

SATIF-16 Shielding aspects of Accelerators Targets and Irradiation Facilities



Treatment of low-energy heavy particle fusion reactions in PHITS

H. Iwase¹, T. Kambara², K. Hagino³, T. Ogawa⁴, T. Furuta⁴, and A. Yoshida²

¹KEK, ²RIKEN, ³Kyoto Univ., ⁴JAEA



Background

of heavy ion collisions in the energy region toward the stopping

- Fusion is one of major component in the reaction cross section
- The low-energy heavy ion fusion occur even below the coulomb barrier
- The sub-barrier fusion is more pronounced for heavier mass collisions



Hagino et al., Prog. Theor. Phys., Vol.128, 6 (2012)



- Revising PHITS by including the low-energy heavy ion fusion cross section explicitly
- It is required providing more precise simulation to some accelerator facilities and experiments
- Previous methods; fusion occurs as results of JQMD simulations
- This methods; the CCFULL fusion cross section is used

CCFULL

Hagino et al., Prog. Theor. Phys., Vol.128, 6 (2012)

- fusion cross section model based on the quantum tunneling of many-body systems
- treats deformation of nucleus, excitation energies, and treats multiple excitations of a nucleus with finite excitation energies
- the Channel Coupling represents fusion cross sections even below sub-barrier





Hagino et al., Prog. Theor. Phys., Vol.128, 6 (2012)

Methods

A. Fusion cross section is explicitly defined by CCFULL

- B. In case of fusion reaction, a composite nucleus of projectile and target nuclei is prepared
- C. Evaporation calculation is performed to composite nuclei by the statistical model GEM



Benchmark data

[2] Kambara et al, Acc. progress report Vol 52, p158 (2019)

- ¹³⁶Xe 10.75 MeV/A + light mass targets
- Measured at E5A beam line, at RIKEN
- Nuclides and their production rate obtained by HP-Ge gamma rays analysis





Projectile energies & Target nuclei



Measured nuclei ^[2]

Nuclei	halflife	unit	Z	N	А	production rate	error
Xe-135g	9.14	h	54	81	135	9.86E-05	2.97E-05
Xe-135m	15.29	m	54	81	135	1.94E-05	6.39E-06
Cs-135m	53	m	55	80	135	4.22E-06	2.01E-06
Cs-136	13.16	d	55	81	136	7.44E-05	3.62E-05
Ba-137m	2.552	m	56	81	137	2.91E-05	1.25E-05
Pr-138m	2.12	h	59	79	138	6.64E-06	2.61E-06
Nd-139m	5.5	h	60	79	139	4.01E-05	1.28E-05
Pm-140m	9.2	S	61	79	140	4.52E-06	1.97E-06
Dy-157	8.14	h	66	91	157	7.75E-06	6.55E-06
Ho-156	56	m	67	89	156	3.95E-05	1.14E-05
Ho-157	12.6	m	67	90	157	5.05E-05	1.53E-05
Ho-158	11.3	m	67	91	158	1.04E-05	3.33E-06

