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MEASUREMENT AND EVALUATION OF NUCLEAR DATA FOR FISSILE AND FERTILE ISOTOPES: AN IMPORTANT TASK OF PRESENT-DAY PHYSICS

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ABSTRACT

This paper considers questions relating to the analysis of neutron cross-section measurements and measurements of transmission functions for heavy isotopes in the unresolved resonance region. It also considers questions connected with the evaluation of group constants. Conclusions are drawn regarding the need to set up new experiments for measuring transmission functions. [16 references]

Considerable progress is now being made with nuclear data for fast reactors. In the early 1970s work carried out largely at the Institute of Physics and Power Engineering (by L.N. Usachev, M.F. Troyanov, M.N. Nikolaev and others), and also abroad, made it possible to formulate criteria for permissible margins of error in nuclear data based on the accuracy required in criticality and breeding parameters. A status was subsequently established for nuclear data which, together with analyses of integral data, led to a re-evaluation of these parameters that unfortunately turned out to be unfavourable [1]. The elucidation of this situation, as reflected in the nuclear constants handbook, at the same time reduced the urgency of the data problem.

Indeed, the development of a future large fast power reactor (the main line of future developments in nuclear power technology) is being held up at present not so much by inaccuracies in nuclear data as by technological problems, against the background of which research into core and blanket physics appears on the whole to have been completed. Nevertheless, it has not so far been possible to work out the basic design features of the fast reactor power plants now in operation (such as BN-350 and BN-600) without direct modelling on critical facilities, and even under these conditions the design specifications have had to allow wide margins for error compensation. Considerable practical difficulties are involved in full-scale simulation of the large BN-1600 plutonium breeder reactor, so that the accuracy of reference data will be a vital factor in determining the reliability of the design calculations [2]. This means that both microscopic and macroscopic experiments aimed at further reducing the uncertainties in the physical parameters of these reactors still have great importance. To see the truth in this one has only to consider a few of the

specific problems concerning nuclear data for uranium and plutonium isotopes in the resonance region of neutron energies. A full enumeration of the tasks facing nuclear physics at the present stage obviously would cover a far greater number of nuclei and comprise a broader range of energies. It is now a matter of urgency to prepare the groundwork for such an enumeration, which would reflect both the present state of nuclear data and new lines of enquiry in reactor physics. All this must be done if we are to counter opinions sometimes expressed concerning the so-called "genre crisis" in the nuclear data field.

Influence of the resonance structure of neutron cross-sections on reactor characteristics. The boundaries of the unresolved resonance region, where the effects of resonance self-shielding are fairly noticeable, depend on the type of nucleus. For ^{238}U the region lies roughly between 5 and 50 keV, while for fissile nuclei it lies between a few hundred electron-volts and 20 keV. Neutron reactions within these intervals make a substantial contribution to the neutron balance in a fast reactor. In the core of a future fast breeder reactor, approximately 70% of ^{239}Pu radiative capture events, 50% of ^{238}U radiative capture events and 30% of ^{239}Pu fission events take place at neutron energies below 20 keV. For this reason resonance self-shielding of the neutron cross-sections for heavy nuclei has a powerful effect on the reactor physics parameters, and a dual effect on the Doppler coefficient of reactivity: through that part of the neutron spectrum which depends on the mean effective cross-sections, and through the temperature dependence of the resonance structure of the neutron cross-sections. At the transition to the blanket zone the effects of resonance self-shielding increase owing to softening of the neutron spectrum, which makes the neutron flux and integral parameter space-energy distribution calculations less reliable, especially as so little attention has been paid to shield physics research on experimental rigs. Finally, we should mention the important role played by the transport cross-section in calculating heat-release fields throughout the reactor. The effect of resonance self-shielding of the total (and transport) cross-section is considerable, and the resultant inaccuracy leads to further uncertainty in determining technological parameters.

A rigorous quantitative evaluation of the different error types associated with the resonance structure of the neutron cross-sections, essential new experiments, the accuracies required in these experiments - all these things call for special methodical analysis which to a large extent has not yet been carried out. However, such an analysis is no easy task, requiring as it does a thorough and detailed study both of the relevant nuclear and reactor physics problems, and of questions related to the evaluation and preparation of group constants. Some of these matters have already been considered [3-8]. In what follows we shall confine ourselves to a number of rough evaluations of specific nuclear data inaccuracies and to recommendations for setting up the required experiments.

