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CONSISTENCY OF MICROSCOPIC EVALUATIONS AND INTEGRAL EXPERIMENTS FOR CHROMIUM, IRON AND NICKEL

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CONSISTENCY OF MICROSCOPIC EVALUATIONS AND INTEGRAL EXPERIMENTS FOR CHROMIUM, IRON AND NICKEL

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The new version (TsYaD-2) of the files of evaluated neutron cross-sections for natural isotopic mixtures of chromium, iron and nickel [1] is based mainly on experimental data published before 1983 and physical models used for interpolation and extrapolation of the cross-sections. The main focus of attention was the fast reactor neutron spectrum energy region (E_n = 1 keV-4 MeV), although in many cases the representation of cross-sections for neutrons with higher energies, such as for example the fusion reactor neutron spectrum, is perfectly satisfactory. A description of the basic evaluation methods and the experimental data base used is given in Refs [2 and 3]. The results of microscopic experiments on fast critical assemblies containing large amounts of chromium, nickel or stainless steel [4] and the available neutron spectra of different degrees of hardness were used to test the microscopic cross-section files. In this paper we intend to consider the characteristics of the evaluated data files which have an important role in neutron physics calculations for fast reactors and fusion reactors.

RESOLVED RESONANCE REGION

In order to give a correct account of the cross-section structure, a cross-section representation based on resolved resonances was used up to the maximum possible energies. Since these upper resonance region boundaries are different for the s-, p- or d-wave systems of the same isotope, pseudoisotopes were used artificially to introduce different upper boundaries for the various waves. Thus, in the case of the iron file the cross-sections are represented for s-resonances of ^{56}Fe in the region from 10^{-5} eV to 850 keV and for p- and d-resonances in the region from 10^{-5} eV to 500 keV, which makes it

possible to reproduce correctly the cross-section self-shielding factors over a wide energy range. For such a wide range there is a noticeable dependence of the potential scattering radius on the energy. Since the format does not allow for the introduction of this dependence, it was modelled by introducing a remote resonance lattice, with the number and neutron widths of these resonances being selected on the basis of the description of the average cross-section level for the whole resolved resonance region.

All this made it possible to give a fairly realistic description of the resonance structure and cross-section self-shielding factors for the total cross-section up to energies of 500-850 keV and for the capture cross-section up to E_n = 200-350 keV.

It should be noted that the deviations from the format caused by the introduction of pseudoisotopes are minimal and evidently do not require any serious changes to the processing programs.

In order to calculate the cross-sections from the resonance parameters for even-even isotopes of $^{54,56}Fe$, $^{50,52}Cr$ and $^{58,60}Ni$ in the s-wave resonance region, the Reich-Moore formalism is recommended. Since during the work on the files, it was not possible to use the Reich-Moore formalism in the existing format of the ENDF-5 file, the Reich-Moore parameters were recorded in the format adopted for the multi-level Breit-Wigner formalism and then the GRUKON [5] program package was used for calculation of the cross-sections from the parameters in the Reich-Moore formalism.

Thus, the main limitation of the construction material files in the TsYaD-2 evaluation in the resolved resonance region is that they do not always process the existing standard processing programs.

UNRESOLVED RESONANCE REGION

For even-even isotopes, the upper boundary of the unresolved resonance region was selected up to the inelastic scattering threshold. The average resonance parameters for calculating cross-sections in the unresolved

resonance region were initially evaluated by averaging the parameters in the resolved resonance region and then correcting them using the EVPAR program [6], taking into account the simple physical dependencies of the average distances between the levels and the widths on the spin, parity and energy and comparing them with the available experimental data on average neutron capture cross-sections. The possible contribution of the f-wave was effectively taken into account by increasing slightly the average radiation widths for the d-wave.

Among the limitations of the construction element files of the TsYaD-2 evaluation is the fact that for the natural isotopic mixture in the unresolved resonance region, the contribution gives a large number of level systems for the individual isotopes which slows down and complicates the processing of cross-sections in cases where it is necessary to take account of the cross-section resonance structure in the unresolved resonance region.

