International Atomic Energy Agency

INDC(CCP)-209/L

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EVALUATION OF NEUTRON INELASTIC SCATTERING CROSS SECTIONS FOR CHROMIUM

V.V. Vozyakov, V.M. Bychkov, V.P. Lunev and V.I. Popov

Translation from Nuclear Constants 4(48) 44(1982)

Translated by the IAEA
October 1983

IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

Reproduced by the IAEA in Austria
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83-05937

L83-21847
Translated from Russian

UDC 539.172.4

EVALUATION OF NEUTRON INELASTIC SCATTERING CROSS-SECTIONS FOR CHROMIUM

V.V. Vozyakov, V.M. Bychkov, V.P. Lunev and V.I. Popov

The nuclear level excitation functions and non-elastic (sic) and inelastic cross-sections for natural chromium were re-evaluated on the basis of recent experimental data, theoretical calculations and previously evaluated cross-sections for the (n,p), (n,pn), (n,α) and (n,2n) reactions. The evaluated cross-sections are compared with ENDF/B-V cross-sections. Data received from elsewhere have been incorporated into the Soviet library of evaluated data.

A complete file of evaluated neutron cross-sections for a natural mixture of chromium isotopes was established at the Nuclear Data Centre of the USSR State Committee on the Utilization of Atomic Energy in 1977 [1], and incorporated into the evaluated data library there with the number 2013. The inelastic scattering cross-sections in that file were evaluated solely from the results of theoretical calculations.

New experimental work [2-5], the fifth version of the ENDF/B library (ENDF/B-V) [6], and the importance of the neutron constants for chromium, a material used extensively in reactor construction, made it appear necessary to review the inelastic scattering cross-sections and the total cross-sections for inelastic interactions. This was made possible through advances in the development of theoretical methods of describing nuclear interactions. The energy region for the evaluation runs from the inelastic scattering threshold to 20 MeV.

PARTIAL CROSS-SECTIONS FOR NEUTRON INELASTIC SCATTERING ACCOMPANIED BY EXCITATION OF DISCRETE LEVELS

Natural chromium contains four stable isotopes: 4.35% ^{50}Cr, 83.79% ^{52}Cr, 9.50% ^{53}Cr and 2.36% ^{54}Cr. The evaluation was performed for the twelve levels listed in Table 1. All the available discrete levels of the chromium isotopes from the energy of the first level, ^{53}Cr, to 2 MeV were considered. Above

2 MeV, only the levels of the isotope ^{52}Cr were taken into account, the contribution from excitation of the levels of the remaining isotopes being represented by the average cross-section. Inelastic scattering accompanied by excitation of levels with energies above 3 MeV was related to the continuum region. Thus, two types of inelastic scattering cross-section were obtained: the discrete level excitation cross-section and the continuum cross-section. The total inelastic scattering cross-section is simply the sum of these two.

When evaluating the excitation functions of the discrete levels for neutron inelastic scattering the experimental data in Refs [2-5, 7-10] and calculations of the contributions of both compound and direct processes were taken into account. Experimental work (Table 2) on the characteristics of the radiation detected can be divided into two categories according to whether neutrons or the accompanying gamma radiation were recorded. The processing and analysis of experimental results of the latter type are not so simple, as not only the evaluated levels and the applicable standards but also information about cascade processes must be taken into account. Reference [3] is distinguished by the fact that a small energy spacing is used, so the energy behaviour is described in detail and even the near-threshold region is measured. The errors in the experimental data of these papers vary between 15 and 50% (Figs 1, 2).

Calculation method

The neutron cross-sections were calculated in terms of the optical model of nuclear reactions. The contribution by direct processes to inelastic scattering was calculated by the strong channel coupling method [11], that of compound processes in terms of the Tapel-Weidenmüller model [12] with the penetration factors being calculated on the basis of the spherical optical model. The parameters of the optical potential*/

$$\left.\begin{array}{ll} V_o = 48{,}7 - 0{,}33E_n; & r_o = r_s = r_{so} = 1{,}25; \\ W_s = 7{,}2 + 0{,}66E_n; & a_o = 0{,}65; \\ & a_{so} = 0{,}65; \\ V_{so} = 7{,}5; & a_s = 0{,}43 \end{array}\right\} \qquad (1)$$

*/ The amplitudes of the potential (1) are given in MeV, the geometric parameters in Fermi units.

