CHEMKIN-PRO

Chlorine Plasma Modeling

Plasma etching offers environmentally efficient, precise and accurate methods for surface cleaning and etching in the industrial, medical, and energy sectors. As miniaturization and environmental factors play greater roles as business drivers, etching's role also grows as an attractive alternative to wet cleaning and etching. CHEMKIN-PRO is well suited for modeling plasmas. For treating non-equilibrium plasmas, the plasma models allow specifying different temperatures for the neutral gas, electrons, ions, and surfaces. CHEMKIN-PRO provides efficient capabilities for handling energy and managing ion-assisted reactions with a Bohm-flux correction model.

Setting Up a Low-Pressure Plasma Etching Simulation

This chlorine plasma's gas-phase chemistry[1] considers the electron impact reactions that result in dissociation and ionization of chlorine. The gas-phase species list contains seven species: Cl_2, Cl, Cl* (chlorine atoms in a metastable electronically excited state), Cl_2+, Cl+, Cl- and E. The gas-phase reactions include electron collisions with Cl_2, leading to vibrational and electronic excitation, dissociation, ionization, and dissociative attachment. Electron reactions with Cl include electronic excitation into a number of excited states, including Cl* formation and ionization.

The gas-phase reaction mechanism also includes electron collisions with Cl-, leading to electron detachment, electron collisions with Cl* leading to ionization, and gas-phase neutralization of Cl- with Cl+ and Cl_2+ ions. All the reactions are irreversible, since this is a non-thermal plasma, where the gas-phase electron production is balanced primarily by surface recombination reactions. The rates for the electron-impact reactions depend on the electron energy, rather than the neutral gas temperature. The surface mechanism for reactions occurring on the reactor wall[2] address the electron-ion neutralization and chlorine atom recombination. It includes neutralization of Cl+ and Cl_2+ with electrons (subject to the Bohm criterion), de-excitation of Cl* and radical recombination reactions for Cl to Cl_2.

[1] E. Meeks and J. W. Shon, “Modeling of Plasma-Etch Processes Using Well Stirred Reactor Approximations and Including Complex Gas Phase and Surface-Reactions”, IEEE Transactions On Plasma Science, 23(#4): 539-549 (1995).

[2] E. Meeks, J. W. Shon, Y. Ra, P. Jones, “Effects of Atomic Chlorine Wall Recombination: Comparison of a Plasma Chemistry Model With Experiment,” JVSTA 13(#6): 2884-2889 (1995).

The neutralization and de-excitation reactions are non-site specific, but the recombination reactions are described in terms of open and Cl-covered sites. Although this example problem does not include surface etching reactions, such reactions could be introduced. In any case, surface recombination and neutralization reactions can be quite important in determining the characterizing low-pressure plasmas. All the surface reactions are treated as irreversible.

Results

Figure 1 shows the electron temperature as a function of power for this chlorine plasma. The electron temperature shows only small changes over the large variation in plasma power, since most of the power is transferred into ionization and dissociation rather than electron heating. However, as the plasma power drops, the electron temperature rises as the plasma nears extinction, since there are fewer electrons and electron-driven events.

