Theoretical cross sections of tantalum on neutron induced reactions

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Abstract. Neutron-induced cross-sections for the stable isotope $^{181}$Ta, in the energy region up to 20 MeV have been calculated. Statistical model calculations, based on the Hauser-Feshbach formalism, have been carried out using the TALYS-1.0 and were compared with available experimental data in the literature and with ENDF/B-VII, $T = 300$ K; JENDL-3.3, $T = 300$ K and JEFF-3.1, $T = 300$ K evaluated libraries.

1 Introduction

With the advent of fast computers, software that simulates nuclear reactions is able to play an increasingly important role in nuclear data. It is possible to provide an exact computational scheme for sophisticated nuclear models, not only new ones but also those that have been lying on the shelf for decades and only now become amenable for numerical implementation. Large scale comparisons with measurements are within reach. TALYS is a nuclear reaction program created at NRG Petten, the Netherlands, and CEA Bruyères-le-Châtel, France. The purpose of TALYS is to simulate nuclear reactions that involve neutrons, photons, protons, deuterons, tritons, $^3$He, and $\alpha$ particles in the 1 keV to 200 MeV energy range. Predicted quantities include integrated, single and double-differential cross sections, for both the continuum and discrete states, residue production and fission cross sections, $\gamma$-ray production cross sections, etc. Nuclear cross section data can be obtained by three different ways on the basis of experimental measurement, theoretical model calculations and evaluation data files. Experimental cross section data in the range 15-20 MeV are not available for all neutron induced reactions on Tantalum isotopes however, there is only a limited number of data for at the energy range $<15$ MeV [1-4].

2 Calculation Methods

The high-energy end of the ejectile spectra are described by preequilibrium emission, which takes place after the first stage of the reaction but long before statistical equilibrium of the compound nucleus is attained. It is imagined that the incident particle creates step by step more complex states in the compound system and gradually loses its memory of the initial energy and direction. The default preequilibrium model of TALYS is the two-component exciton model [5,6]. We recall the basic formula of [5] for the exciton model cross section,

$$
\frac{d\sigma_{EM}}{dE_k} = \sigma_{CF} \sum_{p_\pi} \sum_{p_\nu} w_k(p_\pi, h_\pi, p_\nu, h_\nu, E_k) 
$$

where $p_\pi$ ($p_\nu$) is the proton (neutron) particle number and $h_\pi$ ($h_\nu$) the proton (neutron) hole number, $\sigma_{CF}$ is the compound formation cross section, and $S_{pre}$ is the time-integrated strength which determines how long the system remains in a certain exciton configuration. The initial proton and neutron particle numbers are denoted $p_\pi^0$ and $p_\nu^0$, with $Z_p(N_p)$ being the proton (neutron) number of the projectile. In general, $h_\pi = p_\pi$ and $h_\nu = p_\nu - p_\nu^0$, so that the initial hole numbers are zero, i.e., $h_\pi^0 = h_\nu^0 = 0$ for primary preequilibrium emission. The preequilibrium part is calculated by Eq. (1), using $p_{\pi}^{eq} = p_{\nu}^{eq} = 6$, whereas the remainder of the reaction flux is distributed through the Hauser-Feshbach model. In addition, the never-come-back approximation is adopted. The emission rate $w_k$ for ejectile $k$ with spin $s_k$ is given by

$$
w_k(p_\pi, h_\pi, p_\nu, h_\nu, E_k) = \frac{2s_k + 1}{\pi^2 h^3} \mu_k E_k \sigma_{inv}(E_k) 
\times \frac{\omega(p_\pi - Z_k, h_\pi, p_\nu - N_k, h_\nu, E_k)}{\omega(p_\pi, h_\pi, p_\nu, h_\nu, E^{inv})},
$$

where $\sigma_{inv}(E_k)$ is the inverse reaction cross section as calculated from the optical model, and $\omega$ is the two-component particle-hole state density. The full reaction dynamics that leads to Eq. (1) is described in Refs. [5,6]. We here restrict ourselves to the formulas given above since they contain the model- and parameter-dependent quantities. The expression for $S_{pre}$ contains the adjustable transition matrix element $M_2$ for each possible transition between neutron-proton exciton
configurations. A proton-neutron ratio of 1.6 for the
squared internal transition matrix elements was adopted
to give the best overall agreement with experiment, i.e.,
$M_{\text{NN}}^2 = M_{\text{NN}}^2 = 1.6M_{\text{NN}}^2 = 1.6M_{\text{NN}}^2$. Partial level density
parameters $g_n = Z/17$ and $g_v = N/17$ were used in the
equidistant spacing model for the partial level densities.

