JAEA Contract Work for Fiscal Year 2007 (H19)

Study on Collisions of Atoms, Molecules and Ions:

Analytic Expressions for Reaction Cross Sections of He Atoms and Ions (IV)

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Contents

Introduction

- Purpose: Formulation of analytic expressions for atomic and molecular collision cross sections to enhance the JEAMDL database
- Earlier work of present series: Cross sections for collisions of He atoms and ions with light atoms and molecules, treated in Chaps. A–D, ORNL-6086/V1 (1990) ('Redbook')
  - A: Electron capture collisions
  - B: Electron capture into excited states
  - C: Excitation and spectral line emission
  - D: Ionization and production of charged particles

Introduction (2)

- Present work treated:
  - Reactions in Chaps. E–G of Redbook; some of them including new data
  - Some reactions in Chap. A with new data
  - New reactions not included in Redbook
- New data in the last two categories:
  - Collected by Imai at Kyoto University

Reactions Treated

- Projectile electron loss or stripping collisions (Chap. E): 11
- Electron detachment collisions (Chap. F): 5
- Dissociative collisions (Chap. G): 7
- Revision of earlier fits (Electron capture): 6
- New reactions (Transfer ionization, charge exchange, electron detachment, projectile excitation): 13
- Total number of reactions treated: 42

Methods

- Re-evaluation and reformulation of earlier expressions in JAERI-Data/Code 95-008 and 96-024
- New formulation for new reaction data
- Functional forms: Green-McNeal formula and its modifications, having good rising and asymptotic behavior for atomic collision cross sections, thus allowing extrapolation
- Fitting: Made with ALESQ code

Functional Forms

- Basic relations

$$f_1(x;\ c_1, c_2) = \sigma_0 c_1 (x/E_R)^{c_2}$$

$$f_2(x;\ c_1, c_2, c_3, c_4) = f_1(x;\ c_1, c_2) \Big/ \left[1 + (x/c_3)^{c_2+c_4}\right]$$

$$f_3(x;\ c_1, c_2, c_3, c_4, c_5, c_6) = f_1(x;\ c_1, c_2) \Big/ \left[1 + (x/c_3)^{c_2+c_4} + (x/c_5)^{c_2+c_6}\right]$$

$$\cdots$$

$$\cdots$$

Functional Forms (2)

- In the expressions of the previous slide,

$$\sigma_0 = 1\times 10^{-13}\ \text{cm}^2$$

$$E_\text{R} = \begin{cases} 99.27\ \text{keV for He} \\ 74.80\ \text{keV for } ^3\text{He} \end{cases}$$

$$x = E - E_\text{th} \text{ or } \left(E - E_\text{th}\right)/a_i$$

$$E = \text{projectile energy in keV/amu}$$

$$E_\text{th} = \text{threshold energy in keV/amu}$$

Functional Forms (3)

- Fitting functions (Examples)

$$m = 3,\ n = 3:\ \ \sigma = f_2(E_1;\ a_1, a_2, a_3, a_2)$$

$$m = 4,\ n = 4:\ \ \sigma = f_2(E_1;\ a_1, a_2, a_3, a_4)$$

$$m = 4,\ n = 6:\ \ \sigma = f_2(E_1;\ a_1, a_2, a_3, a_4) + a_5 f_2(E_1/a_6;\ a_1, a_2, a_3, a_4)$$

$$m = 6,\ n = 6:\ \ \sigma = f_3(E_1;\ a_1, a_2, a_3, a_4, a_5, a_6)$$

. . .

Results

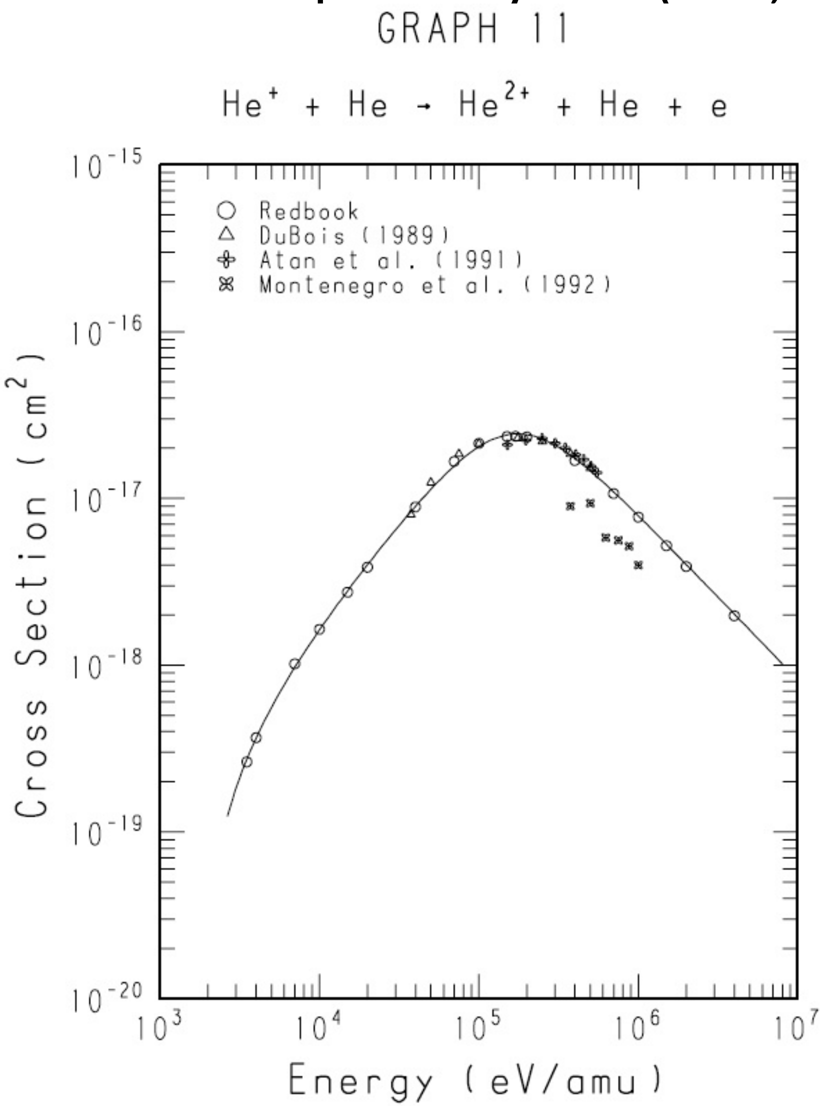
- Table. Parameters of analytic expressions (Example rows)

