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Electron Collision Cross Sections of Mercury

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Abstract

In this paper, we propose a new collision cross section set for mercury which revises the original set summarized by Hayashi in 1989. Hanne reported three excitation collision cross sections (6^3P_0, 6^3P_1, 6^3P_2) determined from an electron beam experiment in 1988. As a matter for regret, no attentive consideration was given to combining these three excitation cross sections with the cross section set of Hayashi. Therefore we propose a new set where these three excitation cross sections are included. In this study, other two excitation cross sections (6^1P_1, 6^3D_3) except for the three excitation collision cross sections (6^3P_0, 6^3P_1, 6^3P_2) are taken from the original set of Hayashi. The momentum transfer cross section and the ionization collision cross section are also taken from Hayashi. A Monte Carlo Simulation (MCS) technique is applied for evaluating our new cross section set. The present results of the electron drift velocity and the ionization coefficient are compared to experimental values. Agreement is secured in relation to the electron drift velocity for $1.5\,\mathrm{Td} < E/N < 7\,\mathrm{Td}$ and to the ionization coefficient for $400\,\mathrm{Td} < E/N < 3000\,\mathrm{Td}$, where E/N ($\mathrm{V \cdot cm^2}$) is the reduced electric field, E (V/cm) is the electric field, N (1/cm^3) is the number density of mercury atoms at 0 ℃, 1 Torr, E/N is also equal to $2.828 \times 10^{-17}\, E/p_0$ from the relation of the ideal gas equation, p_0 (Torr) is gas pressure at 0 ℃, 1 Torr = 1.33322×10^{-2} N/cm^2 and 10^{-17} V/cm^2 is called 1 Td. Thus it is ensured that our new cross section set is reasonable enough to be used up to 100 eV when considering with the electron drift velocity and the ionization coefficient.

Keywords:

mercury, electron collision cross section, excitation collision cross section, Monte Carlo simulation

1. Introduction

Mercury is the only metal kept in a state of liquid at ordinary temperatures, and has widely been utilized in electrical equipment such as light sources, switches, vacuum pumps, thermometers, etc. Mercury, cadmium, arsenic, and lead are regarded as environmental pollutants recently, and mercury is, above all, said to be the gravest pollutant. For this reason, its use is prohibited in industry. Despite the above, mercury, with which none of adequate substitutes for a strong emission source of ultraviolet ray can hardly be found, is still a prominent source of fluorescent light since no adequate substitute for a strong emission source of ultraviolet ray can be found.

The new collision cross section set is based on the set summarized by Hayashi [1], except with three excitation collision cross sections (6^3P_0, 6^3P_1, 6^3P_2) based on the experimental data of Hanne [2]. Remarkable difference is noticed in a portion of the built-up 6^3P_1 cross section. Evaluation of the proposed collision cross section set is made by means of the MCS. Concurrently with this, comparison is made with the experimental values of the electron drift velocity and ionization coefficient by others [3-9].

A rapid rise is noticed in the momentum transfer cross section of the mercury in the range from 0.05 eV to 0.2 eV. Then a monotonoic decrease is made after the cross section reaches a peak value of 2×10^{-14} cm^2 [1-3, 7-9]. The momentum transfer cross section is completely different in its shape with respect to Ramsauer gases such as Ar, Kr and Xe. However in this study detailed results brought about from the problems of the cross section are not considered as a matter of course, because the high region of electron energy is to be exclusively dealt with in this paper.

The electron collision cross section set of mercury has been reported by Rockwood [10], Nakamura [4], Liu [11], Hayashi [1], Sakai [12] and England [9]. In this paper, the validity of the proposed electron cross section set is shown by comparing the present MCS calculation with the experimental swarm data.

