DEVELOPMENT OF CALCULATION TOOLS: CALCULATION OF CROSS SECTIONS FOR 50,52CR UP TO 60 MEV
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The activation cross sections of the isotopes ^{50,52}Cr in the excitation-energy range up to 60 MeV have been analyzed as part of a general investigation [1-5] of the reaction mechanisms of fast neutrons at low and medium energies. This analysis results also enabled a stringent test of models for the above-mentioned nuclear processes, although our primary aim was to comply with the needs of a sound, complete and reliable neutron-induced cross section data library to address safety and environmental issues of the fusion programme [6]. Thus, in order to gain insight into this problem, we have analyzed these activation cross sections using the parameter databases obtained previously by global optimization within the computer codes TALYS [7] and EMPIRE-II [8], as well as a local parameter set within the STAPRE-H code [9] using the pre-equilibrium emission (PE) model Geometry-Dependent Hybrid (GDH). No fine tuning was done to optimize the description of the nucleon emission for all the cases, but for STAPRE-H a consistent set of local parameters has previously been established or validated on the basis of independent experimental information of, e.g., neutron total cross sections, proton reaction cross sections, low-lying level and resonance data, and gamma-ray strength functions based on neutron-capture data. The comparison of various calculations, including their sensitivity to model approaches and parameters, has concerned all the activation channels for which there are measured data. It was thus avoided the use of model parameters which have been improperly adjusted to take into account properties peculiar to specific nuclei in the decay cascade. This work has had to be done for the four isotopes since the consistency of model calculations can be proved only by consideration of at least all stable isotopes of an element. This point is of particular importance for the Cr isotopes due to a known model inconsistency found by EC/JRC scientists within the trial [10] to describe unitary the (n,p) and (n,2n) reaction cross sections up to the incident energy of 20 MeV. This lack of consistency remains also within the more recent work of Han [11] which stops at the incident energy of 20 MeV while more data are known up to 40 MeV. Actually the complexity and difficultness of this analysis for the Cr isotopes have been proved even as an unsolved sample case within the EMPIRE-II manual (Ref. [8], pp. 171-172).

<u>The global predictions</u> provided by TALYS-1.0 and EMPIRE-II v.2.19 up to 60 MeV for ^{50,52}Cr are shown in Figs. 2-4, in comparison with the experimental data available at lower energies. One may note that the above-mentioned model inconsistency [10] is still surrounded by these calculated results, the (n,p) and (n,2n) reactions being suitable described by using the TALYS code, deeply involved in the EAF/EFF development, only in the case of the isotope ^{52}Cr. The very few data sets available above 20 MeV but below 40 MeV neutrons on ^{50,52}Cr are also not described except four ^{52}Cr(n,2n)^{51}Cr reaction cross section data. On the other hand the EMPIRE-II results decrease systematically faster with energy than the TALYS ones. Under these conditions the correctness of model predictions for the incident energies up to 60 MeV is rather questionable. Thus, the overview of the calculated activation cross sections shows that an analysis based on a consistent local parameter set is necessary in order to explain the differences between the experimental, calculated and evaluated cross sections.