were selected on the basis of a description of the angular distributions of elastically and inelastically scattered neutrons with initial energies of 1.5–7 MeV for the isotope ^{52}Cr [13] and of the total cross-section for a natural mixture of chromium isotopes in the range 3–15 MeV (Nuclear Data Centre estimate). The total cross-section for the natural mixture of chromium isotopes over the energy range 2.5–15 MeV is shown in Fig. 3. Averaged dependences $\sigma_t(E)$ are given for an averaging range width of 0.5 MeV. Comparison shows that the curves diverge by as much as 5-6% in the 3-6 MeV region, whereas under other conditions the discrepancy is 1-3%. In order not to clutter up the diagram we have not entered Foster's data, which, within the given accuracy limits, are the same as the curves shown here. Leaving aside the detailed structure of the total cross-section in this paper (since the search for optimum optical parameters calls for a smoothed curve) we can state that from this point of view the quality of the evaluation of the total cross-section in the first TsYaD (Nuclear Data Centre) version (TsYaD-1) [1] is satisfactory. The total cross-sections calculated with the optical parameters obtained are also shown in Fig. 3. Note that with this set of parameters it is not possible to reproduce the experimental values of the neutron force functions for S and P waves, so renormalized penetration factors have been used to calculate the level excitation functions for incident neutron energies below 2.5 MeV. These factors were selected so that they matched, at E_n = 0.1 MeV, the experimental force functions (S_o for even, S_1 for odd partial waves) taken from Ref. [14] (Table 3) and merged smoothly at an energy E = 2.5 MeV with the penetration factors of an optical model having the potential parameters (1) which are given above.

A selection of penetration factors of this kind makes it possible to avoid the sharp increase in the excitation function of the individual levels in optical calculations for iron [15] and chromium nuclei. Nevertheless, some questions remain unanswered as regards ways of interpolating experimental sticking probabilities in the process of joining them with the optical values and to the position with respect to energy of the joining point.

The direct excitation of collective levels of even-even nuclei was calculated in terms of the strongly coupled channel method [16] with the above parameters (1) of the optical potential. Since the excitation of the 2_1^+ state is explicitly taken into account, the value of the imaginary part is reduced by 20% so that the total cross-section will agree with the results of spherical-model calculations. The values of the dynamic deformation parameter β_2 are taken from Ref. [11]. For nuclei with odd atomic masses the contribution of direct processes was evaluated by a model of weak coupling between an odd particle of momentum and parity J^π and an even core. Hence, the excited states of the odd nucleus form a multiplet of states $\{J^\pi \otimes 2^+\}$ due to the excitation of a 2^+ even-even core. The cross-sections for direct excitation of each member of the multiplet may be represented in the form

$$\sigma^{dir}_{I_f^\pi} = \sigma^\lambda(I_i \rightarrow I_f) = \frac{2I_f+1}{(2\lambda+1)(2I_i+1)}\,\sigma^\lambda(0 \rightarrow \lambda), \qquad (2)$$

where $\sigma^\lambda(0 \rightarrow \lambda)$ is the cross-section for direct excitation of the collective state with momentum λ in the even-even nucleus and $\sigma^\lambda(I_i \rightarrow I_f)$ is the cross-section for direct transition from the initial state I_i to the final state I_f of the odd nucleus.

The calculated level excitation cross-section was calculated as the sum of the cross-sections $\sigma_{I^\pi}(E) = \sigma^{I^\pi}_{comp}(E)R + \sigma^{dir}_{I^\pi}$, where $\sigma^{I^\pi}_{comp}$ is the cross-section calculated according to the statistical scattering model and $\sigma^{dir}_{I^\pi}$ is the contribution of direct processes. Since an optical potential with a reduced imaginary part was used in the strongly coupled channel method, a correction R was introduced to account for the difference between the absorption cross-section for the strongly coupled channel method σ_a^{sc}, and the analogous cross-section for the spherical model, σ^{opt}: $R = \sigma_a^{sc}/\sigma_a^{opt}$. As an example, we give the values of the correction R for the 1.434 MeV level of ^{52}Cr: for $E_n = 1.5$ MeV, R = 0.92; for $E_n = 2$ MeV, R = 0.96; for $E_n = 2.5$ MeV, R = 0.986; and for $E_n = 3$ MeV, R = 1. At energies above this last known level of the residual nucleus a statistical description of the density of states in a Fermi-gas model with the parameters of Ref. [17] was used.

Results

Figures 1 and 2 give our version of an evaluation of the excitation function together with experimental data and the evaluation results for the fifth version of ENDF/B [6]; the underlying principle of the evaluation was a comparison of the set of experimental points with the calculation results. The evaluated curves for almost all the levels considered were plotted on the basis of calculated results, in the first place because they did not conflict with the experimental data, and secondly because they yielded a reasonably reliable curve in those regions where such data were not available. The latter statement is based on experience gained in evaluating excitation cross-sections for the 1.434 MeV level of ^{52}Cr. We used data from Ref. [3], but disregarded the structure in the $\sigma_{exc}(E)$ curve, as we believed the uncertainties in that experiment to be quite large. An experimental verification of this structure would be desirable.

