LXCAT: A WEB-BASED, COMMUNITY-WIDE PROJECT ON DATA NEEDED IN MODELING LOW TEMPERATURE PLASMAS

LC Pitchford, on behalf of the LXCat team¹

LAPLACE (Laboratoire Plasma et Conversion d'Energie); CNRS and Université de Toulouse; Toulouse, France

LXCat (for ELECtron SCATtering) is an open-access website for exchanging data related to ion and electron transport and scattering cross sections in cold, neutral gases. Such data are essential for the modeling of low temperature plasmas. At present, 22 databases contributed by groups around the world can be accessed on *LXCat*. On-line tools enable importing and exporting data, plotting and comparing different sets of data, and for downloading data.

In this presentation I will focus on the status of the data available for electrons on *LXCat*. For the most part, these data are in the form of "complete" sets of cross sections, compiled or calculated by different contributors and covering a range of energies from thermal up to about 1 keV. "Complete" in this context means that the cross section data are detailed enough to yield an accurate steady-state energy distribution for electrons subjected to the combined influences of a uniform electric field and collisions with a uniform background gas. Thus, these data can be used directly in a Boltzmann equation solver to calculate electron transport and rate coefficients as a function of electron temperature (for Maxwellian distributions) or as a function of E/N or average electron energy (for nonMaxwellian distributions). The on-line Boltzmann solver, BOLSIG+, allows easy conversion of cross section data to transport and rate coefficients useful for fluid modeling of low temperature plasmas in pure gases or in gas mixtures if a complete set of cross sections are also available for each component in the mixture. Partial sets of cross sections are also available on *LXCat*.

Validation is a key issue. To this end, the LXCat team has been making systematic intercomparisons of cross section data and comparisons of calculated and measured swarm parameters – first for the noble gases as was reported in a series of poster presentations at the Gaseous Electronics Conference in 2011, then for common molecular gases (H₂, N₂ and O₂) as reported at the GEC in 2012, and work is now in progress on the validation of data for more complex molecules (H₂O, CO₂, CO, CH₄ and CF₄). Databases of measured swarm parameters (electron mobilities, diffusion coefficients, ionization and attachment rates,...) are also available on LXCat.

Anyone willing to contribute to this project is very welcome to take part.

¹ As of February 2013, contributors to public databases on *LXCat* are : J de Urquijo, AA Castrejón-Pita, JL Hernández-Ávila, E Basurto (Mexico); LL Alves and CM Ferreira (Portugal); I Bray (Australia); K Bartschat, WL Morgan, AV Phelps, L Viehland and O Zatsarinny (USA); S Biagi and Quantemol (J. Tennyson and D Brown) (UK); JP Boeuf, MC Bordage, S Chowdhury, GJM Hagelaar, S Pancheshnyi, LC Pitchford, V Puech (France); I. Kochetov, A. Napartovich (Russia); Y Itikawa (Japan); and A. Stauffer (Canada). S Pancheshnyi conceived of and designed the database structure and website, and B Chaudhury has contributed valuable technical assistance.

References

[1] S Pancheshnyi, S Biagi, MC Bordage, GJM. Hagelaar, WL Morgan, AV Phelps, and LC Pitchford, "The *LXCat* project : Electron scattering cross sections and swarm parameters for low temperature plasma modeling", Chem. Phys, 398, 148 (2012).