

Scaling of hollow cathode magnetrons for ionized metal physical vapor deposition

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Ionized metal physical vapor deposition is being increasingly used to deposit diffusion barriers and Cu seed layers into high aspect ratio trenches for microelectronics fabrication. Hollow cathode magnetrons (HCMs) represent a technology capable of depositing metal over large areas at pressures of a few millitorrs. The fundamental mechanisms of these devices are not well understood and so their optimization is difficult. In this article, results from a two-dimensional computational investigation of HCMs are discussed to illuminate scaling issues. The hybrid model incorporates algorithms whereby transport coefficients for use in fluid equations are derived using a kinetic simulation. The goal is to enable the fluid algorithms in the model to be able to more accurately represent low pressure operation. The consequences of power, pressure, and magnitude and orientation of applied magnetic fields were investigated. The authors found that the magnetic field configuration significantly affects the magnitude and distribution of fluxes incident on the substrate. A study of the Cu seed layer deposition process, carried out using a feature scale model, correlates changes in plasma properties with conformal deposition into trenches. © 2006 American Vacuum Society. [DOI: 10.1116/1.2335864]

I. INTRODUCTION

As the number of devices per die increases and their critical dimensions decrease, the RC time delay resulting from the finite resistance and capacitance of the metal interconnect wiring becomes an increasingly important consideration in optimizing the performance of integrated circuits. As a consequence, copper is the material of choice for interconnect wiring because of its lower resistance compared to aluminum. Although copper is typically deposited using electrochemical plating processes, diffusion barriers and Cu seed layers on the surface of high aspect ratio ($>5:1$) trenches and vias are typically deposited using physical vapor deposition.¹

Ionized metal physical vapor deposition (IMPVD) is increasingly being used to deposit these diffusion barriers and Cu seed layers.²⁻⁴ IMPVD typically improves bottom and sidewall coverages in the trench compared to conventional PVD due to there being a larger fraction of ionized species arriving at the wafer. In a typical IMPVD reactor, a dc voltage applied to a magnetron target accelerates ions into the target with energies of several hundred eV resulting in sputtering of the target material. An inductively coupled^{5,6} or electron cyclotron resonance plasma^{7,8} is often used as a secondary power source to increase the fraction of the metal species incident on the substrate that is ionized.

The hollow cathode magnetron (HCM) has been developed as an alternate IMPVD technology.⁹ The HCM relies on magnetic fields to generate a high-density plasma at low pressures ($\leq$ a few millitorrs) within the volume of a cup-shaped cathode target. The magnetic field is oriented parallel to a portion of the inner surface of the vertical walls of the target. This creates a closed $E \times B$ drift parallel to the cathode surface that reduces charged particle losses. The magnetic field also captures secondary electrons emitted from the cathode surface, producing an ionization source near the target surface which increases the plasma density near the cathode. The end result is efficient utilization of ions in sputtering of the cathode target. The HCM differs from conventional planar magnetrons in that a high-density plasma ($>10^{11} \text{ cm}^{-3}$) may be generated throughout the volume of the reactor.

A challenge in using PVD for Cu seed layer deposition is obtaining sufficient sidewall coverage in high aspect ratio features. Deposition of a continuous Cu seed layer of a critical thickness is essential to attaining a void-free fill of the feature when using electrochemical deposition. Poor sidewall coverage can be compensated by increasing the PVD seed layer thickness. The usefulness of this approach is limited by the amount of Cu overhang, the lateral overburden at the top of features, which leads to formation of seams and keyholes during electroplating. The ion and neutral energy distributions of the fluxes incident onto the substrate in the PVD process must be tailored to achieve conformal seed layer deposition with minimum overhang.

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The HCM is an attractive plasma source for obtaining the control necessary to insure highly conformal and uniform barrier coatings and seed layers. This results from the ability to geometrically configure the magnetic field of the HCM for a given operating pressure and power to control the uniformity of fluxes (copper species and ions) to the substrate, the ionization fraction, and their angular distributions. The use of plasma equipment models to aid in development and analysis of IMPVD processes, as in the HCM, is made difficult due to their low operating pressure where the mean free path of the gas particles is commensurate with the dimensions of the reactor. In this regime, purely fluid models may be less accurate and so one is motivated to employ kinetic or hybrid models. In this regard, kinetic simulations, such as particle-in-cell employing Monte Carlo collisions^{10,11} or direct simulation Monte Carlo,^{12,13} are attractive computational techniques, though they are also computationally intensive at the high plasma densities of IMPVD systems which requires resolution of short Debye lengths. Hybrid simulations^{14,15} which approach the accuracy of kinetic simulations and are less computationally expensive may be acceptable compromises for the conditions of IMPVD reactors.

In this article, results from a computational investigation of a HCM reactor are discussed. The model employed in the investigation uses a newly developed computational technique in which a Monte Carlo simulation for ion and neutral transport (IMCS) is integrated with fluid based transport modules with the goal of improving the accuracy of the model at lower pressures where the Knudsen number (λ/L or mean free path divided by characteristic dimension of the reactor) is large (a few tenths or more). In this model, the ion and neutral velocity distribution functions obtained from the IMCS are used to calculate transport coefficients which are then employed in momentum conservation equations for neutrals and ions. The consequences of varying power, pressure, and magnetic field magnitude and distribution on plasma properties during Cu IMPVD will be discussed. A feature scale model was used to assess the consequences of these process parameters on deposition of seed layers into trenches.

The model employed in this investigation is described in Sec. II. Results from our parametric investigation are discussed in Sec. III. Our concluding remarks are in Sec. IV.

II. DESCRIPTION OF MODEL

The model employed in this investigation is a modification of the two-dimensional Hybrid Plasma Equipment Model (HPEM).¹⁵ The modules of the HPEM used in this investigation are the electron energy transport module (EETM), the fluid kinetics module (FKM), and the plasma chemistry Monte Carlo module (PCMCM). The FKM solves continuity, momentum, and energy equations for all ion and neutral species and Poisson's equation for the electric potential. For electrons, the continuity and energy equations are solved. For charged transport in the static magnetic fields of the HCM, all transport coefficients are expressed as tensors.

Fluxes of energetic particles to surfaces are transferred to the PCMCM where the transport of sputtered and reflected atoms is modeled by Monte Carlo techniques.¹⁶ The PCMCM kinetically resolves the transport of sputtered atoms and reflected neutrals from the target, producing the nonequilibrium density of "in-flight" species prior to thermalizing to the bulk fluid.

The results from the FKM and PCMCM are transferred to the EETM where a Monte Carlo simulation (MCS) is used to track the trajectories of secondary electrons emitted from the cathode. The results of the MCS, electron impact source functions for ionization and excitation, and injected charge are transferred to the FKM. The process iterates until a converged solution is obtained. When the plasma properties converge, the PCMCM is run one last time while also including the volumetric sources of excited and ionized species. This produces the energy and angular distributions for neutrals and ions striking surfaces. The Monte Carlo feature profile model (MCFPM) then uses these distributions at the wafer to predict deposition profiles.¹⁷

The IMCS is incorporated within the FKM. The logic of the IMCS is as follows. Species (e.g., electrons, ions, and neutrals) transport can be kinetically described by the Boltzmann equation and this method provides the most accurate solution at low pressures. Unfortunately, this tends to be computationally intensive, particularly when solving Poisson's equation where the accuracy of the resulting densities must be high. As a result, moments of Boltzmann's equation are taken in order to construct the continuity equation (first moment), momentum equation (second moment), and the energy equation (third moment) producing the fluid hydrodynamic equations. In principle, the moments of Boltzmann's equations are exact solutions applicable to arbitrarily low densities if only the distribution functions are known with which the moments are taken.

The IMCS is a kinetic simulation that produces, in principle, exact particle velocity distributions functions throughout the reactor. These distributions functions are used to derive the transport coefficients used in the fluid equations (moments of Boltzmann's equation). The logic is that with these kinetically derived transport coefficients, the resulting solution should be more accurate at lower pressures since nonequilibrium effects are better captured. This technique could, in principle, dispense with the fluid simulation if the IMCS was sufficiently accurate and coupled with Poisson's equation, as in a particle-in-cell simulation. Doing so would require large computational resources. The advantage of only using the IMCS derived transport coefficients in the fluid equations is computational speed. The integration of the velocity distributions used to obtain transport coefficients can tolerate a large amount of noise in the distribution functions because the dependence of the underlying cross sections on speed is slowly varying.

The electron impact source functions, electric and magnetic fields, and the advective flow field are exported from the FKM to the IMCS. Pseudoparticles representing the ions and neutral species are launched from locations in the reactor

with statistical weightings given by the electron impact source functions obtained from the FKM or by gas sources from nozzles. The trajectories of the pseudoparticles are followed in a time dependent fashion using electric and magnetic fields interpolated from the numerical mesh. Surface reactions are represented by sticking coefficients and fractions of species that return from the surface. Particle-mesh algorithms are used to represent ion-ion, ion-radical, and radical-radical collisions. Statistics are collected during each flight of the pseudoparticles and transferred to the mesh to obtain their spatially dependent velocity distribution. With these distribution functions, transport coefficients are computed for use in the fluid equations of the FKM.

Pseudoparticles for each species j are launched in the reactor in accordance with the spatial distribution of the source functions resulting from electron impact and heavy particle collisions $S_j(r, z)$ obtained from the FKM. Particles representing the species injected from nozzles are also launched from inlets based on the specified flow rates. The number of pseudoparticles of species j launched from a given computational cell centered on (r, z) having volume $V(r, z)$ is

$$N_j(r, z) = N_t \frac{S_j(r, z)V(r, z)W_j(r, z)}{\int \left[\sum_i S_i(r, z)V(r, z)W_i(r, z) \right] d^3r}, \quad (1)$$

where N_t is the total number of pseudoparticles being launched, the sum in the denominator is over all the species being initialized, and W_i is a weighting function. The dynamic range of electron impact source functions may span many orders of magnitude. To launch a statistically relevant number of pseudoparticles, the number of particles launched from each cell is weighted by

$$W_j(r, z) = \frac{\log[S_j(r, z)]}{\log[S_m]}, \quad (2)$$

where S_m is the maximum value of all electron impact source functions. The i th particle of species j is then “tagged” as representing,

$$m_{ij} = \frac{S_j(r, z)V_j(r, z)}{N_j(r, z)}, \quad (3)$$

actual particles, with m_{ij} having units of s^{-1} . The pseudoparticles are launched with velocities

$$\mathbf{v}(r, z) = \mathbf{v}_t + \mathbf{v}_a, \quad (4)$$

where $\mathbf{v}_t$ is the thermal velocity randomly selected from a Maxwell-Boltzmann distribution having the local gas (or ion) temperature and $\mathbf{v}_a$ is the local advective velocity obtained from the FKM. Statistics on the volumetric densities $N_j(r, z)$ of each species are then obtained by integrating the time each particle spends in a given computational cell.

