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NUCLEAR STRUCTURE EFFECTS ON CALCULATED FAST NEUTRON REACTION CROSS SECTIONS

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Abstract

The importance of accurate low-lying level schemes for reaction cross section calculations and the need for microscopically calculated levels are proved with reference to fast neutron induced reactions in the A=50 atomic mass range. The use of the discrete levels both for normalization of phenomenological level density approaches and within Hauser-Feshbach calculations are discussed in this respect.

1. INTRODUCTION

The most well-known aspects of the nuclear structure effects on calculated reaction cross sections concern the **nuclear structure approach (NSA) to nuclear reactions** realized within the DWBA or SCC methods. While it is not possible to use at present state the NSA for high accuracy quantitative predictions of the cross sections, these microscopic approaches give the understanding of underlying physics [1].

On the other hand, the statistical features of the spectrum of the nuclear hamiltonian are essential ingredients of any **statistical theory of nuclear reactions** [2], the most illustrative example being the recent formulation of the statistical theory by the Heidelberg group (e.g. [3]). Shell model level densities have been also tested by incorporating them into Hauser-Feshbach evaporation calculations and comparing the results with heavy-ion reaction experimental data (e.g. [4]). Intensive attempts have been done [2,5,6] to derive partial level densities starting from shell model hamiltonian eigenvalues, in order to optimize pre-equilibrium emission cross section calculations near shell closures [7].

Thirdly, the **discrete level microscopic descriptions** of nuclei at low excitation energies can be quite valuable for accurate reaction cross section calculations. Actually, the respective relationship has been mostly used to derive low-lying level spectroscopical data (J^{π}). Comparisons of the experimental populations of the low-lying levels in nucleon induced reactions with the theoretical populations $P(J^{\pi})$ calculated according to the Hauser-Feshbach-Moldauer statistical model of the compound nucleus have been widely used (e.g. [8,9]) to draw conclusions on the spin of the level discussed.

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Discrete level description requirements for accurate calculation of fast neutron reaction cross sections, for the A>100 mass range, have been largely discussed by M.A. Gardner and D.G. Gardner ([10] and references therein). They shown that level information obtained from experiment must be supplemented with that known to be present theoretically, also for improvements on global parameterizations of level densities, predictions of unknown values of the average s-wave neutron resonance spacing, computation of correct radiation widths, inference of absolute E1 and M1 gamma-ray strength functions, and analyses of primary gamma-ray spectra.

In the present work the importance of accurate low-lying level schemes for reaction cross section calculations and the need for microscopically calculated levels are proved with reference to fast neutron induced reactions in the A=50 atomic mass range. The use of the discrete levels both for normalization of phenomenological level density approaches and Hauser-Feshbach calculations are discussed in this respect. Special comments concern related questions rised during the recent Third Research Co-ordination Meeting (RCM) (June 20-22, 1990, IAEA, Vienna) of the IAEA Coordinated Research Programme "Methods for the Calculations of Neutron Nuclear Data for Structural Materials of Fast and Fusion Reactors" (1986-1990). Conclusions equally useful for theoretical works are finally advanced.

2. USE OF THE DISCRETE LEVELS IN DERIVING NUCLEAR LEVEL DENSITY PARAMETERS

In a recent paper [11] a difference of about an order of magnitude has been found among level densities given for the 58Ni nucleus by a Back-Shifted Fermi Gas (BSFG) parameter set [12] and few other predictions. In the absence of s-wave neutron resonance spacing data, the level density parameter a=5.90 MeV-1 and the back-shift Δ=0.08 MeV were got [12] by using an "a-smooth curve" method and **fitting the discrete level numbers** up to **N =14 at E =4.620 MeV** (Table I of [12])(Fig. 1c). The same condition is fulfilled by a set of BSFG parameters [13] adjusted in the limits of the fitted data errors to allow a better agreement between the calculated and experimental reaction cross sections. Rather similar cumulative level numbers (Fig. 1c) and level density (Fig. 2) for the 58Ni nucleus are got by using the BSFG parameters adopted within an extensive analysis [14] of fast neutron induced reactions on 58Ni. It can be seen that one order of magnitude lower level densities would predict the first excited level above 4 MeV ! A first consequence of this shortcoming should be a not continuous behaviour of the neutron reaction cross sections at incident energies just above the last excited level taken into account in the Hauser-Feshbach-Moldauer calculations.

Nevertheless, two aspects have to be pointed out with reference to the BSFG parameters derived in [12,13]. Firstly, they belong to a set of **consistent Hauser-Feshbach model input parameters**, derived or validated by means of various independent types of experimental data. The unitary use of the common pre-equilibrium and statistical model parameters has been also carried out [15,16]. Secondly, the correctness of these parameters is supported by an **unitary account** of a whole body of **related experimental data** for isotope chains of neighbouring elements (e.g. for fast neutron induced reactions on 58Ni, Fig.3[13]).

The usefulness of the discrete level account for the level density parameter establishment is sometimes diminished by the uncertainty on the excitation energy up to which is believed that all discrete levels are experimentally known. Usually, this limit is connected with the lessening of the rather regular exponential