Finally, an effective surface interaction well depth $V = 12$
MeV [5] was used. At incident energies above several
tens of MeV, the residual nuclides formed after binary
emission may have so large an excitation energy that the
presence of additional fast particles inside the nucleus
becomes possible. The latter can be imagined as
strongly excited particle-hole pairs resulting from
the first binary interaction with the projectile. The residual
system is then clearly non-equilibrated, and the excited
particle that is high in the continuum may, in addition to
the first emitted particle, be emitted on a short time
scale. This so-called multiple preequilibrium emission
forms an alternative theoretical picture of the
intrannuclear cascade process, whereby the exact location
and momentum of the particles are not followed, but
instead the total energy of the system and the number of
particle-hole excitations (exciton number). In actual
calculations, the particle-hole configuration of the
residual nucleus after emission of the ejectile, is
reentered as an initial condition in Eq. (1). When
looping over all possible residual configurations,
the multiple preequilibrium contribution is obtained [7-20].

In TALYS, multiple preequilibrium emission is
followed up to arbitrary order; though for 96 MeV, only
the secondary preequilibrium emission is significant. It
is well known that semiclassical models, such as
the exciton model, have had some problems in describing
angular distributions (essentially because the model is
based on a compound like concept instead of a direct
one). Therefore, as mentioned previously, the double-
differential cross sections are obtained from the
calculated energy spectra using the Kalbach
systematics
[11]. To account for the evaporation peaks in the
charged-particle spectra, multiple compound emission
was treated with the Hauser-Feshbach model. In
this scheme, all reaction chains are followed until all
emission channels are closed. The Ignatyuk model [12]
has been adopted for the total level density to account
for the damping of shell effects at high excitation
energies. For preequilibrium reactions involving
deuterons, tritons, $^3$He and $\alpha$ particles, a statistical
contribution from the exciton model is automatically
accounted with the formalism described above.

However, it is well known that for nuclear reactions
involving projectiles and ejectiles with different particle
numbers, mechanisms such as stripping, pickup, and
knockout play an important role, and these direct like
reactions to the continuum are not covered by the
exciton model. Therefore, Kalbach has developed a
phenomenological contribution for these mechanisms
[11], which is included in TALYS. The advantages over
the older method include a better consideration of the
available phase space through normalized particle-hole
state densities and a better empirical determination of the
pickup, stripping, knockout strength parameters,
enabled by the more extensive experimental database
that is now available. It has recently been shown that for
medium and heavy nuclides this method gives a
considerable improvement over the older methods. The
latter seemed to consistently under predict neutron-
induced reaction cross sections involving pickup of one
or a few nucleons.

Fig. 1. The comparison of calculated excitation function using TALYS of $^{181}$Ta(n,n') & $^{181}$Ta(n, el) reaction with available experimental values and evaluated nuclear data files ENDF/B-VI. The values reported in Ref. (21)

Fig. 2. The comparison of calculated excitation function using TALYS of $^{181}$Ta(n,p) and $^{181}$Ta(n,α) reaction with available experimental values and evaluated nuclear data files ENDF/B-VI, JENDL-3.3 and JEFF3.1. The values reported in Ref. (21)
There are only a limited number of experimental cross sections obtained. The results can be summarized and conclude that there is reasonable agreement with ENDF/B-VII.0 code are compared with available experimental data. The results of our calculations using TALYS-1.0 have been carried out up to 20 MeV incident neutron energy. The calculation of TALYS-1.0 code of $^{181}$Ta(n,2n) reaction are in good agreement with the measurements between 12 and 20 MeV Fig. 2. ENDF/B-VII.0 and JENDL-3.3 show important discrepancies in energies < 16 MeV.

### 3.4 (n,α) Reactions

There are only two experiment value for $^{181}$Ta(n,α) Fig. 2. TALYS-1.0 has been used for $^{181}$Ta(n,α) reaction.

### 3.5 (n,2n) Reactions

The calculation of TALYS-1.0 code of $^{181}$Ta(n,2n) reaction are in good agreement with the measurements between 12 and 20 MeV Fig. 3. ENDF/B-VI, JENDL-3.3 and JEFF-3.1 files are in agreement with each other.

### 3.6 (n,3n) Reactions

The calculation of TALYS-1.0 code of $^{181}$Ta(n,3n) reaction are in good agreement with the experimental data Fig. 3. ENDF/B-VI, JENDL-3.3 and JEFF-3.1 files are in agreement with each other.

### References