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2. Calculation method

The MCS [13] is carried out in a uniform electric field where the gap length is 1cm. An electron is released from a center point of the cathode at zero velocity, and 1.0×10^4 electrons are calculated on their trajectory until they reach the anode. Positions and velocities of electron are calculated by Newtonian mechanics at every short duration Δt. The collision time is also calculated by comparing the total collision cross section given by the electron energy of the in-flight electron and a random number at every Δt. The kind of collision is determined by the method of Itoh and Musha [14]. After the collision, the electrons restart with an initial energy that is equal to the electron energy possessed just before the collision minus the energy lost by the electron in the collision. The energy loss of the electrons in collisions with gas molecules is given below.

(a) Momentum transfer collision ; $\varepsilon_{eloss} = \frac{2m}{M}(1-\cos\omega)\varepsilon$ eV.
where m and M : masses of electron and mercury, respectively, ω : scattering angle of electron to the direction of electric field, ε : electron energy possessed just before the collision.

(b) Excitation collision : ε_{exloss} = 4.67 eV (6^3P_0), 4.89 eV (6^3P_1), 5.64 eV (6^3P_2), 6.70 eV (6^1P_1) and 8.86 eV (6^3D_3).
These values are a constant loss for each excitation threshold.

(c) Ionization collision : ε_{iloss} = 10.43 eV.
The value indicates the threshold of ionization.

The data of electron behavior are obtained by the steady state Townsend (SST) sampling in 200 segments of slit section Δx between the cathode and the anode.

The momentum transfer and ionization collision cross sections of Hayashi [1] are adopted in this study, because of the existence of the data covering a wide region ranging from 0.1 eV to 1000 eV. The newest ones adopted about from Hanne [2] are employed as the three excitation cross sections. However to interpolate a lack of data for $\varepsilon > 6$ eV for with these cross sections, extrapolation is made to attain a higher energy level to the extent of 1000 eV. As the method of extrapolation, to be suitable for the experimental values of the electron drift velocity and the ionization coefficient [3-9], the correction of these cross sections is repeated up to about 100 eV that is the maximum value of electron energy distribution in the calculation of MCS to obtain the ionization coefficient at E/N = 3000 Td. These cross sections for $\varepsilon > 100$ eV are estimated smoothly. The two excitation cross sections 6^1P_1 and 6^3D_3 are employed from the original data of Hayashi [1]. The set of cross sections adopted in this study is illustrated in

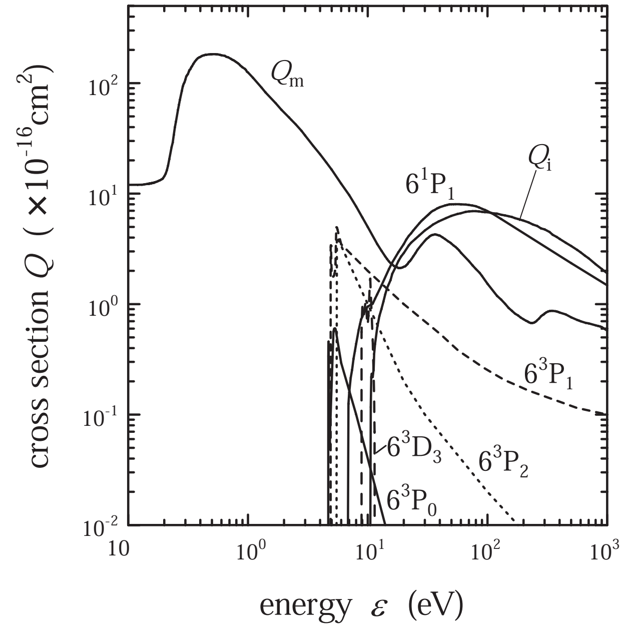

Fig. 1 Electron collision cross section of mercury. (to distinguish the cross sections, the line kind is indicated as for 6^3P_1 (broken line), 6^3P_2 (dotted line) and 6^3D_3 (long broken line).)

Fig. 1.

