Vibrational excitation of a carbon dioxide molecule by electron and positron impacts

M. Takekawa[1]
Institute of Physics, University of Tokyo, 3-8-1 Komaba, Meguro, Tokyo 153-8902, Japan
Atomic Physics Laboratory, RIKEN, 2-1 Hirosawa, Wako, Saitama 351-0198, Japan

An electron (e^-) or a positron (e^+) collision process with a molecule gives us fundamental information of scattering dynamics, relevant to condensed matter physics, radiation physics and so forth. From the point of view of elementary physics, e^-–molecule and e^+–molecule collisions are worth studying not only independently but comparatively as well. In e^- (e^+) scattering from a molecule, one of the important inelastic processes is vibrational excitation, which is the dominant energy loss process of an incident particle below 10 eV. Carbon dioxide (CO_2) is an interesting molecule as a target of the e^- (e^+) collision, since it is one of the simplest polyatomic molecules with the symmetry of $D_{\infty h}$ and the problem of e^-–CO_2 collisions is important for various applications, e.g., planetary atmospheres, plasma chemistry, etc. In the present talk, vibrational excitation of the CO_2 molecule in collision with e^- and e^+ is studied theoretically. The range of incident energy is $2 \leq E \leq 10$ eV for e^- and $2 \leq E \leq 6$ eV for e^+ (it should be noticed that the threshold of positronium formation is 6.7 eV). Each fundamental mode of vibration is treated separately. Main part of this talk and related topics have already been given in [1–3].

CO_2 has three fundamental modes of vibration. The ground state of CO_2 for vibration is denoted as (000) and the lowest excited state of each mode is described as (100) for symmetric stretching, (010) for bending and (001) for antisymmetric stretching. In the present calculation, scattering dynamics is treated by the vibrational close coupling method for each excitation from the ground state to the lowest excited state within the fixed nuclear orientation approximation. In the interaction potential for the e^-–CO_2 collision system, the static and correlation-polarization terms are attractive and an attractive electron-exchange term, which plays an important role in low energy e^- scattering, is also added. On the other hand, the interaction for e^+ impact consists of repulsive static and attractive correlation-polarization potentials and includes no electron-exchange term. As a result, the three attractive interactions are summed up for e^- impact and the repulsive static interaction and the attractive correlation-polarization interaction cancel out each other to a large extent for e^+ impact.

Figure 1 shows the integral cross sections for the excitation of (000) $\rightarrow$ (100) by e^- impact and e^+ impact. The present e^+ impact cross section is compared with the theoretical result obtained by Gianturco and Mukherjee [4] (they treated symmetric stretching mode of vibration only). Although the present e^+ impact cross section is somewhat smaller than that of Gianturco and Mukherjee, the energy dependence of the two data sets are qualitatively similar. The quantitative disagreement between these cross sections is considered to be due to the difference in the accuracy of the molecular wave function used to obtain the interaction potential. It is also noticed that the number of excited states of vibration included for close coupling calculation is 1 in the present calculation and 4

[1]e-mail: mtake@postman.riken.go.jp

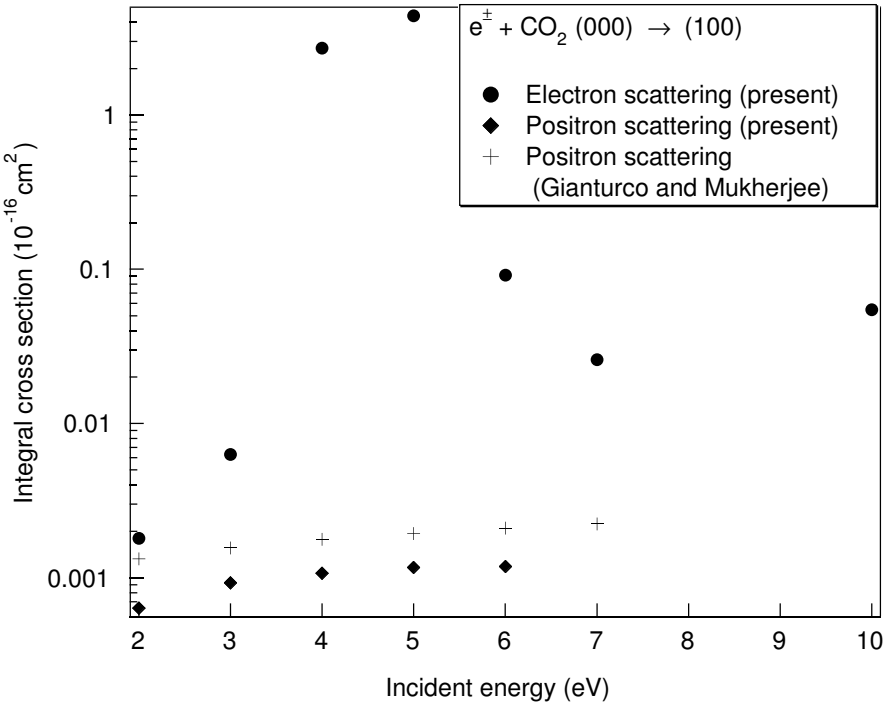

Figure 1. Integral cross sections in units of 10^{-16}cm^2 for (000) $\rightarrow$ (100) excitation of CO_2 by e^- impact and e^+ impact. The present result of e^+ impact is compared with the theoretical result obtained by Gianturco and Mukherjee [4].

in that of Ref. [4]. In the present data of e^- collision, the strong Π_u resonance peak is seen at around 5 eV and no such structure exists in the e^+ collision cross section. The difference of the interactions between the collisions by e^- and e^+ described above results in the different energy dependence of the cross sections.

References

[1] M. Takekawa and Y. Itikawa, *Journal of Physics B*, **31**, 3245 (1998).

[2] M. Takekawa and Y. Itikawa, *ibid*, **32**, 4209 (1999).

[3] M. Kimura, M. Takekawa, Y. Itikawa, H. Takaki and O. Sueoka, *Physical Review Letters*, **80**, 3936 (1998).

[4] F.A. Gianturco and T. Mukherjee, *Journal of Physics B*, **30**, 3567 (1997).