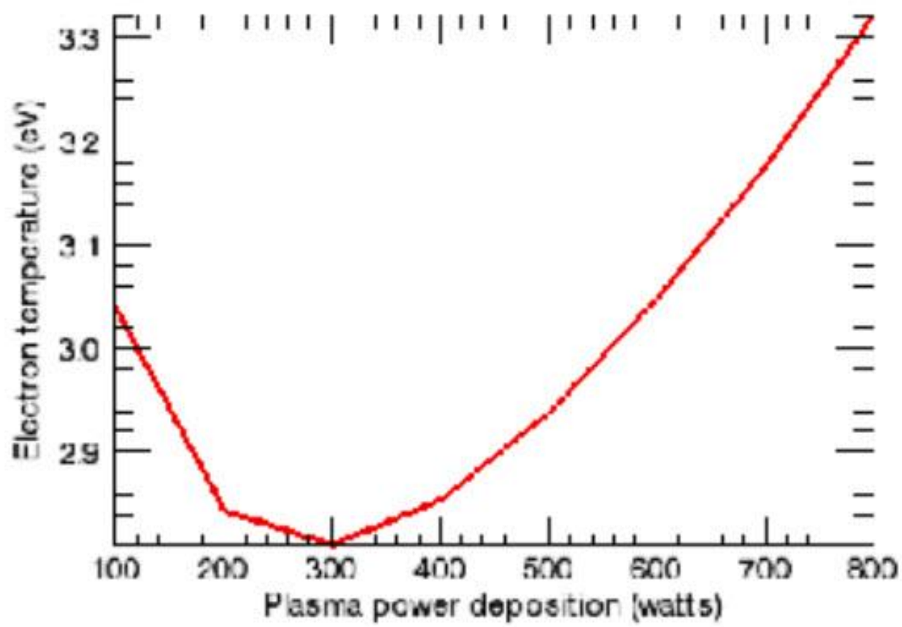

Figure 1. Electron temperatures vs. power.

Figure 2 shows a rate-of-production analysis for the input gas Cl_2. In this case, there are clear major and minor pathways. The primary reaction consuming molecular chlorine is gas-phase reaction #3, which is the electron-impact dissociation to two Cl atoms. Gas reactions #5 and #2, the electron-impact ionization and dissociative attachment reactions of Cl_2, respectively, are minor channels for Cl_2 consumption. The primary reaction producing Cl_2 is surface reaction #4, the reaction between gas-phase and adsorbed Cl atoms producing molecular chlorine in the gas phase. Gas reaction #18, the neutralization reaction between Cl^- and Cl_2^+, and surface reaction #2, the neutralization of Cl_2^+ on the wall, are minor channels for Cl_2 production.

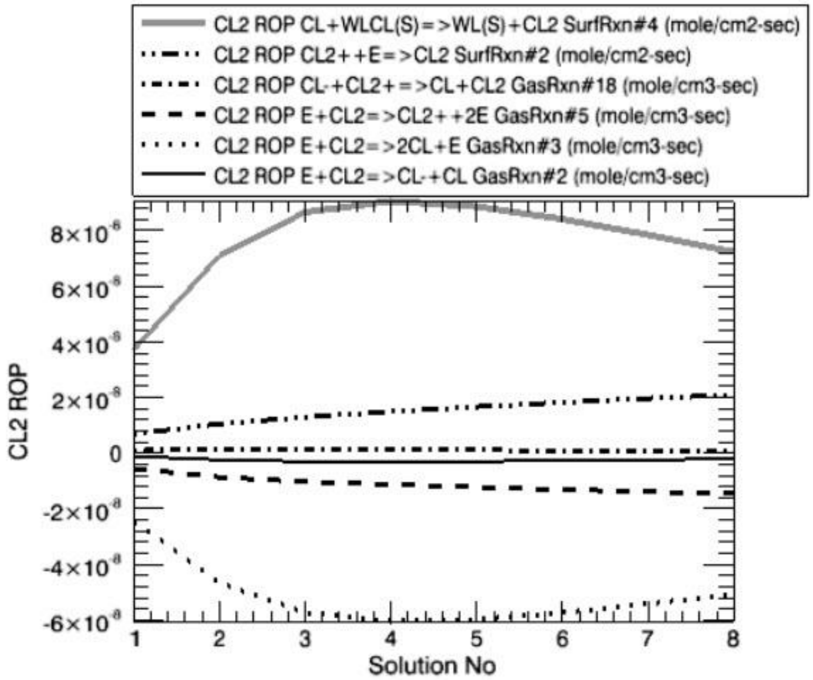

Figure 2. ROP analysis.