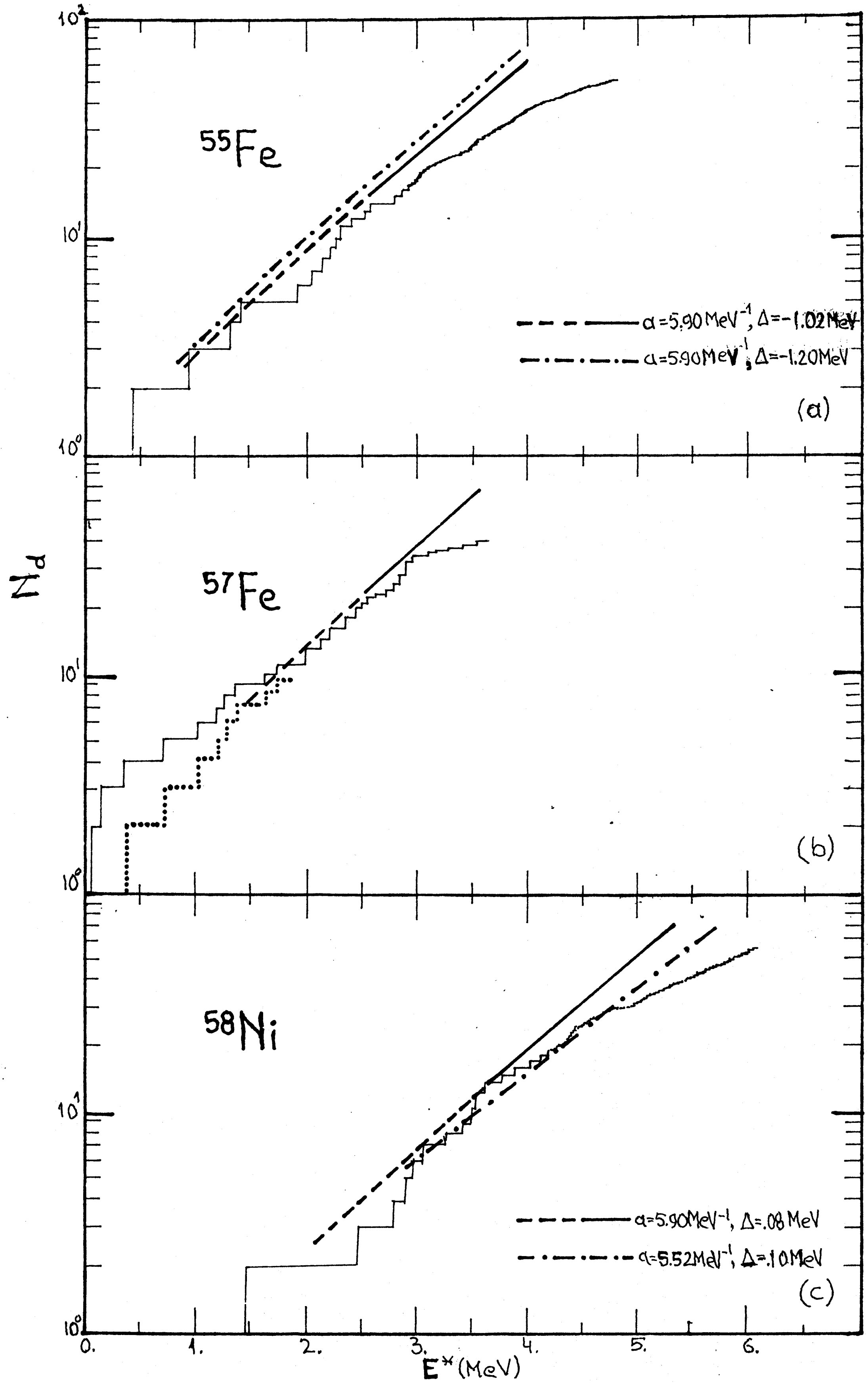

Fig.1. Total number of discrete levels, experimental (Refs. given in [12,13]) and BSFG model description, for 55,57Fe and 58Ni. The dashed lines are predictions for the discrete levels explicitly included in the Hauser-Feshbach calculations [13] (Tables 1 of [12,13]).

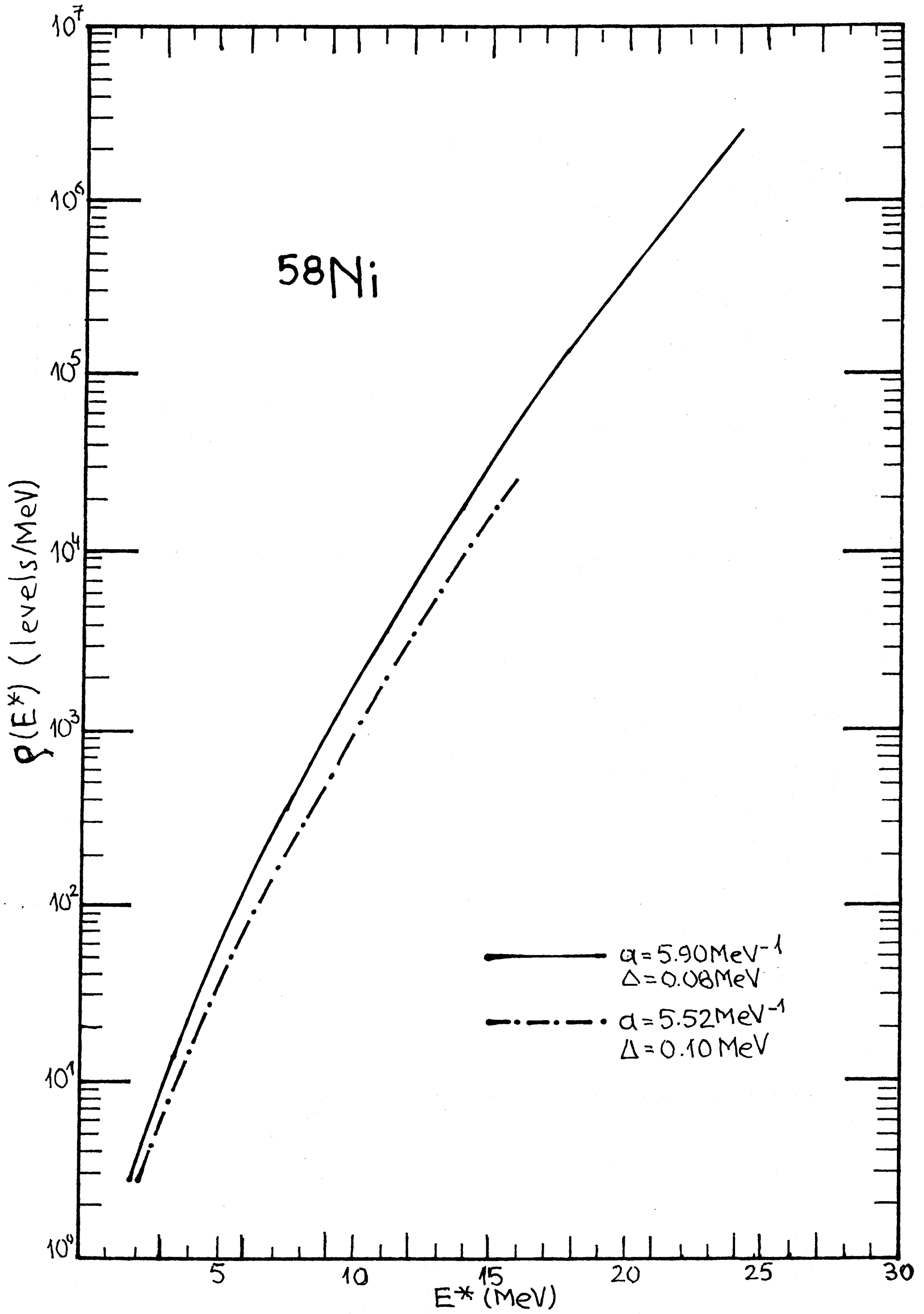

Fig. 2. Calculated nuclear level densities for 58Ni nucleus by using the BSFG parameters of Refs. [12] (full curve) and [14] (dotted curve).