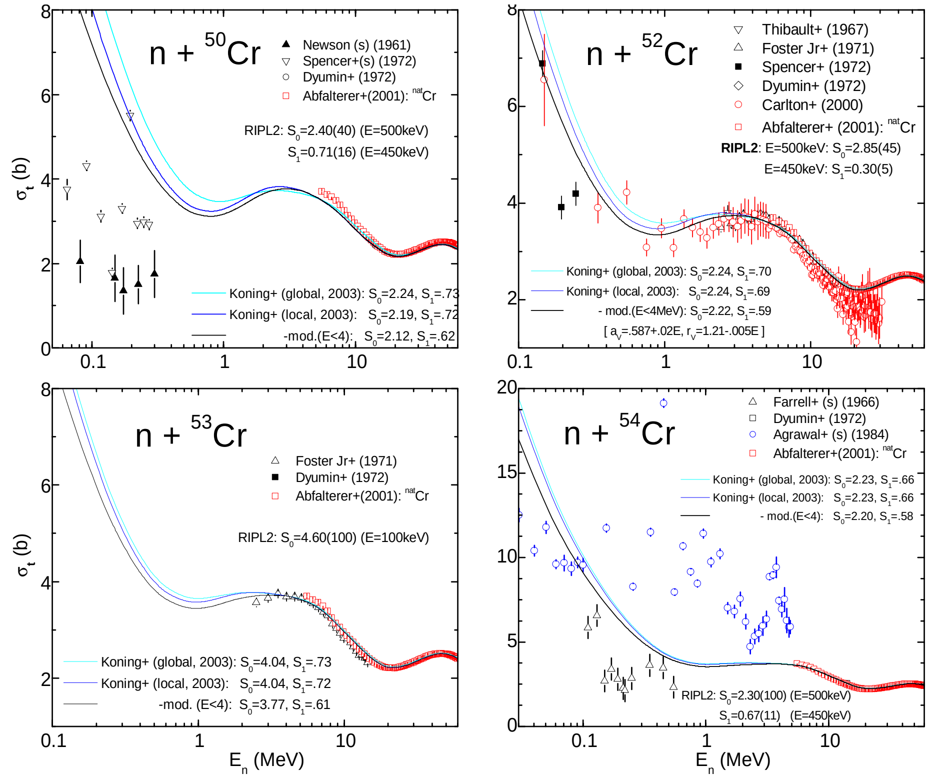

Figure 1. Comparison of calculated and measured neutron total cross sections for all stable Cr isotopes