Group constant errors in the neutron resonance region. A multigroup calculation of the core neutron balance in the so-called B^2 approximation can be carried out rigorously in the sense that it permits accurate preparation of macroscopic group constants, provided the microscopic neutron cross-sections are known. Therefore, when considering inaccuracies in the data for reactor calculations, we must differentiate between the errors in primary nuclear data, errors arising from the approximations used in preparing the group constants, and inaccuracies in evaluation procedures which violate the established formalism or lead to internal inconsistencies from the neutron cross-section theory point of view. In all papers concerned with formulating nuclear data accuracy requirements the last two types of inaccuracy have been assumed to be absent. In other words, it was assumed that the required accuracies were related to the self-shielded average cross-sections or to the average cross-sections, if the resonance self-shielding factors were known exactly. Such a formulation is incorrect for the region of unresolved or poorly resolved resonances, since the uncertainties in the resonance self-shielding factors are comparable with or greater than the errors achieved in the mean cross-section measurements. Experience with experimental evaluations of resonance self-shielding factors indicates that deviations of 10-15% from the standard values are normal.

The task of the experimenters can be characterized most accurately as measuring the effective mean cross-sections as a function of the thickness of a filter sample. Looked at this way a nuclear physics research programme takes on a new meaning. The reformulation of the accuracy requirements for these measurements is obvious: the errors in the measured self-shielded (effective) cross-sections must not exceed the previously established mean cross-section errors, which makes the measurement conditions more rigorous. The situation is complicated by the fact that a high level of evaluation accuracy is needed not only in the self-shielding factors themselves but also in their temperature increments. These it would be possible to determine from measurements of the transmission functions at various sample temperatures. However, this is a complex procedure, and it is therefore more expedient to determine the temperature increments of the resonance self-shielding factors by calculations based on a theoretical model with optimized parameters evaluated from all the available experimental data. Thus we can draw the conclusion (which, generally speaking, is not a new one) that the theoretical model has an important part to play in the task of evaluating group constants.

The situation which has emerged with regard to the measurement and evaluation of group constants for fertile material isotopes in the unresolved resonance region is not altogether satisfactory. Let us begin by looking at the conditions for preparing group constants. The least dangerous of the approximations usually made would seem to be the approximation of constant collision density, although as we come to lower neutron energies local discrepancies can become significant [6].

A physically less acceptable and mathematically poorer approach is the dilution cross-section (σ_o) approximation. The error in this approximation, particularly in the Doppler increments, is hard to predict. At the present stage there is every reason for rejecting both this approach and also the associated subgroup approximation approach, and for going over to a consistent concept with regard to group functions for cross-section distributions $P(\sigma_t)$ and $x(\sigma_t)P(\sigma_t)$ (where σ_x are the partial cross-sections). This more general information on cross-section structure is precisely what is to be found in the results of transmission function measurements:

$$T(n)=(1/\Delta u)\int_{\Delta u} \exp(-\sigma_t n)P(\sigma_t)d\sigma_t \ ;$$

$$T_x(n)=(1/\langle\sigma_x\rangle)\int_{\Delta u} \sigma_x(\sigma_t)\exp(-\sigma_t n)P(\sigma_t)d\sigma_t \ .$$

The same information can be obtained from statistical neutron cross-section theory. Within such a concept, evaluations of all types of data become self-consistent and their extrapolation to high temperatures is justified. Macroconstant preparation then reduces to a successive convolution based on the physical premise of non-correlatability of isotope cross-sections having the numbers i and j:

$$P_{i+j}(\Sigma_t)=\int_0^\infty P_i(\Sigma_t-\Sigma_{tj})P_j(\Sigma_{tj})d\Sigma_{tj} \ ;$$

$$\Sigma_x(\Sigma_t)_{i+j}=\int_0^\infty \Sigma_{xi}(\Sigma_t-\Sigma_{tj})P_j(\Sigma_{tj})d\Sigma_{tj}+\int_0^\infty \Sigma_{xj}(\Sigma_t-\Sigma_{ti})P(\Sigma_{ti})d\Sigma_{ti}-$$

with a subsequent calculation of arbitrary functionals:

$$\langle f(\Sigma_t,\Sigma_x)\rangle=\int_0^\infty f\left[\Sigma_t,\Sigma_x(\Sigma_t)\right]P(\Sigma_t)d\Sigma_t \ .$$