increase of the discrete level total number with the excitation energy increasing. However, this exponential increase can be also affected by specific structure of the low-lying levels. For the medium nuclei real "gaps" could be thus present at excitation energies of 2-3 MeV (even higher for even-even nuclei). Therefore, to make a good choice for the upper number of discrete levels fitted is - sometimes - a difficult task. Theoretical predictions of complete low-lying level schemes can be rather helpful in this respect.

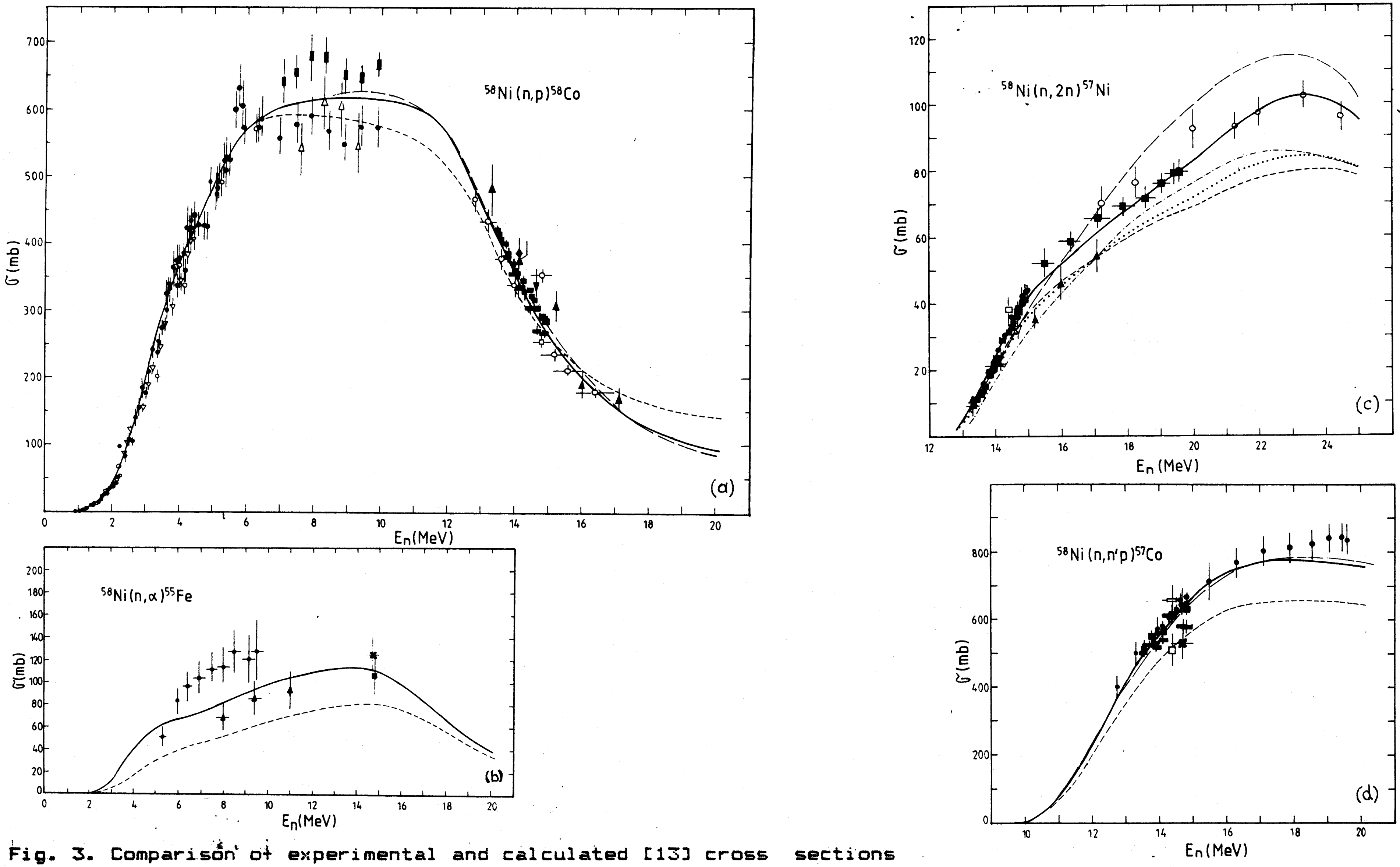

Fig. 3. Comparison of experimental and calculated [13] cross sections of the reactions (n,p), (n,α), (n,2n) and (n,n'p) on the target nucleus 58Ni. For experimental data see [13].

3. LOW-LYING LEVEL STRUCTURE EFFECTS ON HAUSER-FESHBACH MODEL REACTION CROSS SECTIONS

3.1. The 58Ni(n,α)55Fe reaction

An open question rised during the above-mentioned IAEA RCM concerned the rather unusual behaviour of the low energy side of the calculated 58Ni(n,α)55Fe reaction excitation function [17,13]. It has been considered that the change of its slope, before reaching the maximum, does not agree with the statistical theory. The calculated excitation functions of the populations for the first 7 levels of the residual nucleus 55Fe, as well as of the total population of the discrete levels taken into account (14 up to 2.578 MeV excitation energy, Table 1 of [13]) and the continuum population, are shown in Fig. 4a. Each separate excitation function is characterized by a shape in accordance with the Hauser-Feshbach model. It seems that the decreasing of the (n,α) reaction excitation function slope, in the incident energy range E =5-7 MeV, is connected with the much higher population of the ground state of the residual nucleus. This aspect could be explained by the ground state spin 3/2, close to the maximum of the angular distribution of the compound nucleus initial population, and the presence of a similar excited level only at about 1 MeV higher excitation energy.

