PROCESSES AT INTERFACES OF PLASMA AND MOLECULES

Predrag S. Krstić[(1,2,*)]

[(1)] Physics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

[(2)] Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA

[(*)]**krsticp@ornl.gov**

The understanding of fundamental atomic interactions in low temperature plasmas is vital to plasma modeling for many technologies, including ion source development, semi-conductor processing, and magnetic fusion. Typical for these plasmas is existence of nondissociated, though rovibrationally excited molecules, which play important roles in the volume recombination of ions (Molecule Assisted Recombination, MAR, for creation of a detached plasma layer in the boundary plasma), in radiation detection and modeling of planetary plasmas, in plasma chemistry, in transport of momentum and energy in plasma. Most efficient in production of the excited molecules are interactions at the plasma-material interface, either through association or sputtering of the surfaces of the plasma vessels walls, or of dust particles. We study processes in which the initial state of the particle-molecular complex is far from equilibrium, and the final equilibrated system state is only reached via multiple coupled pathways, in which atomic physics and in some cases, solid state processes are intimately intertwined.

We report on a comprehensive study of scattering of hydrogen ions on rovibrationally excited hydrogen molecules as well as of hydrogen atoms on rovibrationally excited hydrogen molecular ions in a range of center of mass energies below 10 eV [1-4]. Total and partial, initial and final rovibrationally state resolved cross sections for excitation, charge transfer, dissociation including dissociative energy spectra and association have been calculated using a fully- quantal, coupled-channel approach. The results have a large importance for modeling of both fusion plasma and planetary atmospheres of the external planets (starting with Jupiter).

Interaction of plasma particles with walls and dusts at low temperatures is mainly localized at the interface of the material and plasma, defining the short time scales, ps to ns, of the cascade interactions. This elucidates the computational pathway for studying these collision processes by classical molecular dynamics (MD), in which localized part of the material is treated as a large classical molecule, made of thousands of atoms. Properly benchmarked MD simulations could provide comprehensive databases for boundary plasma modeling, providing details often not accessible by experiment [5-9].

The key issues for surface experiments on carbon based materials are erosion, reflection, impurity transport in the plasma, deposition, hydrogen uptake and removal. There is a need to determine the composition of eroded species such as hydrocarbon molecules and radicals, their rovibrational state and energy spectra, and their sticking coefficients to surfaces as a function of energy. An expansion of the available erosion database towards low energies (<50 eV) was identified as highly needed. Chemical and physical sputtering cause the erosion of the vessel walls, and degrade plasma performance in applications. Deposition and re-deposition of the sputtered molecules can lead to accumulation of large inventories of non-desired materials.

Well-controlled plasma sources can be used for experimental characterization of sputtering processes [10]. Experiments of this kind were performed recently for the accommodation

coefficients of H2 interacting with polycrystalline carbon surfaces. We have calculated the sputtering yields and reflection coefficients using a distribution of impacting particles that mimics a plasma environment, which can be directly validated by experiment [11].

The accuracy and completeness of the current calculations on both plasma interfacing small, large and ultra-large molecules is by far beyond any other theoretical information on the considered collision systems and range of energies, still limited by the numerous approximations used in the approaches.

Reference

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