Workshop "Collision Data for Plasma Modelling"

Atomic and Molecular Collision Data for Plasma Modelling

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Plasma based technology underpins some of the world's largest industries producing a significant proportion of the world's global commercial products including; computers, cell phones, automobiles, aeroplanes, paper and textiles [1]. Foremost among these is the electronics industry, in which plasma-based processes are indispensable for the manufacture of ultra large-scale integrated microelectronic circuits. According to the Semiconductor Industry Association, worldwide sales of microelectronic components were $247.7 billion in 2006, with plasma etching equipment sales alone generating a market of 3-5 billion dollars per year and plasma CVD more than 5 billion dollars per year. Plasma processing and coating of materials is a key technology in the aerospace, automotive, paper and textile industries employing a work force (directly and indirectly) in excess of 5 million world wide. Since 70-80% of the light on the planet is produced by plasmas, plasma technology also underpins the global lighting industry. With the growing consensus that anthropogenic climate change is now inevitable, plasma technology is set to play a key role in the development of a cleaner and more environmentally conscious world e.g. in toxic waste management, air-pollution detection (and removal) and in the development of fusion as a clean, sustainable energy source. Plasma processing will also play an essential role in the emerging technologies including carbon based electronics, solar cell manufacture and hydrogen storage. The role of plasmas in biomedicine, where they may be used both as a sterilization agent and as a possible surgical tool – with *minimum tissue damage*, is also making rapid progress. Finally, and crucially, plasma technology currently provides the only truly viable methodology for further reductions in the size of structures in integrated circuits (e.g. fabrication of carbon nanotubes) and hence the introduction of nanoelectronics into the market place.

Since plasma processing is such an integral part of the infrastructure of so many industries the growth of technology based economies (vital to the long term global economic growth) will therefore depend upon the development of a strong and innovative plasma research programme. The international plasma research community has recently identified three key 'Grand challenges' to be tackled namely:
(i) The development of atmospheric plasma processing.
(ii) The development of plasmas capable of operating at the micro and nanoscale and
(iii) The adaptation of plasma processing methods that are both more energy efficient and use cleaner technologies (e.g. less atmospheric emissions).

Control of such plasma processing methodologies can only occur by obtaining a thorough understanding of the physical and chemical properties of plasmas. However all plasma processes are currently used in the industry with an incomplete understanding of the coupled chemical and physical properties of the plasma involved. Thus they are mostly 'non predictive' and hence it is not possible to alter the manufacturing process without the risk of considerable product loss. A clear research imperative in the next decade will therefore be to increase our knowledge of the chemical and physical interactions in such plasmas of electrons, ions and radicals with neutral species'. A more comprehensive understanding of such processes will then allow models of such plasmas to be constructed that may be used to design the next generation of plasma reactors, reactors that will:

(i) allow more site specific control of surface reactivity.
(ii) allow smaller feature sizes to be produced (a few tens of nm or less).
(iii) be more efficient in the use of materials in such reactors and
(iv) allow development of new technologies for etching of low k organic materials.

Item (iii) is particularly important since most of the current gases used in the plasma reactors are known *greenhouse gases.* This, in turn, has led to the Kyoto Protocol, one of first global agreements to directly influence industrial production processing, which aims to phase out the use of such feed-gases and seek their replacement with cleaner alternatives. It is also necessary to investigate whether, and how, such gases may be inadvertently synthesized by a plasma process starting from innocuous feedstock gases.

Developing such models and gaining a detailed understanding of the physical and chemical mechanisms within plasma systems is intricately linked to our knowledge of the key interactions within the plasma and thus the status of the database for characterizing electron, ion, photon interactions with those atomic and molecular species within the plasma and knowledge of the reaction rates of such species, both in the gaseous phase and on surfaces of the plasma reactor.

Databases listing atomic and molecular data have been assembled for over 40 years, initially purely in print form and often as lengthy reviews - indeed there are journals that have specialised in such data compilations (for example The Journal of Chemical Physics Reference Data). Some of these databases have acquired international status being widely accessed and by the international community, for example the AMBDAS and ALADDIN databases compiled by the Atomic and Molecular Data Unit as part of the Nuclear Data Section of the International Atomic Energy Agency, Vienna, Austria. There is even a conference series dedicated to the discussion of atomic and molecular databases and their organization - the ICAMDATA (International Conference on Atomic and Molecular DATA) conference series.

