Comparison of EMPIRE-II (2.19) calculations for (n, p) reaction with experimental data in different mass regions

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Introduction

An extensive study of (n, p) reaction cross section data for structural materials over a wide mass region is important for estimating hydrogen gas generation and induced activities in fusion and fission reactors. In the literature, the experimental results for a number of nuclei have been reported. In the present paper we have used EMPIRE-II (ver 2.19) [1] code to explain the available data for the (n, p) cross sections for various structural materials and we report here typical results for few cases in different mass regions. This analysis was carried out over an energy range extending up to 20 MeV.

Calculations and comparison with data

The theoretical calculations carried out for the reactions ^{27}Al(n,p)^{27}Mg, ^{92}Mo(n,p)^{92m}Nb, ^{153}Eu(n,p)^{153}Sm and ^{186}W(n,p)^{186}Ta are presented in Figs. 1-2, along with the available experimental data. Fig 1b and 2a also includes the measurements carried by us [2]. EMPIRE is a modular system of nuclear reaction codes. The code contains the full EXFOR [3] library of experimental nuclear data. The main input parameters to the calculations e. g., nuclear masses, ground state deformations, discrete energy levels and decay schemes, nuclear level densities and moment of inertia, and gamma ray strength function parameters are taken from "Reference Input Parameter Library: RIPL-2" [4] developed at IAEA. The exciton model (DEGAS code) with angular momentum conservation [5,6] is used to describe the particle and gamma ray emissions before the compound nucleus formation and includes the contribution of pre-equilibrium effects in the emission spectra. The particle transmission coefficients for the exciton and Hauser-Feshbach models were generated in the EMPIRE runs via the SCAT-2 optical model code [7]. We used different global and local sets of OMPs and selected the one that fits the data best at all the energies. For neutrons and protons, the optical model potentials of Koning and Delaroche [8] are used. For alphas, the potentials proposed by Satchler [9] have been adopted. The level density was calculated using the dynamic approach specific to the EMPIRE code in which collective enhancements of the level densities due to the nuclear vibrations and rotations were

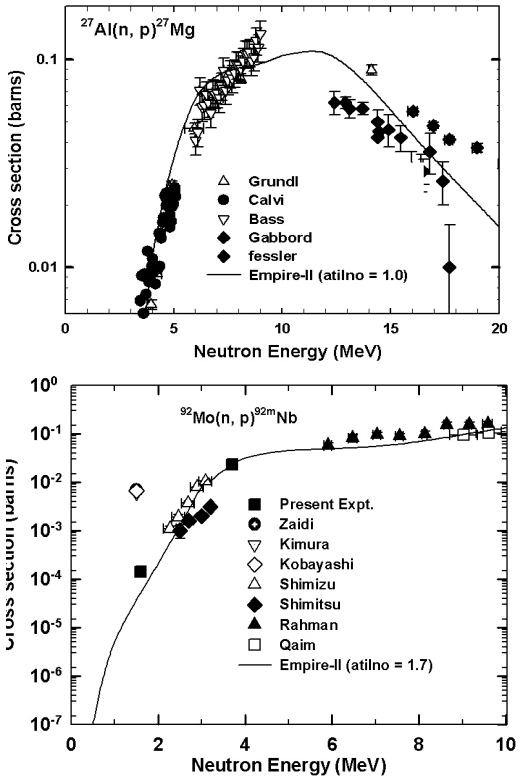

Fig. 1a, 1b: Excitation function for the reactions ^{27}Al(n, p)^{27}Mg and ^{92}Mo(n, p)^{92m}Nb. The solid line represents the EMPIRE-II calculations.

accounted for. The formalism uses the superfluid Bardeen- Cooper-Schrieffer (BCS) [10] model

below the critical excitation energy (when the EMPIRE-specific parameterization of the level density parameter is selected) and Fermi gas model for above the critical excitation energy. With pairing correction $\Delta = 12/A^{1/2}$ and the critical temperature $T_{crit} = 0.567\Delta$, the BCS level densities are calculated from the following expression [11],

$$\rho_{(U,J)} = \frac{(2J+1)\exp\left(\frac{S - J(J+1)}{2\sigma_{eff}^2}\right)}{2\sqrt{2\pi}\left(\sqrt{Det}\right)\sigma_{eff}^3} \quad (1)$$

where,

ρ = excitation energy minus pairing energy

J = nucleus spin , S = entropy of the system

σ_{eff} = effective spin cut off parameter and det is as defined in ref 11.

The EMPIRE-specific energy (temperature) - dependent level density parameter "a" was used which is in the form of

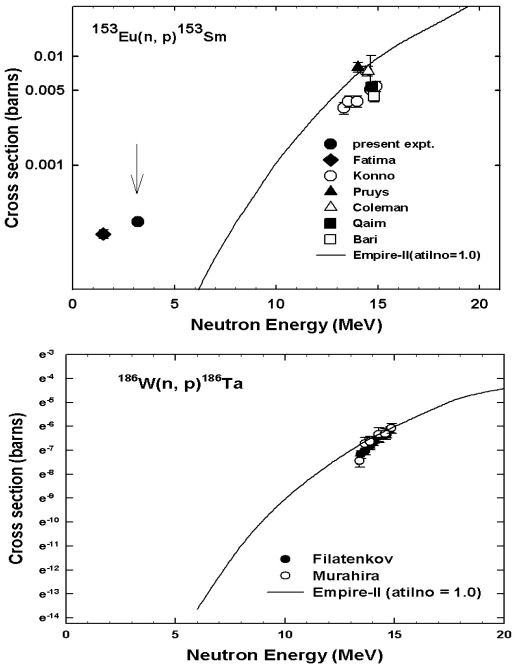

Fig. 2a, 2b: Excitation function for the reactions ^{153}Eu(n, p)^{153}Sm and ^{186}W(n, p)^{186}Ta. The solid line represents the EMPIRE-II calculations.

$$a(U) = \tilde{a}\left(1 + f(U)\frac{\delta_W}{U}\right) \quad (2)$$

where, $f(U) = 1 - \exp(-\gamma U)$, δ_W = shell correction. The asymptotic value of the level density parameter of the level density parameter is then given by

$$\tilde{a} = \eta A + \zeta A^{2/3} F_{surf}\left(\frac{R_{max}}{R_{min}}\right) \quad (3)$$

The various terms have their usual meanings as defined in Ref 12. In the present calculations, Myers Swiatecki shell correction [13] with the following values is used.

η = 0.052268, ζ = 0.13395, and γ = 0.093955 for Z<85.

The cumulative plots of the discrete levels for each nucleus involved in the calculation were produced using the FITLEV option in the code.

Conclusion

In case of ^{92}Mo(n, p)^{92m}Nb reaction, the level density parameter was required to be scaled up by a factor of 1.7. For other reactions ^{27}Al(n, p)^{27}Mg, ^{153}Eu(n, p)^{153}Sm and ^{186}W(n, p)^{186}Ta default value of level density parameter was used. A good agreement is obtained for all the systems. Calculations for various other systems over entire mass region and other reaction channels are also in progress.

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