REGION OF POINTWISE CROSS-SECTION REPRESENTATION, ENERGY AND ANGULAR DISTRIBUTIONS OF SECONDARY PARTICLES

The energy region of neutrons above the inelastic scattering threshold for construction elements is very important for fusion reactors. Since the files are primarily directed towards neutron physics calculations of systems, the main focus in them had to be on the representation of elastic and inelastic scattering processes and (n,2n), (n,pn) + (n,np) reactions and other reactions leading to the escape of neutrons and significant in the energy region up to 15-16 MeV. It is assumed that for activation calculations, a separate library will be created for the facility elements which will contain the activation cross-sections for individual isotopes and the nuclear product decay characteristics. Nevertheless, the main cross-sections leading to activation are given in the TsYaD-2 evaluation completely satisfactorily for the separate isotopes Cr, Fe and Ni.

The evaluation of the level excitation functions for inelastic scattering with an excitation energy of 4-4.5 MeV and of the cross-sections for inelastic scattering was performed using the optical-statistical approach,

taking into account the contribution of direct processes. The files include the level excitation functions for odd isotopes which have a low inelastic scattering threshold and which affect the shaping of the scattered neutron spectrum. Since the total number of discrete levels usually exceeded the number of levels allowed by the format (40 levels), some of the near levels were combined into groups. The angular distributions are given for all the levels in the ^{nat}Fe file, which in many cases are not isotropic in the centre-of-mass system (contribution of the direct processes). In the case of the ^{nat}Cr and ^{nat}Ni files, the angular distributions for all levels of inelastic scattering are taken to be isotropic in the centre-of-mass system.

The shape of the angular distributions of elastic scattering for the ^{nat}Fe file was taken from the ENDF/B-4 library and based on interpolation between the experimental data. The ENDF/B-4 evaluation was also used for the file for $E_n < 1$ MeV and $E_n > 14$ MeV and in the region $1 \leq E_n \leq 14$ MeV the angular distribution evaluation was obtained using the phenomenological approach, whereby the cross-sections were calculated from the optical model and then corrected on the basis of experimental data. Such a correction made it possible to obtain a better description of the observed angular distributions than the calculations by means of the optical model with a single set of parameters. The results obtained in Ref. [7] were used for the evaluation of elastic scattering angular distributions for ^{nat}Ni.

We obtained the evaluation of the cross-section for the (n,2n) reaction and other threshold reactions from the evaluations for separate isotopes in the BOSPOR library [8] (^{nat}Fe) or from calculations using the statistical model with a description of the level densities based on the generalized superfluid nucleus model [9] and taking the pre-equilibrium processes into account (Cr, Ni isotopes).

The evaluation of the inelastic scattering spectra in the region of continuous spectrum excitation energies was made for iron with phenomenological account of the contribution of direct processes and with a temperature

Table

Comparison of neutron displacement cross-sections below the ^{238}U fission threshold in the spectrum for thermal neutron-induced fission of ^{235}U [4]

Material	Experiment b [12]	BNAB-78 b	ENDF/B-4 b	TsYaD-2 b
Fe	0.70 ± 0.02	0.66	0.70	0.66
Cr	0.66 ± 0.02	0.67	0.67	0.67
Ni	0.74 ± 0.02	0.81	0.75	0.76
Stainless Steel	0.69 ± 0.02	0.68	0.70	0.67

description of the compound-nuclear process spectrum. The total neutron emission spectra obtained are in good agreement with the emission spectra measured for E_n = 7, 9, 14 and 26 MeV. This gives reason to hope that in the case of the intermediate energies, the representation of the emission spectra will also be fairly reliable. A pure temperature representation of the secondary neutron spectra was used in the evaluation for the ^{nat}Cr and ^{nat}Ni files. Such a representation permits reasonably good unfolding of the emission spectra for neutrons with an initial energy up to the (n,2n) reaction threshold but for higher energies it strongly distorts the shape of the spectra tending to soften it.

Thus, the limitations of the files in describing secondary neutron spectra include the following:

1. Double differential cross-sections are represented as isotropic over the angle for the continuous part of the spectrum (^{nat}Fe, ^{nat}Cr, ^{nat}Ni) and also in the discrete level region (^{nat}Cr and ^{nat}Ni).
2. Although the temperature representation of the spectra (^{nat}Cr, ^{nat}Ni) is satisfactory for the fast reactor neutron spectrum, changes have to be made to make the representation more realistic for the fusion reactor neutron spectrum.

3. The ^{nat}Fe file does not have data on the secondary gamma radiation emission spectra. The ^{nat}Cr and ^{nat}Ni files have such data where the results of the corresponding ENDF/B-4 evaluation are taken as a basis.