Measured nuclei

Fusion of ¹³⁶Xe+²⁷Al

¹⁴¹ Ho	¹⁴² Ho	¹⁴³ Ho	¹⁴⁴ Ho	¹⁴⁵ Ho	¹⁴⁶ Ho	¹⁴⁷ Ho	¹⁴⁸ Ho	¹⁴⁹ Ho	¹⁵⁰ Ho	¹⁵¹ Ho	¹⁵² Ho	¹⁵³ Ho	¹⁵⁴ Ho	¹⁵⁵ Ho	¹⁵⁶ Ho	¹⁵⁷ Ho	¹⁵⁸ Ho	¹⁵⁹ Ho	¹⁶⁰ Ho	¹⁶¹ Ho	¹⁶² Ho	¹⁶³ Ho	¹⁶⁴ Ho	ⁱ¹⁶⁵ Ho	¹⁶⁶ Ho	¹⁶⁷ Ho	¹⁶⁸ Ho
¹⁴⁰ Dy	¹⁴¹ Dy	¹⁴² Dy	¹⁴³ Dy	¹⁴⁴ Dy	¹⁴⁵ Dy	¹⁴⁶ Dy	¹⁴⁷ Dy	¹⁴⁸ Dy	¹⁴⁹ Dy	¹⁵⁰ Dy	¹⁵¹ Dy	¹⁵² Dy	¹⁵³ Dy	¹⁵⁴ Dy	¹⁵⁵ Dy	¹⁵⁶ Dy	¹⁵⁷ Dy	¹⁵⁸ Dy	¹⁵⁹ Dy	¹⁶⁰ Dy	^{ì61} Dy	¹⁶² Dy	¹⁶³ Dy	^{`164} Dy	¹⁶⁵ Dy	¹⁶⁶ Dy	¹⁶⁷ Dy
¹³⁹ Tb	¹⁴⁰ Tb	¹⁴¹ Tb	¹⁴² Tb	¹⁴³ Tb	¹⁴⁴ Tb	¹⁴⁵ Tb	¹⁴⁶ Tb	¹⁴⁷ Tb	¹⁴⁸ Tb	¹⁴⁹ Tb	¹⁵⁰ Tb	¹⁵¹ Tb	¹⁵² Tb	¹⁵³ Tb	¹⁵⁴ Tb	¹⁵⁵ Tb	¹⁵⁶ Tb	¹⁵⁷ Tb	¹⁵⁸ Tb	^{`159} Tb	¹⁶⁰ Tb	ⁱ⁶¹ Tb	¹⁶² Tb	¹⁶³ Tb	¹⁶⁴ Tb	¹⁶⁵ Tb	¹⁶⁶ Tb
¹³⁸ Gd	¹³⁹ Gd	¹⁴⁰ Gd	¹⁴¹ Gd	¹⁴² Gd	¹⁴³ Gd	¹⁴⁴ Gd	¹⁴⁵ Gd	¹⁴⁶ Gd	¹⁴⁷ Gd	¹⁴⁸ Gd	¹⁴⁹ Gd	¹⁵⁰ Gd	¹⁵¹ Gd	¹⁵² Gd	¹⁵³ Gd	¹⁵⁴ Gd	¹⁵⁵ Gd	¹⁵⁶ Gd	^{`157} Gd	⁻¹⁵⁸ Gd	¹⁵⁹ Gd	¹⁶⁰ Gd	¹⁶¹ Gd	¹⁶² Gd	¹⁶³ Gd	¹⁶⁴ Gd	¹⁶⁵ Gd
¹³⁷ Eu	¹³⁸ Eu	¹³⁹ Eu	¹⁴⁰ Eu	¹⁴¹ Eu	¹⁴² Eu	¹⁴³ Eu	¹⁴⁴ Eu	¹⁴⁵ Eu	¹⁴⁶ Eu	¹⁴⁷ Eu	¹⁴⁸ Eu	¹⁴⁹ Eu	¹⁵⁰ Eu	¹⁵¹ Eu	¹⁵² Eu	¹⁵³ Eu	¹⁵⁴ Eu	¹⁵⁵ Eu	¹⁵⁶ Eu	¹⁵⁷ Eu	¹⁵⁸ Eu	¹⁵⁹ Eu	¹⁶⁰ Eu	¹⁶¹ Eu	¹⁶² Eu	¹⁶³ Eu	¹⁶⁴ Eu
¹³⁶ Sm	¹³⁷ Sm	¹³⁸ Sm	¹³⁹ Sm	¹⁴⁰ Sm	¹⁴¹ Sm	¹⁴² Sm	¹⁴³ Sm	¹⁴⁴ Sm	¹⁴⁵ Sm	¹⁴⁶ Sm	¹⁴⁷ Sm	¹⁴⁸ Sm	¹⁴⁹ Sm	^{`i50} Sm	¹⁵¹ Sm	¹⁵² Sm	¹⁵³ Sm	¹⁵⁴ Sm	¹⁵⁵ Sm	¹⁵⁶ Sm	¹⁵⁷ Sm	158Sm	¹⁵⁹ Sm	¹⁶⁰ Sm	¹⁶¹ Sm	¹⁶² Sm	¹⁶³ Sm
¹³⁵ Pm	¹³⁶ Pm	¹³⁷ Pm	¹³⁸ Pm	¹³⁹ Pm	^{I40} Pm	¹⁴¹ Pm	¹⁴² Pm	¹⁴³ Pm	¹⁴⁴ Pm	¹⁴⁵ Pm	¹⁴⁶ Pm	¹⁴⁷ Pm	¹⁴⁸ Pm	¹⁴⁹ Pm	¹⁵⁰ Pm	¹⁵¹ Pm		^J XE) +) ('	525	5(1))	¹⁶⁰ Pm	¹⁶¹ Pm	¹⁶² Pm
