

Modeling the effect of gaseous impurities in argon glow discharges: A comparative study of H₂, N₂ and O₂

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It is generally established that the working conditions in glow discharges may be considerably affected by the presence of small amounts of molecular gases, such as H₂, N₂ and O₂, in the discharge gas. In order to obtain a better insight in the underlying mechanisms, we have developed a computer model for describing Ar/H₂ [1], Ar/N₂ [2] and Ar/O₂ [3] glow discharges, with typical impurity concentrations varying between 0.1 and 10% (v/v). The species taken into account in the model include electrons, Ar atoms in the ground state and in the 4s metastable levels, Ar⁺ ions, as well as several species characteristic for each gas impurity. In the case of H₂, the extra species are ArH⁺, H⁺, H₂⁺ and H₃⁺ ions, H atoms and H₂ molecules [1]. In the N₂ case, the relevant species include N⁺, N₂⁺, N₃⁺ and N₄⁺ ions, N atoms, N₂ molecules in the ground state and in 6 different electronically excited levels [2]. Finally, in the case of O₂, the following species are considered: O⁺, O₂⁺ and O⁻ ions, O atoms in the ground state and one metastable level, O₂ molecules in the ground state and two metastable levels, and O₃ molecules [3]. In the three cases, the fast electrons are simulated with a Monte Carlo model, whereas all other species are treated in a fluid model. These species interact with each other through various chemical processes. In the Ar/H₂ model, 65 different reactions between the various species were taken into account. In the Ar/N₂ model, 74 different reactions were included, and finally the Ar/O₂ model considers 87 different reactions. Hence, although the three gases are all diatomic in nature, different species appear to be formed in the glow discharge. The Ar/O₂ discharge is especially interesting, because also negative ions (O⁻) are present in the discharge, although still at a lower concentration than the positive ions. Typical results of these models include the density profiles of the various plasma species, the relative importance of their production and loss mechanisms, the ionization and dissociation degree, as well as the effect of the gas addition on the sputtering process.

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- [2] Bogaerts, A. *Spectrochim. Acta, Part B* **2009**, *64*, 126-140.
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The author acknowledges financial support from the EU Marie Curie Research Training Network GLADNET.