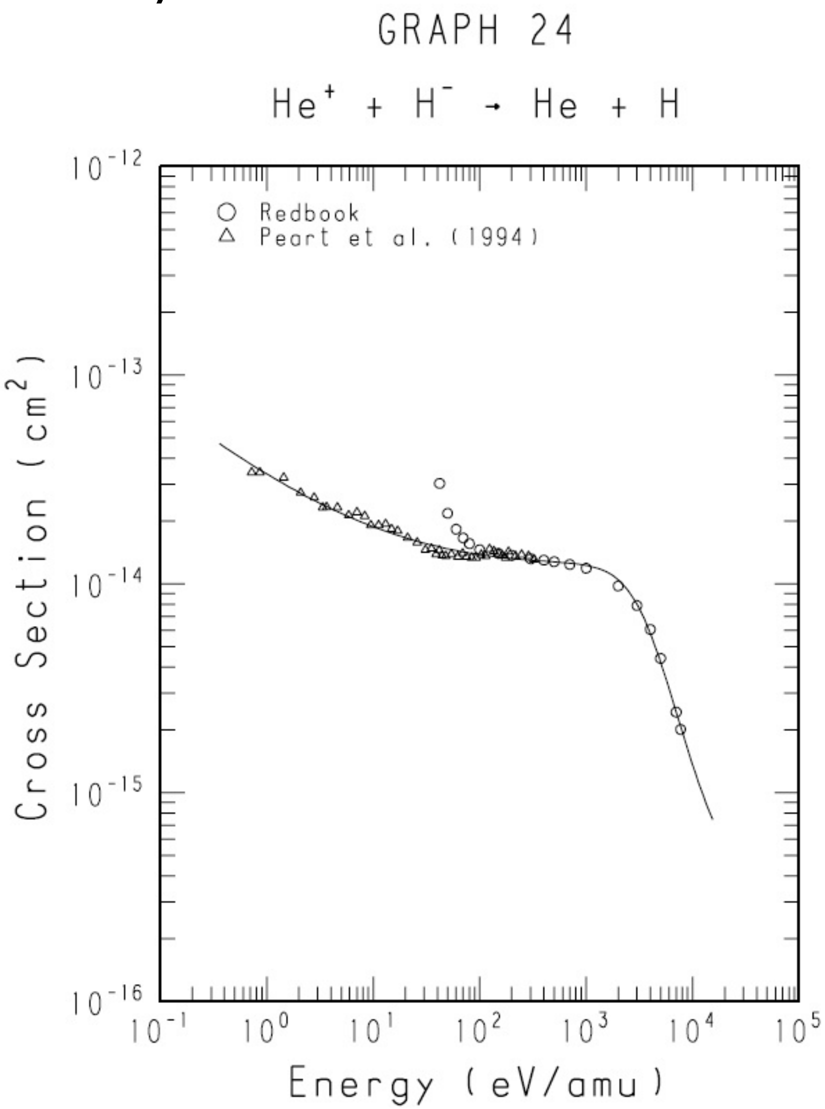
No.	$E_{\min}$	$E_{\max}$	δ_{rms}	$\delta_{\max}$	$E_{\delta_{\max}}$	E_{R}	E_{th}
01	5.00E+01	1.20E+03	2.8	6.1	5.00E+01	9.927E+01	0.00E+00
02	5.00E-01	1.00E+03	3.9	8.7	3.50E+02	9.927E+01	0.00E+00

No.	m	n	$(a_i, i = 1, 2, 3, \ldots, n)$				
01	4	4	2.510E+00	4.550E-02	8.000E+01	1.097E+00	
02	6	6	1.600E+04	2.680E+00	1.300E+00	-6.540E-01	8.470E+00
			9.020E-01				

Results (2)

