-capture$ alpha particle capture;

β^-– beta-minus transformation;

β^+– beta plus transformation;

EC– electronic capture.

The model is based on several basic principles:

– for each element, there is a certain reference minimum value of the mass excess Mz(Z), which corresponds to the lower part of the isotope curve for the element with proton number Z;

– for each element, there is a number of neutrons at which the mass excess is minimal – Nz(Z);

– the deviation of the actual number of neutrons N from Nz(Z) is described by two different branches – left and right. The left branch corresponds to a lack of neutrons, the right branch corresponds to an excess of neutrons;

– in addition to a smooth parabolic shape, local corrections are required that reproduce kinks and features associated with shell effects;

– it is necessary to take into account the evenness of the number of neutrons, because even and odd N give a systematic alternation of mass values.

To organize calculations, simple auxiliary functions are introduced: right linear function (H_i), left linear function (H_d), right transition function (T_i), left transition function (T_d), trapezoidal function (S_i), weighting function for local corrections (K_w), parity function (P).

The position of the peak of the isotope curve (Nz) determines the number of neutrons that provide the minimum mass excess for isotopes with the same Z, and Mz gives the mass excess value for that point.

For this, the left and right coefficients are calculated (K_l, K_r), parabolic part (Sq), and local corrections that are needed to reproduce kinks that are not described by a smooth parabolic dependence (Cl, Cr).

Basic function for calculation $Me(Z,N)$ returns mass excess to MeV summing up all the components:

$$Me(Z,N) = Mz(Z) + Sq(Z,N) + Cl(Z,N) + Cr(Z,N) + 1.088P(N).$$

For conversions between units of measurement and derived quantities, conversion formulas are used.

Mass number:

$$A = Z + N.$$

Atomic mass of a neutral atom:

$$M_a(Z,N) = A + \frac{Me(Z,N)}{931.49410372}.$$

Reverse transition:

$$Me(Z,N) = [M_a(Z,N) - A] \cdot 931.49410372.$$

Nuclear binding energy:

$$B(Z,N) = ZMe(1,0) + NMe(0,1) - Me(Z,N).$$

Energy equivalent of a mass defect:

$$\delta mc^2 = B(Z,N).$$

Mass defect in atomic units:

$$\delta m(u) = \frac{B(Z,N)}{931.49410372}.$$

Specific binding energy:

$$B_A(Z,N) = \frac{B(Z,N)}{A}.$$

The calculation of the reaction energy is carried out according to the general formula

$$Q = \sum Me_2 - \sum Me_1$$

according to which energy is defined as the difference between the mass characteristics of the initial and final states. For changes in the number of neutrons and protons (z_p, n_p) the general entry for radiation would be:

$$Q_{em} = Me(Z,N) - Me(Z - z_p, N - n_p) - Me(z_p, n_p).$$

To capture:

$$Q_{cap} = Me(Z,N) + Me(z_p, n_p) - Me(Z + z_p, N + n_p).$$

Then the main reactions should be represented in separate expressions.

Neutron radiation:

$$Q_n = Me(Z,N) - Me(Z,N-1) - Me(0,1).$$

Neutron capture:

$$Q_{n-cap} = Me(Z,N) + Me(0,1) - Me(Z,N+1).$$

Proton radiation:

$$Q_p = Me(Z,N) - Me(Z-1,N) - Me(1,0).$$

Proton capture:

$$Q_{p-cap} = Me(Z,N) + Me(1,0) - Me(Z+1,N).$$

Alpha radiation:

$$Q_\alpha = Me(Z,N) - Me(Z-2,N-2) - Me(2,2).$$

Alpha capture:

$$Q_{\alpha-cap} = Me(Z,N) + Me(2,2) - Me(Z+2,N+2).$$

A special case is β-processes because the electron and positron are not nuclide components of the (Z,N) type.

