Study of various cross sections of fluorocarbons for plasma modeling applications

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Electron interaction with molecules play a fundamental role in understanding and modelling of atmospheric and industrial plasma. The study of electron impact scattering cross section for fluorocarbons have gained much importance over the years due to its various applications in low temperature plasma and in plasma-assisted fabrication of electronic microcircuits [1]. The interest in the scattering properties of fluorocarbon molecules is due to their application in semiconductor industry as etching agent, and as gaseous dielectric in electrical industry [2]. The electron-impact dissociation of the stable parent molecules such as CF_4,C_2F_6, C_3F_6, C_3F_8,C_4F_6, C_4F_8 and C_5F_8 in the plasma leads to the formation of reactive radicals, CxFy, which are important for the chemical reactions in fluorocarbon-containing plasmas [3]. In general we notice there are actually very less or no studies of electron scattering cross sections of many fluorocarbon molecules/radicals important for plasma applications. Hence, the present study is concerned with the calculation of various cross section of fluorocarbons from the past two and half years and ongoing.

In the pursuit of investigating fluorocarbons, we have produced many useful data for these systems. We have calculated the comprehensive sets of total ionization cross sections for C_2F_x(x=1-6), C_3F_x (x=1-8) [4] and C_4F_x(x=1-8) [5] fluorocarbons species. The elastic, excitation, differential, total and momentum transfer cross sections are calculated for C_2F_2[6], C_3F_4 [7] and C_4F_6 isomers [8] at low energies. We have compared our data with experimental and theoretical results and in general, a good agreement is obtained. Further investigations are in progress for electron collision cross sections of c-C_3F_4,c-C_3F_6, c-C_4F_8 and c-C_5F_8. The binary encounter-Bethe (BEB) [9] method is used to calculate and study the ionization cross section for all the targets and the calculation of orbital parameters (input for BEB model) are carried out using the Gaussian 09 [10] program with different levels of theory. The R-matrix method [11] is used to study and calculate various cross section for fluorocarbons at low energies. In the conference, all the cross section results obtained until date for these fluorocarbons species along with its implications for plasma modelling will be discussed.

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