Data Center for Plasma Properties

Group Research on Procedures for Evaluation of CH4 Collision Processes

Mi-Young Song
This work decide at the Joint IAEA-NFRI Technical Meeting (TM) on Data Evaluation for Atomic, Molecular and Plasma Material Interaction Processes in Fusion in September 2012
Participants recommended group member and molecule at that time.
Group Members:
- Y. Itikawa (Japan)
- Grzegorz P. Karwasz (Nicolaus Copernicus University),
- J. Tennyson (University College London)
- Viatcheslav kokouline(University of Central Florida)
- H. Cho(Chung-Nam National University)
- Y. Nakamura (Tokyo Denki University)
- J.-S. Yoon, M.-Y. Song (National Fusion Research Institute)

Our purpose: To establish the internationally agree standard reference data library for AM/PMI data
1) Experiment (Cho, Karwasz, Nakamura)

- experimentalist cover all processes
- we must check carefully systematic uncertainty of the experimental data what we will be doing before we evaluate the experimental data
- we need swarm experimentalist to evaluate vibrational excitation cross section
- we need experienced person to evaluate electronic excitation cross section

2) Theory (Itikawa, Tennyson, Kokoulin)

- Theorists cover all processes
- Theory should cover some processes because of experiment is so difficult. But theorists don’t give uncertainty. How to solve these problems.
- Few researchers can measure electronic excitation cross section but they cannot analysis because they don’t know radical state. They need theoretical data
General evaluation procedure
Preparatory stage
- Review of previous evaluation paper
- Collection of new paper.
- Define working Scope
- Contents of report
- To shard working part

Evaluation stage
- Analysis method of experiment and theory (characteristics, limitation, uncertainty, method)
- Comparisons of different research group
- Selection (good agreement)

Certified stage
- Check uncertainty
- Combine different collision processes
- Define recommended data of each collision processes
- Agreement of each evaluator
I. Preparatory stage

1. To review of previous evaluation paper
   7) LB Vol17C
2. Define working Scope
   • We don’t have all collision processes and decide working scope. (Electron collision, Photon collision cross section)

3. Contents of report
   • This report includes evaluated data and uncertainty.
   • We will create a report containing a detailed description of the data evaluation methods
   • We suggests researchers future research topic when evaluation with data is impossible

4. What do we do?
   • We list up processes according to Prof. Itikawa’s comment processes LIST
   • We shard working part from the processes list. All coworker decide working part.
5. Define Main evaluator for each process

- First, we specified main evaluator for each process in order to arrange the contents of evaluation. He will collects and adjusts other evaluator’s opinion.
  1. Ionization (dissociative ionization) – [Karwasz]
  2. Total cross section- [Karwasz]
  3. Electron Attachment [Cho]
  4. Elastic + DCS [Cho, Itikawa]
  5. Momentum transfer + DCS [Nakamura, Karwasz, Cho, Itikawa,]
  6. Vibrational excitation + DCS [Kokoouline, Karwasz, Nakamura]
  7. Rotational excitation + DCS [Itikawa, Nakamura, Kokoouline, Tennyson ]
  8. Electron excitation & Dissociation [Tennyson, Kokoouline, Cho, NFRI]
II. Evaluation stage

- Certified data with uncertainty
- Construction of NSRD (National Standard Reference Data) for A+M data for plasma
Analysis method of experiment and theory (characteristics, limitation, uncertainty, method)

It compares with other experimental data of the same process.
- Classification of same group and upgrade data
- near threshold energy
- Few data point
- Maximum position
- shape of cross section

Recent paper confidence
Ionization cross section

UMK DataBase*
Recommend
- L-B total recommended for total and partial, based on Straub et al. (1997) +BEB)

Opinion
- New data (Ward 2011) agree within error bars with L-B

Suggestion
- repeat weighted mean values and give the uncertainty on the recommended data in accordance to adopted statistical procedures
- check agreement with Janev’s, Dose’s and Kunc’s empirical formulae
- get into details of Ward’s partial cross sections
Total scattering cross section
 **Recommend**
  – L-B total recommended at 0.1-1000 eV
  – Born-Bethe fit to Ariyosanghe at 1000-4000 eV
  – MERT elastic below 1 eV

 **Opinion**
  - Zecca/Karwasz @ above 1000 eV underestimated due to lack of retarding field analyser in their apparatus
  - MERT merges well @ 0.1 eV with L-B recommended (=Ferch’s and Lohmann/Buckman exp/ total)

