The LXCat project: electron scattering cross sections and swarm parameters for low temperature plasma modeling

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LXCat is a dynamic, open-access, website for collecting, displaying, and downloading **ELEC**tron **SCAT**tering cross sections and swarm parameters required for modeling low temperature, non-equilibrium plasmas. Contributors set up individual databases, and the available databases include electron-neutral scattering cross sections or swarm parameters. On-line tools include options for browsing, plotting, and downloading data. The electron energy distribution functions in low temperature plasmas are in general non-Maxwellian, and LXCat provides an option for execution of an on-line Boltzmann equation solver to calculate the edf in homogeneous electric fields. LXCat is part of a larger, community-wide effort aimed at collecting, evaluating, and sharing data relevant to modeling low temperature plasmas.

1. Introduction

The modeling of low temperature, non-equilibrium plasmas (LTPs) is centered on the description of electron transport since the energy gained by electrons in the sustaining electromagnetic fields is deposited in these plasmas mainly through electron-neutral collisions. The transport of electrons (and ions) and the coupling of the charged particle transport to electromagnetic fields can be described using different levels of models ranging from macroscopic "fluid models" [1], to "hybrid models" [2], or to detailed kinetic models such as "particle in cell/Monte Carlo collision" (PIC-MCC) simulations [3]. Data needs for modeling depend on the level of description, but in all cases the needs are extensive. For PIC-MCC simulations, electron-neutral scattering cross sections are required input; the information required for fluid models includes electron transport and rate coefficients; and hybrid models use a combination of both kinds of data. Electron transport and rate coefficients are either measured or are calculated by averaging over the electron energy distribution function (edf), which is generally non-Maxwellian and is itself determined by solving the Boltzmann equation using cross section data as input.

There is a growing awareness in the LTP community that some means of collecting, evaluating and sharing data relevant to modeling cold plasmas is necessary [4]. Most modeling groups have their own collections of data and while people are generally willing to share, there has been no convenient way to exchange data except on an informal basis. Often the data concerning the electrons are in the form of compilations of electron-neutral scattering cross sections (up to nominally 1 keV) or tables of swarm parameters (transport coefficient — mobility, diffusion coefficient, ... — and reaction rates, etc.) as a function of E/N, the reduced electric field, the ratio of the electric field strength to the neutral density.

LXCat (pronounced "elec scat" for ELECtron SCATtering) is a dynamic, open-access, website for collecting, displaying, and downloading the electron-neutral scattering cross sections and swarm parameters required for modeling low temperature plasmas. This website is intended to provide storage and access to data related to the electron component of low temperature plasmas as well as on-line tools to facilitate intercomparisons. Anyone willing to contribute data can request an account and instructions for setting up a database on LXCat. The contents and maintenance of the individual databases are the responsibility of the contributors. The LXCat site offers automatic daily back-up and usage statistics, and

archived data is available upon request.

For the users, the LXCat website provides options for browsing through databases, plotting, and downloading selected items from the databases. Also available on the LXCat site is an option for the on-line calculation of electron swarm parameters – electron transport and rate coefficients — in pure gases or in gas mixtures where cross section data for the component species are available in the LXCat databases. The swarm parameter calculation is based on BOLSIG+, an electron Boltzmann equation solver in the two-term approximation [5] and available as freeware [6]. A Monte Carlo simulation tool for LXCat is under development. A small, but growing, database of measured swarm parameters is expected to provide valuable points for comparison.

To be appropriate for use in Boltzmann or Monte Carlo calculations of the edf, the cross section data for a given target species must be complete. "Complete" in this context means that the cross section set be 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 density of neutral, ground-state target species. Accurate is difficult to quantify, but we generally demand that the cross section set, when used in a Boltzmann solver, yield swarm parameters to within 10% in pure gases. The accuracy test is normally conducted by comparison with experiment where available or by sensitivity tests when experiment is not available. In contrast, an incomplete or partial set of cross sections includes information about only one or a subset of the important scattering processes for a given species. Obviously, in different contexts, there could be other criteria for defining a "complete" set of cross sections.

