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The Important Electron Impact Collision Cross Sections with Methane

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Abstract—The electrical discharge plasma in methane is used in many fields of technology and the knowledge of the electron impact cross sections with the molecule of this gas is necessary for the modeling, which represents a good tool for understanding this phenomenon. The main object of this work is a finding the important electron impact cross sections with the methane molecule through the reviewing the theoretical and measured data found in the literature.

Keywords-elastic collision; inelastic collision; electron impact cross section; methane molecule

I. INTRODUCTION

View of recent applications of the cold non-equilibrium thermodynamic plasma in different fields such as medicine and semiconductor manufacturing etc. [1-6]; researchers attention is attracted, experimental and theoretical studies are conducted as [7-20]. The study and the modeling of plasma require the knowledge of the physical processes; these last are based on the elementary microscopic mechanisms such as ionization, excitation, attachment, recombination, dissociation, and elastic collisions. Indeed, it is known that the knowledge of the cross sections of these mechanisms is indispensable to obtain the electron energy distribution function EEDF, the electron transport coefficients, and the rates of the different reactions. In this work we interest to accumulate the cross sections of electronic impact collision with methane found in the literature. Electron collisions with methane are especially important in plasmas. Methane plays a dominant role in the edge plasma region of high temperature plasma apparatus such as a tokamak. The methane CH₄ is the simplest poly-atomic hydrocarbon, and is present in the atmosphere of most planets interstellar surface [21-23]. Low-pressure radiofrequency plasma methane is used in many fields of technology [24-26], this molecular gas is considered to be a good test gas [27], several studies that were experimentally interested for example [28-33], or by numerical (analytical) study by mixing it with other gases such as H₂, N₂, etc. [34-37], or pure [38-42].

II. ELECTRON CROSS SECTION FOR METHANE

When the molecule contains at least three atoms, the number of dissociative excitation channels, ionization and recombination increases drastically. For example, electron impact on the H_2 molecule yields only two fragments, and for CH_4 can produce $CH_3 + H$, $CH_2 + 2H$ (or H_2), CH + 3H (or $H + H_2$), $C + 2H_2$ (or $2H + H_2$), where the atomic and the molecular products both being in excited states (electronic and/or vibratory). The processes of molecular fragmentation lead to a multiplication of molecular species in the plasma and to chains of long reactions before the complete dissociation of the initial molecule is accomplished. The methane molecule is relatively stable and it has four vibrational excitation modes as given in the table I.

TABLE I. Vibrational modes and excitation energies for CH₄ [43]

	Mode	Energy
v_1	Symmetric stretching	0.362
v_2	Twisting	0.190
v_3	Asymmetric stretching	0.374
v_4	Scissoring	0.162

Unfortunately to this day, it there are no effective electron dissociation cross sections of methane to the following channels; (1): CH_3+H , (2): CH_2+H_2 , (3): CH_2+2H , (4): $CH+H_2+H$. The important electron- CH_4 molecule collisions are resumed in table 2.

TABLE II. Electronic impact reactions with threshold energy

Process	Collision	Threshold (eV)
Elastic	$e+CH_4 \Rightarrow e+CH_4$	
Rotational	$e+CH_4 => e+CH_4$	0.0078
Rotational	$e+CH_4 => e+CH_4$	0.013
Vibrational	$e+CH_4 \Rightarrow e+CH_4$	0.162
v ioi ationai	$e+CH_4 \Longrightarrow e+CH_4$	0.362
	$e+CH_4 \Rightarrow e+CH_3+H$	8.8
Dissociation	$e+CH_4 => e+CH_2+H_2$	9.4
Dissociation	$e+CH_4 => e+CH+H_2+H$	12.5
	$e+CH_4 => e+C+2H_2$	14
Ionization	$e+ CH_4 => 2e + CH_4^+$	12.63
	$e+CH_4 => 2e + CH_3^+ + H$	14.25
	$e+CH_4 => 2e + CH_2^+ + H_2$	15.1
Dissociative	$e+CH_4 => 2e + CH^+ + H_2 + H$	19.9
Ionization	$e+CH_4 => 2e + C^+ + 2H_2$	19.6
	$e+CH_4 => 2e + H_2^+ + CH_2$	20.1
	$e+CH_4 \Rightarrow 2e+H^++CH_3$	18.0