Level 1.434 MeV. The isotope ^{52}Cr accounts for the largest contribution to inelastic scattering of neutrons by chromium, so the attention paid by experimenters to this level is understandable. There are experimental data on its excitation function from the actual threshold up to 14 MeV; they have been drawn, for our evaluation, from eight papers published during the past 20 years (see Table 2). The results of Ref. [8] were used for the evaluation after renormalization to the value of the cross-section for iron at the 845 keV level with E_n = 1.2 MeV, which was taken from a Soviet evaluated data file [18]. The reason for this is that the work described in Ref. [8] was performed in the early 1960s and that an obsolete cross-section value of 0.52 b was used as a standard. As Fig. 1 shows, the errors in the experimental data overlap in the vast majority of cases, which makes it easier to draw a mean curve through the set of experimental points. The calculated curve, obtained by the method described in the present paper, differs only insignificantly - within 5% - from the mean curve. The calculated curve was used as the recommended curve. If our version is compared with the third and fourth ENDF/B evaluations, two pecularities will be noted: first, in the region E_n = 1.7-2.2 MeV the results of Ref. [3] are markedly lower than those of Refs [2,4,8,9], a fact which enabled the authors of the evaluation in Ref. [6] to reduce significantly (by about 30%) the evaluated curve in comparison with the fourth version. Although this reduction is not inconsistent with certain experiments [8,9] because of the large errors, it is dictated by the data of Ref. [3] alone. The evaluated ENDF/B-V curve in the region 1.7-2.2 MeV lies at the lower edge of the experimental field. In this paper the shape of the evaluated curve has also undergone a change in a downward direction, i.e. the TsYaD-1 version was approximately the same as the

ENDF/B-IV version on the ascending branch. Since the authors' theoretical calculation results are in significantly better agreement with the data of Refs [2,4,8,9] than with those of Ref. [3], the curve adopted in the fifth version of ENDF/B seems less likely to be correct. The second peculiarity relates to the region $E_n > 8$ MeV, where the contribution of direct processes is dominant; these direct processes, in our opinion, are not correctly accounted for in the fifth ENDF/B version: in the 10-15 MeV region our calculation is corroborated by an experimental point from Ref. [5], whereas the data of the fifth version are 1.5-3 times lower. An incorrect approach in accounting for direct interactions and a certain inconsistency in doing so are characteristic of the authors of the ENDF/B-V evaluation in the case of other discussed levels, too. Thus, for some levels (see Fig. 2, (e)-(k)) the cross-section $\sigma^{dir} = 0$ at energies of about 8, 10 and 15 MeV, which is wrong in principle. In other cases, though, in the region $E_n \approx 7$-15 MeV the contribution of direct processes is significantly overestimated (by a factor of about 2-6).

Level 0.564 MeV. In the ENDF/B-V evaluation the threshold is shown inaccurately, being displaced towards higher energies. In the present paper we adopt the theoretical data, although the descending branch should possibly have been shifted to the right by about 1 MeV to accord with the experimental data. The decision to retain the calculation results was taken for the sake of a more general approach: as noted above, the authors tried to follow the theory as long as no unacceptable inconsistencies arose.

Level 0.783 MeV. The newly evaluated curve is about 40% lower at its maximum than the TsYaD-1 version.

Level 0.835 MeV. No comments.

Level 1.006 MeV. Up to an energy of 5 MeV the difference between our version and ENDF/B-V is insignificant, but beyond that a divergence by a factor of 2-6 is observed, as discussed above.

Level 1.287 MeV. In the region below 2.5 MeV the calculation data should perhaps be increased somewhat to improve agreement with the mean experimental curve. In order to preserve the generality of the discussion the theoretical curve has been retained.

Level 1.539 MeV. The calculated curve is lower almost by a factor of 2 than the experimental one, and the evaluated curve is approximated to the experimental data of Ref. [3]. The reasons for the discrepancy are not explained. Note that the curve of the TsYaD-1 version, based on calculations, also passes below by a factor of about 1.5.

Level 1.973 MeV. No comments.

Level 2.37 MeV (see Fig. 2(g)). The experimental results of four papers are as high as 9 MeV; the data of Ref. [4] are higher by 1.5-2 than the rest, but have a somewhat larger error. That we should distrust Ref. [4], however, is problematic since the data in it agree fairly well with those of other authors for the 1.434 MeV level. The peak of the theoretical curve occupies an intermediate position. The calculation is retained as an evaluation since to aim at lowering the curve to a mean value corresponding to the experiments of Refs [2,3,9,10] would give rise to serious complications with the other levels of this isotope: the excitation functions are reckoned jointly for the system of levels of a particular isotope; a reduction for one level would require a similar reduction for the rest, and this would pose difficult problems in view of the agreement achieved between calculation and experiment, especially in the case of the 1.434 MeV level. The curve of the TsYaD-1 version in the 3-4 MeV region occupied an intermediate position between the curves of TsYaD-2 (present evaluation) and ENDF/B-V.

