IOP Publishing and International Atomic Energy Agency Nuclear Fusion
Nucl. Fusion **48** (2008) 125003 (5pp) doi:10.1088/0029-5515/48/12/125003

A new simple formula for fusion cross-sections of light nuclei

Xing Z. Li, Qing M. Wei and Bin Liu

Department of Physics, Tsinghua University, Beijing 100084, People's Republic of China

E-mail: lxz-dmp@tsinghua.edu.cn

Received 29 April 2008, accepted for publication 3 October 2008
Published 3 November 2008
Online at stacks.iop.org/NF/48/125003

Abstract
The recent ENDF/B VII.0 data are compared with the fitting formula (NRL handbook—Plasma Formulary). The differences between experimental data and the fitting formula for three major fusion cross-sections reveal the need for a replacement to the old 5-parameter fitting formula. The new formula in this paper has only 3 parameters, but its fit with the experimental data is greatly improved because the energy dependence of the incident-channel (deuteron) width is taken explicitly into account through a penetrability function of the Mott form.

PACS numbers: 24.10.−i, 24.30.−v, 25.45.−z

(Some figures in this article are in colour only in the electronic version)

1. Introduction

A formula was published early in 1972 to describe the major fusion cross-sections using only 5 parameters. It was included in a famous handbook, NRL Plasma Formulary, published by the Naval Research Laboratory [1]. It correctly expressed the dependence of the cross-sections on energy, E: the geometric factor ($1/E$ dependence), the Gamow penetration factor ($\mathrm{Exp}[c/\sqrt{E}]$ dependence) and the resonance factor (Breit–Wigner type dependence). Hence it has been widely used by plasma physicists, although Bosch and Hale pointed out in 1992 [2] that this 5-parameter fitting formula did not give the correct results in the low energy region. Bosch and Hale proposed a 9-parameter fitting formula to show the correct dependence based on the R-matrix theory and thousands of experimental data. However, this old 5-parameter formula has still been cited in the later editions of NRL Plasma Formulary [3][1] even 15 years after the publication of the 9-parameter fitting formula. Many plasma scientists are still using this 5-parameter formula.

Moreover, this 5-parameter fitting formula was based on the Breit–Wigner theory, which might not be valid for light nuclei fusion reactions because it was proposed mainly for heavy or intermediate nuclei when fission reactor studies were dominant. The key assumption of Breit–Wigner theory was the compound nucleus model, i.e. the nuclear reaction might be divided into two *independent* steps—the formation of the compound nucleus and the decay of the compound nucleus. This implies that the collisions between the injected nucleon and the nucleons inside the target are strong enough to erase the particle 'memories'. The injected nucleon would become part of the compound nucleus and 'forget' its history. Hence, the decay of the compound nucleus would be totally independent of its formation. When several channels of decay are available, the compound nucleus would tend to decay into the fastest decay channel (the channel with the shortest lifetime). Since the neutron emission channel is the result of the strong nuclear interaction, usually it is the channel with the shortest lifetime. One may expect to see neutron emission after resonant tunnelling if the compound nucleus model remains valid. However, the compound nucleus model is correct only if many collisions occur inside the compound nucleus. This assumption might not be valid in the case of nuclei fusion where no strong collisions occur. The wave function of injected nucleon might still retain a memory of its phase before it is absorbed by the target. With this premise we can develop a better model to describe the fusion reaction between two light nuclei.

2. 3-Parameter model

In order to keep the memory of the phase of the wave function, a spherical square-potential well is assumed to represent the nuclear interaction between the incident projectile and the target nucleus (figure 1). In addition, an imaginary part of the nuclear potential is introduced to represent the effect of

[1] Indeed there was another mistake in the citation of NRL Plasma Formulary. The reference [28] there 'Rept.BNWL-1685 (Brookhaven National Laboratory, 1972)' should be corrected as 'Rept.BNWL-1685 (Pacific Northwest Laboratory, 1972), p 76'. This mistake was pointed out early in 2002 [8].