To get a better insight, the following attempts have been made in this case. A calculation performed by using only the first 4 discrete levels of 55Fe has given a small increase of the (n,α) reaction cross sections between 6 and 10 MeV, due to the overestimation of the first 5 to 10 experimental levels by the adopted level density (full-and-dashed line in Fig. 1a). Two ways can be used starting from this point to get a rather usual behaviour of the (n,α) reaction excitation function. Firstly, an increased nuclear level density, giving a constant level increase from the first excited one (dotted-dash line in Fig. 1a), would also give a constant increase of the excitation function (dotted-dash curve in Fig. 4a). On the other hand, the same qualitative result (dotted curve in Fig. 4a) can be got by taking into account the former level density but changing the ground state spin value from 3/2 to 1/2 (similarly to the first excited state). Therefore, it seems that the (n,α) reaction excitation function shape is given by the specific structure of the residual nucleus 55Fe in the first 1.5 MeV excitation range.

3.2. The 60Ni(n,α)57Fe reaction

A similar and even enhanced change of the slope of the excitation function low energy side is shown by the calculated cross sections for the 60Ni(n,α)57Fe reaction [13]. The same analysis performed as for the previously discussed reaction has also shown (Fig. 4b) usual Hauser-Feshbach populations for all discrete levels. The most important contributions are given now by the first two excited levels, characterized by 3/2 and 5/2 spin values, related to the maximum of the angular momentum distribution of the compound nucleus initial population.

The BSFG level density parameters for the residual nucleus 57Fe have been got [13] by fitting the s-wave neutron resonance spacing $\bar{D}$ and the discrete levels in the excitation range 2 - 2.6 MeV (up to the 24th level at 2.578 MeV). The corresponding level density strongly underestimates the first 9 levels (up to 1.357 MeV, Fig. 1b) but there was no reason to believe that unknown levels are still present up to about 2.6 MeV excitation - the upper point fitted. On the other hand, an attempt to fit all discrete levels in the range 0.4 - 2.6 MeV would

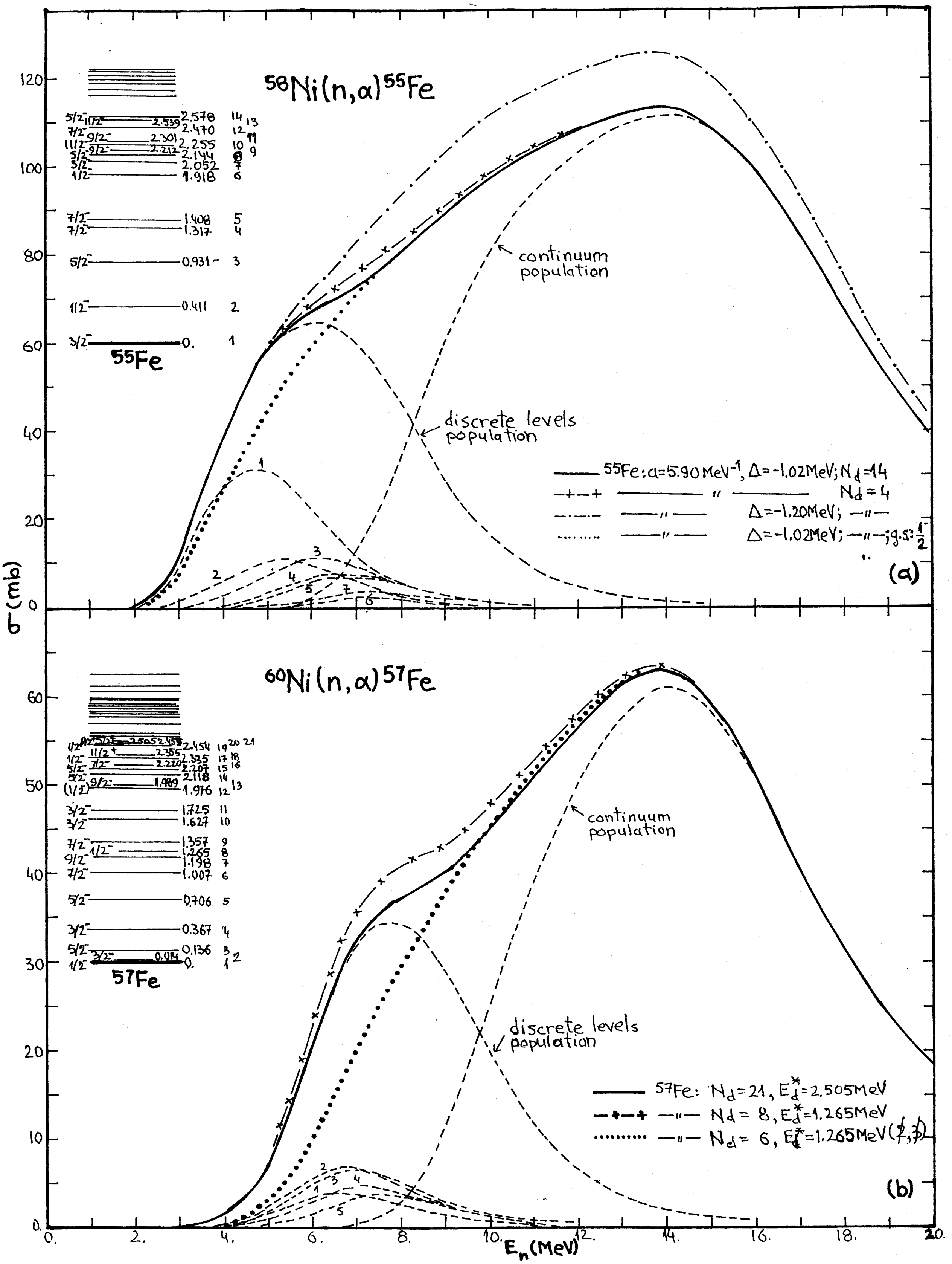

Fig.4. Calculated excitation functions for the (n,α) reactions (curves described in text) on the target nuclei 58Ni (a) and 60Ni (b). Dashed curves are the excitation functions for the population of the first discrete levels of the residual nucleus, the total population of the discrete levels and the continuum population.