Level 2.65 MeV. Again we face the problem of making the experimental data agree with each other. Perhaps their errors are somewhat underestimated. Without the data of Ref. [4], as in the previous case, it would be difficult to understand the tendency of the theoretical curve to fall some way (about 20%) below the experimental curve [3,9].

Level 2.768 MeV. On the ascending branch the theoretical and experimental data agree closely, except for the data from Ref. [4].

Level 2.965 MeV. The experimental data agree as a result of the sharply increased values (by up to about 50%) of the error in Ref. [4], so calculation and experiment do not contradict each other.

TOTAL CROSS-SECTIONS FOR INELASTIC SCATTERING AND INELASTIC INTERACTIONS

The total cross-section for inelastic scattering in the region up to 2 MeV (Fig. 4(a)) was determined as the sum of partial excitation cross-sections of discrete levels. The results of this evaluation are not very different from the curve in the TsYaD-1 version, which is somewhat lower in the region near the threshold and a few per cent higher in the 1.7-2.1 MeV range. As compared with the ENDF/B-V data for the 1.6-2.5 MeV region, this evaluation is higher by about 0.1 b or 10-25%; in the 2.5-3.5 MeV range the curves are practically identical. The experimental value for the inelastic scattering cross-section of 1.4 $\pm$ 0.3 b [19] (Figs 4(b) and 5) was obtained almost 30 years ago, has a large error and lies about 50% above the region of evaluated curves. The recent experimental data of Ref. [3] are 10-20% lower than our estimates.

In view of the dominant contribution by the 1.434 MeV level to the total inelastic scattering cross-section, it should be noted that in order to lower the evaluated curve for this cross-section it would be necessary to reduce the excitation function for the 1.434 MeV level, but as the evaluation of the excitation cross-section for that level shows, there is no basis for doing so (see section headed "Results").

Above 2 MeV the total inelastic scattering cross-section is determined from the expression $\sigma_t^{in} = \sigma_{non} - \sigma_{n,2n} - \sigma_{n,p} - \sigma_{n,pn'} - \sigma_{n,n'p} - \sigma_{n,\alpha} - \sigma_{n,\gamma}$, where σ_{non} is the total cross-section for inelastic interactions. The entire curve $\sigma_t^{in}(E)$ is shown in Fig. 4(b) together with the experimental results. At higher energies our evaluation differs insignificantly from the data of Ref. [20]; at 9.1 MeV there is agreement with the data of Ref. [21], and at 14 MeV with those of Refs [22-25], the value 0.87 $\pm$ 0.08 b [24] being omitted because it is so closely similar to the value σ_{in} = 0.88 $\pm$ 0.04 b [22]. The experimental results of Ref. [26] are higher by a factor of about 1.5. This value would appear to be quite unreliable, as the authors, after determining the differential cross-section at 110°, integrated it on the assumption that inelastic scattering is isotropic.

The total cross-section for inelastic interactions (see Fig. 5) presented here does not come from the thermal energy, but from the threshold energy of the first level of inelastic scattering for chromium, since the cross-section for radiative capture is subject to review. In the 0.4-2 MeV region the total cross-section for inelastic interactions is determined by the expression $\sigma_{non} = \sigma_t^{in} + \sigma_{n,\gamma} + \sigma_{n,p}$, where $\sigma_{n,\gamma}$ varies between 2 and 4 mb and $\sigma_{n,p}$ does not exceed 0.4 mb. In the energy range above 2 MeV, $\sigma_{non} = \sigma_a - \sigma_{el}^c$, where σ_a is the neutron absorption cross-section, σ_{el}^c is the elastic scattering cross-section across the compound nucleus, and both cross-sections were calculated in terms of the optical model. The dependence $\sigma_{non}(E)$ is shown in Fig. 5, as are the experimental data, the results of the ENDF/B-V evaluation, optical-model calculations from Ref. [6] for the establishment of the ENDF/B-V version and calculations from Ref. [10] based on measurement results for σ_t and σ_{el}. The optical-model calculations acquire a special meaning, since the behaviour of the total inelastic interaction cross-section determines the curve for the total inelastic scattering cross-section in the region above 2 MeV, and experimental data for the total inelastic interaction cross-section are few in number and not always reliable; for instance, the value of this cross-section at 2.5 MeV has an error of $\pm$ 22% and is not included in this compilation. In the vicinity of 4.5-8.5 MeV our evaluated curve lies a little below that of ENDF/B-V, the maximum divergence being about 10%; in the remaining region our evaluation is almost the same as the ENDF/B-V data.