Trajectories are advanced by direct integration of velocities between collisions. For neutral species, the trajectories are free flight. For ions, accelerations are included as specified by the local electric and magnetic fields. These fields are obtained by performing a three-dimensional interpolation (r ,

z , and time if there is an ac phase) of the electric fields imported from the FKM. The flight time is determined by

$$\Delta t = \min(\Delta t_r, \Delta t_z, \Delta t_c, \tau), \quad (5)$$

where Δt_r and Δt_z are the times to cross a specified fraction of the computational cell in the r and z directions, Δt_c is the time to the next collision, and τ is a specified fraction of the rf cycle (if applicable). The time to next collision for species j is

$$\Delta t_{\text{col}} = - \left(\sum_k \nu_{jk} \right)^{-1} \ln(1 - r), \quad (6)$$

where ν_{jk} is the collision frequency of species j for process k and r is a random number evenly distributed on (0,1). If a particle collides with a surface during a flight (which results in the particle “appearing” in a solid) the point of intersection of the particle with the surface is back calculated. The particle is then placed at the surface where it is, if applicable, reflected either specularly or diffusively.

Collision dynamics are accounted for by constructing probability arrays for each species j . The arrays are

$$P_{ij} = \frac{\sum_{m=1}^i k_{mj} N'_{mj}}{\sum_{m=1}^{i-\max} k_{mj} N'_{mj}}, \quad (7)$$

where k_{ij} is the effective two-body rate coefficient for the i th heavy particle collision of species j and N'_{ij} is the density of its collision partner. The prime indicates that the maximum density of the collision partner throughout the reactor is used to construct these arrays, thereby implementing a modified null cross section.

When a particle reaches the randomly selected time for a collision, the collision that occurs is determined by selection of another random number r . The collision, which occurs satisfies $P_{i-1j} < r \leq P_{ij}$. Given this choice of collision, the actual occurrence of the collision is denoted by the choice of another random number r ,

$$r \leq \frac{N_{ij}(r, z)}{N'_{ij}}, \quad (8)$$

where $N_{ij}(r, z)$ is the actual local density of the collision partner. This technique allows for null collisions to account for transport of the particle between locations having different densities of the collision partners.

If the collision is an identity changing collision (such as a chemical reaction or charge exchange collision), the particle characteristics are appropriately changed. In the case of thermal chemical reactions in the bulk plasma, the velocities of the products are randomly chosen from a Maxwell-Boltzmann distribution having the local gas temperature. If the reaction is exothermic, this additional energy is accounted for in the reaction products. For charge exchange collisions, the hot neutral retains the original ion's velocity. The rate coefficients for elastic collisions are calculated using Lennard-Jones parameters to simulate hard sphere collisions.

Surface reactions are included using reactive sticking coefficient r_s which specifies the probability that the pseudoparticle reacts with the surface (and is removed from the gas phase). When a particle collides with the surface, a random number is chosen. If $r \leq r_s$, a reaction occurs. If the inequality does not hold, the particle is diffusively reflected from the surface with a speed randomly chosen from a Maxwell-Boltzmann distribution having the wall temperature. If the reaction occurs, another random number is chosen to determine disposition of the particle in accordance with the surface reaction mechanism using the same technique as for gas phase collisions. The particles, which are returned to the gas, leave from the surface with polar angle based on a modified cosine or Lambertian distribution. In the case of ions, the neutralized particle is allowed to return to the plasma with a specified fraction of its incident energy, which allows for specular scattering from the surface.

The reaction mechanism for the Ar/Cu plasma addressed here is the same as that used in Ref. 18 augmented by sputter heating of neutrals as described in Ref. 16. The species for which the temperatures and transport coefficients were computed using the IMCS are Ar, Ar⁺, Cu(²S), Cu(²D), and Cu⁺. The electron-argon collision mechanism includes electron impact excitation of Ar from ground state to excited states 4s and 4p (which are lumped into a single species Ar*) and electron impact ionization (from Ar ground state and Ar*). The electron-copper chemistry includes electron impact excitation of Cu from ground state Cu(²S_{1/2}) to higher excited states ²D_{5/2}, ²D_{3/2}, ²P_{1/2}, ²P_{3/2} [which are lumped into a single species Cu(²D) or Cu*], and electron impact ionization (from Cu ground state and Cu*). The Cu* is quenched by collisions with Cu, Cu*, and Ar. The Ar* reacts with Ar* to produce Ar⁺ and with Cu or Cu* to produce Cu⁺ through Penning processes. Charge exchange reactions play an important role in generating fast neutral fluxes to the target and ionizing Cu atoms before they reach the substrate. The charge exchange reactions also include resonant exchange among the Ar species or the Cu species, which contributes to gas heating. The reaction mechanism used for the MCFPM is the same as that described in Ref. 17, including surface diffusion of Cu atoms.

III. CU IMPVD IN A HOLLOW CATHODE MAGNETRON SOURCE

Our computational investigation was carried out using the reactor geometry shown in Fig. 1, which is our interpretation of the Novellus 200 mm reactor.⁹ The cathode consists of a cup-shaped Cu target with permanent magnets at the sides and at the top. An electromagnetic is located below the permanent magnets. A metal ring and the substrate are electrically floating. Gas is injected radially inward and a pump port surrounds the substrate. Base case conditions are an argon gas pressure of 5 mTorr, cathode power of 10 kW, and gas flow of 125 sccm (sccm denotes cubic centimeter per minute at STP). The magnetic field, also shown in Fig. 1, is configured to be parallel to the inner surface of the cathode, approximately 80 G at the midpoint, and have a cusp at the

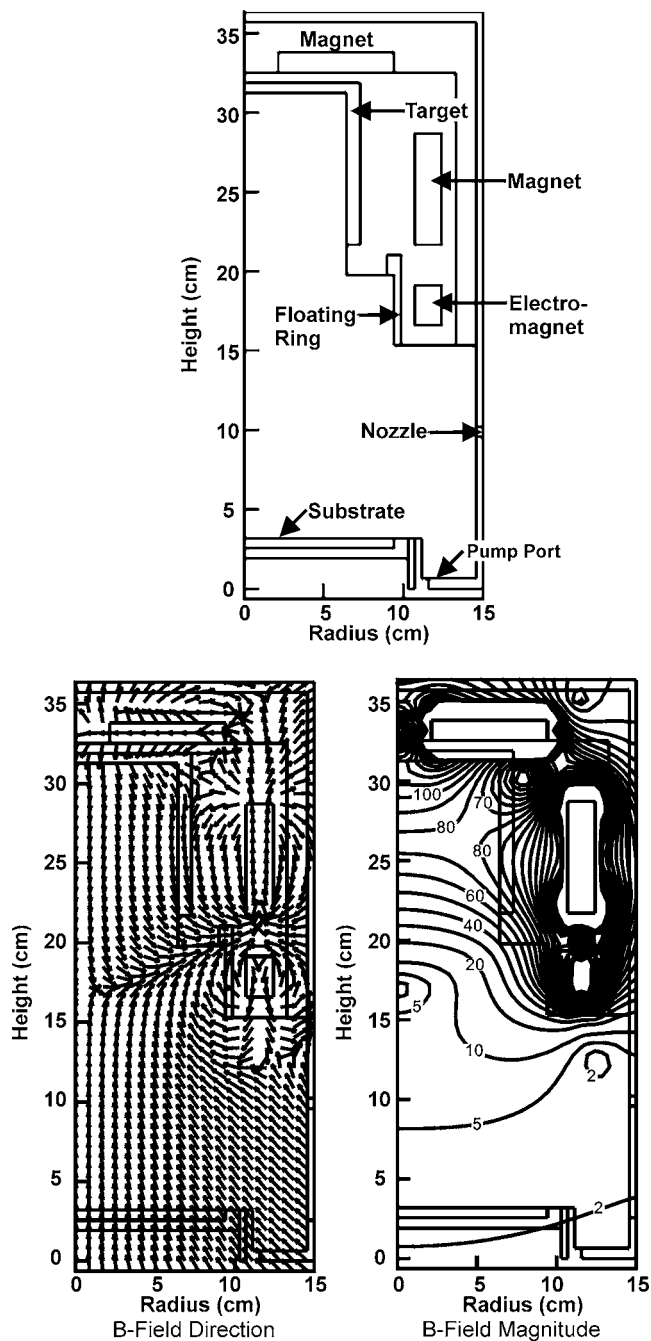


FIG. 1. Schematic of the hollow cathode magnetron source used in this investigation. (a) Components, (b) direction of the magnetic field for a cusp located at 18 cm, and (c) magnitude of the magnetic field for 70 G at the face of the magnetron.

mouth of the cathode. This cusp can be translated in the vertical direction by varying the strength of the electromagnet. The magnetic field is configured to so that the $E \times B$ drift produces a closed loop parallel to the vertical face of the cathode.