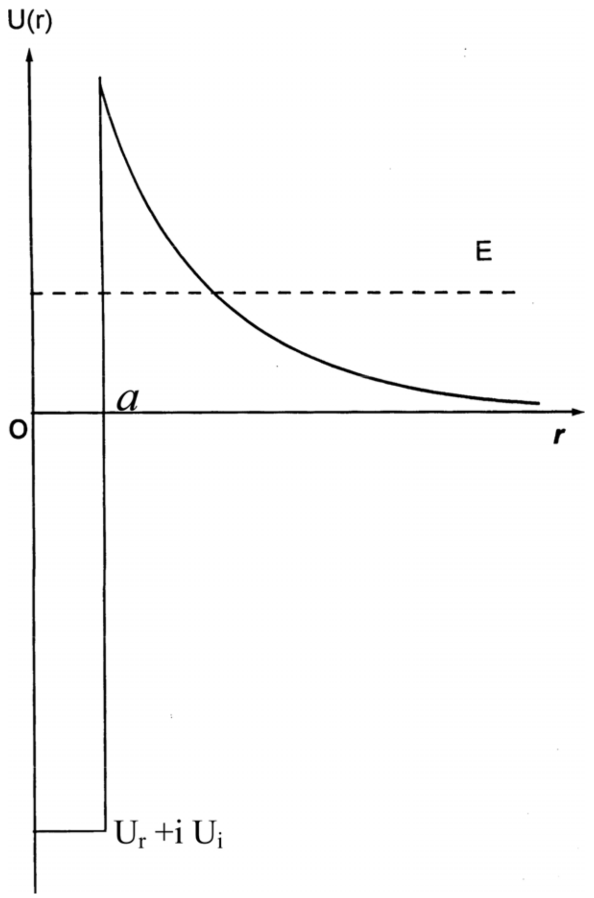

Figure 1. Spherical square nuclear potential well with an imaginary part and Coulomb potential.

absorption on the wave function. Thus, the simplest way to describe the fusion reaction between two light nuclei is a 3-parameter model with U_r (the real part of the nuclear potential well), U_i (the imaginary part of the nuclear potential well), and a (the radius of the potential well) as its parameters. In order to show the dependence of the fusion cross-section on these 3 parameters, this square nuclear potential well is connected to a Coulomb potential (figure 1), which describes the repulsive interaction between two positively charged nuclei when their distance is greater than the radius of the nuclear potential well.

The cross-section of the fusion reaction, $\sigma(E)$, may be written as [4, 5] :

$$\sigma(E) = \frac{\pi}{k^2}\frac{1}{\theta^2}\frac{(-4w_i)}{w_r^2 + (w_i - (1/\theta^2))^2}. \tag{1}$$

Here $1/\theta^2$ is the Gamow penetration factor of the Mott form:

$$\theta^2 = \frac{1}{2\pi}\left(\mathrm{Exp}\left[\frac{2\pi}{ka_c}\right] - 1\right) \tag{2}$$

$k = \sqrt{2\mu E/\hbar^2}$ is the wave number in the region $r > a$ in the centre of the mass system; μ is the reduced mass; $\hbar$ is the Planck constant divided by 2π. w_r and w_i are the real and the imaginary parts of w, which is related to the phase shift, δ_o, as [5]:

$$w = \frac{\mathrm{Cot}[\delta_o]}{\theta^2}$$
$$= k_1 a_c \mathrm{Cot}[k_1 a] - 2\left\{\ln[2ka] + 2C + Re\left[\frac{\Gamma'(-I/ka_c)}{\Gamma(-I/ka_c)}\right]\right\}. \tag{3}$$