 **Suggestion**
  - repeat weighted mean values and give the error bar on the recommended data in accordance to adopted statistical procedures
→ However, there is a huge difference between Rawat et al (2008) and Sharp & Dowell (1967) in total attachment cross section.
Recommend

Not yet

Opinion

- **Sharp & Dowell (1967):** measured the TOTAL attachment cross section using the total ionization method.
- **Rawat et al (2008):** Measurement of absolute cross sections for the formation of H\(^{-}\) and CH\(_{2}\)\(^{-}\) from methane.
- **Hoshino et al (2011):** No absolute measurement, but give relative results for C\(^{-}\), CH\(^{-}\), CH\(_{2}\)\(^{-}\) and CH\(_{3}\)\(^{-}\) anions formed from DEA to CH\(_{4}\). Peak positions of CH\(_{2}\)\(^{-}\) of Sharp & Dowell, Rawat et al, and Hoshino et al agree very well.

Suggestion

- we need to compare the data set and analysis of the experiment method.
- we give the uncertainty on the recommended data in accordance to adopted statistical procedures
Resonance region, $v_1 + v_3$
Resonance region, $v_2 + v_4$
**Recommendation:**
- Curik’s theory, shifted by -1eV at resonance
- Althorpe theory (=Cascella) at threshold

**Opinion**
- elastic MERT + vibrational ≈ exp. Total
- not in disagreement with swarm
- agree very well (within 10%) with Allan 2007 and within exp. declared error bar with Bundschu, Shyn and Tanaka (if renormalized by +30% Tanaka vs. Boesten&Tanaka)

**Suggestion**
- ask their opinion to Curik and Allan
Tentative Recommendation (Karwasz)

- Nakamura’s data @ 1-20 eV
- MERT (Fedus & Karwasz) below 1 eV
- Cho’s analysis of experimental beam data at 20-500 eV

Opinion

- Nakamura’s data in the maximum are intermediate between upper limit (Boesten) and lower (Cho) and in v. good agreement with Allan’s (2007) data
Tentative Recommendation (Cho)

The 7 data sets, given in the table below, are considered to derive the recommended elastic DCS, ICS and MTCS after the following processes:

Opinion

After collecting available elastic cross sections measured experimentally, the following data sets are excluded from the further considerations:

- relative measurements
- data with no uncertainties
- the data points which are too far off the general pattern
- the data points which have no other data points overlapped in the angular and energy region of interest

- average the remaining data to derive the recommended data sets
- estimated the uncertainties of the recommended data
<table>
<thead>
<tr>
<th>Authors</th>
<th>Energy &amp; angular Range measured</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boesten &amp; Tanaka (1991)</td>
<td>1.5-100 eV 10°-130°</td>
<td>Phase-shift fitting to full angle ICS, MTCS</td>
</tr>
<tr>
<td>Bundschu et al (1997)</td>
<td>0.6-5.4 eV 12°-132°</td>
<td>Phase shift analysis ICS, MTCS</td>
</tr>
<tr>
<td>Cho et al (2008)</td>
<td>5-100 eV 10°-180°</td>
<td>ICS, MTCS</td>
</tr>
<tr>
<td>Sakae et al (1989)</td>
<td>75-700 eV 5°-135°</td>
<td>ICS, MTCS Extrapolated by fitting the square of the Legendre polynomials to the experimental values.</td>
</tr>
<tr>
<td>Shyn &amp; Cravens (1990)</td>
<td>5-50 eV 12°-156°</td>
<td>ICS, MTCS Exponentially extrapolating to 180°</td>
</tr>
<tr>
<td>Sohn et al (1986)</td>
<td>0.2-5 eV 15°-138°</td>
<td>ICS, MTCS using phase shift analysis</td>
</tr>
</tbody>
</table>
Tentative Recommendation (Itikawa)

- Below 5 eV: the LB values
- 5 – 100 eV: Cho
- Above 100 eV: Sakae

Uncertainty:
- E ≤ 1 eV: 35%
- 1 < E ≤ 100 eV: 26%
- 100 < E: 10%

To smoothly connect the low-energy side (< 100 eV) and the high-energy one (> 100 eV), the value of LB, instead of Cho, is taken at 100 eV.

To avoid an irregularity, the Sakae's value at 300 eV is excluded.
Opinion

- starts from the recommended data of LB (2003). It gives the cross section at 0.05 to 100 eV. The uncertainty is ±35% below 1 eV and ±25% above 1 eV.

- One new measurement is available. Cho et al., J. Phys. B 41, 045203 (2008). This paper reports the cross section at 5 to 100 eV. Those values agree with the LB data within the uncertainty. But the new measurement has obtained DCS up to 180°. Hence the new values are better than the previous ones.