Fig. 2 is the comparison between the excitation cross sections of 6^3P_0, 6^3P_1 and 6^3P_2 of Hayashi (solid line) and Hanne (broken line). The momentum transfer cross section Q_m is plotted in the same figure. By comparing the two sets of cross sections, it is clear that the threshold regions of the 6^3P_0 cross section curve agree well with each other. However above the peak in the curve, the curve of Hanne reaches a much deeper minimum at approximately 4.8 eV than that of Hayashi. The 6^3P_1

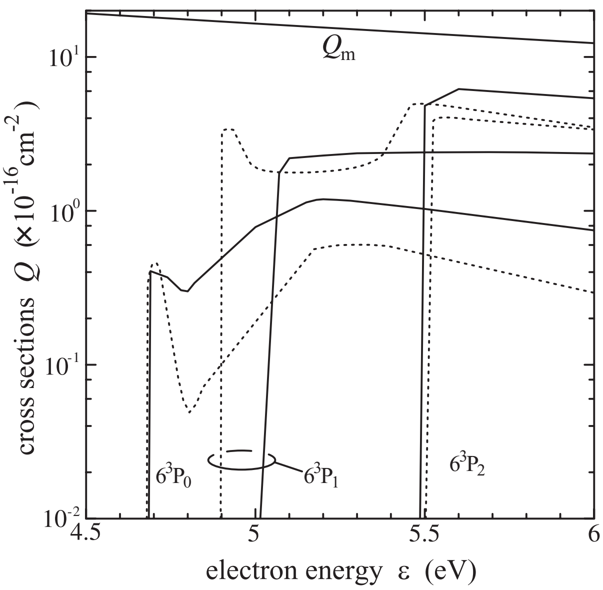

Fig. 2 Excitation collision cross sections (solid line : Hayashi, broken line : Hanne).

cross section curve of Hanne begins to rise upward and almost vertically, starting from 4.9 eV. After reaching the peak, the curve again makes a rise in a direction of the second peak, starting from 5.4 eV. Thus the maximum value is obtained as 5.5 eV. On the other hand, the 6^3P_1 cross section curve of Hayashi makes slower increase than the other curves. After that, the curve approaches a nearly constant value. The 6^3P_2 excitation cross section curves of Hanne are smaller than that of Hayashi in all regions.

3. Results and discussion

3.1 Comparison of excitation collision cross section of mercury

Spatial distributions of excitation are calculated by MCS using each excitation collision cross section of Hayashi and Hanne. Figure 3 shows an example with $E/p_0 = 10\,\text{V/cm} \cdot \text{Torr}$, $p_0 = 1$ Torr. In this figure, the position of the excitation collision occurring in the three- dimensional space is projected perpendicularly onto the two-dimensional plane included in the axis connecting the centers of the cathode and anode. The excitation collision starts on a position at a distance of 0.467 cm from the cathode corresponding to the threshold 4.67 eV of 6^3P_0 and existence of a peak is noticed at 0.5 cm to be continued up to approximately 0.6 cm. Building-up of the second group of excitation collisions occurs beyond the position of 0.9 cm. The first peak is attributed to the peak for 6^3P_0, whereas the highest peak at 0.5 cm complies with the peak for 6^3P_1. The

