Metastable Argon Density Evolution in a Pulsed ICP Discharge

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Abstract—A two-dimensional self-consistent plasma fluid model was developed to study the dynamics of a pulsed power inductively coupled argon discharge. The metastable Ar^* (3P_0 and 3P_2 levels) density evolution during a pulse is governed by volumetric reactions, giving rise to complex spatiotemporal behavior.

Index Terms—Inductively coupled plasma, plasma reactor simulation, pulsed plasma.

I NDUCTIVELY coupled plasmas (ICP) are used for the etching and deposition of thin films in microelectronics manufacturing. Pulsing the plasma power may offer several advantages compared to continuous wave (cw) discharges, such as improved etch rate, selectivity, and/or uniformity, and the amelioration of anomalous etch profiles (e.g., elimination of notching). In order to improve our understanding of pulsed plasmas and elucidate their impact on wafer processing, we have simulated the spatiotemporal plasma evolution. In previous studies, a modular approach was used to simulate cw plasma operation, in which only the "steady state" was of interest [1]. In the present work, however, the coupled equations governing the system were *solved simultaneously* to resolve transients occurring in pulsed plasmas.

Simulations were performed for a two-dimensional (2-D, azimuthally symmetric) reactor of the Gaseous Electronics Conference (GEC) reference cell geometry. The mathematical model included the coupled partial differential equations of "electromagnetics" (to compute the self-consistent power deposition profiles), electron energy balance (to compute the electron temperature), and ion and neutral species mass balances (to compute the density of Ar^+ and Ar^*). The electroneutrality constraint was used instead of the Poisson equation. Since the sheath is extremely thin, boundary conditions were applied at the geometric location of the wall. The argon chemistry was the same as before [2]. A "composite" state was used to represent the long lived metastables $({}^{3}P_{0}$ and ${}^{3}P_{2}$ levels). Metastable reactions included production by excitation of ground state Ar, and destruction by two-step ionization and quenching by electrons to the resonant states. Three-body reactions were negligible under the low operating pressure. The governing equations were discretized in space

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using a Streamine Upwind Petrov Galerkin (SUPG) finite element method. The resulting set of stiff ordinary differential equations was integrated in time using an implicit solver based on backward difference formulae. Results were visualized on a 1 GHz Dell Windows NT workstation using Tecplot (Amtek Engineering, Inc., Bellevue, WA). Operating parameters were: peak power of 300 W at 13.56 MHz, pressure of 20 mtorr, gas flow of 20 sccm of pure Ar, pulsing frequency of 10 kHz, and duty ratio of 0.5. Plasma power was square-wave modulated, i.e., the power was on at full strength for the first 50 μ s and off to zero for the remaining 50 μ s of each pulse. Results shown below correspond to the periodic steady state. Only half of the reactor, and only the domain occupied by the gas phase, is shown in each frame.

Fig. 1 (upper left corner) shows the location of the planar 5-turn coil and the power deposition profile 50 μ s after the start of the pulse. The electromagnetic (EM) field is attenuated in the high-density plasma and power is deposited within the skin depth of ~ 1 cm below the quartz window. The metastable diffusion time is a few ms, much longer than the pulse period. Thus, the evolution of metastable density during a pulse, Fig. 1 ($T = 5-100 \ \mu s$), is governed by volumetric reactions. Metastable quenching by electrons to resonant states has a time constant of several μ s for an electron density of 5×10^{11} cm⁻³. At the start of the active glow, Fig. 1 ($T = 5 \ \mu s$), the Ar^{*} density is larger in the periphery of the reactor due to destruction of metastables in the core during the afterglow of the previous pulse. The metastable density then begins to rise forming a peak in the plasma core, as production of metastables by excitation picks up ($T = 10-50 \ \mu s$). As the metastable density rises, so do destruction reactions which bring about a quasi-steady-state of the metastable density ($T = 40, 50 \ \mu s$). In the afterglow, Fig. 1 ($T = 52-100 \ \mu s$), the production (by ground state excitation) rate decreases sharply owing to the large threshold (11.56 eV) and the fact that the electron temperature plummets. This leads to a dramatic decrease in metastable density in the discharge core mainly due to step-wise ionization (which has a lower threshold of 4.14 eV) in the early afterglow (T =52, 55 μ s) and quenching in the late afterglow ($T = 60-100 \ \mu$ s). There is a faster depletion rate of metastables at the core, since electrons are much more abundant there. The density profile at 100 μ s is identical to that at 0 μ s (not shown), at the periodic steady state.

In conclusion, the transient behavior of argon metastables in a pulsed ICP discharge displays intricate profiles derived from the fact that plasma chemical processes dominate over diffusion.

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Fig. 1. Power deposition profile (upper left corner) and argon metastable density profiles for various times T during a pulse of period 100 μ s (power in W/m³, densities in cm⁻³). Profiles are at periodic steady state. Each unit of the horizontal (r) and vertical (z) axes is 1 cm long. Note change of metastable density scale for each frame.

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