Experience has shown that with approximately 100 nodes in a histogram representation of the functions $P(\sigma_t)$ and $\sigma_x(\sigma_t)$, primary information distortions are unidentifiable, and the problem can be raised of representing nuclear physics information relating to $P(\sigma_t)$ and $\sigma_x(\sigma_t)$ in the form of additional files, or perhaps in the form of approximating functions.

Theoretical models of neutron cross-sections and algorithms for calculation of functionals

The next step in the process of evaluating group constants - the theoretical model and the calculation algorithm - plays an exceptionally important role in the processing of the primary physical data. For example, the primary treatment of experimental data on transmission functions can be performed by the method of approximating functions (especially by the sub-group method) so as to have a direct evaluation of the cross-section moments. However, a more exhaustive analysis having a much higher scientific and practical value is based on the use of the neutron cross-section theory. Without a means of theoretical

calculation the very idea of creating an evaluated nuclear data library is inconceivable. Therefore, what gives rise to criticism is that the well-known ENDF/B system, whose format is taken as standard for international exchange, is based on formal algorithms for representation of data (on the basis of given parameters cross-section files are calculated, to which "correction backgrounds" need to be added) [9]. The approach to the problem of evaluation of files developed under the guidance of V.A. Kon'shin [10] with the use of physical models is more correct and efficient.

The main problem of analysing neutron data for heavy nuclei in the resonance region concerns the applicability of the single-level and multi-level formalisms. As we know, in the case of non-fissile heavy nuclei in the resonance region for neutron energy, it is legitimate to use a simple theoretical model (Breit-Wigner formalism) because of the comparatively low level density and weak inter-resonance interference effect. Consequently, the analytical technique whereby one considers the Doppler broadening can be used. The method of calculating functionals developed on this basis in Ref. [11] uses numerical integration over the level-statistical distributions of the fixed state with the application of few-point quadrature formulae, followed by convolution of the superposition of states by the sub-group method. This method is efficient when preparing group constants for non-fissile isotopes. Similar methods have been developed abroad, but their use in the case of fissile nuclei is not acceptable from the physical standpoint because of the strong inter-resonance interference effects. Nevertheless, all studies involving the calculation of the cross-section functionals for fissile nuclei are based on the Breit-Wigner formalism with allowance being made for the Doppler effect through Ψ - and X - functions in the approximation of a weak pair interference of resonances.

This problem was first solved within the framework of the multi-level R-matrix theory (Reich-Moore formalism) by the Dubna group when processing transmission functions for fissile isotopes [12, 13]. They developed a method of statistical modelling of the neutron cross-section structure which had only been used before within the framework of the Breit-Wigner formalism. The main difficulty in using the R-matrix formalism in this problem was the large amount of computer time needed for the numerical method of calculating the Doppler broadening. In order to overcome this difficulty, the present author suggested the idea of considering the Doppler effect also on the basis of the statistical test method. The algorithm for evaluation of the functions $P(\sigma_t)$ and $\sigma_x(\sigma_t)$ and of the various functionals of the observed cross-sections involves realization of a random selection of parameters for the resonance set (superposition of the levels of all the necessary states) over a sufficiently wide lethargic interval ΔU, followed by obtaining the statistics by means of multiple neutron "emission" from given points u_i (with step Δu) having a spread with respect to the random Doppler broadening function. The point of this is that the detailed

scanning required in this approach is determined by the criterion of the number of points on the Doppler width (and not on the resonance width at zero temperature), and for an actually chosen step $\Delta u = 20$ MeV the error due to piecewise linear representation of the Doppler function plays virtually no part. Thus, by consistently applying the Monte Carlo method to calculate the cross-section functionals we can get rid of the problem of quadrature formulae and reduce the calculation error to the error of test statistics, which can be evaluated easily.

