State-by-state emission spectra fitting for non-equilibrium plasmas: OH spectra of surface barrier discharge at argon/water interface

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A novel method of state-by-state fitting of OH(A $^2\Sigma^+ \rightarrow$ X $^2\Pi$) spectra is introduced and applied to a special case of surface dielectric barrier discharge (DBD) in contact with water level. The resulting Boltzmann plot revealed three groups of OH(A $^2\Sigma^+$) - *hot group*, *cold group*, and group influenced by isoenergetic vibrational energy transfer OH(A $^2\Sigma^+$, v'=1$\rightarrow v$'=0). The state-by-state fitting is incorporated in the *massiveOES* software package and available for free to the scientific community. The linearity of the problem ensures low computational demands - the whole fit for one spectrum takes few seconds on a usual office computer. The Boltzmann plot was extensively analysed, the three groups were decoupled and the of OH production pathways were investigated.

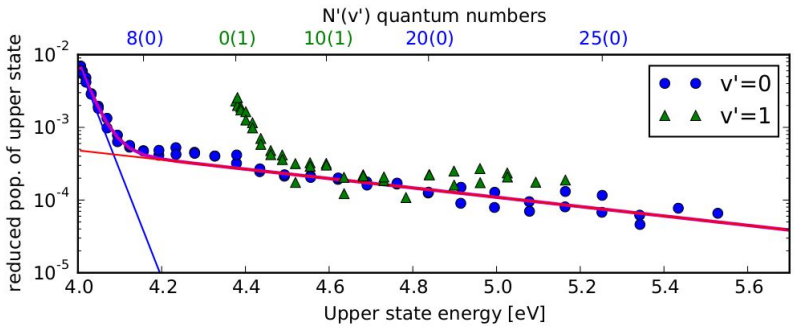

Figure: The population distribution of OH(A $^2\Sigma^+$) rotational states and two-exponential fit. The corresponding temperatures are $T_{rot}^{low} = 340 \pm 30$ K and $T_{rot}^{high} = 7800 \pm 550$ K.

Recently, the interest in discharges in contact with water increased enormously [1]. Often, the discharges are ignited in a noble gas and the atoms and water fragments are the only available spectral signature. In such cases, the spectrum of hydroxyl radical (OH) may seem attractive for neutral gas thermometry. This contribution brings an extensive analysis of OH(A $^2\Sigma^+ \rightarrow$ X $^2\Pi$) spectrum obtained on special case of kHz driven surface DBD in contact with water. As other groups, we have observed a spectrum that may be interpreted as a superposition of emission from several groups of OH. We have distinguished three groups - *cold group*, best observable for low N' quantum numbers, *hot group*, best observable for higher N' quantum numbers and the third group influenced by isoenergetic vibrational energetic transfer OH(A $^2\Sigma^+$, v'=1$\rightarrow v$'=0), best observable for $9 \leq N' \leq 13$. The unusual accuracy of our Boltzmann plot (see the figure) was enabled by the novel method of state-by-state fitting. This approach combines spectral simulation and traditional Boltzmann construction procedure. A synthetic spectrum is simulated for each rovibronic upper state, including the instrumental broadening and matched with the measurement. Best-fitting linear combination is then searched for. This functionality was incorporated to the *massiveOES* software package [2,3,4].

Acknowledgements

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References

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[2] J. Voráč et al. Plasma sources sci. technol. **26**.2 (2017) 025010.
[3] J. Voráč et al. submitted to J. Phys. D: Appl. phys.
[4] massiveOES software package https://bitbucket.org/OES_muni/massiveoes