fast quenching of singlet oxygen molecules by ground state o atoms at high temperatures [[1]](#footnote-1)\*)

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Oxygen plasma can be found in many applications as a source of highly active particles: ground state oxygen atoms O(3P) and singlet oxygen molecules O2(a1Δg). Dissociation degree in oxygen plasma can exceed 20% and fraction of O2(a1Δg) can be up to ~15-20% [1, 2]. It is important to reproduce carefully kinetics of atomic and singlet oxygen to be sure in correct simulation of oxygen discharges since all the processes in O2 plasma involving atoms O(3P) and O2(a1Δg) molecules strongly influence on plasma parameters. Besides, while the processes with stable species are well known in many cases, processes with radicals are still poorly studied. Among the latter, one of the most important processes is fast O2(a1Δg) collisional quenching by oxygen atoms O(3P) since it can strongly influence O2(a1Δg) concentration and plasma as whole. This work is focused on detailed study of this process using joint approach that includes both experiment and modelling.

O2 plasma was generated in a quartz tube (length 200 mm and inner diameter 10 mm) at pressures 10 – 100 Torr by using transversal 81 MHz CCP discharge with external electrodes along all tube. To keep surface conditions nearly stable, the electrodes were cooled by water while soft carbon insert provided good thermal contact between tube and electrodes. The rf power input into the plasma was estimated from direct measurements of rf voltage, rf current and phase shift between them. The rf generator could be programmed to operate in continuous and pulsed mode with different rf power modulation depth up to 100%. The used discharge configuration allowed providing high specific energy input that led to high gas temperatures.

The optical emission spectroscopy (OES) methods were basic diagnostics in this research. Mole fraction of atomic oxygen was obtained by actinometry technique [3]. Mole fraction of O2(a1Δg) was obtained by measuring absolute power of O2(a1Δg,v=0) → O2(X3Σg-,v=0) emission at 1.27 µm. The gas temperature values were obtained from comparison of simulated and measured spectra of the A-band O2(b1Σg+,v=0) → O2(X3Σg-,v=0).

Used discharge model considered two scenarios of O2(a1Δg) quenching: i) using standard (“old”) kinetic scheme where the process R1 is fully excluded and ii) including quenching reaction R1:

 O2(a1Δg) + O(3P) → O2(X3Σg-) + O(3P) kq = 3·10-11·exp(-8000/Tgas) cm3/s (R1)

Analysis was based on comparison of the model and experimental results for gas temperature, mole fractions [O(3P)]/N and [O2(a1Δg)]/N which will be presented and discussed. As it turned out, just an inclusion of R1 reaction allows reproducing adequately observed experimental trends (in contrast to the “old” kinetic scheme without R1). Moreover, detailed analysis of the reaction pathways of O2(a1Δg) + O(3P) → O3\*\* indirectly confirms existence of (R1) reaction with high activation barrier ~5000-9000 K.

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