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# HYBRID MONTE CARLO – FLUID MODEL FOR Ar/$N_2$ GLOW DISCHARGES: EFFECT OF $N_2$ VIBRATIONAL LEVELS

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**Abstract**

A computer model has been developed with the aim of investigating the effect of nitrogen impurities in a direct current glow discharge in argon. Particular attention has been devoted to the vibrationally excited states of nitrogen molecules.

**Introduction**

Small amounts of molecular gases such as nitrogen can affect drastically the conditions present in an argon glow discharge. In glow discharge optical emission spectrometry (GD-OES) the changed conditions can manifest themselves in the altered sputtering rates and the modified relative intensities of emission lines, thereby significantly influencing the quantitative analysis [1-3]. In many cases these effects cannot be avoided because the molecular gases are present in the samples themselves as compounds or occluded gas. It is therefore important to understand the effects of such molecular gases in detail. Computer modelling can be very useful in revealing the underlying mechanisms responsible for these effects.

**Description of the model**

Previously [4] we developed a computer model describing Ar/$N_2$ glow discharges with 74 different chemical reactions between the plasma species including electrons, Ar atoms in the ground state and the 4s metastable levels, $N_2$ molecules in the ground state and in six different electronically excited levels, N atoms, $Ar^+$ ions, $N^+$, $N_2^+$, $N_3^+$ and $N_4^+$ ions. Now we have extended this model by taking the vibrational levels of the ground state $N_2$ molecules into account.

Following the model of Lino da Silva et al. [5] we consider 60 vibrational levels. The additional processes involving the ground state molecules are the excitation and de-excitation of vibrational levels by electron impact collisions, the vibration-vibration (V-V) and the vibration-translation (V-T) energy exchange processes in $N_2$-$N_2$ collisions and the V-T energy exchange processes in $N_2$-N and $N_2$-Ar collisions. These processes are summarized in Table 1.

The electrons are simulated with a Monte Carlo model, whereas all other species are treated in a fluid model. The output of one model is used as input in the other models, and the models are solved iteratively until convergence is reached.

Table 1: Kinetics of $N_2(X\ ^1\Sigma_g^+,v)$ molecules

| | | | |
|---|---|---|---|
| $e^- + N_2(X,v)$ | $\rightleftharpoons$ | $e^- + N_2(X,w)$ | e-V |
| $N_2(X,v) + N_2(X,w)$ | $\rightleftharpoons$ | $N_2(X,v+1) + N_2(X,w-1)$ | V-V |
| $N_2(X,v) + N_2$ | $\rightleftharpoons$ | $N_2(X,w) + N_2$ | V-T |
| $N_2(X,v) + N$ | $\rightleftharpoons$ | $N_2(X,w) + N$ | V-T |
| $N_2(X,v) + Ar$ | $\rightleftharpoons$ | $N_2(X,w) + Ar$ | V-T |

**Results**

Calculations have been performed for a Grimm-type glow discharge cell with simplified cylindrical geometry, i.e., a cell length of 1 cm and diameter of 4 mm. Typical operating conditions are a gas pressure of 850 Pa, a discharge voltage of 800 V and an electrical current of 15 mA. The results include the two-dimensional density profiles of several plasma species as well as the electron energy distribution function (EEDF) and the vibrational distribution function (VDF) at different positions of the discharge cell. Information is also obtained on the relative importance of the various processes in the discharge. The effect of $N_2$ concentration in the range of 0.1-10% is investigated.

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