¹³⁴ Nd	¹³⁵ Nd	¹³⁶ Nd	¹³⁷ Nd	¹³⁸ Nd	^{I39} Nd	¹⁴⁰ Nd	¹⁴¹ Nd	¹⁴² Nd	¹⁴³ Nd	¹⁴⁴ Nd	¹⁴⁵ Nd	¹⁴⁶ Nd	¹⁴⁷ Nd	¹⁴⁸ Nd	¹⁴⁹ Nd	136	°X∈) +	14] (1:	50 -	' m)	⁵⁷ Nd	¹⁵⁸ Nd	¹⁵⁹ Nd	¹⁶⁰ Nd	¹⁶¹ Nd
¹³³ Pr	¹³⁴ Pr	¹³⁵ Pr	¹³⁶ Pr	¹³⁷ Pr	¹³⁸ Pr	¹³⁹ Pr	¹⁴⁰ Pr	¹⁴¹ Pr	¹⁴² Pr	¹⁴³ Pr	¹⁴⁴ Pr	¹⁴⁵ Pr	¹⁴⁶ Pr	¹⁴⁷ Pr	136	³ Xe) +	120) (14	48N	Jd)	¹⁵⁵ Pr	¹⁵⁶ Pr	¹⁵⁷ Pr	¹⁵⁸ Pr	¹⁵⁹ Pr	¹⁶⁰ Pr
¹³² Ce	¹³³ Ce	¹³⁴ Ce	¹³⁵ Ce	¹³⁶ Ce	¹³⁷ Ce	¹³⁸ Ce	¹³⁹ Ce	¹⁴⁰ Ce	¹⁴¹ Ce	¹⁴² Ce	¹⁴³ Ce	¹⁴⁴ Ce	¹⁴⁵ Ce	¹⁴⁶ Ce	¹⁴⁷ Ce	¹⁴⁸ Ce	¹⁴⁹ Ce	¹⁵⁰ Ce	¹⁵¹ Ce	¹⁵² Ce	¹⁵³ Ce	¹⁵⁴ Ce	¹⁵⁵ Ce	¹⁵⁶ Ce	¹⁵⁷ Ce	¹⁵⁸ Ce	
¹³¹ La	¹³² La	¹³³ La	¹³⁴ La	¹³⁵ La	¹³⁶ La	¹³⁷ La	¹³⁸ La	¹³⁹ La	¹⁴⁰ La	¹⁴¹ La	¹⁴² La	¹⁴³ La	¹⁴⁴ La	¹⁴⁵ La	¹⁴⁶ La	¹⁴⁷ La	¹⁴⁸ La	¹⁴⁹ La	¹⁵⁰ La	¹⁵¹ La	¹⁵² La	¹⁵³ La	¹⁵⁴ La	¹⁵⁵ La	¹⁵⁶ La	¹⁵⁷ La	101
¹³⁰ Ba	¹³¹ Ba	¹³² Ba	¹³³ Ba	¹³⁴ Ba	¹³⁵ Ba	¹³⁶ Ba	¹³⁷ Ba	¹³⁸ Ba	¹³⁹ Ba	¹⁴⁰ Ba	¹⁴¹ Ba	¹⁴² Ba	¹⁴³ Ba	¹⁴⁴ Ba	¹⁴⁵ Ba	¹⁴⁶ Ba	¹⁴⁷ Ba	¹⁴⁸ Ba	¹⁴⁹ Ba	¹⁵⁰ Ba	¹⁵¹ Ba	¹⁵² Ba	¹⁵³ Ba	¹⁵⁴ Ba			
¹²⁹ Cs	¹³⁰ Cs	¹³¹ Cs	¹³² Cs	¹³³ Cs	¹³⁴ Cs	¹³⁵ Cs	³⁶ Cs	¹³⁷ Cs	¹³⁸ Cs	¹³⁹ Cs	¹⁴⁰ Cs	¹⁴¹ Cs	¹⁴² Cs	¹⁴³ Cs	¹⁴⁴ Cs	¹⁴⁵ Cs	¹⁴⁶ Cs	¹⁴⁷ Cs	¹⁴⁸ Cs	¹⁴⁹ Cs	¹⁵⁰ Cs	¹⁵¹ Cs	¹⁵² Cs		99	100	
¹²⁸ Xe	¹²⁹ Xe	¹³⁰ Xe	¹³¹ Xe	¹³² Xe	¹³³ Xe	¹³⁴ Xe	¹³⁵ Xe	³⁶ Xe	Pr (13	oje ³⁶ X(ctil Ə)	е	¹⁴¹ Xe	¹⁴² Xe	¹⁴³ Xe	¹⁴⁴ Xe	¹⁴⁵ Xe	¹⁴⁶ Xe	¹⁴⁷ Xe	¹⁴⁸ Xe	¹⁴⁹ Xe	¹⁵⁰ Xe		98			