Mi- Song Yong *et al.* [43] confirm that for the dissociative there is no practical measure that distinguishes between (2) and (3) and no direct estimate of (4). Erwin and Kunc. [44], [45] presented a semi-empirical method to estimate the dissociative cross sections, but without including the dissociation to C+2H₂ (or 2H+H₂). Figure 1 represents the cross sections of electron impact collision with methane for: momentum transfer cross

section, rotational excitation cross section for the energies (0.0078 eV and 0.013 eV) eV, vibrational excitation cross section for the energies (0.162 eV and 0.362 eV), the dissociation excitation for the channels: CH_3+H , CH_2+H_2 , CH_2+H_2+H , $C+2H_2$, the ionization into CH_4^+ , and the dissociative ionization cross section for the channels: $H+CH_3^+$, $CH_2^++H_2$, $CH_2^++H_2$, $CH_2^++H_2$, $CH_2^++CH_2$, $H_2^++CH_2$, $H_2^++CH_3$.

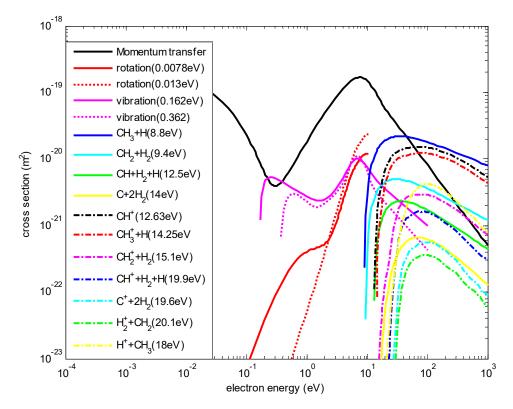


Fig.1: electron impact collision cross sections with methane [25]

III. CONCLUSION

In this study a complete set of electronic impact collision cross sections with methane have been reported. These cross sections are very important for the study of the electrical discharge plasma in methane gas, and can be used especially in the modeling as input data for particle models.

References

- M. A. Lieberman and A. J. Lichtenberg, "Principles of Plasma Discharges and Materials Processing", 2nd edition (New York: Wiley), 2005
- [2] P. Chabret, N. Braithaite, "Physics of radio-frequency plasmas", Cambridge University Press, 2011.
- [3] Djilali Benyoucef, Mohammed Yousfi, "Particle modelling of magnetically confined oxygen plasma in low pressure radio frequency discharge," Physics of Plasmas, vol. 22, no. 1, 2015.
- [4] Jae Young Kim, Sung-O Kim, Yanzhang Wei, and Jinhua Li, "A flexible cold microplasma jet using biocompatible dielectric tubes for cancer therapy," *Applied physics letters*, vol. 96, no. 20, 2010.

- [5] G. J. Kim, W. Kim, K. T. Kim, and J. K. Lee, "DNA damage and mitochondria dysfunction in cell apoptosis induced by nonthermal air plasma," *Applied Physics Letters*, vol. 96, no. 2, 2010.
- [6] K. McKay, F. Iza, and M.G. Kong "Excitation frequency effects on atmospheric-pressure helium RF microplasmas: plasma density, electron energy and plasma impedance," *The European Physical Journal D*, vol. 60, pp. 497-503, 2010.
- [7] Jia Liu, De-Qi Wen, Yong-Xin Liu, Fei Gao, Wen-Qi Lu, and You-Nian Wang, "Experimental and numerical investigations of electron density in low-pressure dual frequency capacitively coupled oxygen discharges," *Journal of Vacuum Science & Technology A: Vacuum, Surfaces, and Films*, vol. 31, no. 6, 2013.
- [8] Driss Raouti, Samir Flazi, Djilali Benyoucef, "Electrical modelling of a positive point to plane corona discharge at atmospheric pressure," *Contributions to Plasma Physics*, vol. 54, no. 10, 2014.
- [9] Mohamed Mostafaoui, Djilali Benyoucef, "Electrical model parameters identification of radiofrequency discharge in argon through 1D3V/PIC-MC model," *Plasma Science and Technology*, vol. 20, no. 9, 2018.
- [10] P. D. Lymberopoulos and D. J. Economou, "Two-Dimensional Self-Consistent Radio Frequency Plasma Simulations Relevant to the Gaseous Electronics Conference RF Reference Cell," *Journal of research of the National Institute of Standards and Technology*, vol. 100, no. 4, 1995.

