Electron collision cross section set of O_2

S Kawaguchi[(*)1], Y Iwabe[1], K Takahashi[1], and K Satoh[1]

[1] *Division of Information and Electronic Engineering, Graduate School of Engineering, Muroran Institute of Technology, Muroran, Hokkaido, 050-8585, Japan*

[(*)] *skawaguchi@muroran-it.ac.jp*

A reliable and detailed electron collision cross section set of O_2 is required for precisely modelling and simulating O_2 containing plasmas. There are numerous studies on electron collision cross sections of O_2 for various processes. In the LXCat [1], seven kinds of self-consistent cross section sets for O_2, which include momentum transfer, excitation, electron attachment, and ionization cross sections, are available. However, the number and the shape of electron collision cross sections in the cross section sets differ from each other. This would yield different values of electron transport coefficients and rate coefficients; therefore, an assessment of the cross section sets is needed by comparing calculated and measured coefficients. The aim of this work is to construct reliable and detailed electron collision cross section set of O_2. The priority for constructing cross section set is to respect measured and theoretically calculated cross sections. The neutral dissociation cross sections and ionization cross sections for excited O_2^+ are carefully considered. The validity of the constructed cross section set is demonstrated by comparing measured and calculated electron transport coefficients in O_2 in a wide range of reduced electric fields.

The present electron collision cross section set consists of one vibrationally elastic momentum transfer, 15 rotational excitation, 15 rotational de-excitation, four vibrational excitation, 10 electronic excitation, 1 ion-pair formation, 3 neutral dissociation, 2 electron attachment, and 4 ionization cross sections. The rotational excitation and de-excitation cross sections were taken from Ridenti *et al.* [2] The vibrationally elastic momentum transfer cross section, q_{vm}, is defined as the sum of elastic momentum transfer cross section, rotational excitation, and rotational de-excitation cross sections. The shape of q_{vm} was determined to follow the q_{vm} measured by Shyn and Sharp [3], Iga *et al*. [4], Sullivan *et al.* [5], and Linert *et al*. [6]. Below 1 eV, the shape of q_{vm} was determined to reproduce the measured electron drift velocity and longitudinal diffusion coefficient at low reduced electric fields. The vibrational excitation cross sections are based on Laporta *et al*. [7]; however, their cross sections were multiplied by 0.31 to reproduce measured electron transport coefficients and modified to follow the measured vibrational excitation cross sections [8-10]. The electronic excitation cross section, q_{ex}, for $a^1\Delta_g$ and $b\,^1\Sigma_g$ was determined to follow q_{ex} measured by Linder and Schmidt [11], Shyn and Sweeney [12], and Wakiya *et al*. [13]. The q_{ex} for $c\,^1\Sigma_u^-$, $A'\,^3\Delta_u$, and $A^3\Sigma_u^+$ was based on Shyn and Sweeney [14]. The q_{ex} for the Schumann-Runge continuum consists of q_{ex} for $1^3\Pi_g$, $B^3\Sigma_u^-$, and 8.87 eV state. The q_{ex} for $1^3\Pi_g$ and 8.87 eV state are based on Shyn *et al.* [15]. The q_{ex} for $B^3\Sigma_u^-$ is based on the BEf scaling result [16], but the shape near its threshold energy is modified to reproduce the measured ionization coefficient. The q_{ex} for $E^3\Sigma_u^-(v'=0)$ and $E^3\Sigma_u^-(v'=1)$ are based on Campbell *et al*. [17] and Suzuki *et al.* [16] A neutral dissociation cross section calculated by Laporta *et al.* [18] was included. Furthermore, we added two kinds of neutral dissociation cross sections the threshold energies of which are 10.5 eV and 12.1 eV. The former is determined to reproduce the sum of q_{ex} for the exsited states ranging from 9.7 to 12.1 eV. The latter is determined to reproduce measured ionization coefficieint and represents the neutral dissociation of superecited O_2 molecules[19]. The dissociative electron attachment cross section and cross section for ion-pair formation ($O^- + O^+$) were determined from total cross section for negative ion formation measured by Rapp and Briglia [20], which was multiplied by 0.74 in this work. Three-body attachment collisions were considered in accordance with Taniguchi *et al*. [21]. The ionization cross sections consists of cross sections for yielding $O_2^+(X^2\Pi_g)$, $O_2^+(A^2\Pi_u)$, $O_2^+(a^4\Pi_u)$, $O_2^+(b^4\Sigma_g^-)$, O^+, and O^{2+}. The ionization cross sections for $O_2^+(b^4\Sigma_g^-)$ and $O_2^+(A^2\Pi_u)$ were obtained from the total emission cross sections for the first negative system of O_2^+ ($b^4\Sigma_g^- \rightarrow a^4\Pi_u$) and the second negative system of O_2^+ ($A^2\Pi_u \rightarrow X^2\Pi_g$) measured by Terrell *et al*. [22], respectively. The ionization cross section for $O_2^+(X^2\Pi_g)$ and $O_2^+(a^4\Pi_u)$ was determined as follows: The sum of cross sections for $O_2^+(b^4\Sigma_g^-)$ and $O_2^+(A^2\Pi_u)$ is subtracted from the total ionization cross section for O_2^+ recommended by Itikawa [23], and the residual cross section is splitted into cross sections for $O_2^+(X^2\Pi_g)$ and $O_2^+(a^4\Pi_u)$ using the branching ratio of cross sections for $O_2^+(X^2\Pi_g)$ and $O_2^+(a^4\Pi_u)$ reported by Doering and Yang [24]. The ionization cross sections for O^+ and O^{2+} recommended by Itikawa [23] were used.