Here, only the S-partial wave is considered because we are interested in the range of low energy. a_c is the length of Coulomb unit: $a_c = \hbar^2/\mu z_1 z_2 e^2$. z_1 and z_2 are the charge numbers of the colliding nuclei, respectively, $C = 0.577\,216$ is the Euler constant, $k_1 = \sqrt{2\mu(E - U_r - iU_i)/\hbar^2}$ is the complex wave number inside the nuclear potential well and $\Gamma(x)$ and $\Gamma'(x)$ are the gamma function and its derivative. w looks like a complicated function of energy E; but its rapidly varying part has been extracted in θ. The remaining dependence on E is the slowly varying part in k and k_1, because the change in energy is less than 1 MeV, which is much smaller than $|U_r|$, since $|U_r| > 10$ MeV. Therefore, we anticipate that the real part of k_1 does not change too much in the range of interest. Usually $|U_i| \ll |U_r|$, so the imaginary part of k_1

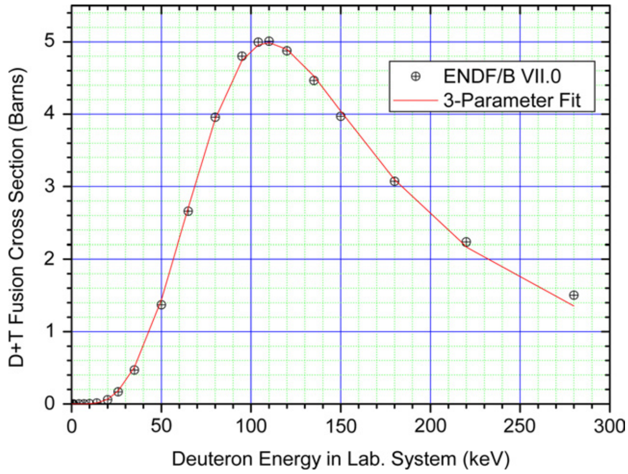

Figure 2. Comparison between D+T fusion data and the 3-parameter fit (solid line).

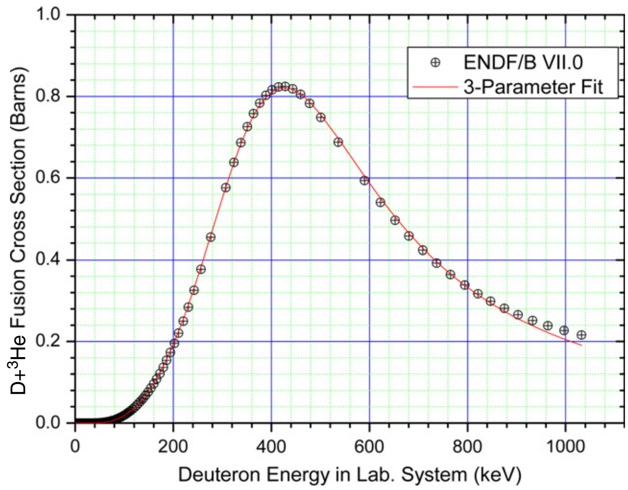

Figure 3. Comparison between D+^{3}He fusion data and the 3-parameter fit (solid line).

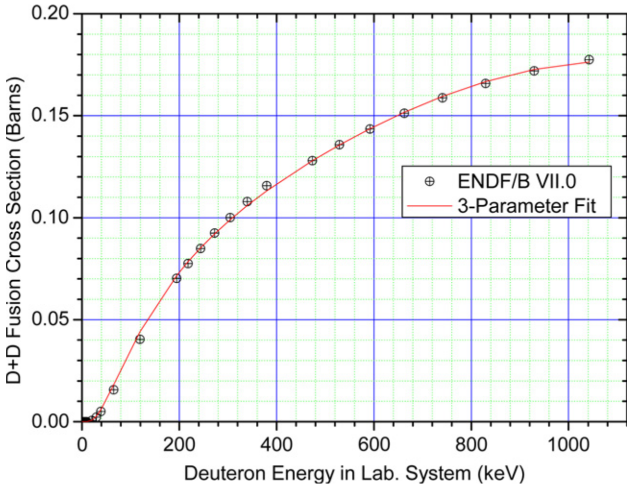

Figure 4. Comparison between D+D fusion data and the 3-parameter fit (solid line).