Typical plasma conditions are shown in Figs. 2 and 3 for the base case. As shown in Fig. 2, the electron temperature T_e has a maximum of 4.5 eV near the face of the cathode, producing a confined region of ionization by bulk electrons inside the cathode having a maximum value of 2.4

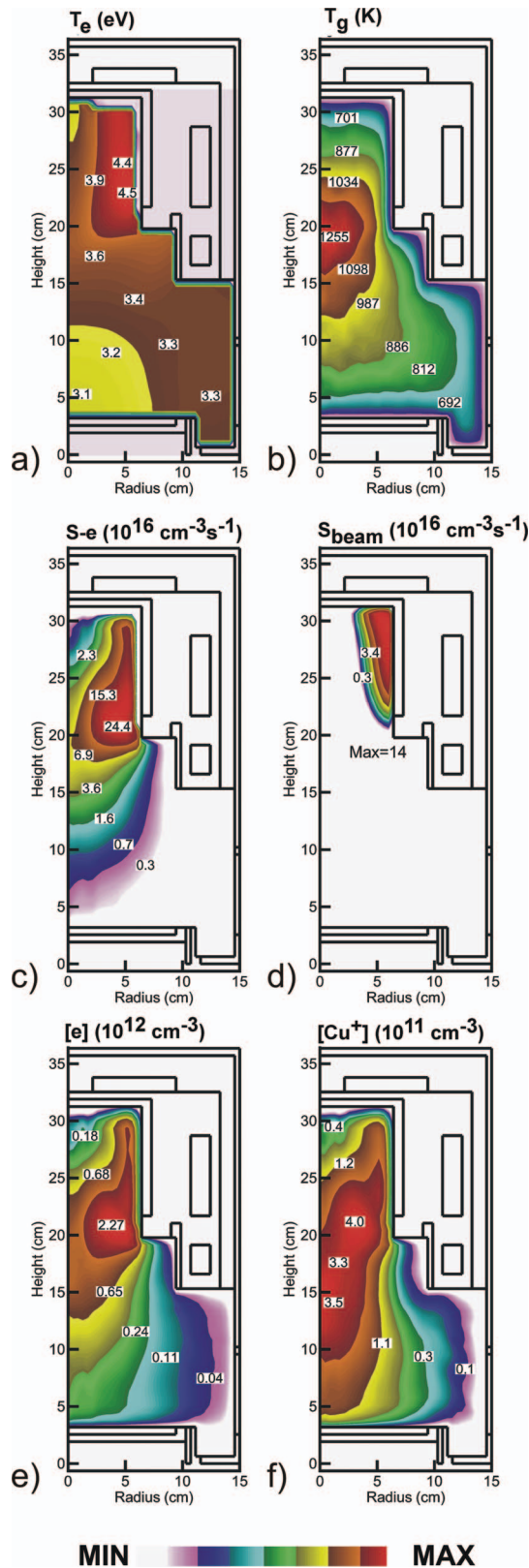


FIG. 2. Plasma parameters for the base case (5 mTorr, 10 kW, 80 G). (a) Electron temperature, (b) gas temperature, (c) ionization source by bulk electrons, (d) ionization source by beam electrons, (e) electron density, and (f) Cu^+ density. The contours are labeled in the units shown at the top of each figure. Other than T_e and T_g , plots have a 2-decade log scale.

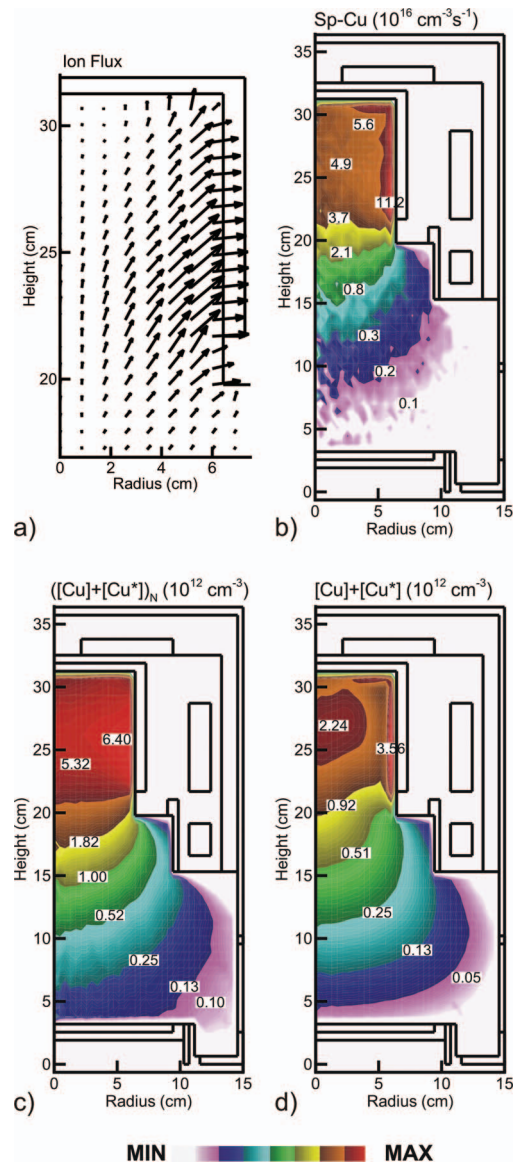


FIG. 3. Plasma parameters for the base case (5 mTorr, 10 W, 80 G). (a) Ion flux vectors, (b) source of thermal Cu resulting from collisions of sputtered Cu atoms, (c) total density of nonthermal Cu atoms, and (d) total density of thermal Cu atoms. The contours are labeled in the units shown at the top of each figure. Plots have a 2-decade log scale.

$\times 10^{17} \text{ cm}^{-3} \text{ s}^{-1}$. In spite of having a low mobility across the magnetic field, T_e persists to the substrate with a value of 3 eV. Ionization by beam electrons resulting from secondary emission from the cathode has a similar peak value, $1.4 \times 10^{17} \text{ cm}^{-3} \text{ s}^{-1}$, but is more tightly confined as these electrons are captured on the magnetic field lines parallel to the cathode. The resulting electron density also has a peak value inside the cathode, $2.2 \times 10^{12} \text{ cm}^{-3}$, extending through the cusp in the magnetic field into the diffusion chamber below. The power deposition of 10 kW is dominantly dissipated by ion acceleration into the cathode; however a non-negligible amount of power is dissipated by gas heating, predominantly by resonant charge exchange collisions, producing a peak gas temperature of 1300 K. The Cu^+ density peaks at about $4 \times 10^{11} \text{ cm}^{-3}$, resulting in about 20% of the ions being Cu^+

and the remainder Ar^+ . The fraction of ions that are Cu^+ increases as the substrate is approached due to charge exchange from Ar^+ and increasing residence time of sputtered Cu atoms as they transition from target to substrate. The longer residence time increases the probability of the Cu atoms being ionized by electron impact.

Ion fluxes to the cathode, the source of sputtered Cu atoms, and the density of nonthermal and thermal Cu atoms are shown in Fig. 3. The magnetron effect concentrates ion flux vectors onto the interior vertical surface of the cathode. The ions arrive at the cathode surface with an energy nearly equal to the cathode voltage (-280 V), sputtering the target, and producing a source of energetic Cu atoms. (The actual distribution of sputtered Cu energies was used in the model as in Ref. 18. The peak energy is approximately 3.5 eV.) Through collisions, the sputtered Cu atoms slow in the gas producing a source of thermalized Cu atoms while heating the collision partners. The nonequilibrium (or in-flight) densities of copper are those atoms sputtered from the cathode that have not thermalized to an energy less than twice the local gas temperature. The density of the nonthermal Cu atoms dominates inside the cathode as few thermalizing collisions occur. As collisions occur during the nonthermal atoms' transit across the reactor, the nonthermal density decreases more rapidly than the density of thermal atoms. Near the substrate, the contributions to the flux of Cu to the substrate are roughly equal between nonthermal and thermal atoms.

The scaling of plasma parameters with pressure results from a competition between increasing confinement of charged particles by the magnetic field at low pressures and more confinement of easily ionized metal atoms by collisions at higher pressures. For example, the electron density for pressures of 1, 2.5, and 10 mTorr is shown in Fig. 4 for a power deposition of 10 kW. (See Fig. 2 for results at 5 mTorr.) The gas flow rate was scaled with pressure to provide approximately the same residence time. The peak electron density does not significantly change over this range of pressures. The spatial distribution of the electrons, however, shifts from being peaked near the cusp of the magnetic field in the throat of the cathode at 1 mTorr to being near the cathode at 10 mTorr where the ionization by beam electrons is largest. The spatial distributions of electron density are nearly the same at higher pressures as at 10 mTorr. The electron density shifts lower into the reactor at lower pressures. This can be attributed to a larger E/N (electric field/gas number density) and higher electron temperature lower in the reactor due to the plasma being more resistive. For example, the cathode voltage required to deliver 10 kW decreases from -630 V at 1 mTorr to -210 V at 10 mTorr. This results in ionization being progressively dominated by collisions in the bulk plasma at lower pressures and beam ionization by secondary electrons near the cathode at the higher pressures, as shown in Fig. 4.

The radially averaged fluxes of Cu, ions, Cu^+ fraction of the Cu flux, and the fraction of the Cu flux, that is nonthermal are shown in Fig. 5. The longer mean free paths of Cu

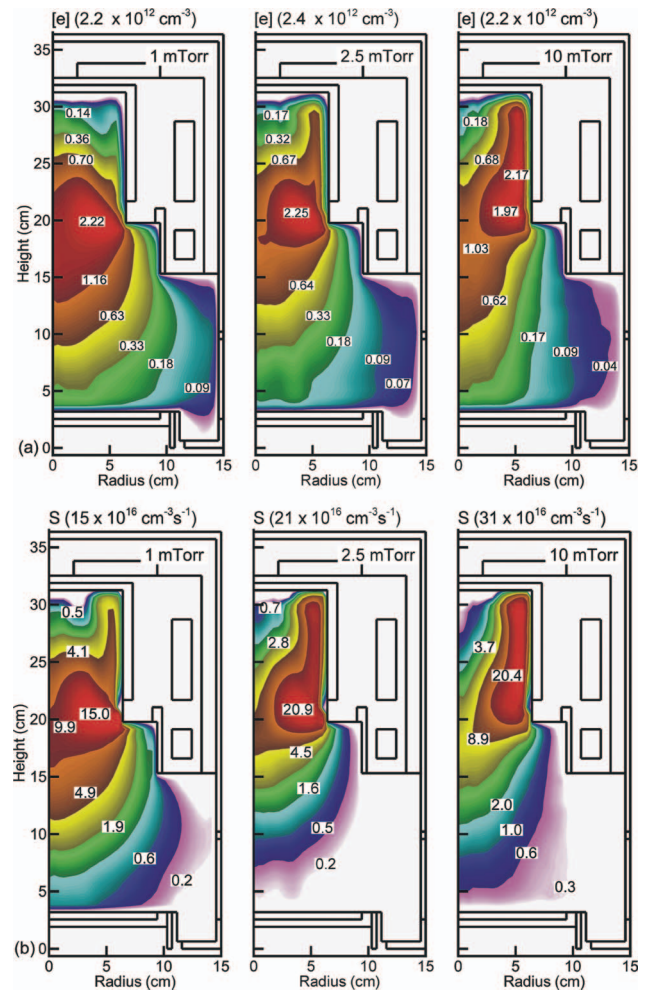


FIG. 4. Plasma parameters as a function of pressure. (a) Electron density and (b) ionization source. The contours are labeled in the units shown at the top of each figure. The plasma density migrates to the axis as the pressure is lowered. Plots have a 2-decade log scale. Color bar is the same as in Fig. 2.

atoms at lower pressures enable a larger fraction of the sputtered flux to reach the substrate as nonthermal atoms. These atoms do not undergo diffusive collisions which would otherwise increase losses to sidewalls. The less collisional transit of the atoms from the target to the substrate also results in there being fewer ionizing collisions (both charge exchange from Ar^+ and electron impact). The end result is that the radially averaged flux of Cu (neutral and ionized) decreases with increasing pressure from 2 to 10 mTorr while the total ion flux and ionized Cu fraction increases. These trends are similar to those found in conventional IMPVD systems.³ As the pressure increases the rate of thermalizing collisions of sputtered copper atoms increases. As a result, the fraction of the total neutral copper flux that is nonthermal decreases with increasing pressure. At pressures below 2.5 mTorr, greater than 95% of the neutral copper flux to the substrate is nonthermal. At pressures above 20 mTorr, the fraction that is nonthermal is less than 1%.