TESTING THE FILES IN INTEGRAL AND MICROSCOPIC EXPERIMENTS

Currently, such data testing is carried out on critical assemblies with a neutron spectrum close to the fast reactor neutron spectrum [4]. As was shown by comparison of the experiments with the calculations for seven uranium critical assemblies with different concentrations of iron, chromium and nickel and neutron spectra with different degrees of hardness, the discrepancies in predicting K_∞ using the 26 group constants system created from the TsYaD-2 evaluation files, range from -0.8% to +2.3% for the different assemblies, from -1% to -5% for the BNAB-78 constants system [10] and from -2.5 to -8% for the ENDF/B-4 constants system (Fig.). The group constants for ^{235}U and ^{238}U in all the calculations were taken from the BNAB-78 system. The share of the spectrum for neutrons above 10 keV for these assemblies was 83-90%.

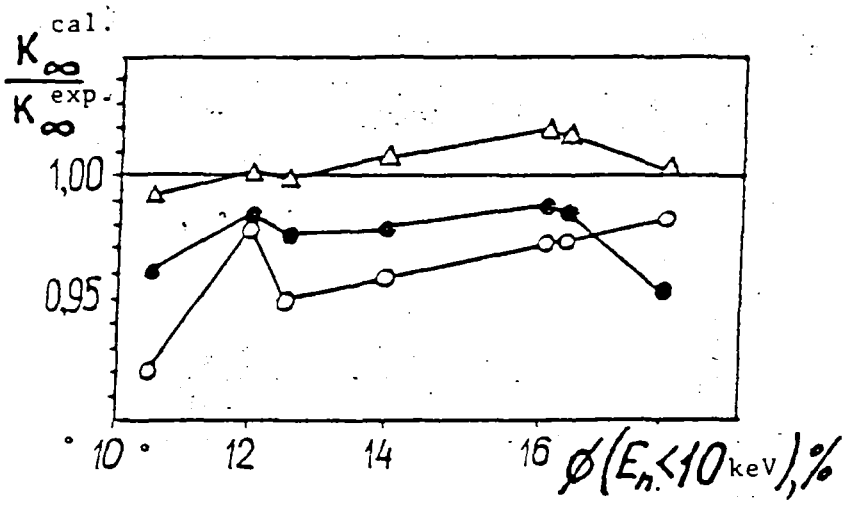

Figure: Relationship of the calculated value for K_∞ obtained using different systems of constants (● - BNAB-78, o - ENDF/B, Δ - TsYaD-2) to the experimental value for critical assemblies of different composition (assemblies 3, 9, 11, 10 and 12 containing stainless steel; 14 - chromium and 7 - nickel). The x-axis indicates the share in the spectrum of neutrons below 10 keV.

The largest deviations in predicting K_∞ occurred for soft assemblies containing a large amount of iron. The authors of Ref. [4] point out that the increase in the capture cross-section for ^{nat}Fe in the TsYaD-2 evaluation in the group 4.65-10 keV from 15.6 mb to 23 mb (ENDF/B-4 value) without any change in the other values lead to an improvement of up to 1% in the accuracy of prediction of K_∞. However, there is no justification for making such a correction to the cross-sections in the TsYaD-2 file now, since the contribution to the capture cross-section in this region for ^{nat}Fe is determined mainly by the first ^{54}Fe resonances, the capture widths of which have been measured fairly accurately [11].

The fact that these data were not available during work on the ENDF/B-4, BNAB-78 and JENDL-2 files and the reliance on experiments with poor resolution resulted in an overestimate of the cross-section in this group by 35-50%.

A comparison of the cross-sections for displacement below the ^{238}U fission threshold in the spectrum for thermal neutron-induced fission of ^{235}U for ^{nat}Cr, ^{nat}Fe and ^{nat}Ni, given in the table, shows that within the limits of error, the theoretical results agree with the available experimental data.

REVISION OF THE CONSTRUCTION MATERIAL FILES OF THE TsYaD-2 EVALUATION

Present plans for revising the construction material files include the following activities:

1. Transfer into the ENDF/B-6 format of all the files and, in particular, the Reich-Moore representation for the s-wave resolved resonance region of even-even isotopes;
2. Improvement in the representation of secondary neutron spectra for the ^{nat}Cr and ^{nat}Ni files.
3. Supplementing of the files with gamma quanta emission spectra necessary for calculation of the energy release and shielding.

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