Applying the principle of correlated selection to this approach, we can obtain the evaluations of functionals at once for several temperatures together with a set of perturbed values for the average resonance parameters. Averaging over resonance statistics is performed by multiple realizations of the random selection of resonances in the Δu interval, which can be shifted in terms of energy for the purpose of "smooth" averaging or can be determined for local evaluation of the average functionals. This method was used with the BEhSM-6 and ES-60 computers and proved to be highly efficient.

The proposed statistical method of considering the Doppler effect can be applied also to the study of the so-called gas approximation. In view of the importance of improving the industrial technology used to fabricate mixed oxide fuel, the Doppler effect as a physical phenomenon affecting the safety parameters of fast reactors should be studied from any angles. Here it is possible to identify the following causes of errors in group constants, which depend on: (1) nuclear physics parameters and model approximations (they are refined by experiments to determine the average cross-sections and transmission functions); (2) preparation of group constants - approximation of constant collision density and the σ_o-formalism (they are refined by detailed calculations); (3) gas approximation and the Debye temperature values (they are refined in slow-neutron measurements of double-differential cross-sections and by calculations by the solid-state theory). With regard to the last effect, we should mention the risk of an error due to the high uncertainty of the Debye temperature and to the latter's dependence on changes in the fuel microstructure and composition during burnup.

Errors in group constant evaluations

The formal procedure for evaluating errors in group constants (neutron cross-sections and resonance self-shielding factors) is to obtain the covariance matrix of the evaluated average resonance parameters and, with the help of sensitivity coefficients, to find the covariance matrix of the group constants. In practice this procedure is not always used since the types of group constant can be evaluated by a variety of methods and calculation procedures. A typical difficulty encountered when evaluating group constant errors is the uncontrolled distortions due to the inaccuracy of the theoretical model. Thus, as was pointed out above, the use of the Breit-Wigner formalism to describe the neutron

data for fissile isotopes is not justified. The fact of model distortion may be less obvious (for example, introduction of a physical hypothesis which is outside the framework of the generally accepted theoretical concepts). Another typical problem is the dependence of the average resonance parameters on neutron energy. In fact, for the R-matrix theory such parameters as the scattering radius and reduced strength functions are external parameters, about which conclusions can be drawn only from the standpoint of a more general theory. These parameters are normally regarded as constants. At the same time, the optical model predicts a monotonic dependence of these parameters on neutron energy.

There is one more important reason for distortion of the evaluations. It occurs during the correction of group constants under inconsistent or statistically unjustified conditions. An example of this is the correction of the group constants for ^{238}U using the integral data on the neutron absorption cross-section on the assumption that the resonance self-shielding factors are exact quantities. This condition led to internal inconsistencies during the evaluation of the group constants for ^{238}U [2]. Refinement of the resonance self-shielding factors in the region of unresolved resonances requires additional information - first of all, from experiments with measurement of transmission functions and, if possible, self-indication functions under conditions where the thicknesses of the indicator sample are extremely small. Experimental data of this type indicate the need for reducing the resonance self-shielding factors of the absorption cross-section for ^{238}U [14]. The evaluations of their temperature increments may also contain systematic errors. In the case of ^{238}U, for example, the author's evaluations of the temperature increments of the effective absorption cross-sections $\Delta\sigma_c$ (300K→2100K) for σ_o = 100b are as follows: 5 mb (46.5-100 keV), 15 mb (21.5-46.5 keV), 45 mb (10-21.5 keV). This is appreciably higher than the tabulated values given in Ref. [2] (3, 10 and 35 mb, respectively). The magnitude of the error evaluated in this case is large for such a well-studied nucleus as ^{238}U. For fissile nuclei there is a greater danger of systematic errors in the resonance self-shielding factors.

The purpose of the present study was to discuss some methodological problems of analysing the set of experimental data available for neutron cross-sections and transmission functions in order to evaluate the parameters of the theoretical model and, on their basis, the group constants in the unresolved resonance region. The conclusion is that it is necessary to carry out new experiments on the measurement of transmission functions. In Refs [15, 16] we have dealt with some specific results of measurements, analysis and evaluation of the neutron data for the case of heavy isotopes.

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