2. Description of the website

LXCat is structured into individual databases, provided by different contributors, and on-line tools for manipulating the data, as illustrated on Figure 1. At this writing, LXCat contains 12 individual cross section databases.

At present, complete or partial sets of electron-neutral scattering cross sections are available in at least one of the databases on LXCat for the

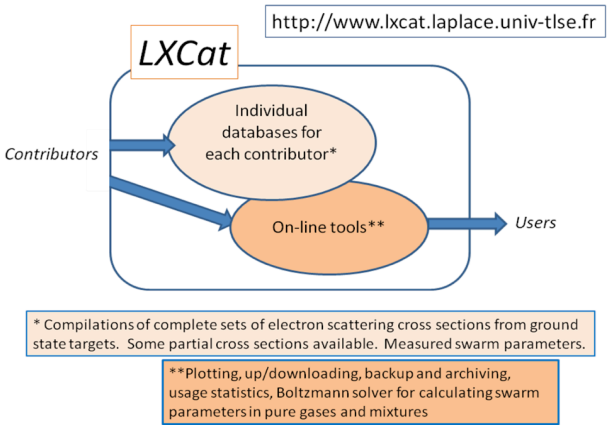

Fig. 1: LXCat project concept.

following 42 target species in their ground state: Ar, C, C_2H_2, C_2H_4, C_2H_6, C_3H_8, CCl_2F_2, CCl_4, CF_4, CH, CH_2, CH_3, CH_4, CHF_3, CO, CO_2, Cl_2, F_2, H, H_2, H_2O, HCl, He, Hg, Kr, Mg, N, N_2, N_2O, NH_3, NO, Na, Ne, O, O_2, O_3, SF_6, SO_2, $Si(CH_3)_4$ or TMS, Si_2H_6, SiH_4, and Xe. Some cross sections are available for electron collisions with atoms and molecules in excited states.

Information for obtaining an account can be found on the LXCat site, and instructions for entering data in the databases are provided with the account information. The contents and maintenance of the invidivual databases are the responsibilities of the contributors. The LXCat website is presently set up to accept electron-neutral scattering cross sections (partial or complete sets) in tabular form and swarm parameters as functions of E/N.

Three levels of comments are included in the LXCat cross section databases (a) comments the database as a whole, (b) comments for each target species and (c) comments for each individual process. The contributors (optionally) provide these comments. For the database as a whole, comments nominally include the names of the contributors with contact information, how the data should be used (two-term Boltzmann, Monte Carlo, etc), and the suggested way to reference the data. For the individual target species, the comments contain, for example, references to publications or websites where the compilations have appeared. Finally, for each scattering process, the comments identify the states involved with references to original data sources as available. All three levels of comments appear in the text of downloaded

data files because keeping proper references with the data is obviously very important. LXCat automatically introduces additional comments. The most recent change date for each cross section is automatically updated if contributors change/delete/upgrade the data. Databases are flagged with the status maintenance if anyone is logged on to the database account or if the data have been changed in the past hour. Note that contributors can manually set the status flag to maintenance or to private. The latter flag is intended to be used while a database is under construction or if the owner wants to take it offline for any reason. The entire website is backed up on a daily basis, and archived versions are available by request.

3. How to use LXCat

Upon first entering LXCat, users can select from a variety of options in the top horizontal tool bar. The options include how to use, databases for browsing through the databases with lists of species and first two levels of comments, cross sections for on-line plotting or downloading of selected data, swarm parameters to access experimental data or to effect an on-line Boltzmann calculation, and notes for more detail on certain related subjects. A Google group has been set up to encourage discussion among users.

