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湿潤空気不純物を含む大気圧プラズマの化学反応
Chemical kinetics of atmospheric pressure plasmas with humid air impurity

村上 朝之
Tomoyuki MURAKAMI

東京工業大学
Tokyo Institute of Technology

Recent results on modelling of gas-phase chemical kinetics in low-temperature atmospheric pressure plasma jets operated in an open-air environment are discussed.

Atmospheric-pressure plasma jets (APPJs) have been gaining attention because of their great potential in various fields, e.g. surface treatment, environmental remediation and bio-plasma applications. In order to understand the underlying operating principles of such systems and to optimize their performance in applications, it is important to know the chemical kinetics of the reactive multi-species plasma. This is a study starting to address this by using a zero-dimensional (0D) time-dependent global simulation of the chemical kinetics in APPJs with a commonly used plasma medicine chemistry, i.e. a helium-based oxygen-mixture (in general, up to 1%) with ambient humid air (the humid air fraction to helium is up to several hundred ppm). Because of the presence of humid air, the plasma tends to produce significant amounts of reactive species and the plasma-induced chemical reactions are complex. So, here, the extended reaction scheme comprises over 1100 elementary reactions among over 60 species; neutral atoms and molecules, metastable species, vibrationally excited molecules, positively and negatively charged ions, various hydrate cluster ions and electrons. The present plasma chemistry model and simulation code have been described in detail in reference [1,2].

Air impurities of 100 ppm with relative humidity of 20–40% crucially change the plasma-induced chemistry from a comparatively simple oxygen-dependent plasma to that of a complex oxygen–nitrogen–hydrogen plasma. The global model reveals that the most pronounced neutral species in a radio-frequency (rf) driven He+0.5%O_2 APPJ are reactive oxygen species, i.e. atomic oxygen (O), singlet delta molecular oxygen ($O_2(^1D)$) and ozone (O_3), and the main ion species are molecular oxygen ions, i.e. O_2^+ , O_4^+ and O_2^-. Addition of the air impurity containing water humidity considerably enhances the electronegativity (negative ion density / electron density), while it decreases the overall plasma reactivity (reactive species density / non-reactive species density) and the densities of reactive oxygen species. However, other potentially important hydrogen and nitrogen reactive species, hydrate cluster ions are created. The global model estimates of the absolute density for reactive oxygen species and helium metastable atoms are in good agreement with experimental measurements in the rf-driven APPJ [3-5].

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