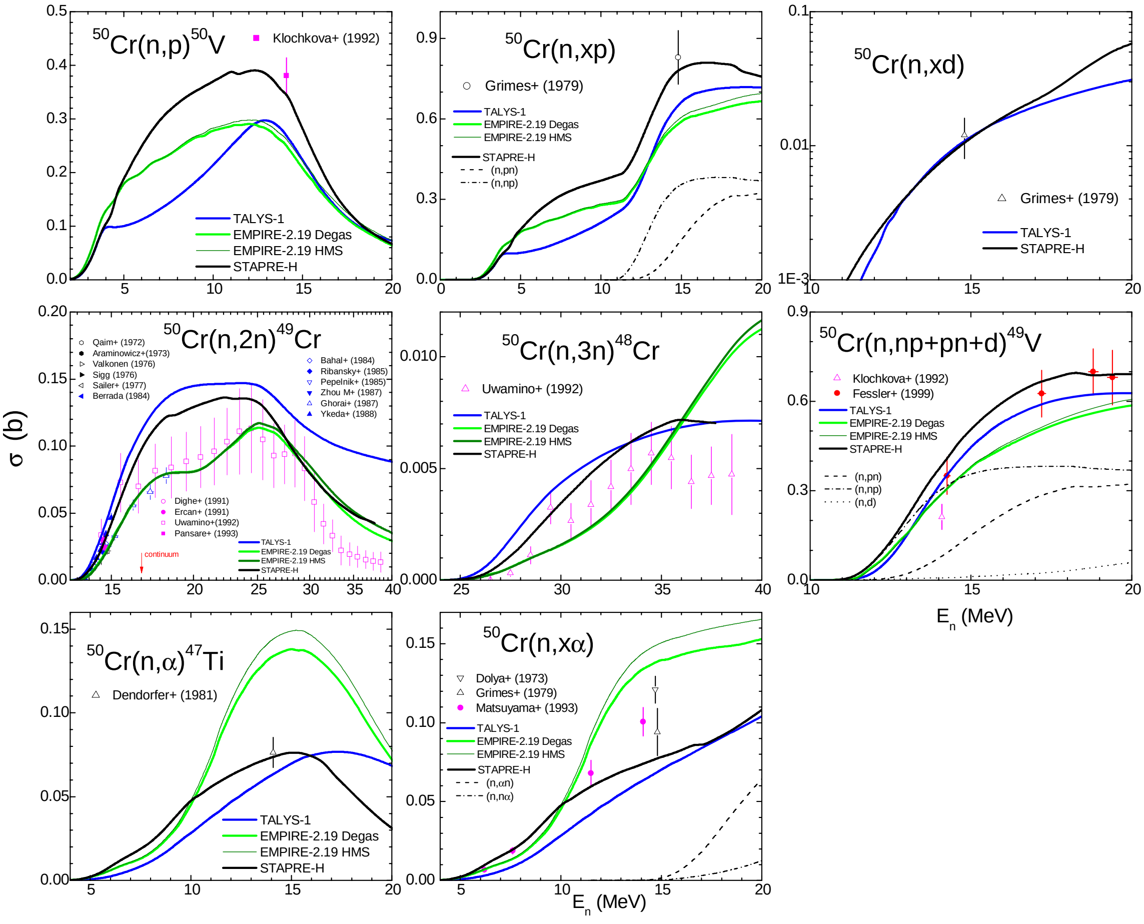

Figure 2. Comparison of calculated and measured activation cross sections for ^{50}Cr isotope.

The neutron optical potential was the first subject of the local parameter analysis. A basic point in this respect is the highlighting that the global potential [12], used by default in both TALYS and EMPIRE codes, does not reproduce the minimum around the neutron energy of 1-2 MeV for the total neutron cross sections of the mass A~60 nuclei. Following also their comment of the constant geometry parameters which may be responsible for this aspect, we have applied the SPRT method by using the RIPL-2 data [13] for the low-energy neutron scattering properties (S_0, S_1, R') and the available measured neutron total cross sections [14] of the neutron total cross sections for ^{50,52,53,54}Cr stable isotopes beyond the neutron energy of even 60 MeV (Fig. 1). A decrease of approx. 7% for this cross section has thus resulted around the incident energy of 1 MeV, corresponding to the average energy of the statistically emitted neutrons. Next, this potential has been involved in the calculation of the corresponding collective inelastic scattering cross sections by means of the direct-interaction distorted-wave Born approximation (DWBA) method, with the local version of the computer code DWUCK4 [15]. The collective state parameters of Han [11] were used in this respect, fractions of the direct inelastic scattering to compound nucleus cross section being obtained as large as approx.11% for ^{50}Cr and approx.7% for ^{52}Cr and decreasing with the energy by approx.50% up to 60 MeV.