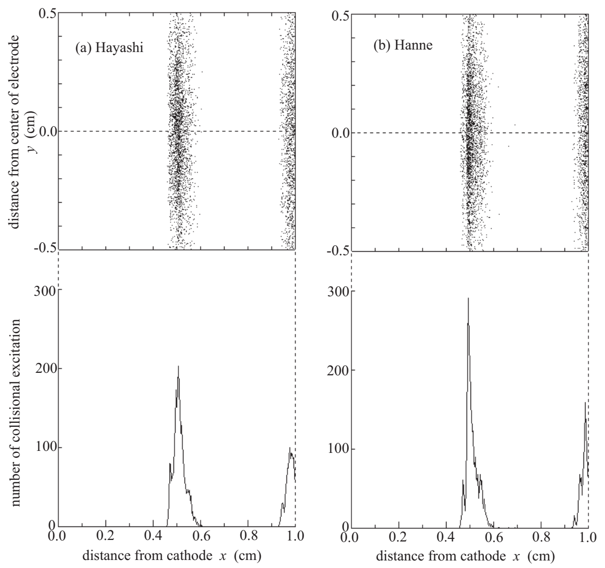

Fig. 3 Spatial distributions of excitation obtained by using cross sections shown in Fig. 2 ($E/p_0 = 10\,\text{V/cm} \cdot \text{Torr}$, $p_0 = 1$ Torr).

Table 1 Occurrence number of the excitation.

Authors		Hanne	Hayashi
Number of Excitation	6^3P_0	950	2185
	6^3P_1	3305	2002
	6^3P_2	121	189
	total	4377	4376

difference between the two cross sections appears distinctly in the spatial distribution. The peak of Hanne is 1.5 times higher than that of Hayashi.

The total number of excitations using the cross sections of Hanne is 4377, whereas that using the data of Hayashi is almost of the same value, 4376. However the numbers of excitations with the Hanne data are of the value of 950, 3305 and 121 for the 6^3P_0, 6^3P_1 and 6^3P_2 excitations, respectively, whereas those from the Hayashi data are 2185, 2002 and 189. These numbers are listed in Table 1. No generation of other excitation or ionization can be seen under such conditions. The energy loss caused by these three excitations is 1.04 times greater using the data of Hanne than that using the data of Hayashi.

3.2 Electron drift velocity

Figure 4 shows the comparison between the present calculated values of electron drift velocity and the experimental values reported by other researchers [3-5]. Although, the present value differs vastly from most of the experimental values obtained for $E/N < 1.5$ Td, it is necessary to consider the influence of thermal motion of the electrons due to energy transfer from mer-

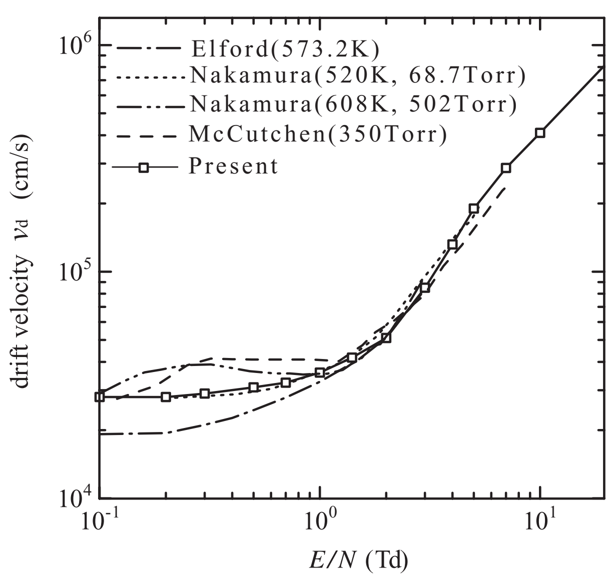

Fig. 4 Comparison between present result and experimental values of the drift velocity reported by other researchers.

