Simulation model for the oxidation of Ru nanolayers under oxidizing/reducing plasma conditions

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A 1D simulation model in COMSOL Multiphysics FEM software is developed to predict the state of the Ru nanolayer under oxidizing/reducing plasma conditions. In COMSOL mathematical models are used to model the full set of radical formation, material fluxes and reaction kinetics of the solid-state chemistry taking place at the surface of and inside the Ru material. Transportation includes the adsorption of H and O radicals produced by the plasma and evaporation of volatile molecules from the Ru surface, and the absorption and penetration of radicals into the Ru bulk and release of matter from the Ru bulk to the surface. Under plasma conditions an adhering monolayer of water at the Ru surface acts as source of penetrating H and O radicals. As it is assumed that the Ru nanolayer is amorphous due to its thickness, interstitial diffusion is modelled where the diffusion constant increases with the interstitial particle size and concentration. Reaction kinetics include recombination reactions of the H and O radicals, the oxidation of Ru to RuO/RuO2¬/RuO3 and the reduction back to RuO2/RuO/Ru and H2O in case of an excess of hydrogen. Oxidation reactions are modelled as Arrhenius equations, and reduction reactions are modelled under irradiation with soft X-rays as driving force using photonic particle interaction statistics. Experimental validation is obtained by exposure and inhouse AR-XPS measurements. We now have achieved a qualitative predictive model with first order quantitative prediction of the oxidation levels of Ru, and our goal is to obtain a full quantitative predictive model in the upcoming months.