- [11] Djilali Benyoucef, Mohammed Yousfi, "Effects of Increasing Magnetic Field and Decreasing Pressure on Asymmetric Magnetron Radio Frequency Ar/O2 Discharges," *IEEE Transactions on Plasma Science*, vol. 41, no. 4, 2013.
- [12] M. Olevanov, O. Proshina, T. Rakhimova, and D. Voloshin, "Ion energy distribution function in dual-frequency rf capacitively coupled discharges: analytical model," *Physical Review E*, vol. 78, no. 2, 2008.
- [13] I. Rafatov, E. A. Bogdanov, and A. A. Kudryavtsev, "On the accuracy and reliability of different fluid models of the direct current glow discharge," *Physics of Plasmas*, vol. 19, no. 3, 2012.
- [14] Djilali Benyoucef, Mohammed Yousfi, "RF discharge characteristics from particle model based on two optimized Monte Carlo methods for collision treatment," XXIX International Conference on Phenomena in Ionized Gases (ICPIG 2009), July 12-17, 2009.
- [15] M Shihab, A T Elgendy, I Korolov, A Derzsi, J Schulze, D Eremin, T Mussenbrock1, Z Donko' and R P Brinkmann, "Kinetic simulation of the sheath dynamics in the intermediate radio frequency regime," Plasma Sources Science and Technology, vol. 22, no. 5, 2013.
- [16] Djilali Benyoucef, "Modélisation particulaire et multidimensionnelle des plasmas réactifs crées par décharge électrique hors équilibre," Diss. Université des Sciences et de la Technologie d'Oran Mohamed-Boudiaf USTOMB, 2011.
- [17] Shinya Iwashita, Giichiro Uchida, Julian Schulze, Edmund Schungel, Peter Hartmann, Masaharu Shiratani, Zoltan Donko' and Uwe Czarnetzki, "Sheath-to-sheath transport of dust particles in a capacitively coupled discharge," *Plasma Sources Science and Technology*, vol. 21, no. 3, 2012.
- [18] Aranka Derzsi, Trevor Laeur, Jean-Paul Booth, Ihor Korolov and Zoltán Donkó, "Experimental and simulation study of a capacitively coupled oxygen discharge driven by tailored voltage waveforms," *Plasma Sources Science and Technology*, 2015, vol. 25, no 1, 2016.
- [19] Djilali Benyoucef, Mohammed Yousfi, "Particle modelling of low-pressure radio-frequency magnetron discharges including the effects of self-induced electromagnetic fields," *Plasma Sources Science and Technology*, 2014, vol. 23, no. 4, 2014.
- [20] M. M. Tur ner, A. Derzsi, Z. Donko, D. Eremin, S. J. Kelly, T. Lafleur, and T. Mussenbrock, "Simulation benchmarks for low-pressure plasmas: Capacitive discharges," *Physics of Plasmas*, vol. 20, no. 1, 2013.
- [21] Robert K. Jones, "Absolute total cross sections for the scattering of low energy electrons by CCl4, CCl3F, CCl2F2, CClF3, and CF4," *The Journal of chemical physics*, vol. 84, no. 2, 1986.
- [22] Xianming Liu and Donald E.Shemansky, "Analysis of electron impact ionization properties of methane," *Journal of Geophysical Research:* Space Physics, vol. 111, no. A4, 2006.
- [23] M. Danko, et al., "Electron impact excitation of methane: determination of appearance energies for dissociation products," *Journal of Physics B: Atomic, Molecular and Optical Physics*, vol. 46, no. 4, 2013.
- [24] Z.Nikitovic, O. Sasic, Z.Lj. petrovic, G. Malovic, Q.Strinic, S. Dujco, Z.Raspopvic and M. Radmilovic-Radjenovic, "Data base modeling plasma devices for processing of integrated circuits", Material Science Forum, Vols 453-454, pp 15-20, (2004).
- [25] Abdelatif Gadoum, Djilali Benyoucef, "Set of the electron collision cross sections for methane molecule. *IEEE Transactions on Plasma Science*, 2018, vol. 47, no. 3, 2018.
- [26] Evangelos Gogolides, David Mary, Ahmed Rhallabi and Guy Turban, "RF plasmas in methane: Prediction of plasma properties and neutral radical densities with combined gas-phase physics and chemistry model," *Japanese journal of applied physics*, vol. 34, no. 1R, 1995.
- [27] D. K. Davies, L. E. Kline, and W. E. Bies, "Measurements of swarm parameters and derived electron collision cross sections in methane. *Journal of Applied physics*, vol. 65, no. 9, 1989.
- [28] S. D. Marcum et al., "Methane dissociation in pulsed dc discharges at high reduced electric field," *Journal of propulsion and power*, vol. 20, no. 2, 2004.

