Surface kinetics in CO_2 plasmas

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CO_2 plasmas are widely studied nowadays due to their importance in a variety of plasma-chemical processes, such as those involved in fuel reforming, production of synthetic fuels and value-added chemicals, iterstellar chemistry, and spacecraft entry in Mars and Venus atmospheres. The interaction of different species with the surfaces play a key role in these applications. Indeed, several processes occur on the surfaces, like vibrational de-excitation and recombination of oxygen atoms, while new chemical reactions or reactions with a different rates can happen on surface with species created in the plasma. A change in behavior of the O-atom gas density with pressure in CO_2 plasmas was recently observed experimentally [1], with a transition of regime around 1 Torr. Measurements of the O atom loss frequency under plasma exposure have shown that this behaviour is caused by a change in the O atom loss mechanisms, which at these pressures are dominated by surface processes [1]. This work addresses this problem and focuses on the heterogeneous recombination of oxygen atoms in CO_2 plasmas at low pressure. A kinetic Monte Carlo (KMC) algoritm is developed to study O-atom recombination on Pyrex surfaces in CO_2 plasmas. The model follows the formalism developed in [2] for pure oxygen plasmas and accounts for the elementary steps of physisorption, chemisorption, thermal desorption, surface diffusion, and recombination both by Eley-Rideal and Langmuir-Hinshelwood mechanisms. The dependences of the atomic recombination probability with the different surface parameters (density of adsorption sites, activation energies of the elementary processes, etc) is presented and discussed in detail. Moreover, surface modification by ion bombardment can change the morphology and composition of the surface and is assumed to be at the origin at the observed change of regime [1,3]. A simplified simulation of these processes within the framework of KMC is presented for the first time.

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References
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