Present and Future Modeling Approaches for Non-Equilibrium Plasma Chemistry at Low and High Pressures*

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Abstract

Modeling of low temperature plasma chemistry has made significant progress during the last five years. This work has been motivated by industrial applications of non-equilibrium plasma chemistry and the need for computer aided design (CAD) tools to help economically optimize those processes. The primary thrust in modeling of low pressure systems has clearly been semiconductor materials processing. The primary thrust in modeling high pressure systems has historically been high power lasers and lighting, however current emphasis is on atmospheric pressure plasma remediation of toxic gases. Although our understanding of the physics of these devices has improved with time, the rapid progress towards first principles CAD tools has in no small part been made possible by the availability of inexpensive high performance computers. For example, in the time required to model a rare gas capacitively coupled radio frequency discharge in 1 dimension 5 years ago, we can now model electromagnetically excited multi-component plasmas in 2 dimensions, an increase in complexity $> 10^3$.

The components of plasma chemistry models in both low and high pressure regimes are basically the same. There are modules for the electric circuitry, electric field, transport of heavy particles and electrons, reaction chemistry and plasma-surface interactions. Perhaps most important, there must be a methodology for generating electron impact rate coefficients by either kinetic or fluid representations of the electron swarm. Although the components of the models are the same in both pressure regimes, the emphases are quite different. For example, in modeling low pressure plasma etching the greatest computational burden is in obtaining the electron energy distribution to generate rate coefficients. In high pressure systems, such as corona and dielectric barrier discharges, the greatest burden is representing the plasma-hydrodynamics of streamer propagation. In either case, as our computational expertise advances, the rate limiting step in providing industrially relevant CAD tools has proven to be the lack of a robust and reliable databases.

In this talk, a brief historical overview of modeling of nonequilibrium plasma chemistry will be given. The current status of the field will be reviewed, with examples from low pressure plasma materials processing, and high pressure lasers and toxic gas remediation. Database and computational needs for further advances will be discussed.

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