Table 1. Parameter list for 3-parameter fit formula.

	D+T	D+^{3}He	D+D (p+T and n+^{3}He)
C_1	−0.5405	−1.1334	−60.2641
C_2	0.005546	0.003039	0.05066
C_3	−0.3909	−0.6702	−54.9932

Table 2. NRL Plasma Formulary 5-parameter list.

			D+D Fusion	
	D+T Fusion	D+^{3}He Fusion	p+T	n+^{3}He
A_1	45.95	89.27	46.097	47.88
A_2	50200	25900	372	482
A_3	1.368×10^{-2}	3.98×10^{-3}	4.36×10^{-4}	3.08×10^{-4}
A_4	1.076	1.297	1.220	1.177
A_5	409	647	0	0

is almost a constant in the range of interest. $\ln(2ka)$ and $\Gamma(-I/ka_c)$ are slow functions of energy, which affect only the real part of w. As a result, the complex function, $w(E)$, may be simplified to

$$w = C_1 + C_2 E_{\text{lab}} + iC_3. \tag{4}$$

The fusion cross-section may be written as

$$\sigma(E_{\text{lab}}) = \frac{\pi}{(2\mu/\hbar^2)E_{\text{lab}}(M_b/M_a + M_b)}\frac{1}{\theta^2} \times \frac{(-4C_3)}{(C_1 + C_2E_{\text{lab}})^2 + \left(C_3 - (1/\theta^2)\right)^2}. \tag{5}$$

We may use experimental data to find these 3 fitting parameters (C_1, C_2, and C_3). In equation (5) and in the definitions of k and k_1, E has been replaced by E_{lab}, the energy of incident projectile in the laboratory system.

$$E_{\text{lab}} = \frac{M_a + M_b}{M_b}E \tag{6}$$

M_a and M_b are the mass of the incident projectile and the target, respectively.

Figures 2–4 are the results of the calculation using this 3-parameter fitting formula (5). Figure 2 is for D + T fusion.

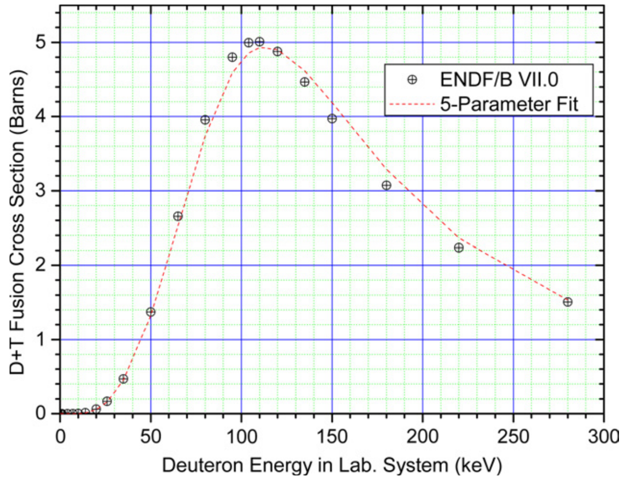

Figure 5. Comparison between D+T fusion data and the 5-parameter fit (dotted line).

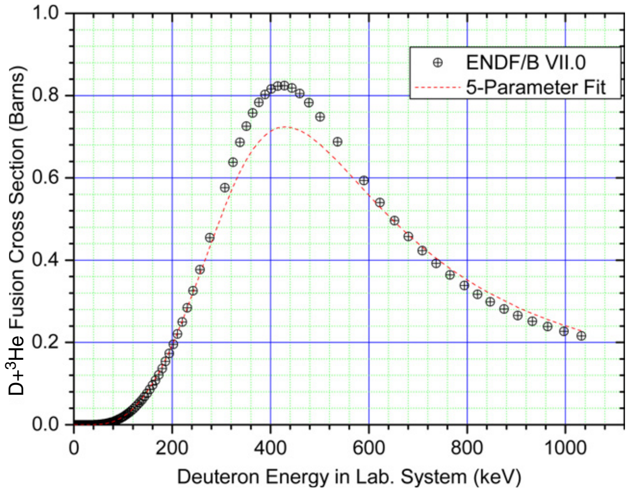

Figure 6. Comparison between D+^{3}He fusion data and the 5-parameter fit (dotted line).