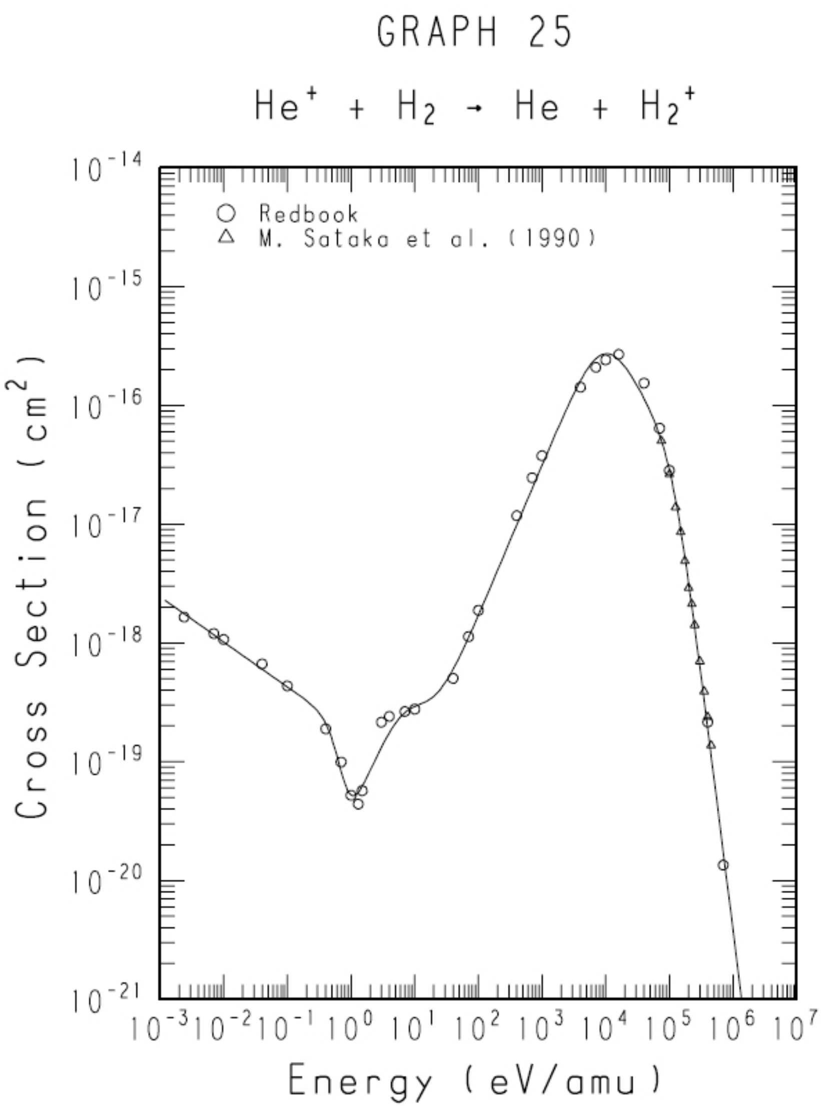
- Examples of Graphs: Projectile electron loss (n=4, δ_{rms}=5.1%); Electron capture by He^+ (n=6, δ_{rms}=4.8%)

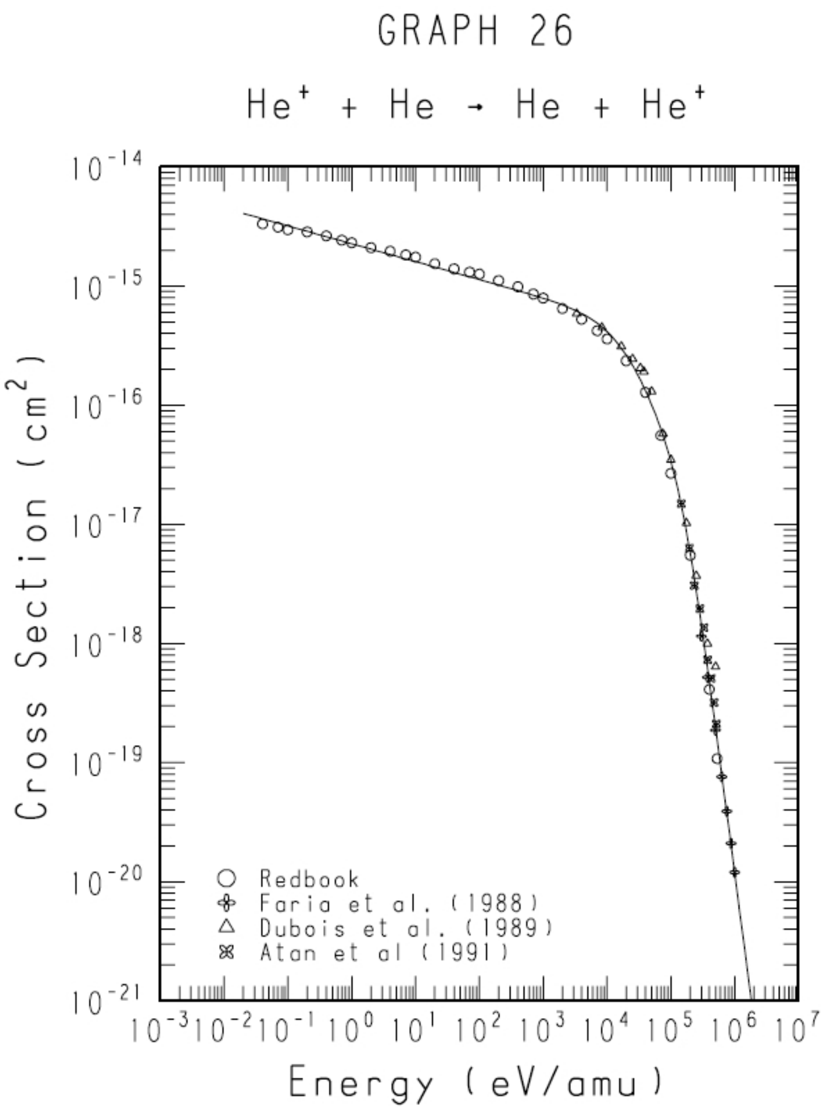




Results (3)