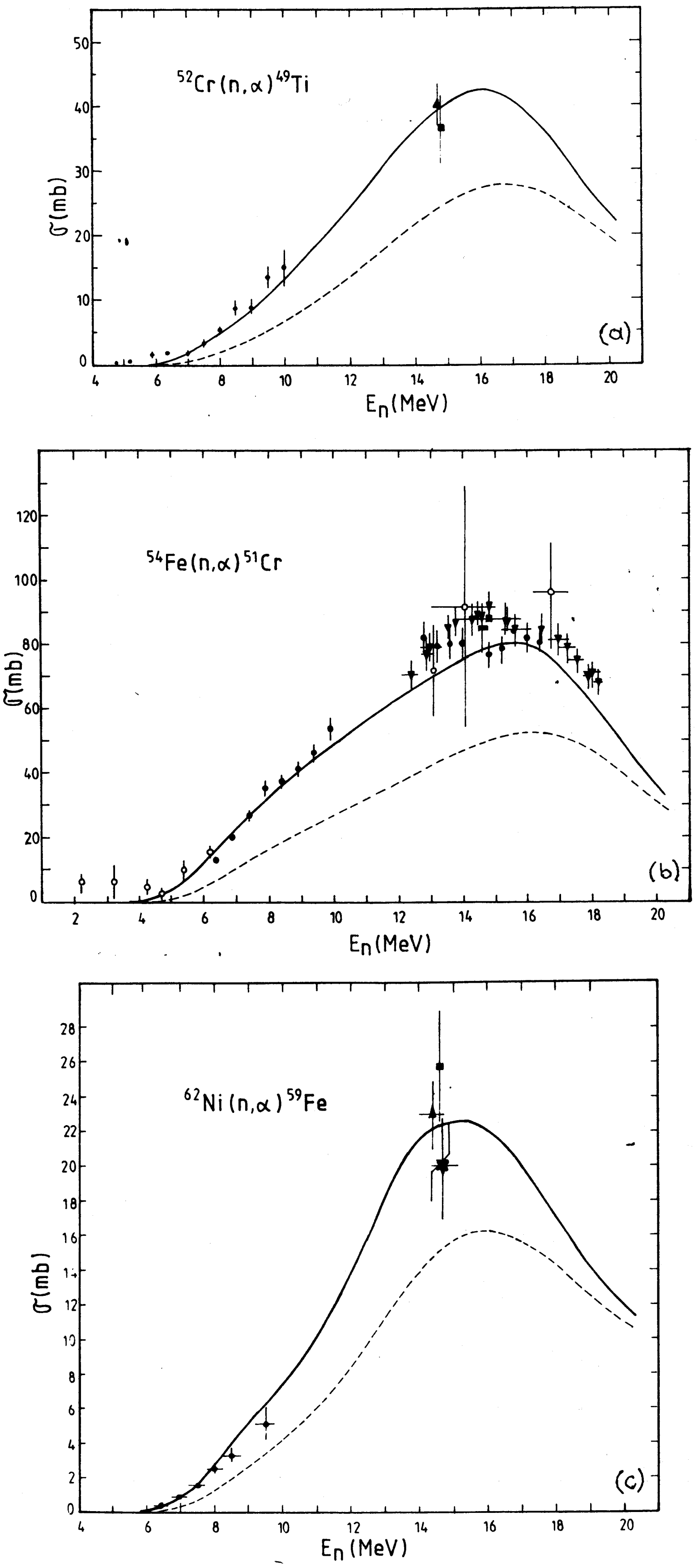

Fig. 5. Comparison of experimental and calculated [13] cross sections of the reaction (n,α) on 52Cr, 54Fe and 62Ni target nuclei. The OMP of McFadden and Satchler [19] (dashed curves) and the same OMP with modified diffuseness parameter (full curves) have been used. For the experimental data see [13].

result in: (a) a value for the level density parameter a quite lower than the smooth empirical curve of this parameter versus the atomic number A, for the range A=40-65 [12], and (b) a much higher calculated $\bar{D}$-value relatively to the experimental one. Therefore, there is a difference between the slopes of the first 9 discrete levels and the adopted level density of the residual nucleus, which could explain the decreased slope of the 60Ni(n,α)57Fe reaction excitation function between 7 and 9 MeV incident energies.

The starting point to prove the above assumption has been an excitation function calculated by using not the 21 discrete levels up to 2.505 MeV excitation energy (full curve in Fig. 4b) but only 8 levels up to 1.265 MeV (crossed-dash curve). It can be seen now that removing the first two excited levels (0.014 and 0.136 MeV, respectively), the rest of 6 levels up to 1.265 MeV (dotted line in Fig. 1b) are just along the predictions of the adopted level density. Taking into account only these 6 discrete levels in the Hauser-Feshbach calculation, the continuous excitation function (dotted curve in Fig. 4b) is finally got. The specific low-lying level structure of the residual nucleus is thus proved responsible for the anomalous behaviour of the low energy side of the 60Ni(n,α)57Fe reaction excitation function.

3.3. alpha-particle optical model potential based on calculated discrete level populations in (n,α) reactions

The **use of a consistent input parameter set** is able to **improve the understanding** of the less documented ones. The (n,α) reaction analysis in the A=50 range [18,13] can be mentioned in this respect, a significant underestimation of the experimental data by the model calculations being attributable to different alpha-particle transmission coefficients in the incident and emergent reaction channels [18]. Thus, the dashed excitation functions for the (n,α) reactions on 52Cr, 54Fe, and 58,62Ni nuclei (Figs. 3b and 5) were got by using the optical model potential (OMP) of McFadden and Satchler [19], however proved to properly describe the alpha-particle total reaction cross sections. Nevertheless, the first MeVs of the calculated excitation functions are mainly determined by the alpha-particle OMP (the neutron and proton OMPs being fixed through the SPRT method and the proton total reaction cross section analysis, respectively, the gamma-ray transmission coefficients being given apart by a gamma-ray strength function analysis, the neutron channel level density being established as mentioned above, and the continuum population being not significant at these incident energies, for the alpha-particle channel). Therefore the alpha-particle OMP diffusibility has been increased with about 20% [13] in order to get the agreement of the calculated (full curves in Figs. 3b and 5) and experimental excitation function low energy side, as the only one free parameter of this analysis. Additional experimental and theoretical work is presently recommended [1] to provide a reliable global OMP for alpha-particles.

3.4. The 52Cr(n,p)52V reaction

The **importance of complete theoretical low-lying schemes** can be also pointed out by the following level density analysis of the 52V nucleus and related discussion of the 52Cr(n,p)52V reaction excitation function.