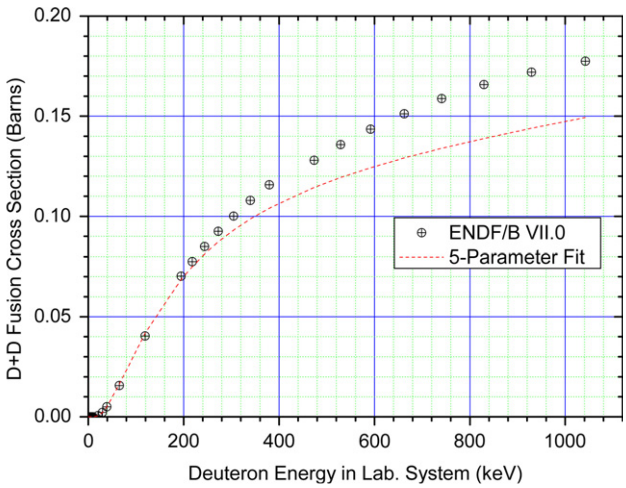

Figure 7. Comparison between D+D Fusion data and the 5-parameter fit (dotted line).

Table 3. D+T fusion cross-section.

Energy in laboratory (keV)	Experimental data (ENDF/B VII.0) (b)	Resonant tunnelling, equation (1) (b)	3-Parameter fit equation (5) (b)	5-Parameter fit equation (7) (NRL Formulary) (b)
0.2	7.43E-39	7.15E-39	7.61E-39	2.83E-40
0.3	4.06E-31	3.90E-31	4.15E-31	2.92E-32
0.4	1.59E-26	1.53E-26	1.63E-26	1.67E-27
0.7	2.51E-19	2.42E-19	2.58E-19	4.80E-20
1	1.03E-15	9.90E-16	1.05E-15	2.66E-16
4	1.16E-06	1.13E-06	1.20E-06	6.57E-07
7	1.54E-04	1.51E-04	1.62E-04	1.07E-04
10	1.73E-03	1.71E-03	1.83E-03	1.32E-03
14	1.14E-02	1.13E-02	1.21E-02	9.47E-03
20	5.97E-02	6.00E-02	6.42E-02	5.34E-02
26	1.68E-01	1.71E-01	1.82E-01	1.57E-01
35	4.70E-01	4.81E-01	5.08E-01	4.53E-01
50	1.37E+00	1.40E+00	1.44E+00	1.32E+00
65	2.66E+00	2.69E+00	2.71E+00	2.53E+00
80	3.96E+00	3.97E+00	3.94E+00	3.74E+00
95	4.80E+00	4.79E+00	4.74E+00	4.59E+00
104	5.00E+00	4.98E+00	4.96E+00	4.86E+00
110	5.01E+00	5.00E+00	4.99E+00	4.93E+00
120	4.88E+00	4.88E+00	4.90E+00	4.90E+00
135	4.47E+00	4.48E+00	4.53E+00	4.62E+00
150	3.97E+00	4.00E+00	4.04E+00	4.19E+00
180	3.07E+00	3.10E+00	3.10E+00	3.29E+00
220	2.23E+00	2.25E+00	2.17E+00	2.36E+00
280	1.50E+00	1.49E+00	1.35E+00	1.53E+00

Figure 3 is for D + ^{3}He fusion, and figure 4 is for D + D fusion. The data points are from ENDF/B VII.0 of the National Nuclear Data Center [6]. (The ENDF/B-VII.0 is the recent evaluated data, but not the experimental one. They correspond to some optimal description of the experimental data including an averaging and extrapolation of the available data.)

