

## 4 - 12 Dissociative Excitation and Vibrational Excitation of $\text{Cl}_2^+$

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Molecular chlorine has attracted a lot of attention in plasma processing<sup>[1]</sup> or in excimer laser<sup>[2]</sup>. It is also of atmospheric and environment interest<sup>[3]</sup>. In these media, electron collisions with chlorine molecules and molecular ions play a central role<sup>[4]</sup>. In our previous work<sup>[5]</sup>, we had firstly studied the direct dissociative recombination (DR) of  $\text{Cl}_2^+$  by theoretical, which is the process where an electron is captured by the molecular ion to form a doubly excited neutral state that dissociates to products. In addition, there are other competing processes occur along with DR. After the formation of chlorine molecule, the incoming electron can also autoionize, returning the target ion to its initial electronic state, either in a state of vibrational excitation (VE), or with enough vibrational energy that the ion dissociates (dissociative recombination-DE). The theoretical studies of the above reactions are valuable in producing accurate models for chlorine plasma processes.

With the potential energy curves and autoionization widths that had been computed by combining electron scattering calculations and ab initio structure calculations in our previous study of DR<sup>[5]</sup>, the reaction dynamics of DE and VE for collisions between electrons and chlorine molecular ions on the four lowest resonant states of all symmetries of chlorine molecule, in the range of 0~10 eV energies, is also investigated by using a local-time-independent approach, where the driven Schrödinger equation is numerically solved. Here, the results of DE and VE of  $\text{Cl}_2^+$  excited from initial vibrational state  $\nu=0$  are separately shown in Figs. 1 and 2. The total VE distribution contributes from the final vibrational state  $\nu=1$  up to  $\nu=19$ , and the cross section contributions of the higher final states shift to higher collision energy, the other follow-up work will be finished soon.

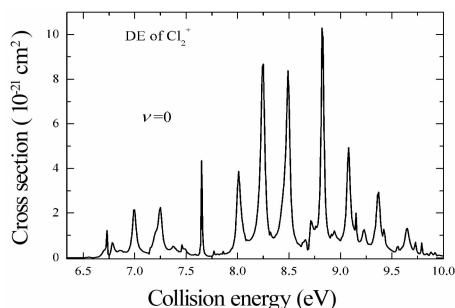


Fig. 1 The dissociative excitation cross section of  $\text{Cl}_2^+$  for  $\nu=0$  initial vibrational state of the target ion.

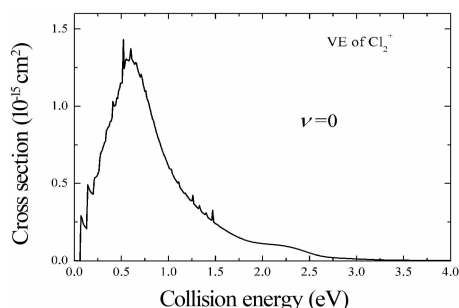


Fig. 2 The vibrational excitation cross section of  $\text{Cl}_2^+$  for the  $\nu=0$  initial vibrational state of the target ion.

Compared with the cross section of the direct DR, is about  $7.2 \times 10^{-15} \text{ cm}^2$  at an energy of 0.01 eV for initial state  $\nu=0$ , the VE cross section for  $\nu=0$  (about  $1.4 \times 10^{-15} \text{ cm}^2$  near the energy of 0.6 eV) is more competitive at low collision energies (smaller than 3.5 eV), while the DE cross section for  $\nu=0$  is more important in the higher energy range larger than 6.5 eV, and it is almost 5 orders of magnitude smaller than DR and VE cross section. Same with DR, the  $^1\Pi_g$  and  $^3\Sigma_g$  resonant states contribute more to the total DE and VE cross section. This means that there is at least one of electronic states of these above resonant states crosses the ionic state close to its vibrational state  $\nu=0$ . Moreover, we believe that the most of sharp peaks in cross sections of DE and VE (Figs. 1 and 2) can be explained with shape resonances formed in the electron-ion scattering, and the other may be created as wave packet is tunneling through a barrier in the potential surface.

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