Numerical optimization of rate coefficientsof chemical reactions in C_4F_8 plasma

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Reliable plasma simulation can be carriedout with a set of accurate chemical reaction rate coefficients that includeevery significant chemical reaction occurred in the plasma. Some of the ratecoefficients can be collected from the literature of theoretical orexperimental researches, but others are hard to achieve. Especially, in theplasma used in the semiconductor industries several hundred reactions should beincluded in the set, but many of them cannot be achieved from literature withhigh accuracy. Some of them have large uncertainty and others should beestimated because they are not found in the literature. Then the researchershave been tuned the estimated rate coefficients until the simulation resultagree with the experiments. This tuning is just trial and error process, butrequires much human effort. In this study numerical optimization software wasdeveloped to tune the rate coefficients with much less human effort thanprevious researches. In the software several numerical optimization algorithmscan be used including steepest descent, Newton, modified Newton andBroyden-Fletcher-Goldfarb-Shanno method. A spatially averaged global plasmasimulator, K-0DPLASMA, was used to simulate plasma while numerical optimizationprocesses. The numerical optimization software was applied to tune a set ofrate coefficients for C_4F_8 plasma which has been used in the etching process ofsemiconductor industries.

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