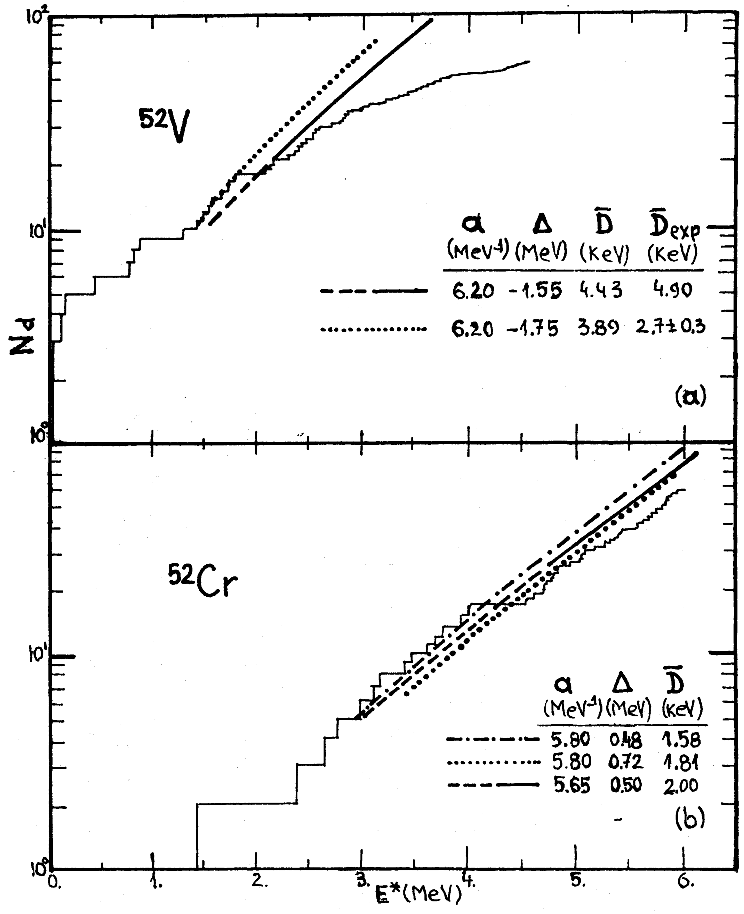

Fig. 6. Same as Fig. 1,
for the 52V and 52Cr nuclei.

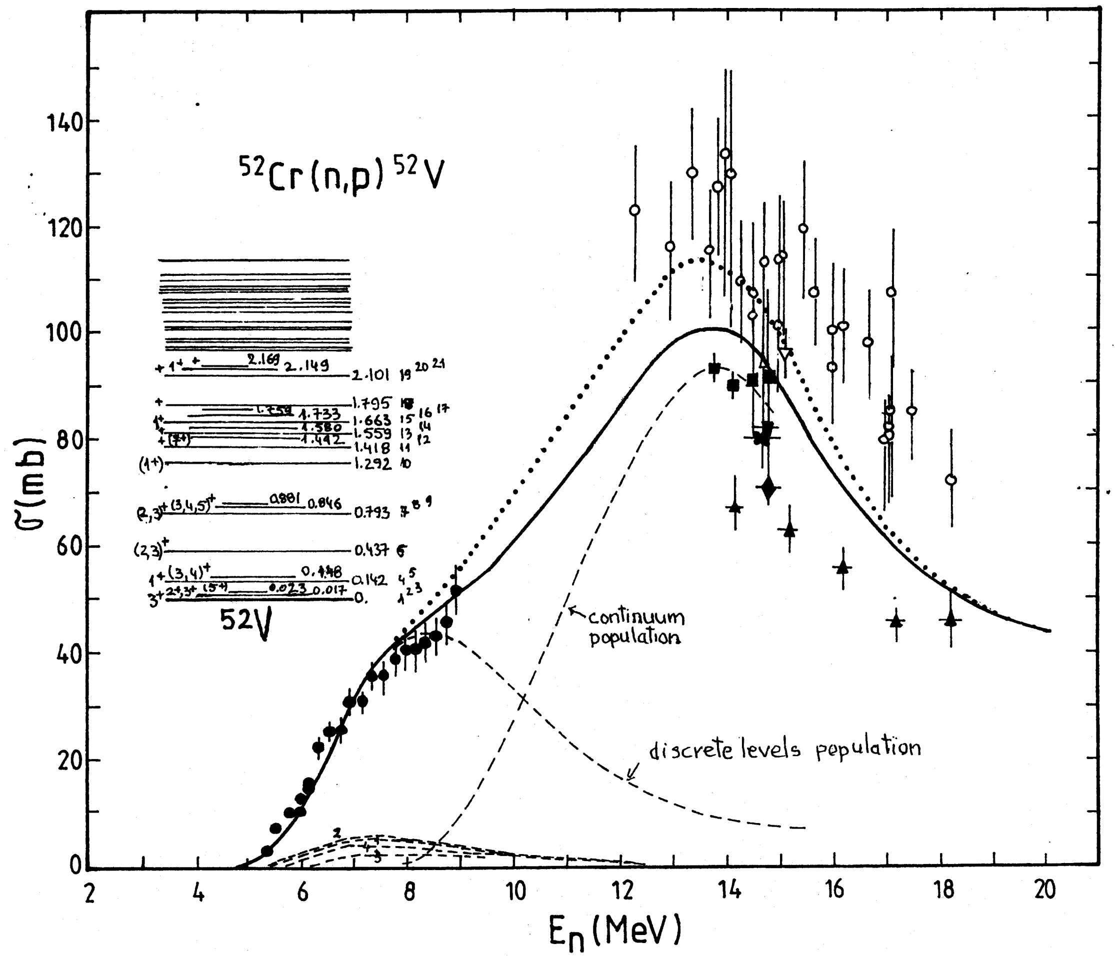

Fig. 7. Same as Fig.4, for the 52Cr(n,p)52V reaction.
For experimental data see [13].