The threshold reaction cross-sections included in the evaluation were taken from the earlier version of TsYaD-1 [1] revised by A.B. Pashchenko, the results of which will be published separately.

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Manuscript received 16 June 1982

Table 1

Evaluated chromium isotope levels

Rel. atom. mass of chromium isotope	Level Energy, MeV	Spin and parity	Rel. atom. mass of chromium isotope	Level Energy, MeV	Spin and parity
53	0,564	$1/2^-$	53	1,539	$7/2^-$
50	0,783	2^+	53	1,973	$9/2^-$
54	0,835	2^+	52	2,37	4^+
53	1,006	$5/2^-$	52	2,647	0^+
53	1,287	$7/2^-$	52	2,768	4^+
52	1,434	2^+	52	2,965	2^+

Table 2. Concise survey of experimental work

Author, laboratory or country, year, reference	Experimental method	Remarks
KORZH, I.A. et al., KGU, 1977 [2]	Neutrons recorded by time-of-flight method	
KARATZAS, P.T., et al., Lowell University, Massachusetts, USA, 1978 [3]	Gamma quanta from (n,n') reaction recorded at 125° angle by time-of-flight method	A correction for the theoretically determined angular distribution was introduced when integrating the differential cross-section for γ-quantum scattering
SMITH, A.B., et al., Argonne National Laboratory USA, 1980 [4]	Neutrons recorded over scattering angle range of 20-160° by time-of-flight method	The authorsof the experiment averaged the results over a 200-keV range so as to obtain a smooth cross-section
WINKLER, G., et al., Institute of Nuclear Physics and Radiation Research Austria, 1980 [5]	Neutrons recorded by time-of-flight method	The angular distributions of elastically and inelastically scattered neutrons over the range of angles 20-130° at E_n = 4-12 MeV was measured for the 1.434 and 4.56 MeV levels of ^{52}Cr
ALMEN-RAMSTRÖM, E.A., Studsvik Energiteknik AB, 1970 [7]	Same	The differential cross-section measured at an angle of 125° was multiplied by 4π
BRODER, D.L., et al., USSR, 1964 [8]	Gamma quanta recorded	The isotope ^{56}Fe was used as a standard for processing with an inelastic scattering cross-section σ_{in} (1.2 MeV)= 0.52b*, E_{level} = 845 keV
VAN PATTER, D.M., et al., Bartol Research Foundation, Pennsylvania, USA, 1962 [9]	Same	A correction for the angular distribution of γ-quanta was introduced in the integration; the inelastic scattering cross-section for ^{56}Fe was used as a standard
KENNEY, W.E., PEREY, F.G., Oak Ridge National Laboratory USA, 1974 [10]	Neutrons recorded by time-of-flight method	

* 1 barn = 10^{-28} m^2.

Table 3. Experimental force functions of chromium isotopes (x 10^{-4})

Isotope	S_0	S_1
^{50}Cr	3,6 ± 0,8	0,33± 0,12
^{52}Cr	2,1 ± 1	0,3 ± 0,2
^{53}Cr	4,5 ± 1	0,15± 0,05
^{54}Cr	2,8 ± 1	0,52± 0,12

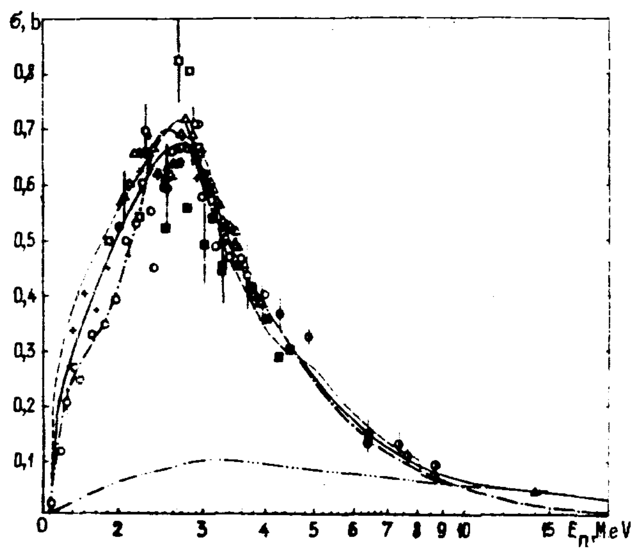


Fig. 1. Excitation cross-section of the 1.434 MeV level for ^{52}Cr (reduced to the content of the isotope in a natural mixture).
Experimental results: ● [2], o [3], △ [4], ▲ [5], ■ [7], + [8], □ [9], ◐ [10].
Evaluation results: --- ENDF/B-IV, 1976; -.- ENDF/B-V, 1979 [6]; —— present paper (TsYaD-1), 1982.
Calculation results: -...- contribution of direct processes.