Additional information/condition

- Focus on heaviest fusion composite of ¹³⁶Xe+²⁷Al and its altered nuclei of Ho and Dy
- Fusion cross section of ¹³⁶Xe + ²⁷Al is calculated by CCFULL
 - Global integration of CCFULL is future work (CCFULL requires deformation parameters and excitation energies of each nucleus, and potential value of composite nucleus)
- For other combination of ¹³⁶Xe + ¹²C, ¹⁴N, ¹⁶O, cross section is not prepared explicitly (original PHITS)

PHITS options

- irqmd = 2 ! (JQMD ver. 2)
- eqmdmin = 3.5 ! (MeV/u)
- eqmdnu = 3.5
- ngem = 2

- ! (MeV/u)
- ! 2:γ emission competes with
 - nucleon emission





All results in one figure



Discussion

- CCFULL improves the accuracy of PHITS calculation of lowenergy heavy ion fusion products by a factor of 2 or more
- Integration of CCFULL into MC is essential for low-energy heavy ion physics and application
- Still discrepancy between data and simulation
 - sum of measured production rate of Ho and Dy nuclei 1.0e-4 supports the number of fusions estimated by CCFULL of 1.2e-4
 - In PHITS, the composite nucleus of ¹⁶³Ho with excitation energy, emits multiple nucleons, which are distributed as other nuclei. The distribution may be improved.

A sensitivity test by limiting the number of nucleon emissions



- only one proton emission restriction changes the result very much

- may indicates a room of improvement of the statistical model of composite nucleus in low energy fusion

Summary

- Fusion cross section of low energy heavy ion may underestimate if classical model is used
- CCFULL improves the accuracy of MC calculation of low-energy heavy ion fusion
- Global integration of CCFULL is the next work
- Other treatment of fusion composite nucleus in this energy region may better represent the data

Thank you very much

hiroshi.iwase@kek.jp

Backups & appendix



Reaction Summary

	Thickness (µm)	Atom	Atomic mass (g/mol)	Atom fraction	Mass density (g/cm3)	Atomic density (/cm3)	Atomic density (/cm3)	Ein (MeV/A)	Eout (MeV/A)	σt (mb)	σ _f (mb)	Σt (cm-1)	Σf (cm-1)	# of interaction	# of fusion	fusion ratio
		н	1.00794	0.256399			0.02237			0.67		0.015		3.73E-05	0.000E+00	0.00
	25	С	12.0107	0.564114			0.04921			2.65	1.33	0.130	0.06545	3.26E-04	1.636E-04	0.50
kapton		N	14.0067	0.051282	1.420000	0.0872	0.00447	10.75	9.04	2.75	1.33	0.012	0.00595	3.07E-05	1.487E-05	0.48
		0	15.9994	0.128205			0.01118			2.78	1.33	0.031	0.01487	7.77E-05	3.718E-05	0.48
		N	14.0067	0.784431			0.0000391			2.56	1.33	0.000100	0.0000520	1.40E-04	7.287E-05	0.52
Air	14000	0	15.9994	0.210748	0.001205	0.0000499	0.0000105	9.04	8.24	2.58	1.33	0.000027	0.0000140	3.80E-05	1.958E-05	0.52
		Ar	39.948	0.004671			0.0000056			3.19	2.07	0.000018	0.0000117	2.51E-05	1.631E-05	0.65
Mylar		Н	1.00794	0.363632		0.0951	0.03460	8.24		0.30		0.010	0.00000	6.29E-06	0.000E+00	0.00
	6	С	12.0107	0.454552	1.380000		0.04325		7.79	2.40	1.33	0.104	0.05752	6.22E-05	3.451E-05	0.56
		0	15.9994	0.181816			0.01730			2.45	1.33	0.042	0.02301	2.55E-05	1.380E-05	0.54
	0.08	AI	26.9815	1.0	2.70	0.0603	0.0603	7.79		2.68	1.33	0.161506	0.0801	1.29E-06	6.412E-07	0.50
	8000	N	14.0067	0.784431	0.001205	0.0000499	0.0000391	7.79		2.32	1.33	0.000	0.0000520	7.26E-05	4.164E-05	0.57
Air		0	15.9994	0.210748			0.0000105		7.31	2.34	1.33	0.000	0.0000140	1.97E-05	1.119E-05	0.57
		Ar	39.948	0.004671			0.0000056			2.89	2.07	0.000	0.0000117	1.30E-05	9.321E-06	0.72
		Н	1.00794	0.363632		0.0774	0.02816			0.06		0.0016	0.00000	9.40E-07	0.000E+00	0.00
	6	С	12.0107	0.454552	1.380000		0.03520	7.31	6.85	2.12	1.33	0.0746	0.04682	4.48E-05	2.809E-05	0.63
Mylar		0	26.9815	0.181816			0.01408	-		2.21	1.33	0.0311	0.01873	1.87E-05	1.124E-05	0.60
	0.08	AI	26.9815	1.0	2.70	0.0603	0.06026			2.38	1.33	0.143	0.08015	1.15E-06	6.412E-07	0.56
		N	14.0067	0.784431			0.0000391			2.10	1.33	0.000082	0.0000520	1.64E-05	1.041E-05	0.63
Air	2000	0	15.9994	0.210748	0.001205	0.0000499	0.0000105	6 85	673	2.12	1.33	0.000022	0.0000140	4.46E-06	2.797E-06	0.63
		Ar	39.948	0.004671	0.001205	0.0000400	0.0000056	0.00	0.70	2.63	2.07	0.000015	0.0000117	2.96E-06	2.330E-06	0.79
Electrode	15	AI	26.9815	1.00	2.70	0.0603	0.0603	673	4 98	1.87	1.33	0.113	0.0801	1.69E-04	1.202E-04	0.71
210011000					2	0.0000		0.70	4.00							