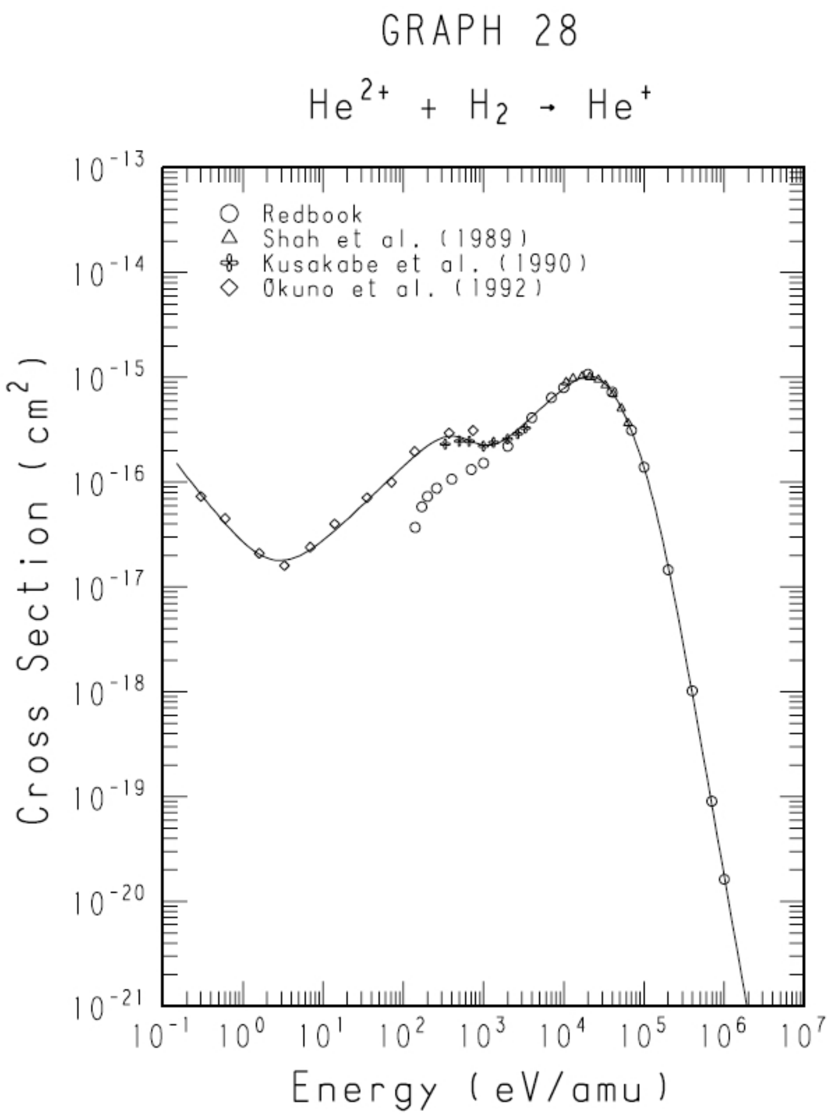
- Electron capture by He^+ (n=11, δ_{rms}=15%; n=6, δ_{rms}=17%)