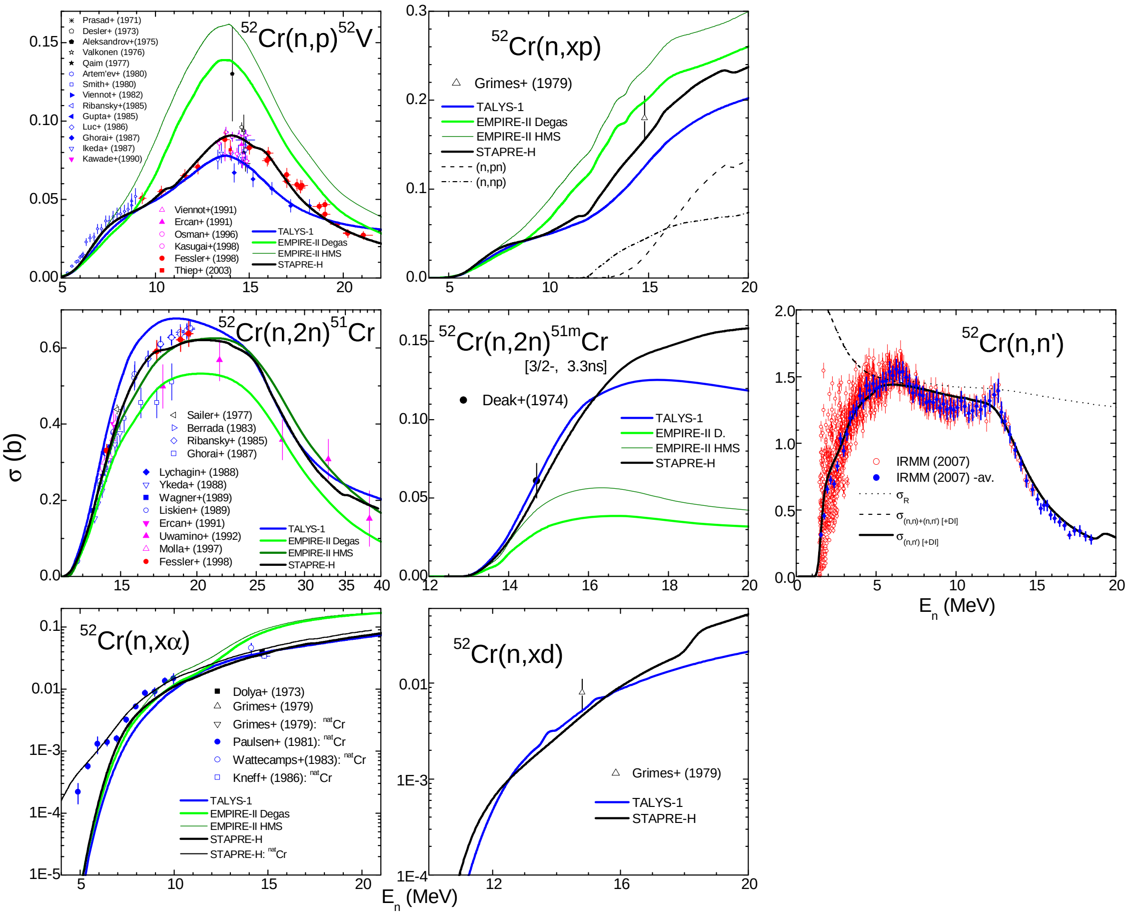

Figure 3. Comparison of calculated and measured activation cross sections for ^{52}Cr isotope.

<u>The proton optical potential</u> [12] was also modified on the basis of a comparison of calculated and measured cross sections of (p,n) reaction on ^{51}V target nucleus as well as the corresponding (p,γ) reaction data. At the same time, the electric dipole <u>γ-ray strength functions</u> $f_{E1}(E_\gamma)$ which are used for the calculation of the γ-ray transmission coefficients, have been obtained by means of a modified energy-dependent Breit-Wigner (EDBW) model [16]. Moreover, systematic EDBW correction factors F_{SR} were obtained by using the experimental average radiative widths $\Gamma_{\gamma 0}^{exp}$ of the *s*-wave neutron resonances, and assuming that $F_{SR}=\Gamma_{\gamma 0}^{exp}/\Gamma_{\gamma 0}^{EDBW}$. Next, the $f_{E1}(E_\gamma)$ thus obtained were checked by calculation of capture data.

Finally a suitable description has been obtained, in the limits of the more recent data, of all activation cross sections for the Cr stable isotopes (Figs. 2-4). The good agreement of the calculated cross sections with the more recent data between 14 and 21 MeV solved thus the model inconsistency pointed out previously. The basic point in this respect has been the use within the PE model of an advanced particle-hole state density [17]. On the other hand, the predictive power of the local-approach model calculations has been just proved by the overestimation of measured cross sections for $^{50}Cr(n,2n)^{49}Cr$ reaction above 15 MeV (Fig. 2) in quite close agreement with results [18] of the most recent integral data analysis. The present consistent model calculations have also pointed out the questionable saturation of the excitation functions of (n,n'p+d) reaction on $^{53,54}Cr$ isotopes, showing the need of additional measurements.