The smooth curves are based on this 3-parameter fitting formula equation (5). The least-square method was applied to find the best fit parameters in table 1. From these parameters we may estimate resonance energies, $E_0 \approx -C_1/C_2$ (in units of keV). They are 97.46 keV, 372.95 keV and 1189.6 keV for D+T, D+^{3}He and D+D, respectively, in the laboratory system. We added the experimental cross-section data of the $(\mathrm{D+D} \to \mathrm{p+T})$ and $(\mathrm{D+D} \to \mathrm{n+{}^3He})$ reactions in order to obtain the total cross-section for D + D fusion reactions.

3. Comparison with NRL 5-parameter fitting formula

It would be interesting to compare the results of the 5-parameter fitting formula in the NRL Plasma Formulary.

$$\sigma_5(E_{\mathrm{lab}}) = \frac{A_5 + (A_2/((A_4 - A_3 E_{\mathrm{lab}})^2 + 1))}{E_{\mathrm{lab}}[\mathrm{Exp}(A_1/\sqrt{E_{\mathrm{lab}}}) - 1]}. \qquad (7)$$

Here, E_{lab} is the energy of the incident deuteron in units of keV, and $\sigma_5(E_{\mathrm{lab}})$ is in units of barn. Five parameters, A_1, A_2, A_3, A_4 and A_5, are listed in table 2 [1, 3].

Figures 5, 6 and 7 are for D+T, D+^{3}He, D+D fusion cross-section, respectively, using the 5-parameter fitting formula (dotted line). It is evident that this 5-parameter fit does not fit the peak values for the case of D+^{3}He and D+D fusion cross-section. This 5-parameter formula is able to fit the peak value of the D+T fusion cross-section, but it fails to fit the low-energy data (compare columns 2 and 5 of table 3). The resonant tunnelling model (column 4) fits the data much better. Now we can see the importance of the $(-1/\theta^2)$ term in the denominator of equation (5), which makes the 3-parameter fit better than the 5-parameter fit.

Table 3 shows the calculations based on equations (1) and (5) in columns 3 and 4. The resonant tunnelling model of equation (1) provides a good description of the fusion process, and equation (5) is a good approximation to equation (1). In table 4, three physical quantities, U_{r}, U_{i} and a are given for two cases based on equations (1), (2) and (3).

4. Discussion on astrophysical S-function

The new formula for fusion cross-section (equation (1)) provides an alternative expression of astrophysical S-function, which is defined as

$$S(E) \equiv \frac{k^2}{\pi}\frac{(\mathrm{Exp}(2\pi/ka_{\mathrm{c}}) - 1)}{2\pi}\sigma(E) = \frac{-4w_{\mathrm{i}}}{w_{\mathrm{r}}^2 + \left(w_{\mathrm{i}} - \frac{2\pi}{(\mathrm{Exp}(2\pi/ka_{\mathrm{c}})-1)}\right)^2}. \qquad (8)$$

This S-function was introduced to extract the fast energy dependence in order to discuss the slow varying factor which was considered dependent on the *intrinsic* nuclear property only. In 1936, soon after the Bohr's Compound Nucleus Model, Breit–Wigner proposed the formula to describe the resonant feature of the compound nucleus. Based on the Breit–Wigner formula, we may have

$$S_{BW}(E) = \left(\frac{2}{C_2}\right)\frac{\Gamma_{\mathrm{a}}}{(E - E_0)^2 + ((\Gamma_{\mathrm{a}} + \Gamma_{\mathrm{in}})/2)^2}. \qquad (9)$$

Here, E_0 is the energy of resonance. Γ_{a} is the absorption width and Γ_{in} is the incident-channel width. These parameters

Table 4. 3 parameters of nuclear potential well.