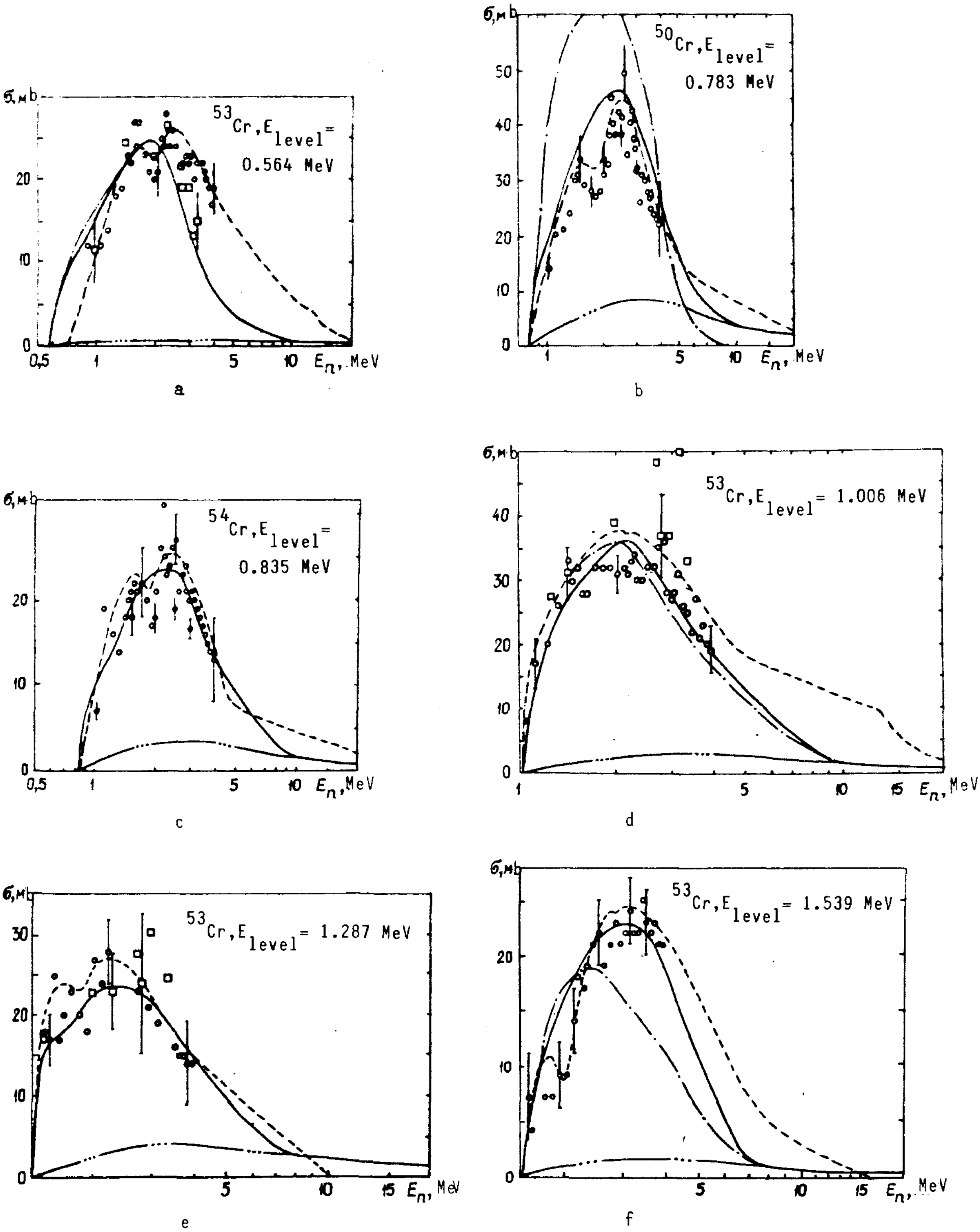
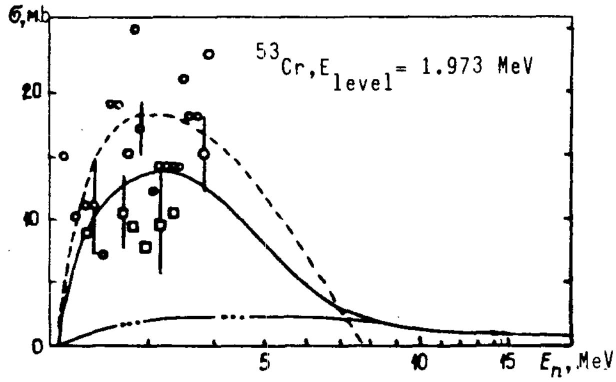


Fig. 2. Level excitation cross-sections for chromium isotopes with relative atomic masses of 50, 53 and 54 (the cross-sections are reduced to the content of these isotopes in a natural mixture). Experimental results: ● [2]; o [3]; □ [9]; ◐ [10]. Evaluation results: -...- contribution of direct processes; --- ENDF/B-V [6]; -.- Ref. [1] (TsYaD-1); —— present paper (TsYaD-2).