Beta-minus:

$$Q_{\beta^-} = Me(Z,N) - Me(Z+1,N-1).$$

Beta-minus:

$$Q_{\beta^+} = Me(Z,N) - Me(Z-1,N+1) - 2m_e c^2.$$

Electronic capture:

$$Q_{EC} = Me(Z,N) - Me(Z-1,N+1).$$

also

$$m_e c^2 = 0.51099895069 \text{ MeV}.$$

Thus, these basic dependencies are completely sufficient to create a complete model of mass excess and its changes based on the number of nucleons alone.

3. RESULTS

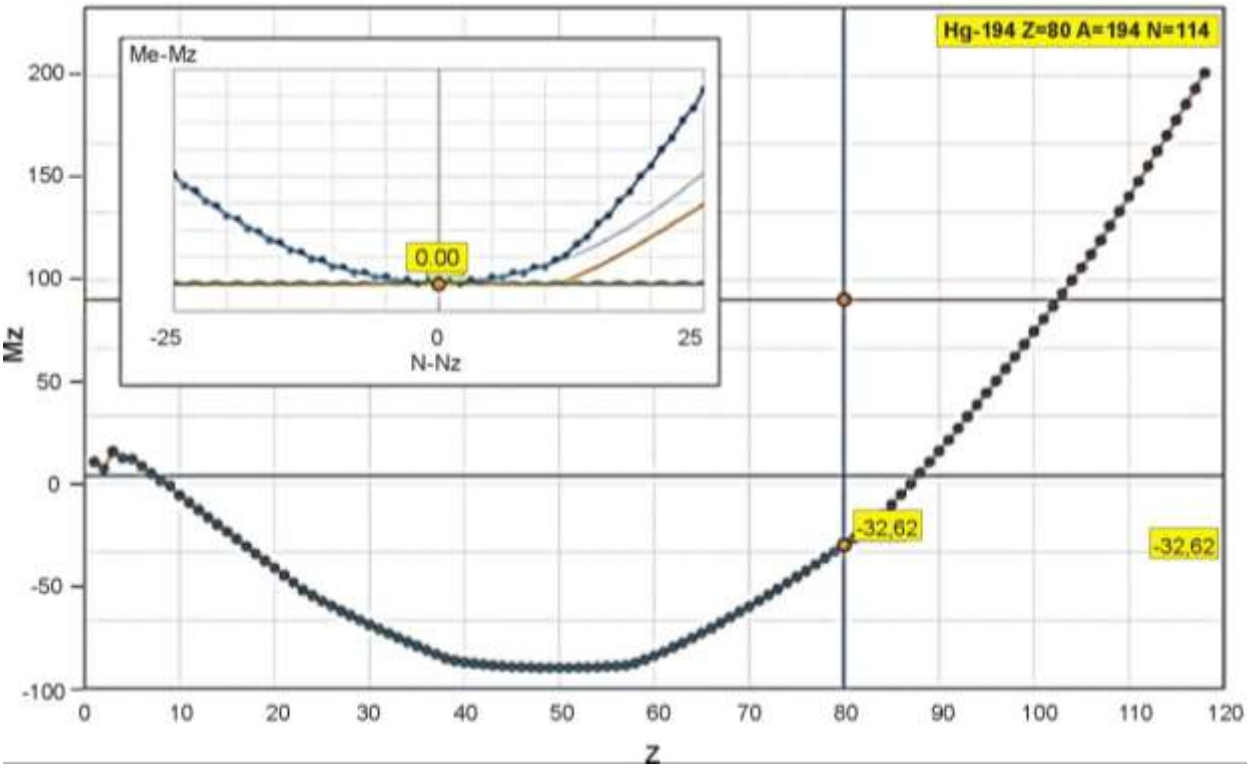


Fig. 1. Minimum excess mass value

Fig. 1 shows one of the basic dependencies of the model – the minimum excess mass value for the elements. In fact, this is a reference line that defines the lowest part of the mass surface for each value of Z. It is needed so that the model does not simply count individual isotopes, but reproduces the general shape of the nuclear stability region.