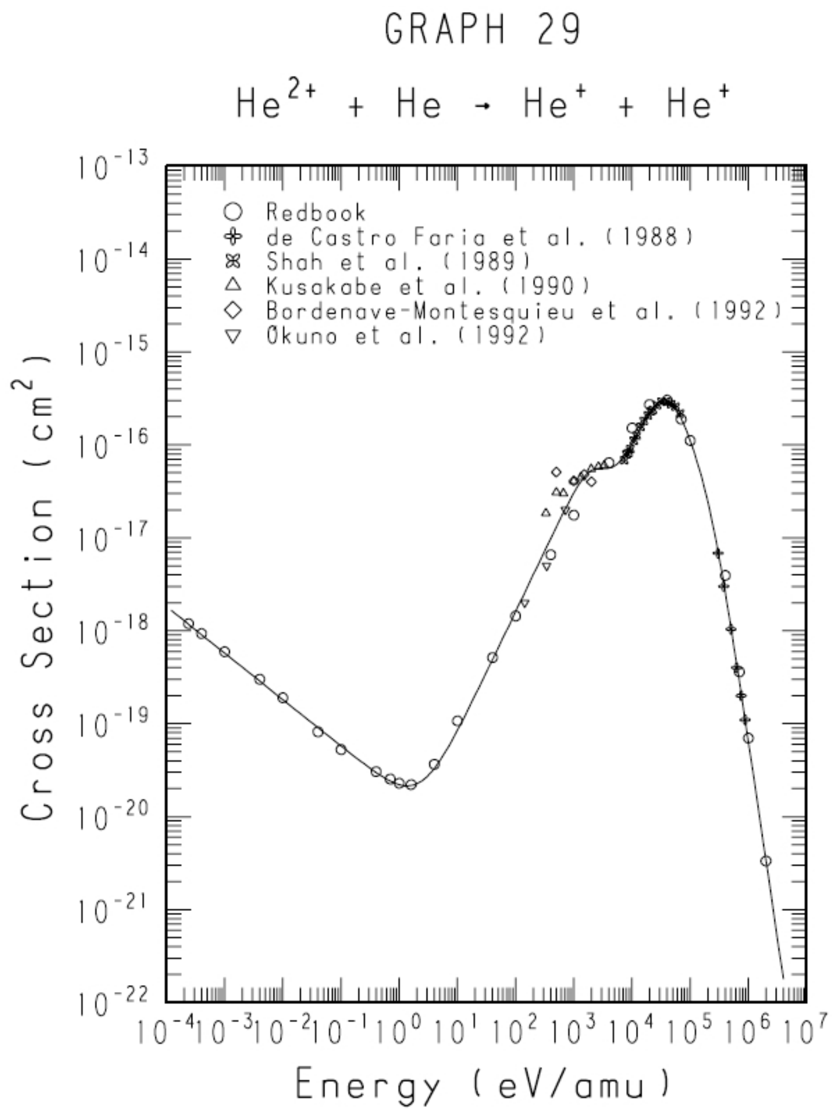




Results (4)

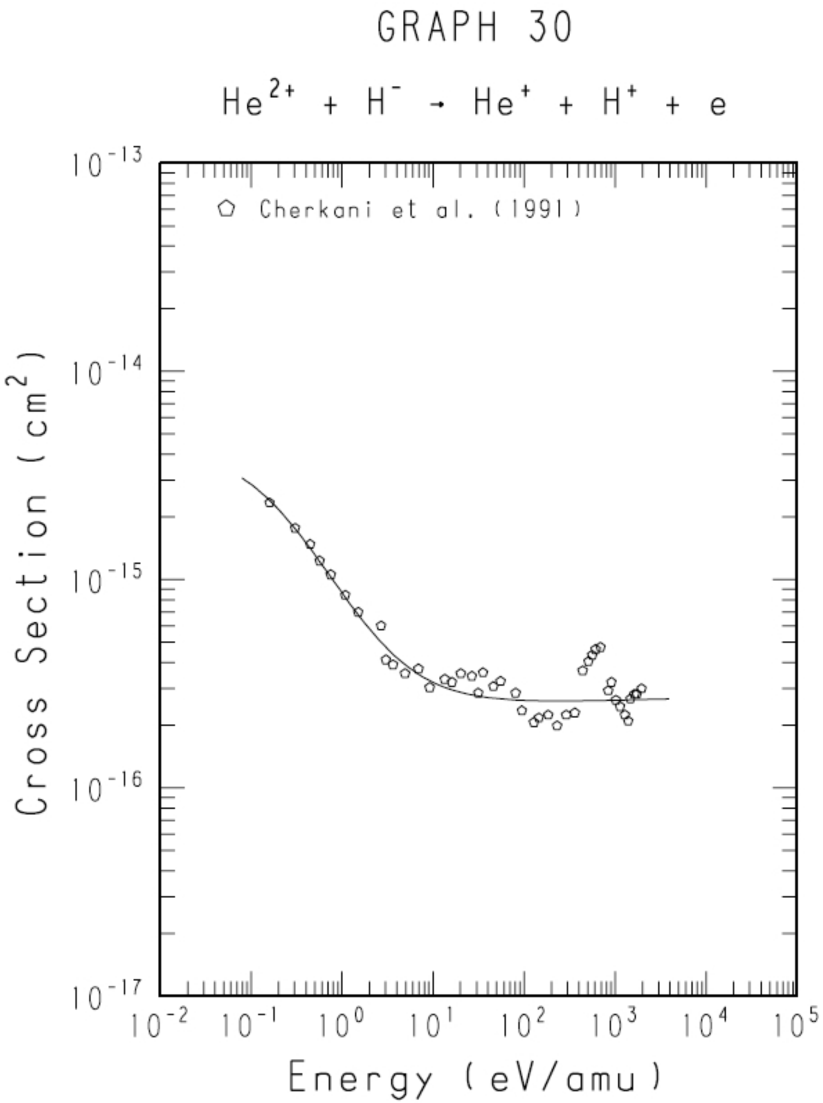
- Electron capture by He^{2+} (n=10, δ_{rms}=7.8%; n=11, δ_{rms}=20%)