We calculated the electron drift velocity, ionization coefficient, electron attachment coefficient, effective ionization coefficient, and longitudinal diffusion coefficient in O_2 by Monte Carlo simulation. It is found that the electron transport coefficients calculated from the cross section sets obtained from LXCat do not necessarily reproduce the measured electron transport coefficients [25-30]. The cross section set reported by IST-Lisbon well reproduces the measured transport coefficients compared to the other cross section sets; however, the calculated ionization coefficient is higher than measured data above 400 Td. The electron transport coefficients calculated from the present cross section set were found to agree with measured data in a wide range of reduced electric fields. This indicates the validity of the present cross section set of O_2.

[1] LXCat [https://nl.lxcat.net/].
[2] M. A. Ridenti, L. L. Alves, V. Guerra, and J. Amorim, *Plasma Sources Sci. Technol.* **24** (2015) 035002.
[3] T. W. Shyn and W. E. Sharp, *Phys. Rev. A* **26** (1982) 1369.
[4] I. Iga, L. Mu-Tao, J. C. Nogueira, and R. S. Barbieri, *J. Phys. B: At. Mol. Phys.* **20** (1987) 1095.
[5] J. P. Sullivan, J. C. Gibson, R. J. Gulley, and S. J. Buckman, *J. Phys. B: At. Mol. Opt. Phys.* **28** (1995) 4319.
[6] I. Linert, G. C. King, and M. Zubek, *J. Phys. B: At. Mol. Opt. Phys.* **27** (2004) 4681.
[7] V. Laporta, R. Caliberto, and J. Tennyson, *Plasma Sources Sci. Technol.* **22** (2013) 025001.
[8] C. J. Noble, K. Higgins, G. Wöste, P. Duddy, P. G. Burke, P. J. O. Teubner, A. G. Middleton, and M. J. Brunger, *Phys. Rev. Lett.* **76** (1996) 3534.
[9] I. Linert and M. Zubek, *J. Phys. B: At. Mol. Opt. Phys.* **39** (2006) 4087.
[10] T. W. Shyn and C. J. Sweeney, *Phys. Rev. A* **48** (1993) 1214.
[11] F. Linder and H. Schmidt, *Z. Naturforsch. A* **26** (1971) 1617.
[12] T. W. Shyn and C. J. Sweeney, *Phys. Rev. A* **47** (1993) 1006.
[13] K. Wakiya, *J. Phys. B: At. Mol. Phys.* **11** (1978) 3931.
[14] T. W. Shyn and C. J. Sweeney, *Phys. Rev. A* 62 (2000) 022711.
[15] T. W. Shyn, C. J. Sweeney, A. Grafe, and W. E. Sharp, *Phys. Rev. A* 50 (1994) 4794.
[16] D. Suzuki, H. Kato, M. Ohkawa, K. Anzai, H. Tanaka, P. Limão-Vieira, L. Campbell, and M. J. Brunger, *J. Chem. Phys*. **134** (2011) 064311.
[17] L. Campbell, H. Tanaka, H. Kato, S. Jayaraman, and M. J. Brunger, *Eur. Phys. J. D* **66** (2012) 26.
[18] V. Laporta, R. Caliberto, and J. Tennyson, *Phys. Rev. A* **91** (2015) 012701.
[19] Y. Hatano, *Phys. Rep.* **313** (1999) 109.
[20] D. Rapp and D. D. Briglia, *J. Chem. Phys.* **43** (1965) 1480.
[21] T. Taniguchi, K. Kawamura, S. Sakamoto, and H. Tagashira, *J. Phys. D: Appl. Phys.* **15** (1982) 1187.
[22] C. A. Terrell, D. L. Hansen, and J. M. Ajello, *J. Phys. B: At. Mol. Opt. Phys.* **37** (2004) 1931.
[23] Y. Itikawa, *J. Phys. Chem. Ref. Data*, **38** (2009) 1.
[24] J. P. Doering and J. Yang, *J. Geophys. Res.* **102** (1997) 9691.
[25] B.-H. Jeon and Y. Nakamura, *J. Phys. D: Appl. Phys.* **31** (1998) 2145.
[26] B.-H. Jeon and Y. Nakamura, *IEEJ Trans. Fundam. Mater*. **118** (1998) 874.
[27] K. Yoshida, H. Tagashira, T. Ohshima, H. Ohuchi, and Y. Kishimoto, *J. Phys. D: Appl. Phys*. **29** (1996) 2124.
[28] S. A. J. Al-Amin, H. N. Kucukarpachi, and J. Lucas, *J. Phys. D: Appl. Phys.* **18** (1985) 1781.
[29] D. R. Nelson and F. J. Davis, *J. Chem. Phys*. **57** (1972) 4079.
[30] T. Rasmus, E. Kalev, P. Peeter, R. Jüri, P. Toomas, and J. Indrek, *Phys. Scr*. **98** (2023) 045613.