Perspectives of the some computer methods using for the transactinide experimental and theory data treatment

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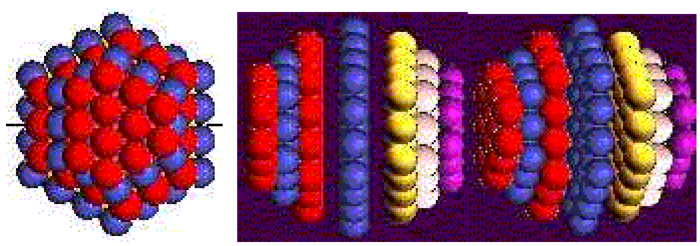
Spontaneous radioactive decay of nuclear belongs to that category of the natural phenomena which reasons, by virtue of complexity of objects, have not received a strict scientific explanation yet. The advanced interest to this phenomena, as having major significance in human life, results, on the one hand, in accumulation of the comprehensive experimental material and, with another hand, in the plenty of theories about its physical nature. On the basis of theories the different mathematical models are created for experimental data processing and the nuclear behavior predicting. Computer modelling is modern and quickly developing method for the complicated physical and chemical processes studying, both for the treatment of the experimental data bulk, and for the theoretical researches. Therefore it seems to be useful to apply some computer methods to the radioactive decay processes investigating.

Spontaneous radioactive decay such as α -decay and spontaneous fission are the properties intrinsic in main to heavy nucleus: actinides and transactinides. One of the problem in modern nuclear physics and radiochemistry is to establish dependence between nuclear composition and half-life of radioactive isotopes and to predict stability of still undiscovered nucleus. Theoretical calculations of nucleus stability are based on the two main physical models: 'liquid -drop' and shell model [1]. The essence of these models is reduced to consideration of nuclear binding energy and calculations for α-particles or fragment particles after spontaneous fission of the potential barrier penetration probability that radioactive decay constant is depended on.

Properly process of nuclear disintegration is described by "liquid-drop" model. On analogy to a drop of a liquid any small distortion of the nuclear sphere will be associated with the surface tension and Coulomb energies increasing so the total nuclear binding decreasing. The main conclusion of this model was that fissionability of nucleus may be expected to correlate with parameter Z^2/A . By several semiempirical energy equations this parameter was calculated as 45-49. Thus all nuclei with $Z^2/A > 49$ are expected to undergo fission instantaneously and limit is set to the synthesis of transuranium elements at $Z \approx 110\text{-}120$.Thought the liquid-drop model explains many features of the nuclear disintegration process some of the experimentally facts could not be interpreted in this framework, especially the "magic numbers" of protons and neutrons at which nucleus are most stable and existence of heavy and superheavy elements. Dependence between number of the nucleons in nucleus and its stability is well described by the shell model, where shell structure in nuclei is proposed as analogous to the electron structure in atoms. The quantum calculations of energy levels showed that the filled shells have numbers of neutrons or protons equal to "magic numbers" and that nuclei are more stable which compositions are closer to the filled shells. Influence of the "shell effects" is important for all nuclei, however for the heaviest nuclei the most essentially. The introduction of the shell term in the formula for energy of a nucleus [2] has essentially improved the convergence between calculations and experimental data of the nuclear stability . Theoretical calculations using the unified "drop-shell" model has allowed to predict an opportunity of existence of unknown stable superheavy nuclei - "islands of stability", presumably in the area of Z=114. The experiments which have been carried out by scientists from Lawrence Berkeley National Laboratory (USA) , Flerov Laboratory in Dubna (Russia) and Research Center Rossendorf (Germany) have confirmed theoretical prediction [3] . Though the "island of stability" is not achieved yet, experimenters have precisely shown, that influence of neutron environment with N=162 (the next filled shell predicted) on half-life of the synthesized nucleus already is observed [4] . Here interests of theorists closely adjoin to interests of experimenters as on the basis of theoretical predictions of "islands of stability" the new techniques of synthesis were development and new superheavy elements have been produced.

Nevertheless it seems to be noticed that functional dependence between nuclear composition (Z and A) and stability of isotopes is so complicated that in correspondence mathematical models semiempirical functions and parameters are usually used and sometimes experimental and calculation data are diverging. In this connection it seems to be useful to apply computer modelling methods to the treatment of the heavy elements experimental data and theoretical models complement and evolving.

For that purposes we selected database and interactive graphics computer methods and created the programs RADCHEM 1.0 and RADCHEMGRAF 1.0 presented here. RADCHEM 1.0 is the database containing as experimental data about isotopes (half-life, a kind of radioactive decay, decay energy characteristics, products of decay etc) as theoretical models explaining received experimental data. Submitting the data in such form is convenient for statistical and correlation analysis. So the investigations for actinides isotopes showed, that at the specified sampling of the unstable nucleus configurations by the probability theory and combinatorial numerical method the correlation between half-life and number of matching of protons and neutrons laid out above the last filled shell could be observed. RADCHEMGRAF 1.0 is the 3D-graphic program for the visual representation and analysis of several computed configurations of nuclei. As shown on the figure nucleus are imaged using mathematical model of “spheres density packing” (as more corresponded to nuclear “liquid drop –shells” model).



Figures 1-3. Surface energy differences for number of configurations for actinides isotopes calculated by the RADCHEMGRAF 1.0 also correlated with its stability.

We believe that the development of presented computer method lead to carry out more accurate calculations and to obtain further information, which could be supplement to the theoretical models. Then it will be perspective to apply RADCHEM 1.0 and RADCHEMGRAF 1.0 for education of specialists in radiochemistry as information resource and visual aids . For this purposes it seems to be very useful to replenish RADCHEM 1.0 with data for transactinides and we hope that TAN 03 Conference open up opportunities to make it.

References

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