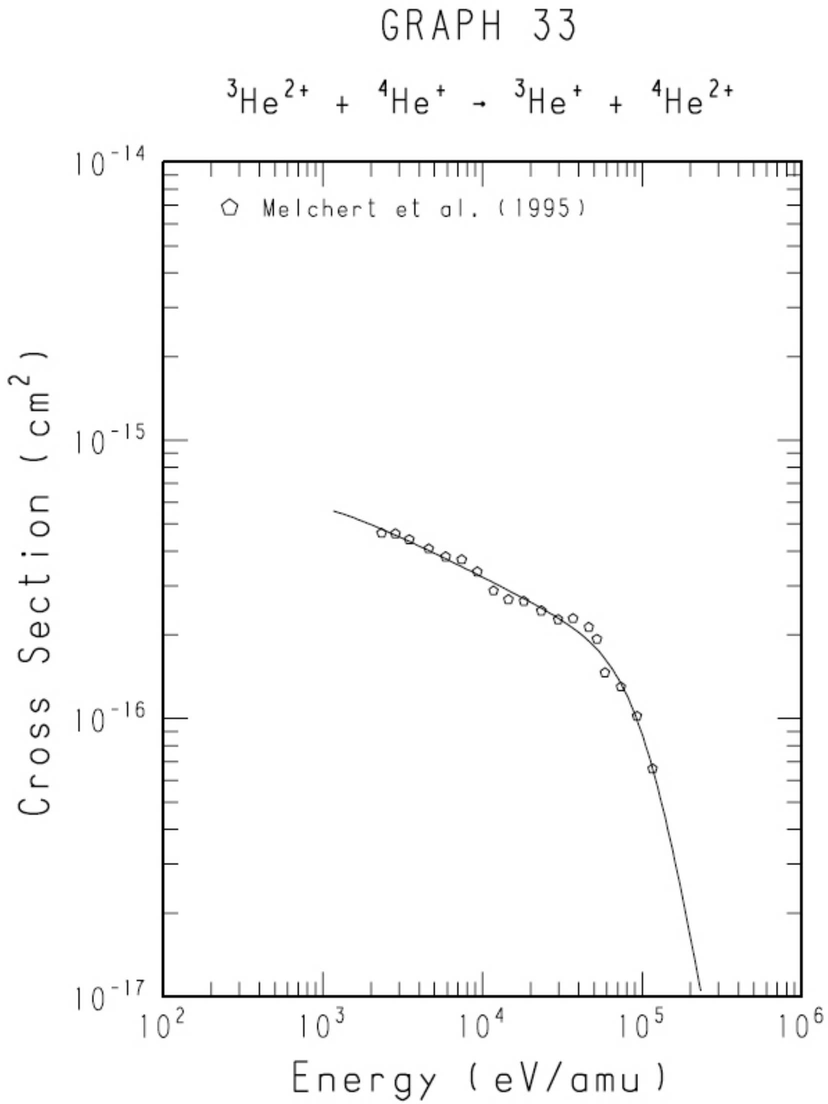




Results (5)

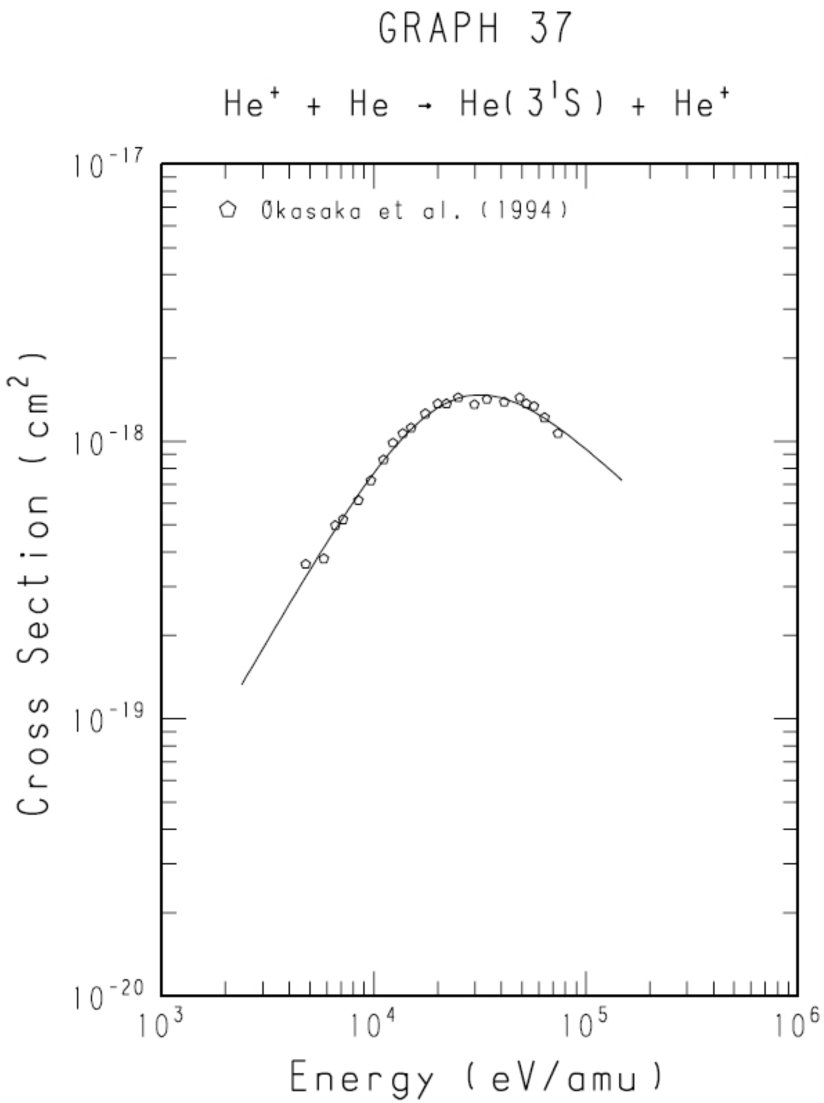
- Transfer ionization (n=6, δ_{rms}=19%), Single capture by $^3He^{2+}$ (n=6, δ_{rms}=5.6%)