The total neutral copper flux (thermal and nonthermal) and copper ion flux to the substrate as a function of radius are shown in Fig. 6(a) for different pressures. At pressures of

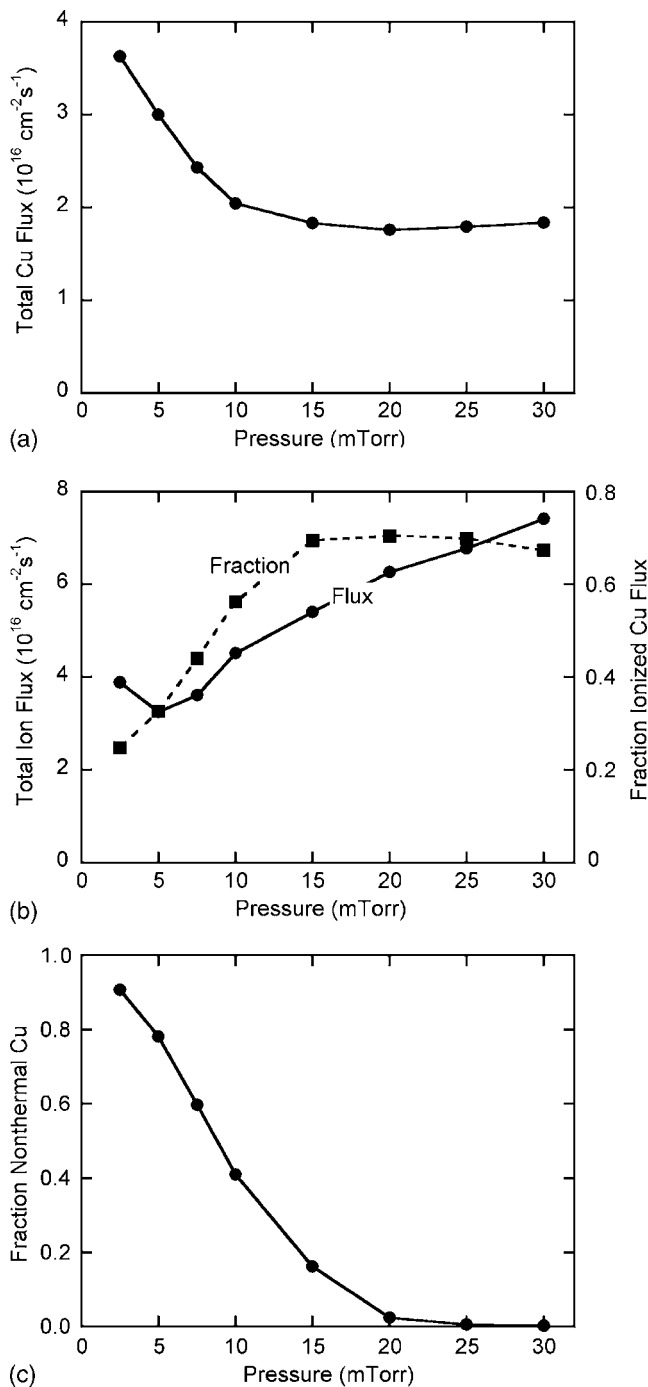


FIG. 5. Flux parameters averaged over the wafer as a function of pressure. (a) Total flux of Cu (neutrals and ions), (b) total ion flux and fraction of the Cu flux that is ionized, and (c) fraction of neutral Cu flux that is nonthermal.

1, 2.5, and 10 mTorr, the neutral fluxes are fairly uniform and, with the exception of 10 mTorr, are dominated by the nonthermal flux. The ion fluxes are also fairly uniform at 1 and 2.5 mTorr but become center weighted at 10 mTorr. This results from the more highly confined source of ionization (see Fig. 4) that aligns with the cusp of the magnetic field in the center of the reactor.

The ion energy distributions (IEDs) for Cu^+ obtained from the IMCS at different heights in the reactor at 3 mTorr and a

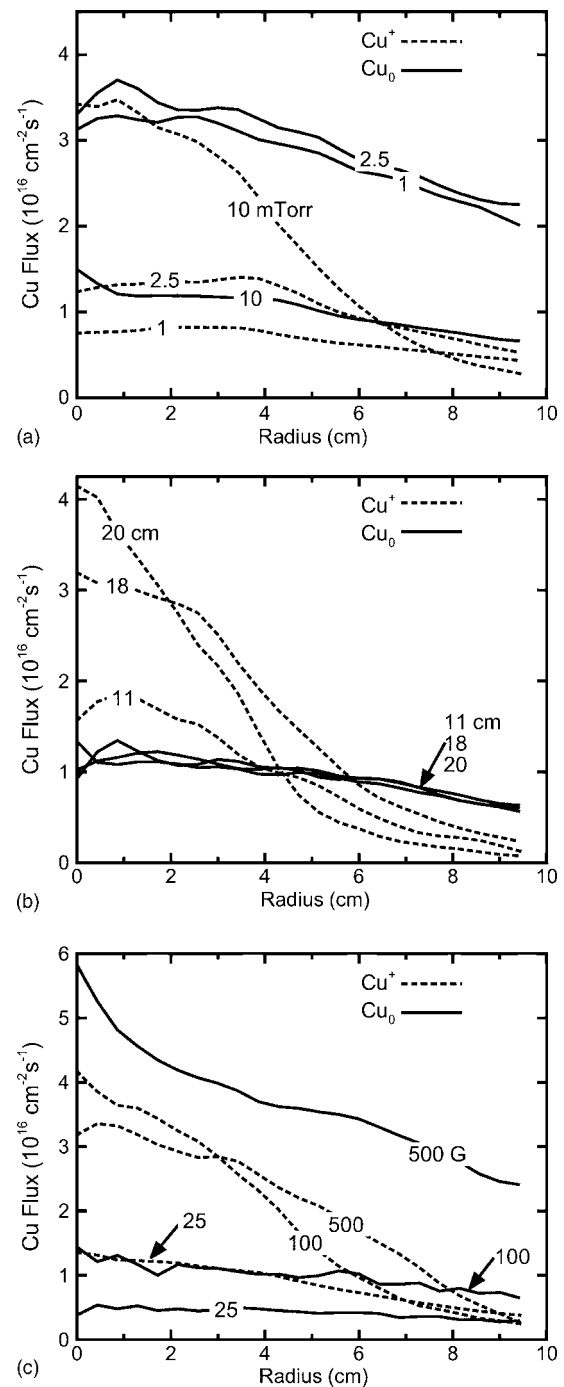


FIG. 6. Cu flux onto the wafer as a function of radius for different (a) pressures, (b) cusp locations, and (c) magnetic fields. Cu_0 is the total flux of copper neutrals (thermal and nonthermal).

radius of 3.5 cm are shown in Fig. 7. In the center of the reactor near the peak of the plasma potential ($h=16$ and 20 cm) the IEDs are nearly thermal at low energies with a high energy tail, displaying a two-temperature distribution. The lower temperature results from newly ionized thermal Cu atoms. The higher temperature results from ionized nonthermal Cu atoms and drift in the radial ambipolar electric field. At larger heights in the reactor ($h=24$ and 28 cm) ions are accelerated towards the cathode, elevating both the low

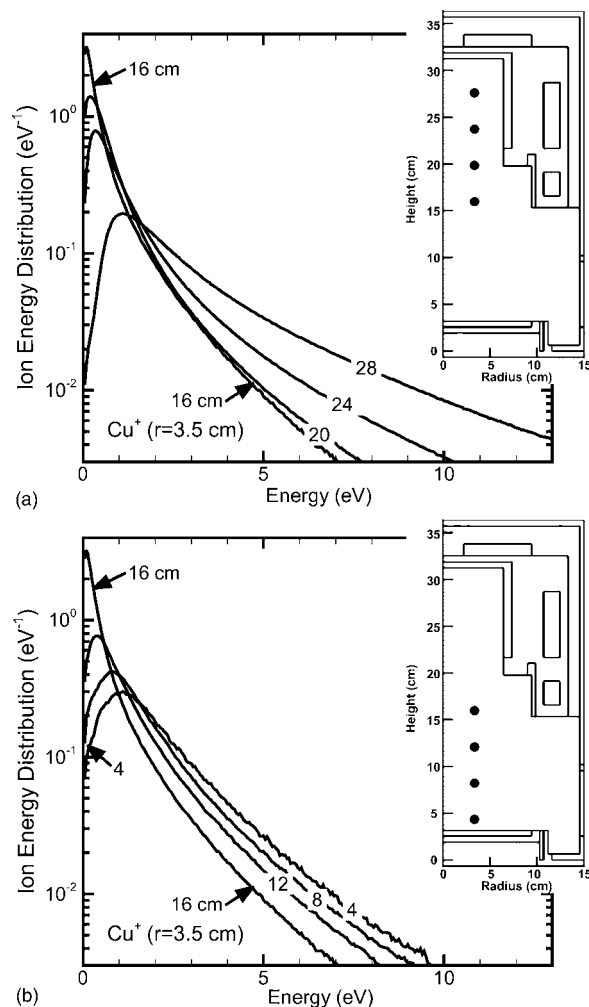


FIG. 7. Ion energy distributions for Cu^+ at 3 mTorr and a radius of 3.5 cm at different heights (h) in the reactor. (a) Heights of 16–28 cm and (b) heights of 4–16 cm.

and high temperatures. Similarly, moving lower in the reactor ($h=12$, 8, and 4 cm) the IEDs also heat as ions are accelerated in the increasing electric fields as the negative floating potential of the substrate is approached.