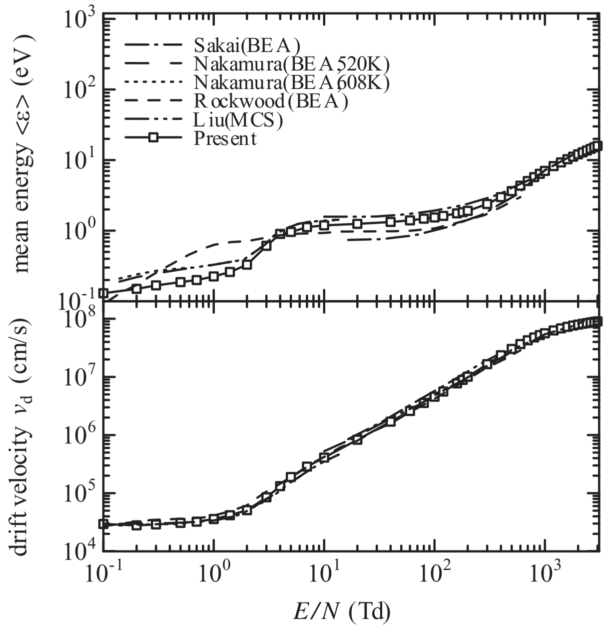

Fig. 5 Comparison between present results and other calculation values of mean energy and drift velocity.

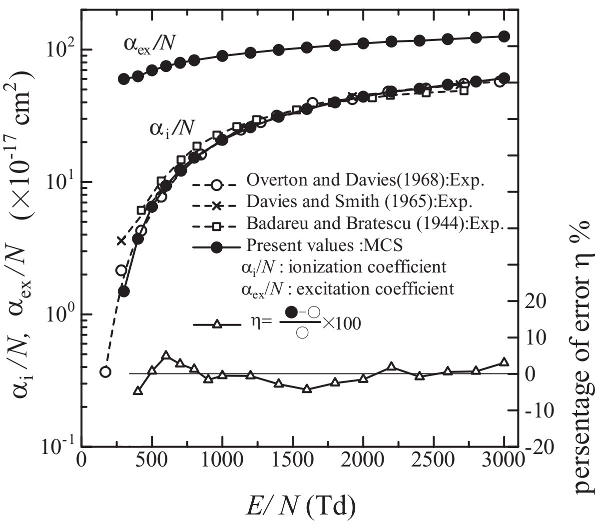

Fig. 6 Obtained ionization and excitation coefficients.

cury atoms. Furthermore Nakamura *et al.* [15] made mention of the existence of the pressure dependence in the drift velocity of the mercury. Thus increase was noticed with the value of the density ratio of the mercury molecules to the mercury atoms with respect to the gas temperature [4], that is, they described the gas pressure varies depending on the gas temperature. In the present calculation, no consideration is taken for this thermal motion in the collision process. Meanwhile in $E/N \geqq 1.5$ Td, the calculations are closely consistent with the values obtained from the experiments.

Figure 5 shows the comparison between the present results and other calculations of the electron mean energy and drift velocity [10 – 12,15]. Although the mean energy of the present results is lower than the values previously obtained in the region $E/N < 3$ Td, it is almost identical with the other calculations for $E/N \geqq 3$ Td. This difference originates from the cross sections used. However, the drift velocity is in agreement with the other results for 0.1 Td < E/N < 2000 Td.

3.3 Ionization coefficient

Figure 6 shows the ionization coefficient α_i/N in the reduced electric field ranging from 200 Td to 3000 Td calculated by MCS for comparison with experimental results. The present data are consistent with those of Overton *et al.* [6] covering a wide region, with differences less than ±5 % for $E/N > 400$ Td. However a distinct difference arises for $E/N < 400$ Td, where the values of Overton are approximately 1.4 times higher than the present values. Sakai *et al.* [12] obtained results similar to those of the present study, and it is interpreted that the discrepancy is due to Penning ionization by metastable atoms of mercury in the experiment. This is a significant effect at such low E/N. Penning ionization is not included in our MCS.

Furthermore, the calculated excitation coefficient α_{ex}/N is shown for reference in Fig. 6.

4. Conclusion

A new electron collision cross section set for mercury was based on the cross section sets of Hayashi and Hanne is investigated. The evaluation of the new collision cross section set is made by MCS, and comparison of the electron drift velocity with the ionization coefficient is also made. The results are in agreement with the previously reported experimental results within a few percent. Thus it is ensured that the new cross section set is reasonable enough to be used with the energies up to 100 eV, when considering the electron drift velocity and the ionization coefficient.

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