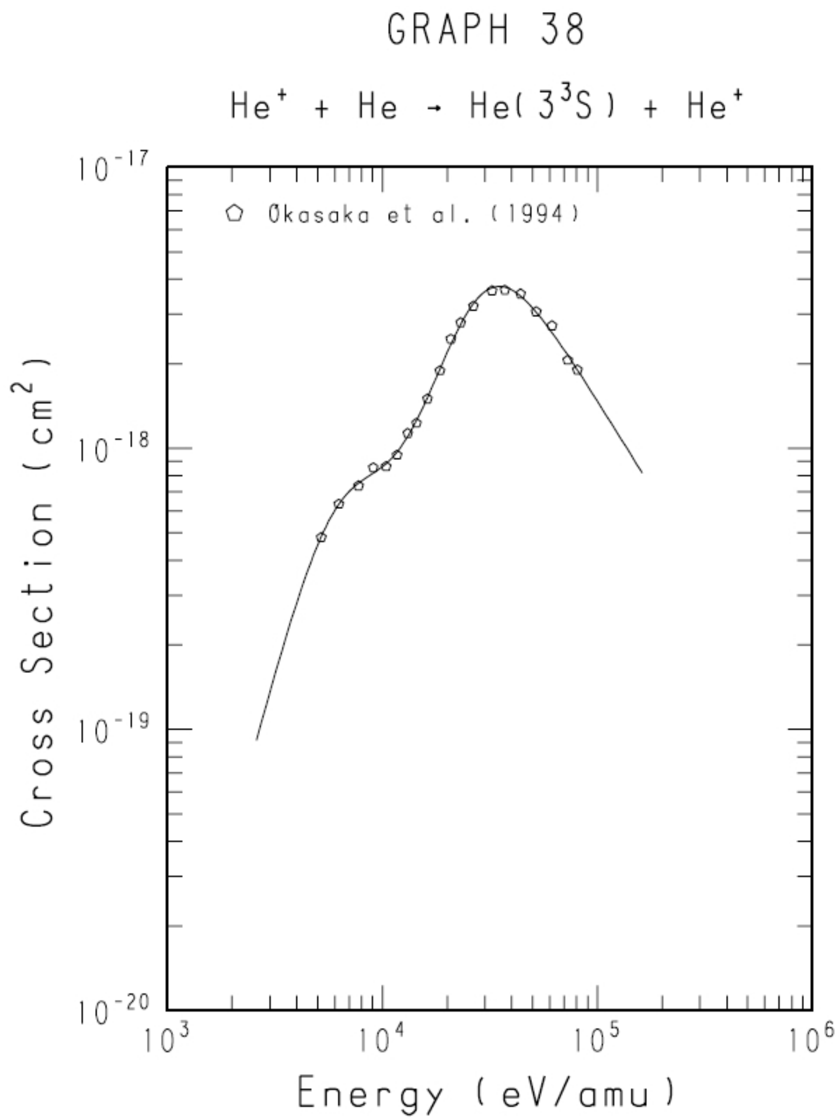




Results (6)

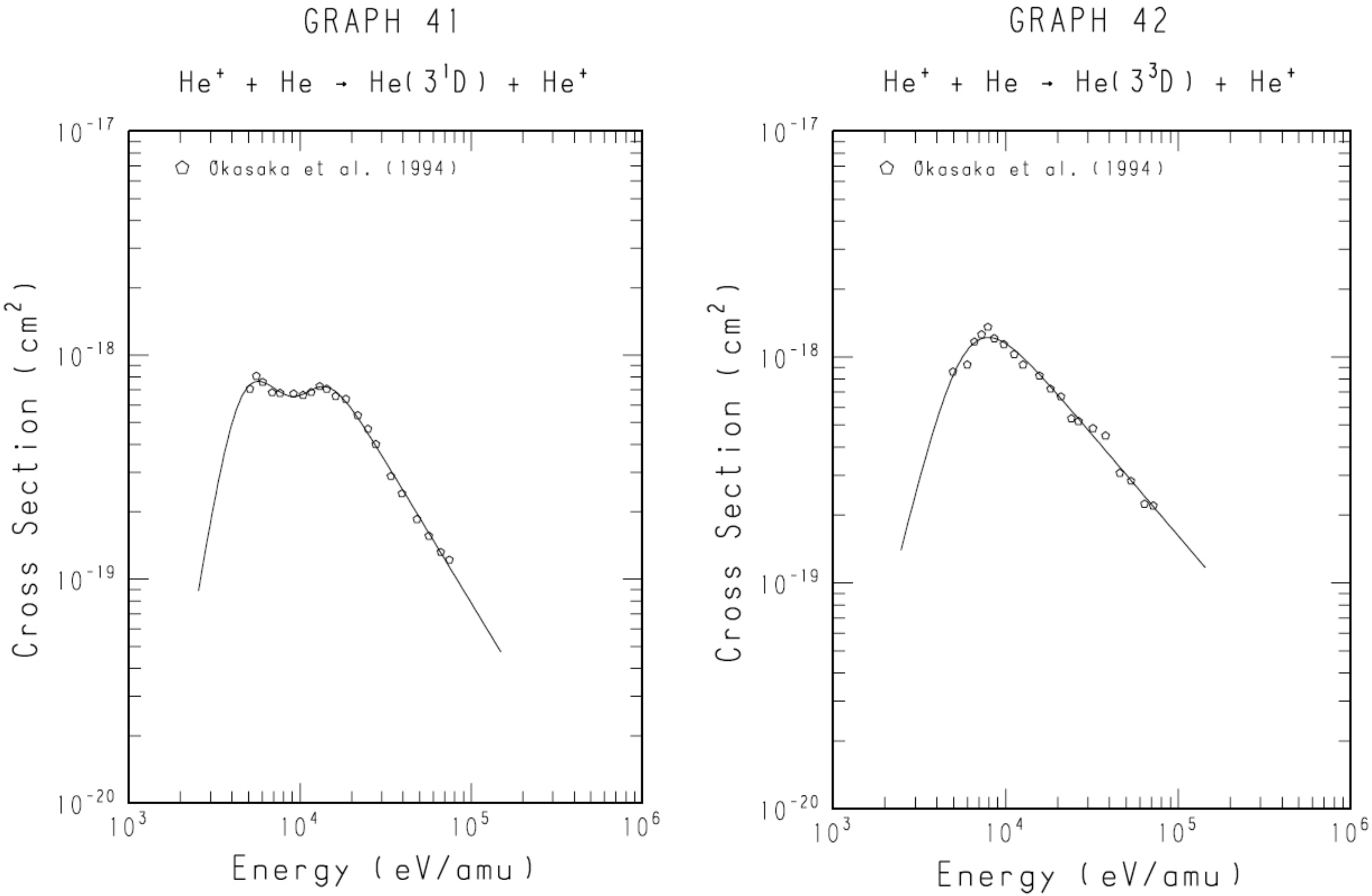
- Projectile excitation (n=4, δ_{rms}=4.6%; n=6, δ_{rms}=2.6%)