In the case of the nucleus 52V there are two rather unlike experimental $\bar{D}$-values (see [12,13]), their usefulness in the establisment of the of the level density parameters being thus reduced. In the fit of the discrete levels there were two possibilities, shown in Fig. 6a. A **comprehensive shell-model study** of A=48-52 nuclei [19] **has allowed to take into account** as they are the gaps around 1.0 and 2.0 MeV excitation energies, respectively. Therefore, the number of 21 levels at 2.169 MeV have been used [13] both to get the level density parameters (full curve in Fig. 6a) and into the Hauser-Feshbach calculations (full curve in Fig. 7). By using the second level density parameter set shown in Fig. 6a for 52V, the calculated excitation function of the 52Cr(n,p)52V reaction is increased with more than 10% (dotted curve in Fig. 7). On the other hand, the proper consideration of the residual nucleus discrete levels and the level density at the low-energy end has allowed a correct descriptions of the "bump" of this excitation function around the 7 - 8 MeV incident energy.

A questionable choice could be however considered the level density parameters for the 52Cr nucleus (Fig. 6b). 26 discrete levels up to 4.838 MeV excitation energy have been taken into account [13], but there was not clear the physical meaning of the 0.5 MeV gap above 4.0 MeV excitation. The final choice (full curve in Fig. 6b) is more an intermediate one than a basically supported assumption. It has been validated by the consistent analysis of the all available (n,p), (n,) and (n,2n) reaction experimental data (Figs. 7, 5a, 8). A particular significance has the calculated 52Cr(n,2n)51Cr reaction excitation function above 16 MeV incident energy [20,13], in clear disagreement with the experimental data known at the calculation time but closely supported by a recent and careful experiment [21].

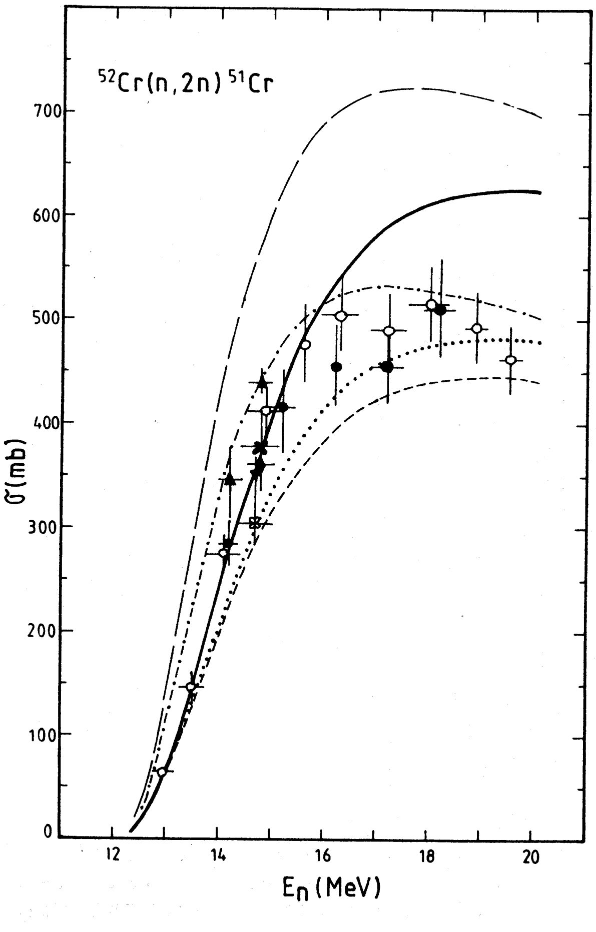

Fig. 8. Same as Fig. 3, for the 52Cr(n,2n)51Cr reaction[13].

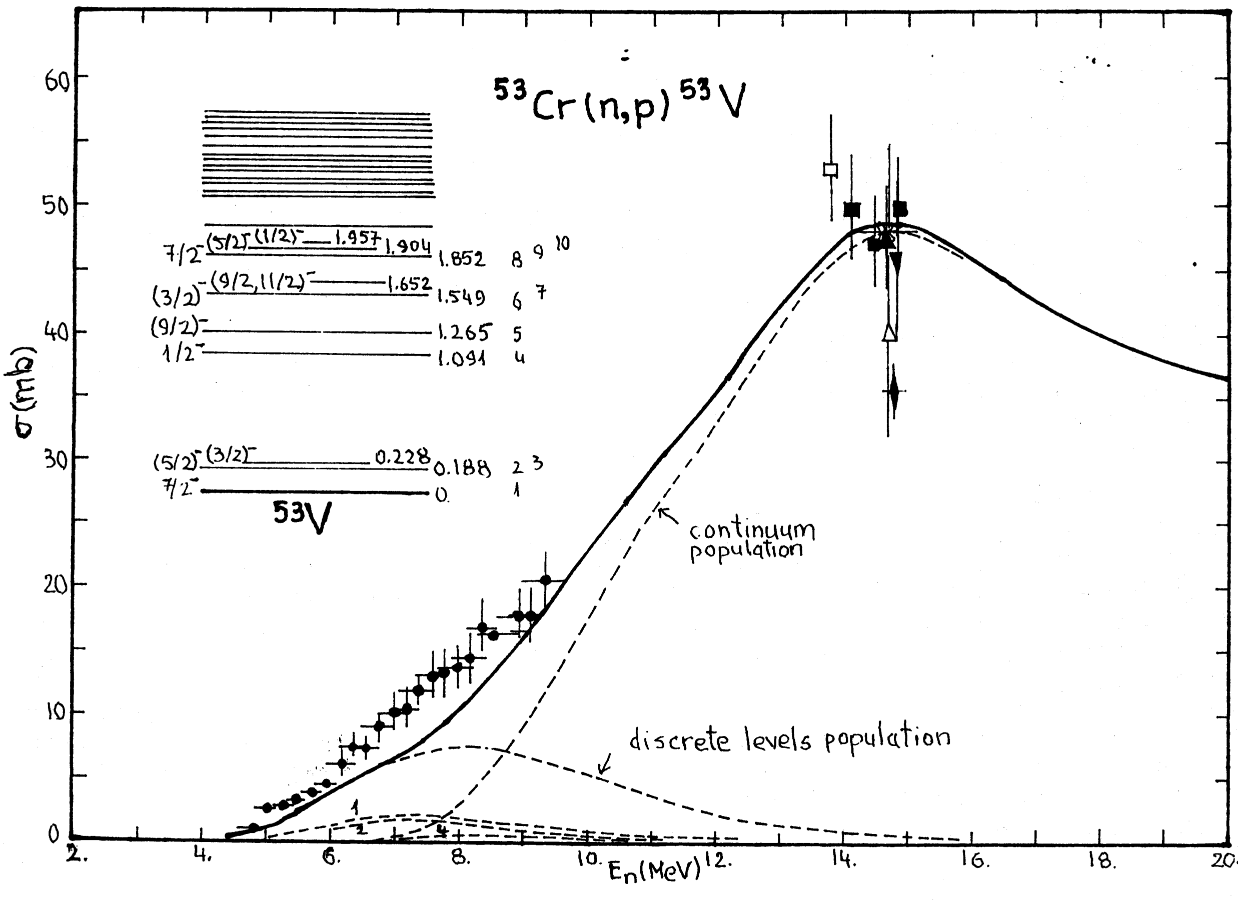

Fig. 9. Same as Fig. 7, for the 53Cr(n,p)53V reaction.