The neutral energy distributions (NEDs) for ground state Cu^2S and metastable Cu^2D are shown in Fig. 8 at different heights in the reactor. At all heights, there is a high energy tail extending to 3–4 eV which represents the nonthermal sputtered atoms. Somewhat counterintuitively, the most thermal distributions are found deep in the cathode ($h=20$ and 28 cm). Upon approaching the substrate ($h=4$ and 12 cm), the low energy thermal portion of the NEDs diminishes. This trend is likely the result of a larger fraction of the neutrals having undergone charge exchange reactions as their average residence time increases during their transit from the cathode to the substrate. With the exception of deep in the cathode ($h=20$ and 28 cm), the Cu^2S is generally hotter than the metastable Cu^2D . This is likely a result of the sputtered atoms being exclusively in the ground state. The Cu^2D atoms are therefore created by electron impact exci-

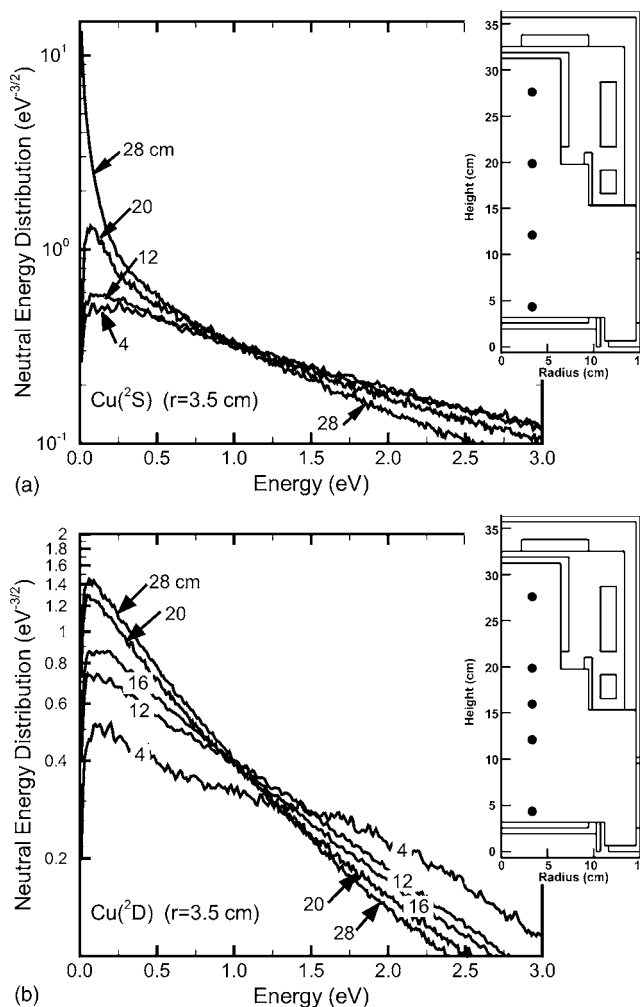


FIG. 8. Neutral Cu energy distributions at 3 mTorr and a radius of 3.5 cm at different heights (h) in the reactor. (a) Cu^2S and (b) Cu^2D .

tation of Cu^2S which, after a finite residence time in the reactor, will have undergone at least a few thermalizing collisions.

IEDs for Cu^+ high in the reactor ($h=24$ cm) inside the cathode and above the substrate ($h=4$ cm) are shown in Fig. 9 at a radius of 3.5 cm for different pressures; the operating conditions (e.g., power and magnetic field) are otherwise the same. High in the reactor, the IEDs are relatively independent of pressure below 6–10 mTorr. Above 10 mTorr, the IEDs become less thermal by losing the lowest energy component. This trend is a result of an increasing bulk electric field at these intermediate pressures. As the pressure increases, the plasma transitions from having a maximum density on the axis to having a maximum density nearer the cathode, as shown in Fig. 4. This occurs while the maximum value of the plasma density decreases. To deliver the same power, the bulk electric field increases to compensate for the lower conductivity. The end result is heating of the bulk ions. This is somewhat counterintuitive as the increase in pressure increases the electron collision frequency which, for magnetized electrons, should increase the cross field conductivity.

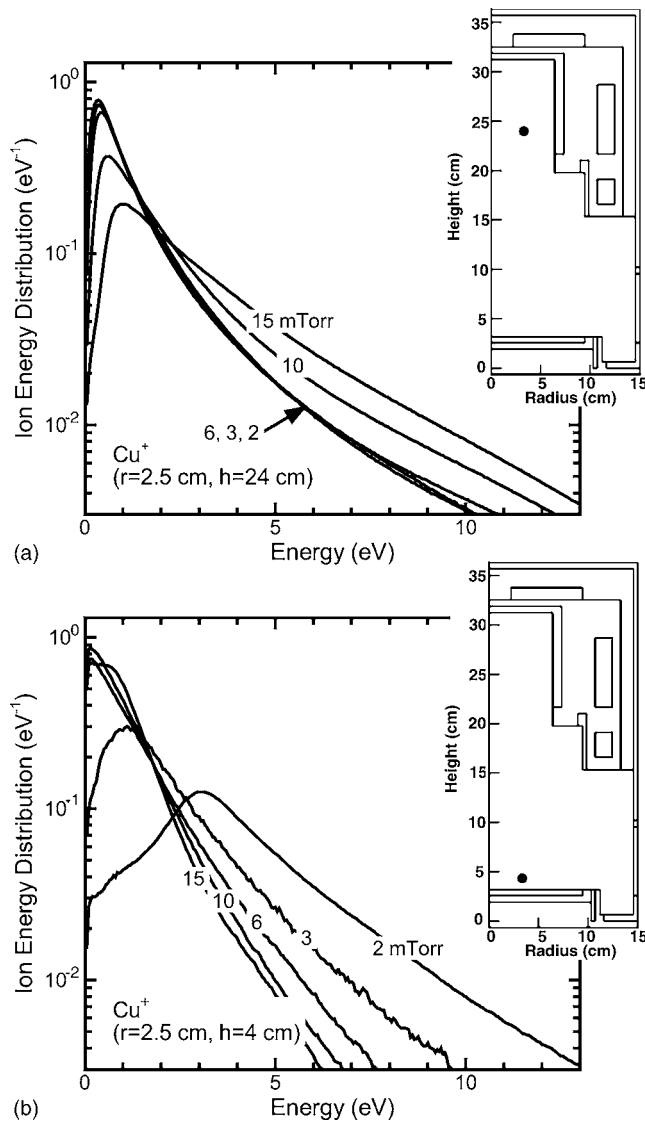


FIG. 9. Ion energy distributions for Cu^+ for different pressures at a radius of 3.5 cm at a height of (a) 24 cm and (b) 4 cm.

Although the electron collision frequency does increase, it is still small compared to electron cyclotron frequency for many tens of Gauss.

The trend for the change in the shape of the IEDs with changing pressure near the substrate is opposite from that inside the cathode. Near the substrate, the IEDs become less thermal with decreasing pressure. The substrate is electrically floating and so there is no net current to the substrate. As a result, there is little increase in bulk electric fields in the vicinity of the substrate with increasing pressure as there is higher in the reactor. The heating of the IEDs as the pressure decreases reflects an increase in the floating potential (more negative) of the substrate. At pressures below 5 mTorr, the IEDs take on a beamlike appearance, resulting from a collisionless acceleration through the presheath.

Ion energy and angular distributions (IEADs) for all ions striking the substrate and averaged over the substrate are shown in Fig. 10 for 3, 6, and 15 mTorr. At 15 mTorr, the

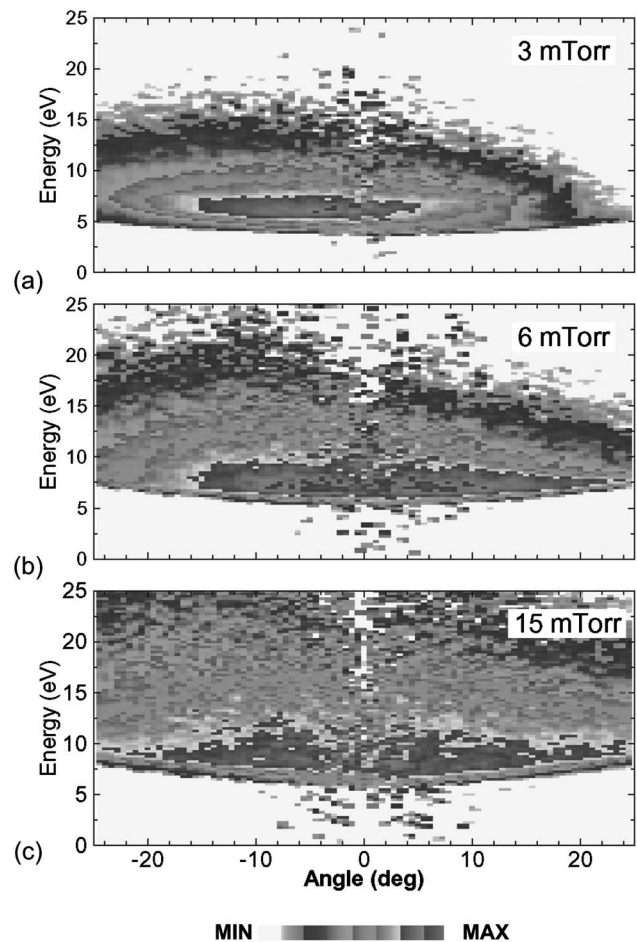


FIG. 10. Total ion energy and angular distributions averaged over the wafer for (a) 3 mTorr, (b) 6 mTorr, and (c) 15 mTorr. The contours are a log-scale over two decades. The angular distributions become less symmetric at low pressure due to the divergence of the ions emerging from the cusp.

angular distribution is nearly symmetric. At lower pressures, the distribution becomes angularly asymmetric. This trend results from the plasma below the cusp becoming more concentrated along the axis as the pressure decreases, as shown in Fig. 4. For example, at 3 mTorr, the plasma becomes almost jetlike as ions emerge through the cusp towards the substrate. Since the probability of collisions is low, the divergent trajectories of the ions are preserved to the substrate and so produce the angularly asymmetric IEAD. As such, the location of the cusp in the magnetic field is an important parameter for controlling the angular distributions of ions to the substrate.