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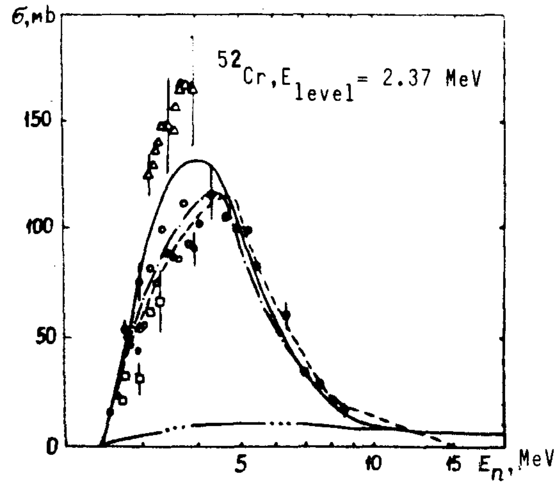

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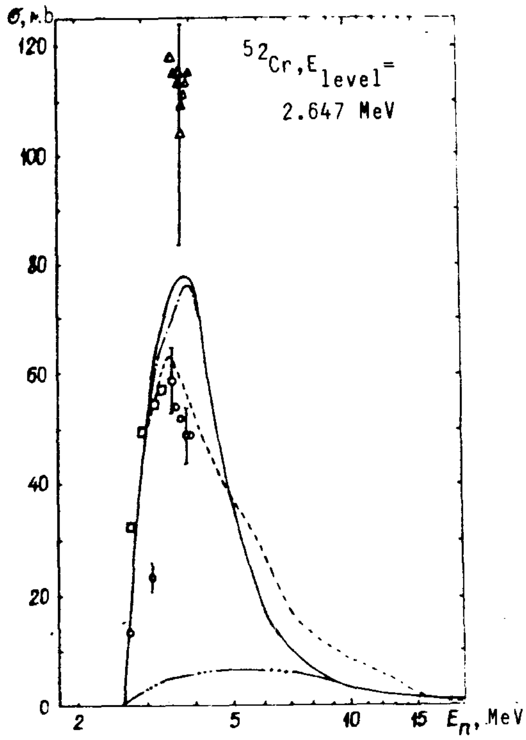

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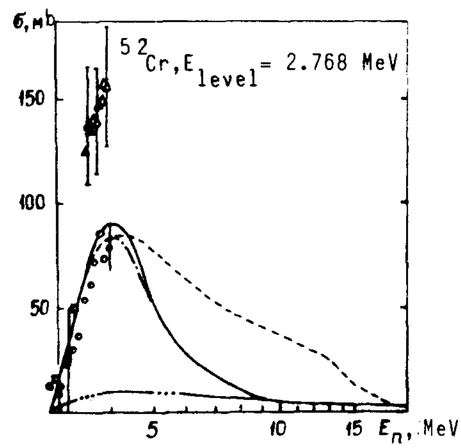

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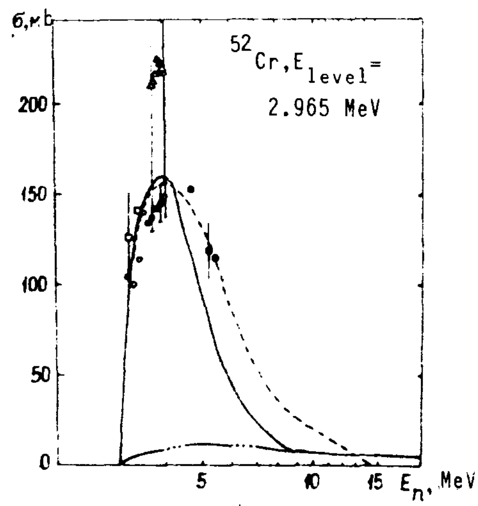