Any database must fulfill several basic pre-requisites.
1. It should be comprehensive with a full listing of experimental and, where applicable, theoretical results. Often it is assumed that the most recent results are the most accurate – this is often not the case since often both experimentalists and theoreticians publish ‘calibration data’ when designing new apparatus/codes. This data is used to illustrate the general operational performance of their system prior to conducting research on new systems. Such ‘calibration data’ is seldom of the same rigorous quality as the original data against which it is compared while subsequent data (often on previously unstudied systems) is performed with greater rigour. Replacing such ‘calibration data’ in a database for older data is therefore often a mistake and is often not the intention of the authors.

2. Any database should provide a critical review of the presented data. Many experiments have limitations which should be clearly stated in the database. Some experiments have recognised systematic errors which, while not precluding their use, should be allowed for when comparing with other data (both experimental and theoretical).

3. Any database that aims to be adopted by an applied community should include a list of recommended values. These may be subject to compilers’ bias (often the choice of which data set to adopt is a question of ‘gut feeling’ based on the experience and personal knowledge of the authors providing the data). Therefore it is necessary to have some method by which databases may be compared with one another.

Funding for databases is, despite the recognition of their importance by users, woefully inadequate receiving little support from research agencies. Therefore all too often a database once compiled, rapidly become out of date and is all too often discarded for the adoption of recent data even if this data has not been critically evaluated against earlier data.

It is therefore important for the fundamental research communities, the providers of such data, to assemble, update and police such databases. This is no longer as complicated as it was a decade ago. Most publications are accessible online and most authors place their data on home pages and in archives, hence adding new data to existing data is considerably easier than in the past, for example the **Gen**eral **I**nternet Search **E**ngine for Atomic Data (GENIE) developed as part of the International Atomic Energy Agency facility for collisional atomic data for fusion and atomic physics research. Such electronic access also provides a model for discussing new data and an important method for peer review. In the future electronic databases should provide the opportunity for authors to both add their latest results to the database and provide a forum for discussing such data, e.g. through a weblog (widely used by students and younger researchers today in other contexts). Such procedures should allow future databases to be constructed more easily, be maintained more regularly and accessed more commonly by users who may be confident of the standards and accuracy of the data provided. It should also be possible to add to such databases access to 'simple' theoretical tools that will allow the user to evaluate cross sections for targets and scattering processes for which experimental data is not yet available.

Nevertheless in the last decade considerable progress has been made and, through closer collaboration between the fundamental research community and the applied plasma community, a greater appreciation of the major problems to be addressed by both communities has been realized. Central to this is the assembly and maintenance of central databases that reviews and recommends standard datasets. Examples include those dedicated to fusion such as the aforementioned AMDAS, ALADDIN and GENIE databases maintained and developed by the Atomic and Molecular Data Unit of the International Atomic Energy Agency [1] and those directed at atmospheric chemistry and astronomy [2-6] which may provide such a service for the plasma community allowing experimentalists and modelers to benchmark one another's work and ultimately provide a better understanding of the plasma, in turn allowing better control of the plasma parameters and thence refinement of the products of the plasma processing.

These databases will be complemented and expanded by the recently funded European Framework VII e-infrastructure that will provide a comprehensive database for atomic and molecular physics; the Virtual Atomic and Molecular Data Centre (VAMDC). This aims to provide a 'one stop' data resource that will support researchers across a wide range of fields, including the plasma community [7]. In developing VAMDC it will be essential to ensure links between the date users and the data providers are fostered and endure over a long period. The presentational format of the data, the methodology of access and crucially, the provision of help support' must be developed by collaboration between data users and providers. Users must be made more aware of the need to cite and adequately recognizer the providers of data if we are to ensure that funding for basic research to generate such data is maintained. Similarly data providers must be made aware of where the data is being used and be made aware of what the critical data requirements are and, through sensitivity analysis, determine what is an adequate error bar on the presented data sets. VAMDC therefore seeks to engage with the plasma community and is hence supporting this workshop at XX ESCAMPIG 2010, within which the requirements and advice of the plasma community may be conveyed to the VAMDC project.

Reference

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