	D+T	D+D (p+T and n+^{3}He)
U_r	-40.69 MeV	-48.52 MeV
U_i	-109.18 keV	-263.27 keV
a	5.1×10^{-15} m	7.0×10^{-15} m

were considered the intrinsic nuclear property only which was supposed to be independent on the penetration factor, because the compound nucleus model assumed two independent stages of the nuclear reaction (penetration and independent decay). This assumption affected Duan's parametrization in 1972. As was alluded to in the earlier paper of Bosch and Hale, the energy dependence of those energy widths should be taken into account in order to obtain the better fit with the cross-section data. In 1992 Feshbach intended to introduce this energy dependence through the Coulomb wave functions for the charged particle injection, but it was mentioned only in the appendix by a few lines [7]. Equation (8) gives the explicit energy dependence of the energy width if we assume

$$\Gamma_{in} = \frac{2}{C_2}\frac{2\pi}{(\mathrm{Exp}(2\pi/ka_c) - 1)}, \tag{10}$$

and

$$\Gamma_a = -\frac{2}{C_2}w_i = -\frac{2}{C_2}C_3. \tag{11}$$

The height of the resonance peak depends on matching of these two energy widths. Only if

$$\Gamma_a \approx \Gamma_{in}, \tag{12}$$

the peak of the cross-section of resonance would reach its maximum value. It can be shown that $w_i \propto -(\tau_{flight}/\tau_{life})$ is the ratio of the flight-time to the lifetime inside the nuclear potential well. When the incident energy of a charged particle is very low, the incident width becomes very small. If there is a resonance at this low energy, then this matching between the absorption width and the incident width would require a very long lifetime inside the nuclear potential well.

5. Conclusion

The 5-parameter fit formula in NRL Plasma Formulary may be replaced by the 3-parameter fit formula (equation (5)) based on the resonant tunnelling model. We may rewrite it as a unified formula:

$$\sigma(E_{lab}) = -16389C_3\left(1 + \frac{m_a}{m_b}\right)^2 \times \left[m_a E_{lab}\left[\mathrm{Exp}\left(31.40 Z_1 Z_2\sqrt{\frac{m_a}{E_{lab}}}\right) - 1\right]\left\{(C_1 + C_2 E_{lab})^2 + \left(C_3 - \frac{2\pi}{[\mathrm{Exp}\,(31.40 Z_1 Z_2\sqrt{m_a/E_{lab}}) - 1]}\right)^2\right\}\right]^{-1} \tag{13}$$

with 3 adjustable parameters (C_1, C_2 and C_3) only. In (13), m_a and m_b are the mass number for the incident and target nucleus, respectively (e.g. $m_a = 2$ for incident deuteron); E_{lab} is in units of keV and σ is in units of barn. The upper-limit energies for the validity of the parametrizations is about 1 MeV under which the S-wave approximation is valid.

Acknowledgments

This work is supported by The Ministry of Science and Technology (Fundamental Research Division), Natural Science Foundation of China (#10475045) and Tsinghua University (Basic Research Fund (985-II)). Encouragement from Sood, D. D. and his IEAE colleagues since 1999 has been important in developing this model. The authors are grateful to the reviewers for their comments which improved this paper.

References

[1] Book D.L. 1980 *NRL Plasma Formulary* (Washington DC: Naval Research Laboratory) p 44 revised

[2] Bosch H.S. and Hale G.M. 1992 *Nucl. Fusion* **32** 611

[3] Huba J.D. 2007 *NRL Plasma Formulary* (Washington DC: Naval Research Laboratory) p 44 revised

[4] Li X.Z., Tian J., Mei M.Y. and Li C.X. 2000 *Phys. Rev.* C **61** 024610

[5] Li X.Z., Liu B., Chen S., Wei Q.M. and Hora H. 2004 *Laser Part. Beams* **22** 469

[6] Chadwick M.B. *et al* 2006 ENDF/B-VII.0: Next generation evaluated nuclear data library for nuclear science and technology *Nucl. Data Sheets* **107** 2931–3060

[7] Feshbach H. 1992 *Theoretical Nuclear Physics (Nuclear Reactions)* (New York: Wiley) p 226

[8] Li X.Z. 2002 *Fusion Sci. Tech.* **41** 63