3.5. The 53Cr(n,p)53V reaction

The calculation of this reaction excitation function is the only one of the consistent nuclear model analysis of fast neutron reaction data of A=50-64 nuclei [13], failling in the description of the low-energy experimental data (Fig. 9). Due to the lack of the J^{π}-values for levels above the excitation energy of ≈2.0 MeV, only 10 and 11 discrete levels have been taken into account in the Hauser-Feshbach calculations for the nuclei 53V and 53Cr, respectively (Fig. 10). It seems to us that the gap of about 1.0 MeV in the presently known low-lying level scheme of 53V is responsible for the large disagreement between the calculated and experimental 53Cr(n,p)53V reaction cross sections between 7 and 8 MeV incident energies. Theoretical works similar to [19] but for the 53V nucleus should be obviously of a great help in this analysis.

4. CONCLUSIONS

Accurate low-lying level schemes are quite important for the **correct establisment** of the **nuclear level density parameters. Confident statistical model calculation results,** highly determined by these parameters, are also conditioned by correctness of the discrete levels taken into account (especially when the continuum population is

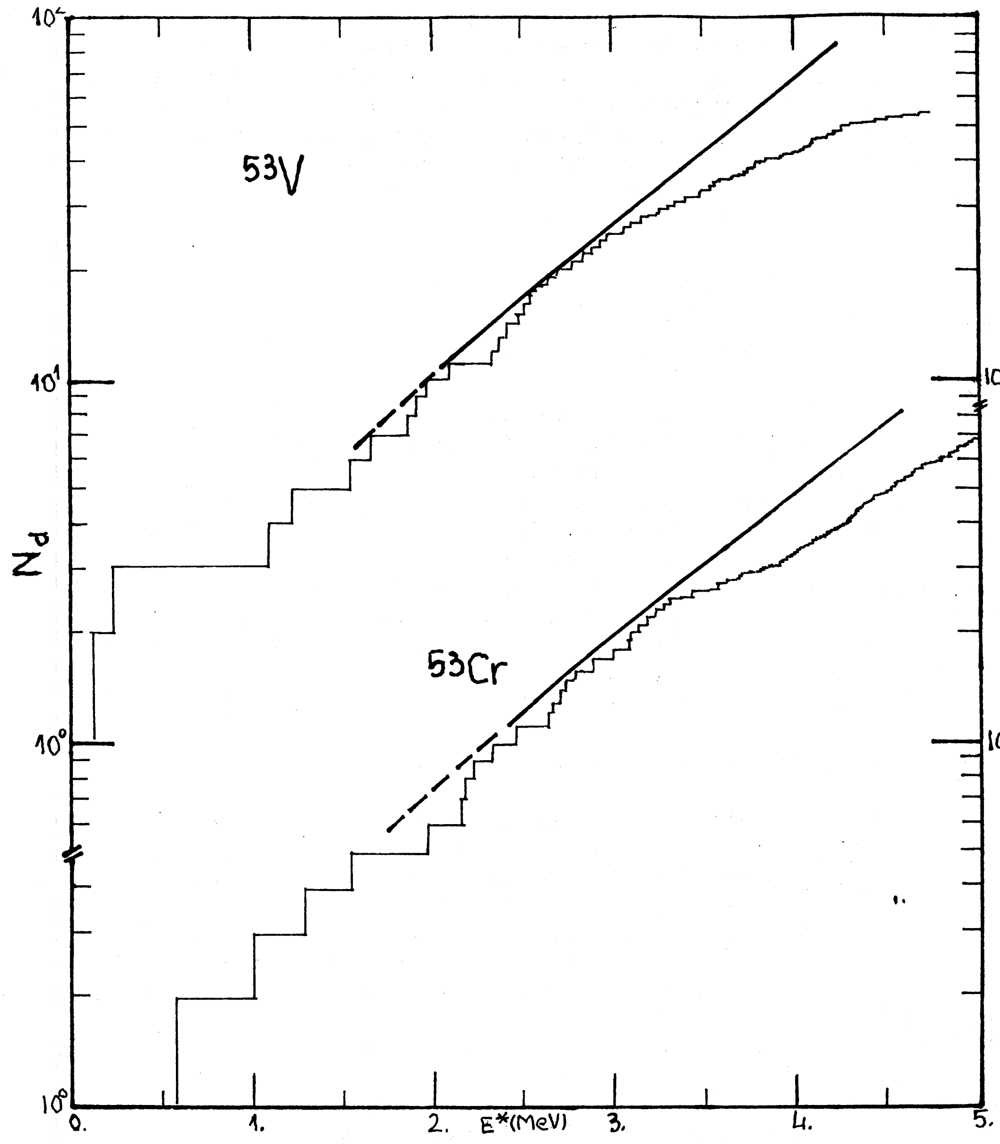

Fig. 10. Same as Fig.1, for the 53V and 53Cr nuclei.

less significant) as presently shown for fast neutron reactions in the A=50 range. The **usefulness of theoretical low-lying level schemes** is even more increased in the case of high accuracy reaction cross sections required by nuclear technology applications.

The recommendations of the recent IAEA RCM includes as a highly desirable a <u>ready-to-use file of discrete level schemes and spectroscopic informations</u> (a similar super-recommended set of average neutron resonance spacings, also for testing and normalization of level density approaches, is already under development within ENEA-Bologna). It seems that a <u>complementary file of microscopical level schemes</u> could be equally valuable for both:

(a) experimentally well-known nuclei, suggesting the energy limit of the all discrete level believed to be known, and

(b) nuclei apart from the beta-stability valley, for which experimental are scarce or even missing.

To this end, each theoretical work should indicate the limit up to which are given all the calculated levels in rather good agreement with the available experimental data.

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