Plasma parameters (electron density, electron source function, and ionization fraction) are shown in Fig. 11 as a function of the location of the cusp in the magnetic field. The cusp heights are $h=11$, 18, and 20 cm. The radial distribution of the fluxes of neutral and ionized Cu to the substrate for cusps having these heights is shown in Fig. 6(b). The total fluxes are shown in Fig. 12 as a function of height of the cusp. When the cusp is located low in the reactor ($h=11$ cm), electron impact source functions and the peak in the charged particle densities are located above the height of

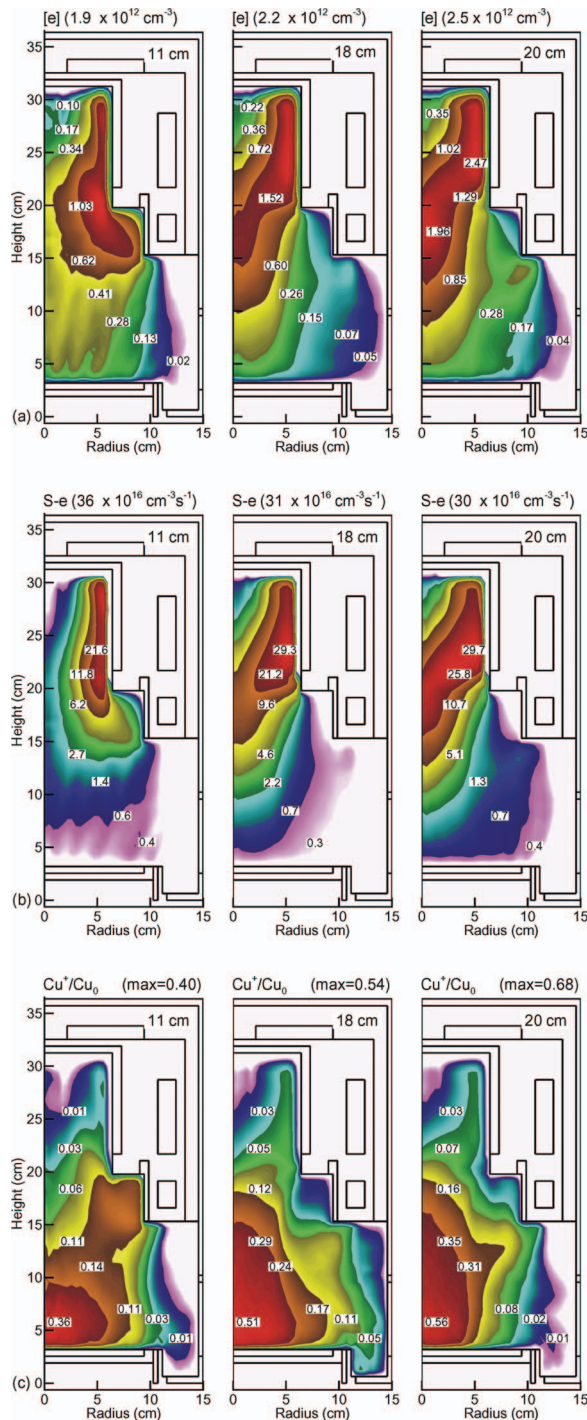


FIG. 11. Plasma parameters as a function of the height of the cusp in the magnetic field. (a) Electron density, (b) ionization source, and (c) ionization fraction of Cu. The contours are labeled in the units shown at the top of each figure. The plasma density migrates to the axis as the cusp is raised. The plots have a 2-decade log scales. Color bar is the same as in Fig. 2.

the cusp. For these conditions, the ionization sources and charged particle densities tend to peak off axis near the cathode where the ionization by beam electrons and the electron temperatures are the highest. There is a moderate amount of focusing of the plasma towards the axis by the cusp as the ion flux nears the substrate. The end result is that the ion flux

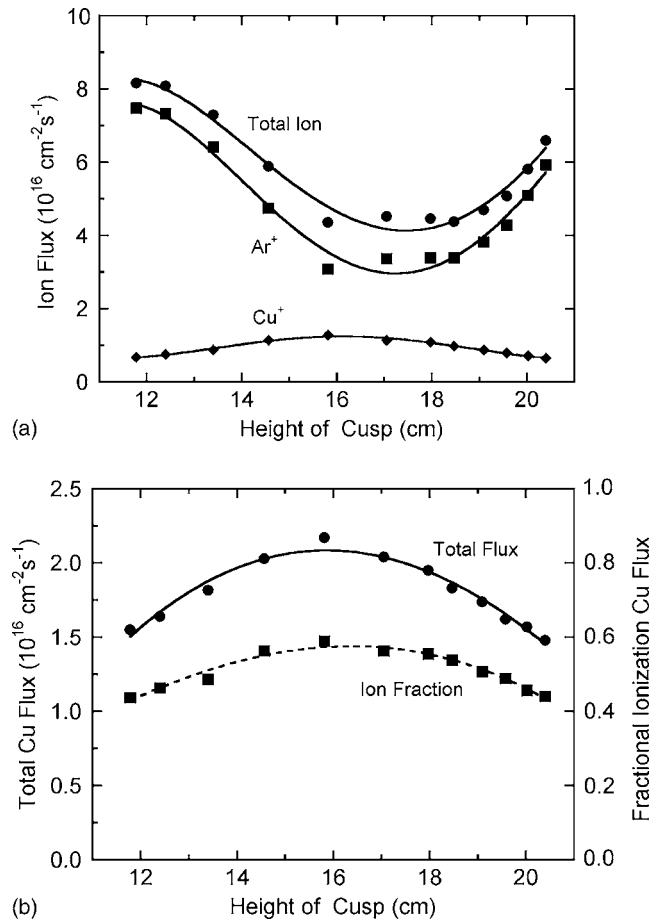


FIG. 12. Flux parameters averaged over the wafer as a function height of the cusp. (a) Ion fluxes and (b) total flux of Cu (neutrals and ions) and fraction of neutral Cu flux that is ionized.

to the substrate has a moderately center peaked profile. As the cusp is raised higher in the reactor ($h=18$ and 20 cm), the focusing of the source of ionization and of the ion density towards the axis is more severe. This results from the increasing magnitude of the transverse component of the magnetic field near the cathode preventing radial expansion of the plasma. The end result is that the radial profile of the ion fluxes to the substrate is more center peaked as the height of the cusp increases. The peak electron density in the reactor increases from $1.9 \times 10^{12} \text{ cm}^{-3}$ for $h=11$ cm to $2.5 \times 10^{12} \text{ cm}^{-3}$ for $h=20$ cm. This is only a moderate change which is likely a consequence of the total power being constant.

The radial distribution and magnitude of the neutral copper flux to the substrate are nearly independent of the location of the cusp, as shown in Fig. 6(b). The source of Cu neutrals is sputtering of the target. The total rate of sputtering is largely determined by the total power of ions incident onto the cathode. Since the total power is held constant, the total production of Cu atoms is approximately the same as is rarefaction by gas heating. The subsequent trajectories of the sputtered neutrals are not affected by the magnetic field. The change in neutral Cu flux to the substrate is then determined by the likelihood that the Cu atoms are ionized prior to

reaching the substrate. As shown in Figs. 11(c) and 12(b), the ionization fraction increases towards the center of the reactor as the cusp moves upwards, a consequence of the ion density being focused towards the axis. However, when averaged over the wafer, the ionization fraction does not significantly change.

The total ion flux (sum of Cu^+ and Ar^+) is a minimum for a cusp height of about 17 cm which also corresponds to a maximum in the total Cu flux. At these intermediate cusp heights, the flux of Ar^+ goes through a minimum whereas that of the Cu^+ goes through a maximum. The minimum in the total ion and Ar^+ flux occurs while the peak electron density is increasing and the total power is constant. The increase in the peak electron density with increasing cusp height (see Fig. 11) results from the transport of electrons in the magnetic field which geometrically concentrates the plasma density on axis. The total inventory of the plasma does not appreciably change. The minimum in the ion flux reaching the substrate indicates that the total ionization efficiency may also be passing through a minimum. The cause of the decrease in ionization efficiency may result from the change in magnetron voltage required to maintain constant power as the cusp height is increased. The cathode voltages are -280 , -210 , and -190 V when the cusp is located at 11, 16, and 20 cm, respectively.

Another parameter that may be used to optimize the fluxes to the substrate is the absolute magnitude of the magnetic field. For example, the total ion density, Cu nonthermal density, and ion flux vectors are shown in Fig. 13 for magnetic fields of 25, 100, and 500 G. Neutral and ion fluxes to the substrate are shown in Fig. 6(c) for these magnetic fields. The total fluxes to the substrate are shown in Fig. 14 as a function of magnetic field strength. The pressure (10 mTorr) and cathode voltage (-200 V) are held constant. As the magnetic field strength increases the peak ion density also increases from $1.0 \times 10^{12} \text{ cm}^{-3}$ for $B=25$ G to $5.8 \times 10^{12} \text{ cm}^{-3}$ for $B=500$ G. Further increases in the magnetic field produce a small decrease of peak ion density to, for example, $5.6 \times 10^{12} \text{ cm}^{-3}$ for $B=2000$ G. These changes in ion density track the change in total power (for fixed cathode voltage) as the magnetic field is changed, shown in Fig. 14(c). These trends results from the shorter penetration distance of secondary beam electrons emitted from the cathode as the magnetic field increases. The Larmor radius decreases from 0.25 cm for 25 G to 0.12 mm for 500 G, thereby trapping secondary electrons closer to the target and producing more efficient ionization. As the magnetic field further increases, the smaller Larmor radius becomes a liability as electrons are lost back to the cathode and ionization efficiency decreases.

