Understanding the interaction of energetic particles with fusion reactor first walls: from binary collision physics to bond conjugation chemistry

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Thermonuclear fusion reactors have a very special and complicated environment for interactions between the fusion plasma and the wall materials [1]. While the central plasma is fully ionized and contains high-energy keV electrons and ions, the edge regions of the plasma that are in contact with the wall material are much cooler and contain a rich potpourri of electrons, atoms, molecules and radicals. These impact on the materials with energies ranging from a few eV to a few keV, depending on position in the reactor and plasma conditions. Understanding the ways in which these particles interact with the fusion first wall material is a crucial issue in the development of commercially viable fusion power plants, as both too high material erosion, and too high deposition of radioactive tritium to the wall materials, may be showstoppers for the reactor operation. Hence the fusion science community has long attempted to obtain an understanding of the fusion plasma-wall interactions.

The original approach used for modelling the plasma-wall conditions came from high-energy radiation physics, where solution of the classical two-body scattering integral for purely repulsive interatomic potentials is routinely used to determine the sputtering yield and penetration depths of high-energy ions. This approach has been widely used to examine fusion reactor plasma-wall interactions. However, by the late 1990's it became clear it cannot possibly explain the experimentally observed high sputtering of carbon by low kinetic energy (a few eV) incoming D ions. Around 2000, we showed using molecular dynamics and many-body reactive interatomic potentials, which describe chemical bonding, that this carbon sputtering can be understood based on a new kind of special physico-chemical endothermal sputtering reaction, "swift chemical sputtering" [2]. We later showed using both classical and quantum mechanical MD simulations that the mechanism is distinct from both binary collisions and conventional chemical reactions [3]. Most recently, we have shown that in binary plasma-facing materials such as BeC not only the nearest-neighbour bonds but also the conjugation of chemical bonds needs to be considered to properly describe fusion reactor plasma-wall interactions.

In this talk, I will overview this development of understanding from nuclear collision physics to complex bonding chemistry, and give some recent results on swift chemical sputtering of metals [4] and metal carbides [5].

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