Selecting the option cross sections and then plot, for example, brings up the list of databases on the left. When the user selects one or more (or all) databases and clicks on update list, the list of species for which data are available in the selected databases appears on the right. By selecting one or more species (and subsequently clicking on update list), the user is shown all the individual scattering processes for the selected databases/species combinations, and plots can be generated for selected subsets of the data in the lists. The plotting and downloading tools are useful for making comparisons (and have helped us identify mechanical errors that have crept into the various data compilations over the years). Cross section data can be selected and downloaded in a simple tabular format with a file header containing all descriptive comments and reference information provided by the contributors as described above. Users are requested to reference the database and the original references, where provided, in all publications making use of these data.

An especially useful feature in LXCat is the on-line version of BOLSIG+ [5] which solves for the electron energy distribution function in the classical two-term approximation whereby the angular dependence of the edf in velocity space is assumed to be well-described by the sum of an isotropic and a cosine (with respect to the direction of the electron acceleration in the electric field direction) component. Swarm parameters and other useful quantities are calculated in BOLSIG+ by averaging different quantities over the edf. A good comparison of calculated and measured swarm parameters provides validation that the input cross section set is complete.

Selecting the option swarm parameters offers the possibility of browsing through the experimental database or calculating swarm parameters using BOLSIG+. Selecting calculate brings up again the list of databases on the left and species on the right, and selecting one or more species from the list calls up a dialog window for the on-line execution of BOLSIG+. The user then selects the range of values of E/N for the calculation and the components of the gas mixture and their relative concentration. The calculation is rapid and results appear in graphical format, and these swarm parameters can be downloaded in a convenient table form, with a text header giving the data used in the calculation. BOLSIG+ can optionally be used to rate coefficients in an equilibrium (Maxwellian) plasmas.

Plasma modelers are confronted with the question of equivalence between swarm parameters and the coefficients needed for fluid models which seek to describe physical situations where there are density gradients, electric field gradients, physical boundaries, and other complications. Further questions arise concerning the exact definition of swarm parameters in different experimental configurations where electron number changing collisions (eg attachment and ionization) are present. While the latter questions have been discussed at length (see, for example, [7]) and are fairly well understood at this point, questions of equivalence of swarm parameters with coefficients used in fluid models merits further discussion. Concerning swarm parameters in different experimental situations, BOLSIG+ distinguishes between the calculations of swarm parameters in Pulsed Townsend (PT, exponential

growth in time) configurations and Steady-State Townsend (SST, exponential growth in space) configurations. That is, when electron number changing processes (attachment and ionization) are present, BOLSIG+ assumes that only the magnitude, and not the shape, of the edf changes in time or in space, and the Boltzmann equation is rewritten to solve for the normalized distribution function. Where it is not possible to assume simply PT or SST to describe the growth of the electron density, the corresponding Boltzmann equation is difficult to solve directly, and a Monte Carlo approach is usually preferred. The on-line version of BOLSIG+ assumes a Pulsed Townsend configuration; the freeware version of BOLSIG+ offers the option of a Steady-state Townsend configuration. The upcoming Monte Carlo option will have more flexibility.

As an example, the comparison of electron-Ar cross sections made in [8] led to the discovery that a more recent publication of Hayashi's momentum transfer cross section is significantly different than in the source previously used and is much more consistent with other compilations. These comparisons of calculated swarm coefficients for electrons in Ar are an important step in evaluating the utility of the available sets. Future comparisons of Boltzmann calculations with experiments will serve as effective evaluations and recommendations to users. Results from some comparisons with experiment will be reported at the Plasma Data Exchange workshop to be held at the Gaseous Electronics Conferences in the USA in November 2011.

4. Conclusions

The question of the reliability of cross section sets made available by data sites such as LXCat encompasses isssues of accuracy of transcription and presentation, timeliness, consistency, completeness, as well as of accuracy and energy resolution. Additional data - both measured swarm data and cross section data - are being added to LXCat as new contributors are joining the project and as resources are available. The development of new tools is underway and users should check back from time to time for updates.

LXCat is available at http://www.lxcat.laplace.univ-tlse.fr.; a sister website for ion transport data is also on-line: www.icecat.laplace.univ-tlse.fr.

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