- Above 100 eV, two sets of experimental data are available. Sakae et al., J. Phys. B 22, 1385 (1989) at 75 – 700 Ev Iga et al., Phys. Rev. A 61, 022708 (2000) at 100 – 500 eV Both the sets of cross sections agree with each other within the combined uncertainties. At 100 eV, however, the two sets of data are significantly larger than the cross sections in the lower-energy region (i.e., LB and Cho). The difference between the largest one (Iga) and the smallest one (Cho) is outside of their combined uncertainties.
Opinion

- Three evaluator give different opinion
- Need more discussion
- Ramsure minimum
• **Tentative Recommendation** (Karwasz)
  1) Nakamura’s data @ 1-20 eV
  2) MERT (Fedus&Karwasz) below 1 eV
  3) Cho’s analysis of experimental beam data at 20-500 eV
• **Justification:**
  1) Nakamura’s data in the maximum are intermediate between upper limit (Boesten) and lower (Cho) and in v. good agreement with Allan’s (2007) data
• **Opinion**
• :1) repeat weighted mean values and give the error bar on the recommeded data in accordance to adopted statistical procedures
  2) await the theoretical analysis of DCS at 5-20 eV to confirm/exclude adopted MTCS at its maximum
  3) explain difference between MT and higher MT cross sections (according to Schmidt) in Boltzman analysis
  4) check the recommended set of cross sections with Monte Carlo and Boltzmann vs swarm drift coefficients
Tentative Recommendation (Cho)

- The 7 data sets, given in the table below, are considered to derive the recommended elastic DCS, ICS and MTCS after the following processes:

Opinion

- The situation is the same as for elastic scattering. The same principle is applied to the determination of the recommended data.
Tentative Recommendation (Itikawa)

- Below 5 eV the LB values
- 5 – 100 eV Cho
- above 100 eV Sakae

Uncertainty:
- \( E < 5 \text{ eV} \) 20%
- \( 5 \leq E \leq 50 \text{ eV} \) 26%
- \( 50 \text{ eV} < E \) 10%

To smoothly connect the low-energy side (< 100 eV) and the high-energy one (>100 eV), the value of Sakae is taken at 75 eV and above.

Opinion

- The situation is the same as for elastic scattering. The same principle is applied to the determination of the recommended data.
Opinion

- Three evaluator give different opinion
- We need more discussion
- Ramsure minimum
- Ask to Prof. Nakamura (swarm method)
- **Recommend**
  - Not yet

- **Opinion**
  - From the comparison of the theoretical results (and also a comparison of the DCS obtained from theory and experiment) we cannot definitely recommend any values.

  - Muller et al., J. Phys. B 18, 3971 (1985) : DCS were derived with the deconvolution of the vibrationally-elastic peak in the electron energy loss spectra. (No ICS)
  - As a representative, the values of McNaughten et al. and Brescansin et al. are compared with each other. There is a good agreement below 10 eV, but not above
  - Tennyson calculated rotational excitation cross section: W. J. Brigg and J. Tennyson (To be published, 2013).
Recommend

- Not yet

Opinion

- Both Winters and Perrin et al are total (not neutral) dissociation cross sections including dissociative ionization cross section.
- There are no uncertainties given in both data sets except one standard deviation in Winters.
- Dissociation into neutral fragments is related excitation processes and we need calculation of excitation cross section.
III. Certified stage

- How to show the uncertainty
  - find correct uncertainty (each data)
  - uncertainty evaluation

- Beat value vs Weight average (10%, good agreement)

- We define recommended data of each collision processes.
<table>
<thead>
<tr>
<th>ionization</th>
<th>Total cross section</th>
<th>ES &amp; MT</th>
<th>Attachment</th>
<th>Excitation</th>
</tr>
</thead>
</table>
| • Be careful: low energy range and light ion  
• To comparison TICS with sum of PICS | • To check minimum position and maximum position  
• To comparison experiment data with sum of all processes | • Careful review the angle of DCS because of ES & MT is obtained integrate of DCS | • Not yet | • Not yet |
1\textsuperscript{st} GM: 23 - 25 January 2013, Gunsan, South Korea

2\textsuperscript{nd} GM: 25 - 27 June 2013, Deajeon, South Korea

3\textsuperscript{rd} GM: 23-24 September 2013, Open university, UK
• Derived research

→ Swarm research for the evaluation of Vibrational excitation
→ BEB calculation for the evaluation of ionization
→ DCS measurement (10-180 degree) for elastic, momentum transfer, vibrational excitation
→ Theoretical research for excitation