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Modeling of low-temperature plasmas: some case studies of different modeling approaches

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In this talk, some examples will be given of different modeling approaches, used in our group. Special attention will be put on input data, needed for the models. As an example of fluid modeling, we will illustrate the detailed plasma chemistry in a DBD used for gas conversion purposes. In this model, a large number of different species (various molecules, radicals and ions, besides the electrons) are included, which can all react with each other. For all these species, transport coefficients need to be defined, as well as reaction (sticking) probabilities at the walls. Moreover, energy-dependent cross sections and thermal rate coefficients have to be defined for all the electron reactions and the heavy particle reactions, respectively. These data are typically not available for the more exotic plasma species, so that certain assumptions have to be made. The second example is for particle-in-cell – Monte Carlo collisions simulations, developed for magnetron discharges in argon/oxygen and argon/nitrogen gas mixtures, used for the reactive sputter-deposition of metal oxide and nitride layers. In this modeling approach, the behavior of the electrons, the various ions and energetic neutrals is described by Newton's laws, and their collisions are treated by the Monte Carlo procedure. Again, energy-dependent cross sections for the various collisions are required. The last example is for hybrid Monte Carlo – fluid modeling, based on the HPEM code developed by Kushner and coworkers. It is applied to an ICP in $Ar/Cl_2/O_2$, used for Si etching. Besides the plasma behavior, also the etching (and deposition) process is described, for which a large number of data (etch and sticking probabilities and sputter yields) are required. We try to obtain accurate values for these data by molecular dynamics simulations. Results of the latter simulation method will also be presented.