Cross Sections and Transport Properties of Negative Ions in Rare Gases

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Negative ions determine kinetics of electronegative plasmas [1] and their presence may change critically the nature of plasmas (examples of obvious changes can be seen in [2]). Ion-Ion plasmas [3] have very distinct characteristics. Numerous applications relay on electronegative reactive gases including plasma etching [4], atmospheric plasmas for biomedical application [5], and many more. Furthermore, negative ions may be used directly, for example to reduce the charging [6] of high aspect ratio structures or to be converted to fast neutrals with the aim to achieve fast neutral etching [7]. Modeling of such processes requires either cross sections or transport data or both.

The purpose of this work is to provide plasma modelers with cross section data and transport coefficients that may be used in simulations of plasmas containing negative ions. It is important to represent properly the effect of detachment on the transport coefficients, as detachment is a nonconservative process.

We have determined a set of cross sections for negative halogen ions in rare gases based on the available experimental transport data [8,9] in a wide range of reduced electric field E/N of 1 Td - 1000 Td by employing a standard swarm technique. The resulting momentum transfer cross section is supplemented by detachment cross section [10,11] that was



Figure 1. Cross sections for F⁻ in Xe.

used from the threshold around 6 eV up to 100 eV. As an example of obtained cross sections, in fig. 1 we show the derived momentum transfer cross section for F^- in Xe.

The procedure used here to determine the cross sections is to apply first the MTT which is fast albeit with limited accuracy to fit the cross sections until the transport data fit the experimental results. In the next step further, but always slight adjustments are made to have a good agreement between experimental data and MC calculations which provide exact results. Normally, the disagreement between MTT and MC (and thereby experimental) results was within 11% for all gases.

The cross sections provided here should be employed with the assumption of isotropic scattering and are very accurate in the region covered by the experiments. We have extrapolated data to somewhat higher energies based on behavior of similar ions in similar gases and by the addition of reactive processes so a relatively complete set was derived which can be used in modeling of plasmas by both hybrid, PIC (particle in cell) and fluid codes [1,12]. It is important to note that so far the data presented here and other similar results were interpreted by using interaction potentials [13] which while producing results of high accuracy is not directly applicable in plasma modeling. As both hybrid and PIC models involve MC simulations for collisions and as applications to plasma etching devices requires control of negative ions in the afterglow or for neutralization [7,14] the data for cross sections of negative ions found in argon-fluorocarbon mixtures are of great importance.

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