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Numerical modeling of the KrCl* kinetics in pulsed discharges

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Rare-gas and rare-gas-halide molecules are well known to be efficient sources of VUV and UV radiation for many potential applications in areas such as microelectronics, water purification, bacterial decontamination of surfaces, medical treatment or photodimerisation. For biomedical applications, it is of interest to use radiation in the UV-C range (200-280 nm), corresponding to the absorption cross section of DNA. In this context KrCl* molecules, emitting at 222 nm, are of special interest. Formation of these molecules is favored in non-equilibrium discharges operating at relatively high pressure, and up to now, they have been mainly produced in capacitive discharges [1] or in dielectric barrier discharges (DBD) [2]. By "capacitive" discharge we mean one in which a capacitor is discharged through a gas gap between metal electrodes, and where the current through the gas gap is initiated by an external trigger – photons, for example [3]. It has been experimentally demonstrated that high power output can be obtained in capacitive discharges, although at a rather low efficiency, whereas low output power but high efficiency can be achieved in DBDs. In the last few years, a new family of non-equilibrium, high-pressure plasma devices has been developed: the so-called micro-discharges. These discharges, characterized by sub-millimeter dimensions, allow the production of stable plasmas at high pressure and high power loading and can be operated in arrays of different geometry. As a result, they could combine the advantages of capacitive discharges and of the DBD for the realization of efficient, high power UV sources. Our long-term goal is to quantify their performance and optimize these different discharge sources of UV radiation.

The results presented in this communication are from a zero-dimensional kinetic model of KrCl* molecule formation in the capacitive and DBD discharge configurations mentioned above. The model is self-consistent in the sense that the discharge current, calculated from the kinetic model, is introduced in a circuit model to obtain the voltage across the gas gap at each time. The purpose is to obtain a deeper understanding of the physical processes limiting the output power and efficiency of each excitation schemes. The model takes into account electrons, three electronically excited atomic krypton states, the Kr_2* excited molecular sates, the Kr^+ and Kr_2^+ ions, the vibrationnally and electronically excited states of Cl_2 molecules, the Cl_2^+ and the Cl^- ions, and the KrCl* excited state. All these species react between themselves and with the Kr and Cl_2 ground state through 68 kinetic reactions. The interactions between electrons and others species are calculated through the solution of the Boltzmann equation using the classical two-term approximation. The electrical circuit consists of a storage capacitance coupled to the discharge through an inductance and a resistance. For DBD the storage capacitance is the capacitance of the dielectric barrier whose value is fully determined by the geometry of the device and by the value of the permittivity of the dielectric material. We used a value of 74 pF, corresponding to the value of an experimental set-up implemented at LPGP. For capacitive discharges, the value of the capacitance is a free parameter and values as high as 100's nF can be used for high energy

deposition. However, in the present work we use the same value of the capacitance, 74 pF, for the capacitive discharge and for the DBD to get insights on the role played by the dielectric barrier on the discharge properties for the same applied voltage. Experimentally, these conditions correspond to situations where the plasmas appear to be homogeneous, justifying our use of a zero-dimensional model for these initial studies.

Examples of the results obtained are shown in Fig. 1. The temporal evolution of the KrCl* population is shown parametrically as a function of the total pressure for a Cl_2 concentration of 3% for a capacitive discharge (left panel) and for a DBD (right panel) operating with the same applied voltage. For capacitive discharges, Fig.1a shows that the maximum value of the KrCl* population is a decreasing function of the total pressure, while for DBD excitation, Fig. 1b, an optimum value is achieved for a pressure of about 100 mbar. It should be emphasized that, for capacitive discharges, we find only one peak in the KrCl* population and the correlated 222 nm emission for all pressures and Cl_2 concentrations studied. The behavior is quite different for DBD excitation; at high total pressure and high chlorine concentration, we find two peaks in the the 222 nm emission which are correlated with two discharge current pulses. Details of the predicted discharge voltage and current waveforms for different conditions will be presented along with a discussion of the predicted pressure dependence. Finally, it should be mentioned that this general behavior is in good agreement with the measurements performed on the different experimental devices under study at LPGP and that more detailed one and two dimensional modeling studies are underway.

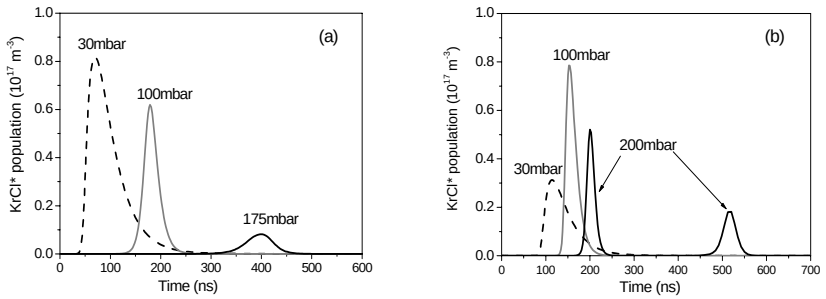

Fig. 1: Temporal evolution of the KrCl* population for a Kr-Cl_2 mixture at 3% Cl_2 for an applied voltage of 2 kV. Fig. 2a: capacitive discharge, Fig. 2b: DBD

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