The increase in ion density and power with increasing magnetic field produces a higher rate of sputtering and an increase in the density of Cu. This trend is shown in Fig. 13(b) where the nonthermal Cu density is shown. The peak nonthermal density increases from $3.1 \times 10^{12} \text{ cm}^{-3}$ at 25 G to $1.7 \times 10^{13} \text{ cm}^{-3}$ for $B=500$ G. The peak nonthermal Cu density decreases to $1.3 \times 10^{13} \text{ cm}^{-3}$ for $B=2000$ G. The

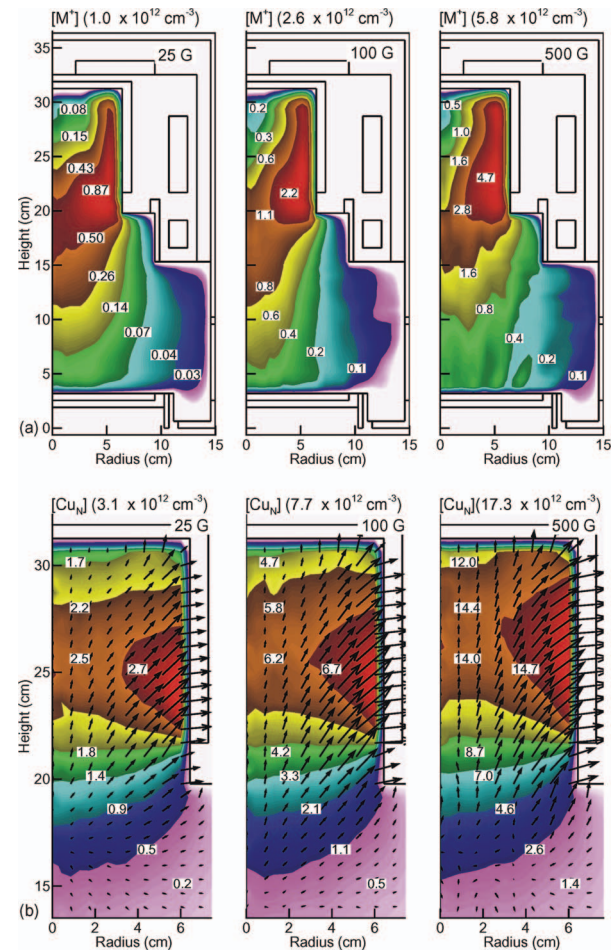
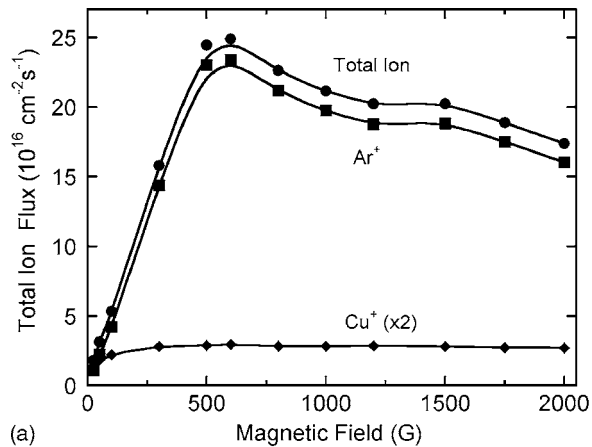


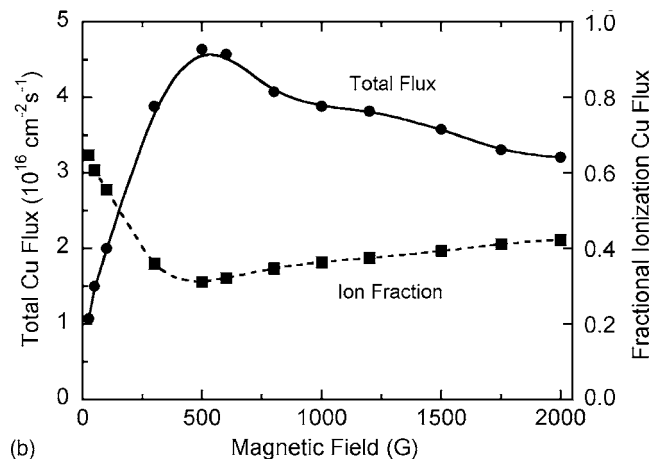
FIG. 13. Plasma parameters as a function of the magnitude of the magnetic field. (a) Total ion density and (b) density of nonthermal Cu atoms with ion flux vectors superimposed. The contours are labeled in the units shown at the top of each figure. The plasma more uniformly covers the surface of the cathode as the magnetic field is increased.

distribution of ion flux onto the cathode becomes more uniform as the magnetic field increases to 500 G. This trend is a consequence of the $E \times B$ forces, which are largely parallel to the cathode, beginning to dominate over the ambipolar forces. As a result, the peak in the nonthermal Cu density moves progressively to higher locations in the cathode as the magnetic field is increased.

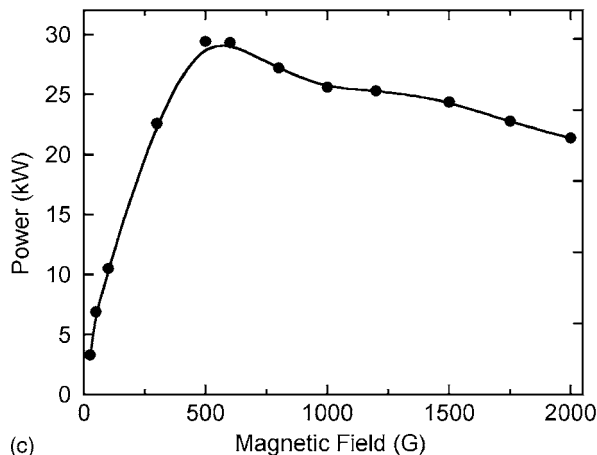
The total fluxes to the substrate as a function of power are shown in Fig. 15. When keeping the pressure and magnetic field constant, the spatial distributions of densities and fluxes change little as a function of power. What changes do occur can be attributed to the increasing rarefaction due to gas heating as the power increases and so the changes resemble the trends for decreases in pressure. The total ion flux to the substrate increases nearly linearly with power deposition as does the total Cu flux. The ionization fraction does, however, decrease with increasing power as it does with a decrease in pressure. The decrease in ionization fraction can be attributed to the increasing rarefaction due to gas heating. The lower rate of scattering of Cu atoms after they are sputtered from the cathode as the gas density decreases with increasing



(a)



(b)

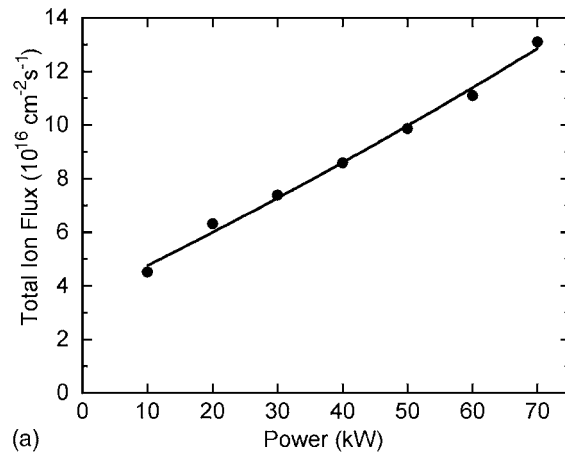


(c)

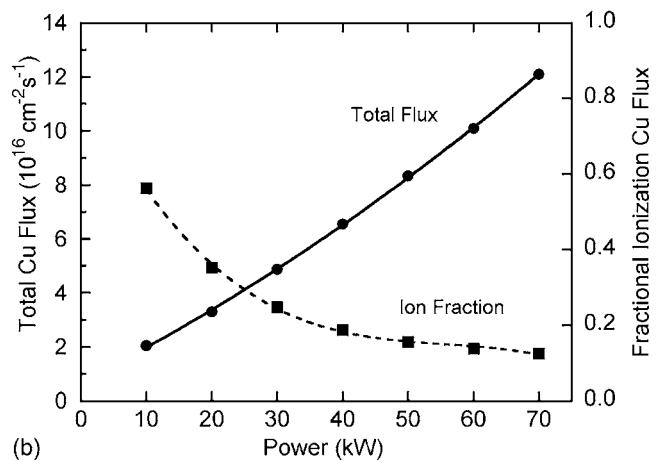
FIG. 14. Flux and plasma parameters averaged over the wafer as a function magnetic field for constant cathode voltage. (a) Ion fluxes, (b) total flux of Cu (neutrals and ions) and fraction of neutral Cu flux that is ionized, and (c) discharge power. The plasma density and power increase with increasing magnetic field due to more efficient ionization and reduced diffusion losses.

power results in a shorter residence time and lower likelihood for there to be ionizing electron collisions.

Similar trends for plasma properties occur when changing the magnitude of the magnetic field while holding the total power deposition constant. For example, plasma properties are shown in Fig. 16 for the HCM operating at 5 mTorr when varying the magnitude of the magnetic field while



(a)



(b)

FIG. 15. Flux parameters averaged over the wafer as a function of power. (a) Total ion flux and (b) total flux of Cu (neutrals and ions) and fraction of neutral Cu flux that is ionized.

keeping the power deposition constant at 10 kW. The spatial distribution of the plasma when changing the magnetic field qualitatively behaves the same as when the voltage is fixed. With increasing magnetic field, the $\mathbf{E} \times \mathbf{B}$ forces at the face of the cathode become more influential and the distribution of the ion flux across the face of the cathode becomes more uniform. The maximum in plasma density also moves towards the cathode. Both of these trends are similar to those shown in Fig. 13 for fixed voltage. As when holding the voltage constant and increasing the magnetic field, the confinement of the plasma improves, utilization of the secondary electrons as ionization sources improves, and so the peak ion density increases, as shown in Fig. 16(a). The peak ion density increases from $1.9 \times 10^{12} \text{ cm}^{-3}$ at $B=35 \text{ G}$ to $4.1 \times 10^{12} \text{ cm}^{-3}$ at $B=450 \text{ G}$. As when holding the voltage constant, the peak gas temperature increases with increasing magnetic field from 1360 K for $B=35 \text{ G}$ to 3100 K for 450 G, a consequence of the increase in momentum transfer from the increasing ion density.

Due to the improved confinement, better utilization of secondary electrons as an ionization source and increase in ion flux, the magnitude of the cathode voltage required to dissipate 10 kW decreases with increasing magnetic field,