1

sum

	Number of	Ratio
Possible fusion	FUSION	to
	per source	total
136Xe + 12C	2.262E-04	0.37
136Xe + 14N	1.398E-04	0.23
136Xe + 16O	9.578E-05	0.16
136Xe + 40Ar	2.796E-05	0.05
136Xe + 27Al	1.215E-04	0.20

1.13E-03 6.112E-04

	Mate	erial Ato	oms	Density (g/cm³)	Atomic mass (g/mol)	Atom fractio n	Atomi c densit yN	Thick ness (µm)	E at Front (MeV/	E at Back (MeV/	σ _t (b)	σ _{fuss} (b)	Σ (cn)	Σt n-1)	Σ _{fuss} (cm- 1)	# c inte s	of total raction per ource	# of total interactio ns per source	# of fusion per source	# of fusion per source (actual)	
1	Kapt	ton I		1.42	1.0079 4 12.010 7			25	10.75	9.04											
			N		14.006	0.784															
Mat I	erial D	Material	Th	iickness (μm)	Density (g/cm³)	E at Front (MeV/A)	E at Bac (MeV/A)	k dE (MeV	: (m /A) (m 平均	ft (mb b) 平均 间	Aton dens N (/cm	nic ity c x1/ 1 ³) 2	љN 0^{- 24}	σtN ×10^ 4}	N (-2 (Σı cm-1) 平均值	Σ _{fuss} (cm-1) 平均值	# of total interactio ns per source (formula)	# of tota interactio s per source (actual)	l per source (formula)	# of fusion per source (actual)
	1	Kapton		25	1.42	10.75	9.04	1.7	1												
	2	Air	1	4000	0.00121	9.04	8.24	0.8	0												
	3	Mayler		6	1.38	8.24	7.79	0.4	5												
	4	Air	1	8000	0.00121	7.79	7.31	0.4	8												
	5	Maylar		6	1.38	7.31	6.85	0.4	6												
	6	Air	:	2000	0.00121	6.85	6.73	0.1	2												
	7	Al		15	2.70	6.73	4.98	1.7	5 1.9	92 1.33	6.02E	+22 1.16	6E-01	7.99E	-02	0.116	0.080	1.74E-04	1.82E-04	1.20E-04	1.27E-04
	8	Air			0.00121	4.98	4.85	0.1	3												
1	9	Maylar			1.38	4.85	4.35	0.5	0												
1	0	Air			0.00121	4.35	3.81	0.5	4												
1	11	Maylar			1.38	3.81	3.29	0.5	2												