- [29] K. Gluch, P. Scheier, W. Schustereder, T. Tepnual, L. Feketeova, C. Mair, S. Matt-Leubner, A. Stamatovic, T. D. Märk, "Cross sections and ion kinetic energies for electron impact ionization of CH4. *International Journal of Mass Spectrometry*, vol. 228, no. 2-3, 2003.
- [30] Michel Geleijns, Ad van der Avoird, Paul E. S. Wormer, and Nadine Halberstadt, "Photodissociation of the methane—argon complex. II. Vibrational predissociation dynamics, spectral linewidths and fragment state distributions," *The Journal of chemical physics*, vol. 117, no. 16, 2002.
- [31] Safa Motlagh and John H. Moore, "Cross sections for radicals from electron impact on methane and fluoroalkanes," *The Journal of chemical* physics, vol. 109, no 2, 1998.
- [32] Cechan Tian and C.R. Vidal, "Electron impact dissociative ionization and the subsequent ion-molecule reactions in a methane beam," *Chemical physics*, vol. 222, no 1, 1997.
- [33] V.A. Ukraintsev and I. Harrison, "Methane dissociative chemisorption on Pt (111) explored by microscopic reversibility," *Surface Science Letters*, vol. 286, no. 3, 1993.
- [34] A. A. Sebastian and J. M. Wadehra, "Time-dependent behaviour of electron transport in methane–argon mixtures. *Journal of Physics D: Applied Physics*, 2005, vol. 38, no 10, 2005.
- [35] S. F. Yoon, K. H. Tan, Rusli, and J. Ahn, "Modeling and analysis of hydrogen-methane plasma in electron cyclotron resonance chemical vapor deposition of diamond-like carbon," *Journal of applied physics*, vol. 91, no 1, 2002.
- [36] B. Farouk and K. Nagayama, "Particle simulation of CH 4/H 2 RF glow discharges for DLC film deposition," In: AIP Conference Proceedings. American Institute of Physics, 2001.
- [37] F J Gordillo-Vazquez, C Gomez-Aleixandre and J M Albella, "Influence of the excitation frequency on CH4/H/H2 plasmas for diamond film deposition: electron energy distribution function and atomic hydrogen concentration," *Plasma Sources Science and Technology*, vol. 10, no. 1, 2001
- [38] Maurizio Masi, Carlo Cavallotti and Sergio Carra', "Different approaches for methane plasmas modeling," *Chemical engineering science*, vol. 53, no. 22, 1998.
- [39] Evangelos Gogolidest, Cyrille Buteaut, Ahmed Rhallabi and Guy Turban, "Radio-frequency glow discharges in methane gas: modelling of the gas-phase physics and chemistry," *Journal of Physics D: Applied Physics*, vol. 27, no. 4, 1994.
- [40] A. Rhallabi and Y. Catherine, "Computer simulation of a carbon-deposition plasma in CH/sub 4," *IEEE transactions on plasma science*, vol. 19, no. 2, 1991.
- [41] K. Matyash, R. Schneider, A. Bergmann, W. Jacob, U. Fantz, P. Pecher, "Modeling of hydrocarbon species in ECR methane plasmas," *Journal of nuclear materials*, vol. 313, 2003.
- [42] Chien-Wei Chang, Mohammad Davoudabadi, and Farzad Mashayek, " One-dimensional fluid model of methane plasma for diamond-like coating," *IEEE transactions on plasma science*, vol. 38, no. 7, 2010.
- [43] Mi-Young Song, Jung-Sik Yoon, Hyuck Cho, Yukikazu Itikawa, Grzegorz P. Karwasz, Viatcheslav Kokoouline, Yoshiharu Nakamura, and Jonathan Tennyson, "Cross sections for electron collisions with methane," *Journal of Physical and Chemical Reference Data*, vol. 44, no. 2, 2015.
- [44] D. A. Erwin and J. A. Kunc, "Electron-impact dissociation of the methane molecule into neutral fragments. *Physical Review A*, vol. 72, no. 5, 2005.
- [45] D. A. Erwin and J. A. Kunc, "Dissociation and ionization of the methane molecule by nonrelativistic electrons including the near threshold region," *Journal of Applied Physics*, vol. 103, no. 6, 2008.