Results (7)

- Projectile excitation (Continued) (n=6, δ_{rms}=4.0%; n=4, δ_{rms}=6.8%)



Final Remarks

- During these four years, we have re-evaluated or newly formulated analytic expressions for a total of 210 reaction cross sections of He ions and atoms colliding with light targets.
- Some more sets of cross section data, collected at Kyoto University, should be fitted by analytic expressions.
- All these expressions should be published in a JAEA-Code/Data Report.

Acknowledgments

- I have worked on the formulation of analytic expressions for JEAMDL, for 26 years since 1982.
- One of the followers of mine will continue the work from the next fiscal year.
- On this occasion, I sincerely thank to all the members that supported me at the former JAERI and JAEA, especially Drs. Nakai, Shirai (deceased), Sataka, Kubo and Nakano.

Appendix: Publications of Our Work

1. Y. Nakai, T. Shirai, T. Tabata and R. Ito, "Cross sections for charge transfer of hydrogen atoms and ions colliding with gaseous atoms and molecules," At. Data Nucl. Data Tables **37**, 69 (1987).
2. T. Tabata, R. Ito, Y. Nakai, T. Shirai, M. Sataka and T. Sugiura, "Analytic cross sections for charge transfer of hydrogen atoms and ions colliding with metal vapors," Nucl. Instr. Meth. **B31**, 375 (1988).
3. Y. Nakai, T. Shirai, T. Tabata and R. Ito, "A semiempirical formula for single-electron-capture cross sections of multiply charged ions," Phys. Scr. **T28**, 77 (1989).

Appendix: Publications of Our Work (2)

4. T. Tabata, R. Ito, T. Shirai, Y. Nakai, H. T. Hunter and R. A. Phaneuf, "Extended scaling of cross-sections for the ionization of H, H2 and He by multiply charged ions," At. Plasma-Mater. Int. Data Fusion **2**, 91 (1992).
5. R. Ito, T. Tabata, T. Shirai and R. A. Phaneuf, "Analytic cross sections for collisions of H, H_2, He and Li atoms and ions with atoms and molecules. I," JAERI-M 93-117 (1993).
6. R. Ito, T. Tabata, T. Shirai and R. A. Phaneuf, "Analytic cross sections for collisions of H, H_2, He and Li atoms and ions with atoms and molecules. II," JAERI-Data/Code 94-005, (1994).

Appendix: Publications of Our Work (3)

7. R. Ito, T. Tabata, T. Shirai and R. A. Phaneuf, "Analytic cross sections for collisions of H, H_2, He and Li atoms and ions with atoms and molecules. III," JAERI-Data/Code 95-008 (1995).
8. R. Ito, T. Tabata, T. Shirai and R. A. Phaneuf, "Analytic cross sections for collisions of H, H_2, He and Li atoms and ions with atoms and molecules. IV," JAERI-Data/Code 96-024, (1996).
9. T. Tabata and T. Shirai, "Analytic cross sections for collisions of H^+, H_2^+, H_3^+, H, H_2, and H^- with hydrogen molecules," At. Data Nucl. Data Tables **76**, 1 (2000).
10. T. Shirai, T. Tabata, and H. Tawara, "Analytic cross sections for electron collisions with CO, CO_2, and H_2O relevant to edge plasma impurities," At. Data Nucl. Data Tables **79**, 143 (2001).

Appendix: Publications of Our Work (4)

11. T. Shirai, T. Tabata, H. Tawara and Y. Itikawa, "Analytic cross sections for electron collisions with hydrocarbons: CH_4, C_2H_6, C_2H_4, C_2H_2, C_3H_8, and C_3H_6," At. Data Nucl. Data Tables **80**, 147 (2002).
12. T. Tabata, H. Kubo and M. Sataka, "Formulating analytic expressions for atomic collision cross sections," JAERI-Res. 2003-015 (2003).
13. T. Tabata, T. Shirai, M. Sataka and H. Kubo, "Analytic cross sections for electron impact collisions with nitrogen molecules," At. Data Nucl. Data Tables **92**, 375 (2006).