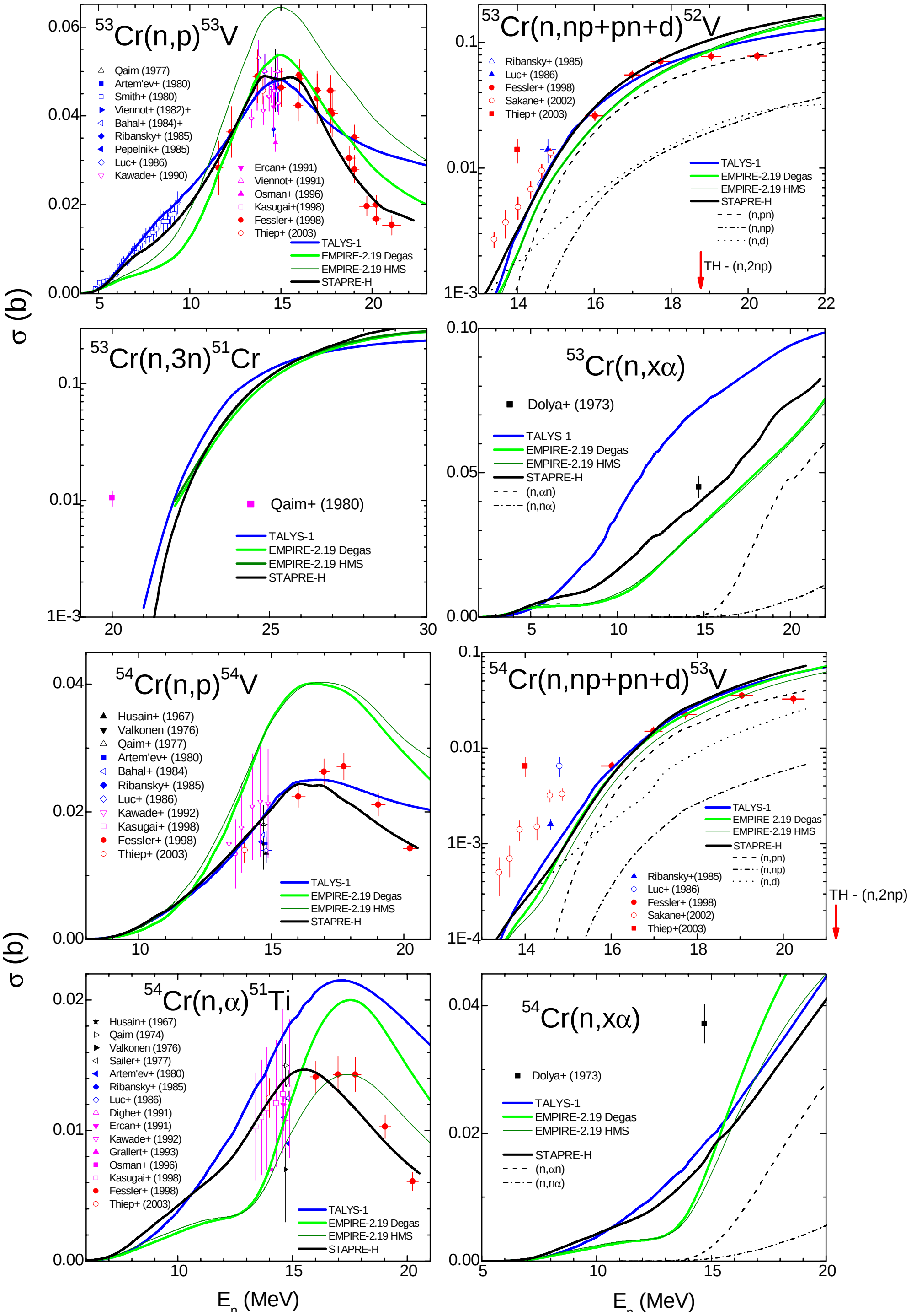

Figure 4. Comparison of calculated and measured activation cross sections for $^{53,54}Cr$ isotopes.

Since no free parameter was involved in the GDH calculations while the same common parameters of OMP and nuclear level density were used in the DWBA, GDH and HF model calculations, the proper description of a large body of data without free parameters validated both the adopted nuclear model assumptions and parameter set. Actually it resulted to be of rather equal importance the agreement with both the data for, e.g., the (n,p) and (n,2n) reactions around the neutron energy of 14 MeV, and the (n,xn) data above 20 MeV. The former is critical for the check of partial level densities which trigger the PE calculated data, while the latter makes possible the analysis of basic assumptions of PE model within an enlarged energy range.

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