k

Fig. 2. Conclusion

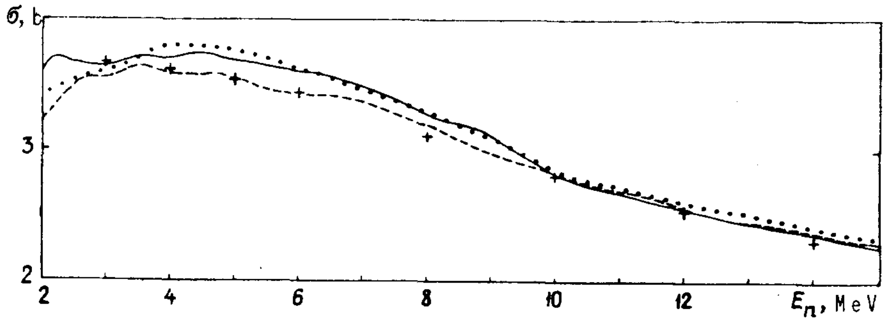

Fig. 3. Total cross-section for a natural mixture of chromium isotopes (averaged curves) according to the measurements of:
--- S. Siryaks, 1970 (corresponds to the TsYaD-1 evaluation);
—— KEDAK-2 library, 1975; ... F. Perey, 1973 [10] (corresponds to ENDF/B-V); + calculation in terms of optical model with parameters (1).

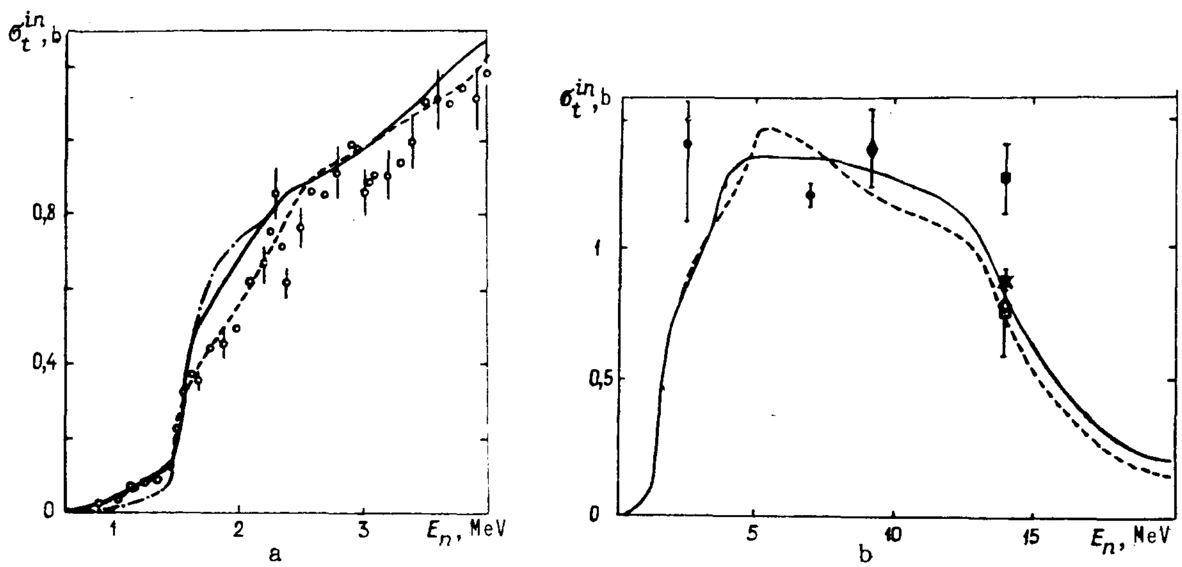

Fig. 4. Total inelastic scattering cross-section for a natural mixture of chromium isotopes. Data from: —— present paper (TsYaD-2);
--- ENDF/B-V; -.-. [1] (TsYaD-1). Experimental results:
o [3]; ● [19]; ◐ [20]; ◆ [21]; x [22]; ◇ [24]; □ [25]; ■ [26].

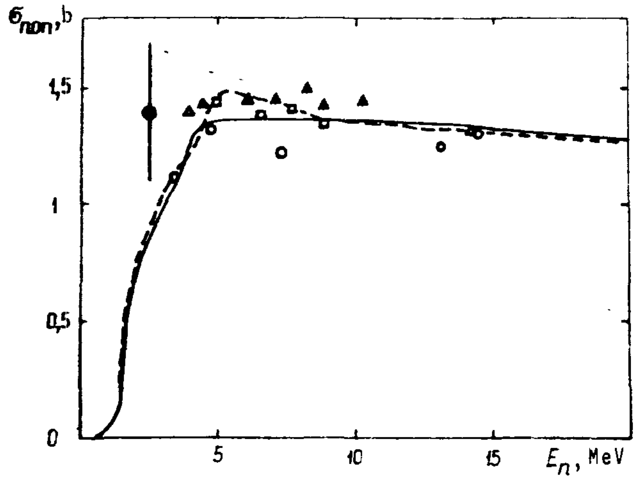

Fig. 5. Total inelastic interaction cross-section for a normal mixture of chromium isotopes. Experimental results: ● [19]; □ [10]; o [27]. Evaluation results: △ [6] (calculation); —— present paper; ---- ENDF/B-V.