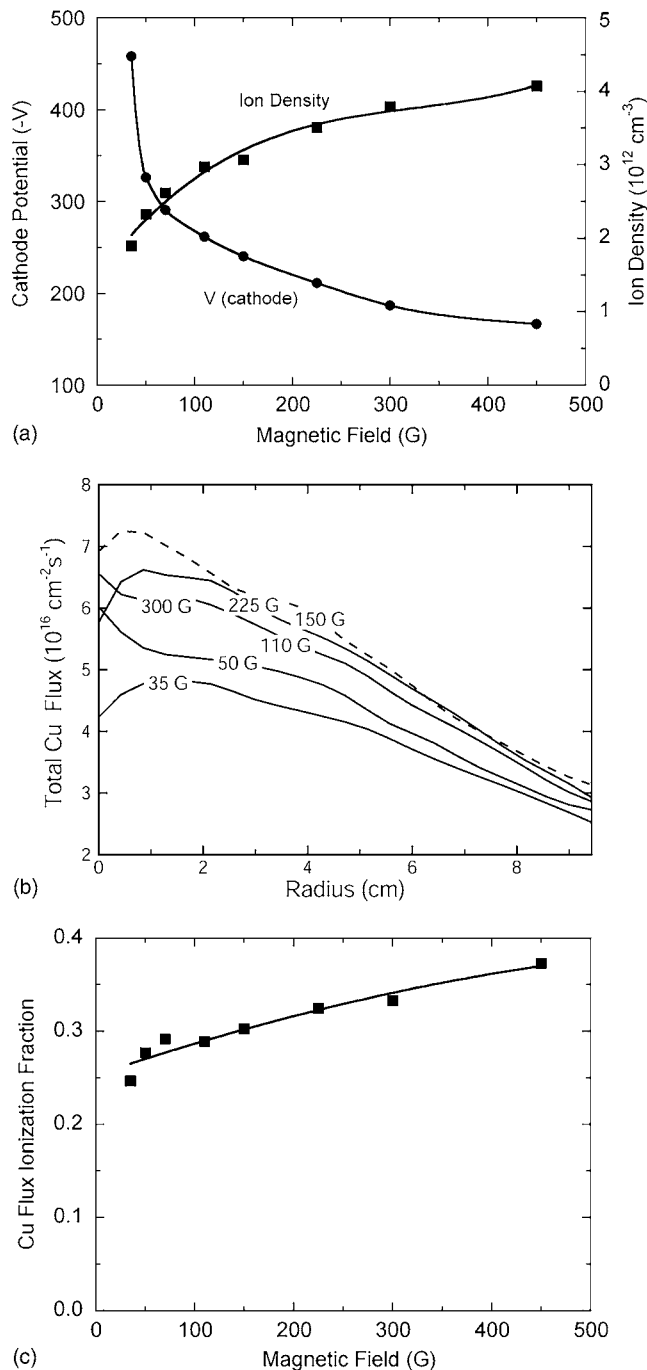


FIG. 16. Plasma parameters as a function of radius on the substrate for increasing the magnetic field while keeping total power deposition constant (5 mTorr, 10 kW). (a) Maximum ion density and cathode voltage, (b) total Cu flux to the substrate as a function of radius (the dashed line is for 150 G), and (c) ion fraction of the Cu flux to the substrate. The decrease in ion sputtering probability with decreasing cathode voltage compensates for the increase in ion flux, resulting in a decrease in the Cu flux at large magnetic field.

also shown in Fig. 16(a). The magnitude of the cathode voltage decreases from -460 V for $B=35 \text{ G}$ to -167 V for $B=450 \text{ G}$. This decrease in voltage has an important effect on the Cu fluxes to the substrate. In spite of the increase in plasma density and increase in ion flux to the cathode, the magnitude of the total Cu flux to the substrate, shown in Fig.

16(b) as a function of radius, does not proportionately increase. The Cu flux increases with increasing magnetic field up to about 150 G and decreases for larger magnetic fields. This trend results from the lower sputtering probability of ions arriving at the cathode with lower energies as the cathode voltage becomes less negative.

The ionization fraction of the Cu flux to the substrate, shown in Fig. 16(c), does not change with increasing magnetic field in proportion to the increase in total ion density. This trend results from the increasing rarefaction and decrease in residence time of the Cu flux with increasing gas temperature as the magnetic field increases. The end result is a decrease in the likelihood for ionizing collisions by Cu atoms transiting from cathode to the substrate. The increase in plasma density (which should produce more Cu ions) and decrease in Cu scattering (decreases likelihood for ionization) are roughly compensating, producing only a small increase in the Cu flux ion fraction at large magnetic fields.

IMPVD is dominantly used to deposit barrier coatings and seed layers into trenches and vias. These layers are typically a few to tens of nanometer thick. The quality of the deposition is often measured by the conformality or uniformity of the thickness of the layers on the sidewalls compared to the bottom of the trench. Since the top of the trench has a larger view angle to the plasma than the bottom of the trench, it is common for the deposited layer to be thicker at the top of the trench. When filling the trench using IMPVD, this disparity in deposition rates can lead to the top of the trench being closed prior to the trench being filled. This results in there being a void, often referred to as a keyhole.

To assess the influence of plasma parameters on the quality of the Cu seed layer, we will use the ratio η between the thicknesses of the deposits on the sidewall at the top of the trench and on the bottom of the trench. η , which ideally should be unity, will be quoted when the film thickness is approximately 25 nm . Values of $\eta > 1$ indicate a more PVD or neutral dominated deposition where depositing species arrive more isotropically onto the substrate and so there is a thicker deposition at the top of the trench where view angles are larger. Values of $\eta < 1$ indicate a more ion dominated deposition with depositing species arriving with more anisotropic trajectories producing more deposition on the bottom of the trench.

Cu seed layers deposited onto SiO_2 are shown in Fig. 17(a) for increasing times during a deposition at 3 mTorr , yielding a value of $\eta=1.8$. This value of η indicates conditions which more resemble PVD than IMPVD. η as a function of gas pressure is shown in Fig. 17(b). η initially increases from 1.3 to 2.0 as the pressure increases from 1 to 4 mTorr . As the pressure increases further, η decreases, reaching unity at approximately 20 mTorr . At low pressures, the fractional ionization the Cu flux is low and deposition is dominated by nonthermal neutrals (see Fig. 5). These neutrals have anisotropic trajectories due to their origin deep in the hollow cathode which produces a narrow view angle to the substrate. As a consequence, there is adequate deposition on the bottom of the trench and η is near unity. In this re-

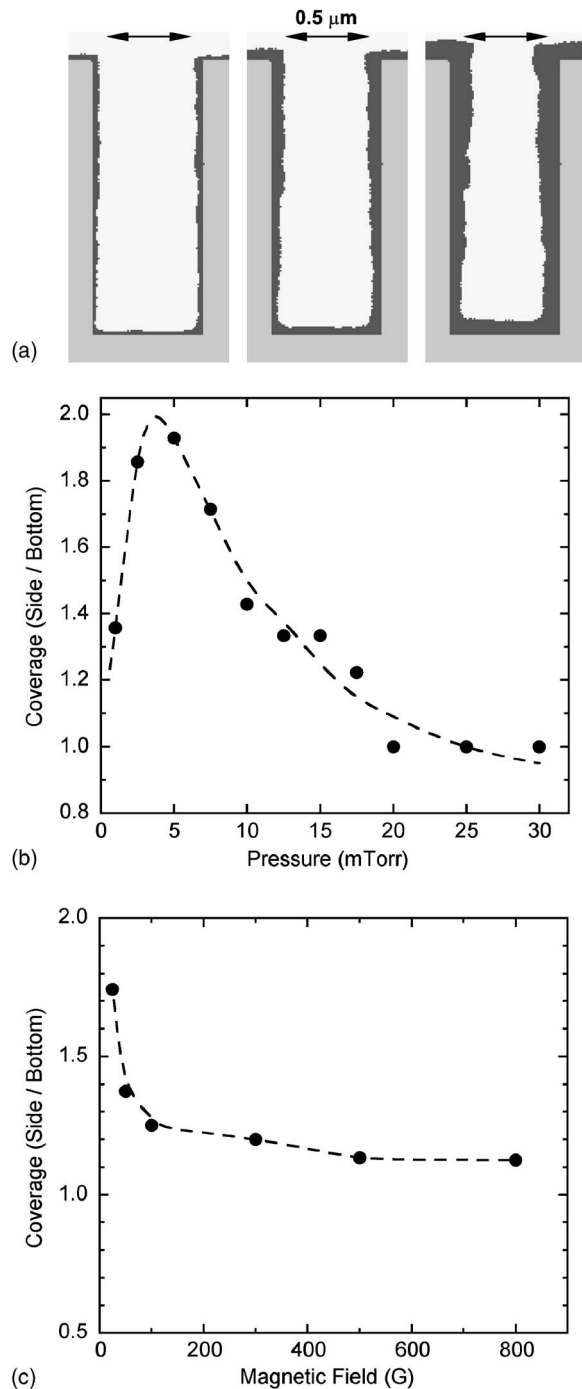


FIG. 17. Seed layer properties as obtained from the MCFPM. (a) Seed layers in a trench for different times during a deposition at 5 mTorr. Coverage (side-to-bottom thickness ratio) as a function of (b) pressure and (c) magnetic field.

gard, the anisotropic neutral flux appears similar to an ion flux. As the pressure increases towards 4–5 mTorr, the Cu flux is still dominated by nonthermal neutrals; however, their trajectories are now more isotropic due to collisions. Deposition begins to look somewhat PVD-like with thicker films at the top of the trench and so η increases. At pressures exceeding 5–10 mTorr, the ionization fraction of the Cu flux increases above 0.6 and the deposition flux becomes more

anisotropic. The end result is a decrease in η . Note that the floating potential for these conditions is at most only a few tens of volts. As a result, sputtering by the larger flux of Ar^+ is not an important process in determining the conformality.

η as a function of magnetic field strength is shown in Fig. 17(c). η decreases from 1.7 to 1.2 for magnetic fields up to 100 G, after which η is nearly constant for larger magnetic fields. Based solely on the ionization fraction, one might expect η to increase with increasing magnetic fields up to 500 G since the ionization fraction of the Cu flux decreases [as shown in Fig. 14(b)]. The opposite trend can be attributed to the increasing rarefaction of the gas. As the magnetic field increases at constant voltage, the total power deposition increases, resulting in an increase in gas temperature and decrease in gas density. The fraction of the Cu flux incident onto the substrate that is nonthermal (and so anisotropic) increases with magnetic field, thereby having the same effect as increasing ion fraction. As the nonthermal component of the Cu flux dominates the deposition, its contribution to conformality also dominates over that of the ions.

IV. CONCLUDING REMARKS

A hybrid modeling approach has been developed in which the ion and neutral transport coefficients and temperatures are kinetically derived and implemented in fluid equations, thereby, extending their applicability to low-pressure IM-PVD systems. A Monte Carlo simulation was also used to assess the consequences of process parameters on the conformality of seed layers. The model was used to investigate plasma properties and seed layer properties for Ar sputtering a Cu hollow cathode magnetron target. The uniformity, magnitude, and composition (i.e., ionization fraction) of the flux can be controlled by judicious choice of power, pressure, magnetic field configuration, and magnetic field amplitude. In optimizing the flux to the substrate at low pressures, the location of the ion sources within the hollow cathode and the location of the magnetic field cusp become increasingly important. In the absence of proper placement, the ion flux may arrive at the substrate with dominantly off axis trajectories. These off axis trajectories could result in the ion angular distribution being skewed from vertical. The conformality of the seed layer (i.e., side-to-bottom coverage), although sensitive to the copper ionization fraction, is also sensitive to the fraction of the Cu flux that is nonthermal. The nonthermal flux originates in the hollow cathode and so arrives at the substrate with anisotropic trajectories resembling the ion flux. In the absence of an appreciable bias on the substrate, the ion energies are not large enough to produce significant sputtering. As such, conditions that produce large nonthermal copper fluxes produce conformality similar to those that have large ionization fractions

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