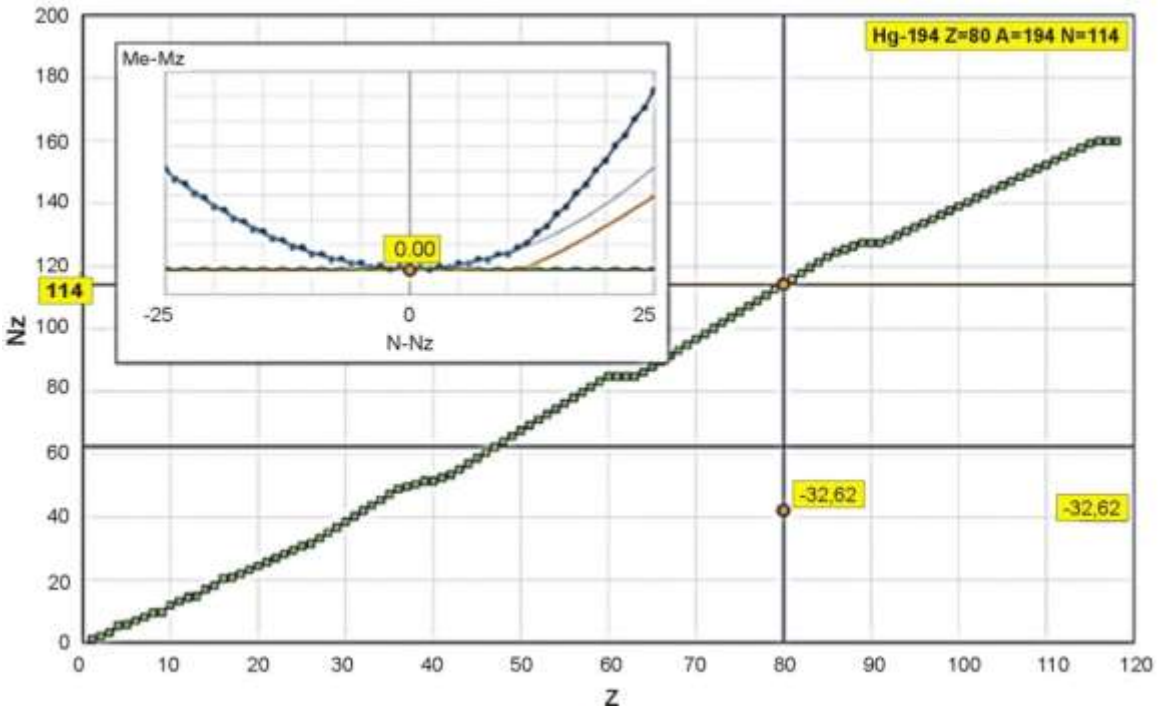


Fig. 2. The value of the optimal composition

Fig. 2 shows the definition of the optimal composition of the nucleus. The function Nz determines the number of neutrons that corresponds to the minimum mass excess for a given Z. This is important because stable isotopes do not lie simply on the line N = Z. For heavy elements, the stability region shifts towards the excess of neutrons, and the model must take this into account.

CONCLUSIONS

As a result of the work, the main nuclear properties of isotopes were studied, modern approaches to modeling nuclear transformations and predicting the properties of isotopes were analyzed, and the advantages and limitations of semi-empirical, macroscopic-microscopic, microscopic, and statistical models of nuclear masses were analyzed.

The use of a phenomenological parametric model as a basis for calculating the mass excess of isotopes, using a minimum number of physically justified parameters, is justified.

The structure and parameters of the model of the main nuclear transformations are agreed upon and a calculation algorithm based on this model is proposed.

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ПРОГНОЗУВАННЯ ЯДЕРНИХ ВЛАСТИВОСТЕЙ ІЗОТОПІВ

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Розглянуто створення програмної моделі для прогнозування ядерних властивостей ізотопів на основі феноменологічної параметричної моделі ядерних мас. Модель дозволяє розраховувати масовий надлишок, оцінювати енергію зв'язку. Сформульовано основні вимоги до програмної реалізації моделі, визначено структуру вхідних і вихідних даних, описано математичні залежності для розрахунку масового надлишку та похідних ядерних характеристик.