Fixing the parameter set for reactive sputtering modelling

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It can be stated without exaggeration, that modelling of reactive magnetron sputtering is a complex task. Several approaches have been developed to model the process, ranging from analytical models over semi-empirical to complete PIC-MC (Particle-In-Cell/Monte-Carlo) models. The choice of the modelling parameters is a key issue for all simulations. The parameters related to reactive magnetron sputtering are however, not easily collected. The variation between for example the calculated and/or experimental metal sputter yield available in literature is quite large. This variation limits the accuracy of the model. Therefore it is essential to study the influence of the parameter set on the goodness-of-fit between model and experiment.

Based on an existing model [D. Depla et al. J.Phys D: Appl. Phys 2007] experimental hystereses, i.e. oxygen pressure-flow curves, were fitted using a parameter set based on experiments and SRIM simulation. For several different targets, a large number (>3x10⁴) of simulations per target/oxygen combination was performed, based on a random variation within the experimental error interval of several parameters. Due to the experimental input, giving strong limitations to several parameters, only a minor amount of simulations showed a good fit with the experiments. A relationship between some parameters was found which gives insight in the impact of each parameter on the simulation. These relationships enable to pinpoint the parameter set for each target/oxygen combination. In this way reasonable suggestions can be made on the material dependency of hard-to-collect parameters such as the chemical reactivity of implanted reactive gas ions in the target. Even more, predictions can be made for the reactive sputtering behaviour of different target/reactive gas combinations.

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