Computer simulation of mass-selective plasma-source ion implantation

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The use of plasma source ion implantation (PSII) for impurity sensitive substrates such as semiconductors has been slow to be adopted due to the difficulty of producing low impurity plasmas. In this work the feasibility of producing impurity-free plasmas for PSII using a mass filtering technique is investigated. In this method, an ion cyclotron resonance (ICR) cell is incorporated into a plasma processing reactor to selectively expel unwanted ions. The implementation of ICR in ion implantation is subject to a number of complications, such as ion–neutral collisions, plasma shielding of excitation fields, and nonhomogeneities of the magnetic field. A numerical simulation of ICR-based mass filtering for PSII to investigate these effects has been developed. Mass filtering is potentially effective over a wide range of magnetic field configurations at the pressures typically used for PSII.

I. INTRODUCTION

Ion implantation of materials is usually accomplished using one of two basic systems. The first method utilizes ion beams, produced by a particle accelerator that are directed into a substrate. With this method, it is difficult to uniformly implant objects with nonplanar topography. The beam technique offers an advantage in that mass selection, primarily obtained using magnetic fields to bend the beam, permits one to isolate the desired ion species for implantation. However, the beam technique is a line of sight process, thereby requiring beam rastering and target manipulations to achieve uniform implantation. The second method, plasma source ion implantation (PSII) is a non-line-of-sight technique in which the target is immersed in a plasma.[1] In PSII, a plasma sheath surrounds the target. Ions accelerated through the sheath bombard all surfaces of the target without the need for active techniques such as beam rastering or target manipulation. However, PSII suffers from the fact that all ions in the plasma, including impurities, are accelerated to the substrate. PSII has therefore not yet been employed commercially for impurity-sensitive implantations, such as some processes used for semiconductor fabrication.

In this work, we numerically demonstrate a mass filtering technique based on ion cyclotron resonance[2] (ICR), which can effectively separate or expel undesired ion species at the operating pressures commonly used by PSII. The use of the ICR principle has already been examined for mass spectrometry in both the Omegatron[3] and Fourier transform mass spectrometry[4] (FTMS) devices, as well as for isotope separation systems. This mass filtering technique has also been recently discussed by Hatakeyama using an analytic formulation, which does not consider the effects of collisions or nonuniformities.[5] Using a mass filtering technique, the range of applications for PSII could be broadened considerably. For example, pure plasmas for implantation could be produced for PSII in the microelectronics industry to generate low-energy ions (~1 kV) for shallow implants. Higher-energy implants, used, for example, in silicon-on-insulator technology,[6] can also be easily combined with rapid thermal annealing using PSII. Recent results using PSII for shallow implant junctions appear to be quite promising.[7] In Sec. II, we will discus the mechanics of the PSII/FTMS system. Our model will be described in Sec. III, followed by an analysis of PSII/FTMS scaling in Sec. IV.

II. A PSII/FTMS SYSTEM

PSII involves the applications of a series of high negative-voltage pulses to a substrate immersed in a plasma. The response of the plasma to this voltage pulse is the formation of a non-neutral sheath around the target and the acceleration of ions into the target. The number of ions collected during the pulse, their energy, and their angular distributions are determined by the characteristics of the plasma, substrate, and voltage waveform. A schematic of a possible PSII system that includes a FTMS cell is shown in Fig. 1. The parallel plate FTMS cell is placed above the target to be implanted, along with a magnetic field coil system. In this embodiment, the plasma is produced in a source region well above the substrate, while the FTMS cell mass filters the plasma immediately above the substrate. The filtered plasma adjacent to the substrate will act as the ion source for final implantation.

Typical PSII plasmas to date have been formed with a filament discharge. The high-voltage pulse is applied between the target stage and the chamber walls. The quantity of interest is the dose or fluence (ions/cm^2) that is implanted in the target. The variables that control the dose (and the dose rate, which is often also important) are the value of the acceleration pulse voltage, the pulse width, and the number of pulses per second. The energy of the incoming ions also determines the range or depth profile, with which the ions are implanted into the substrate. Other types of plasmas could be used, however. Electron cyclotron resonance (ECR) generated plasmas, because of their associated magnetic fields,

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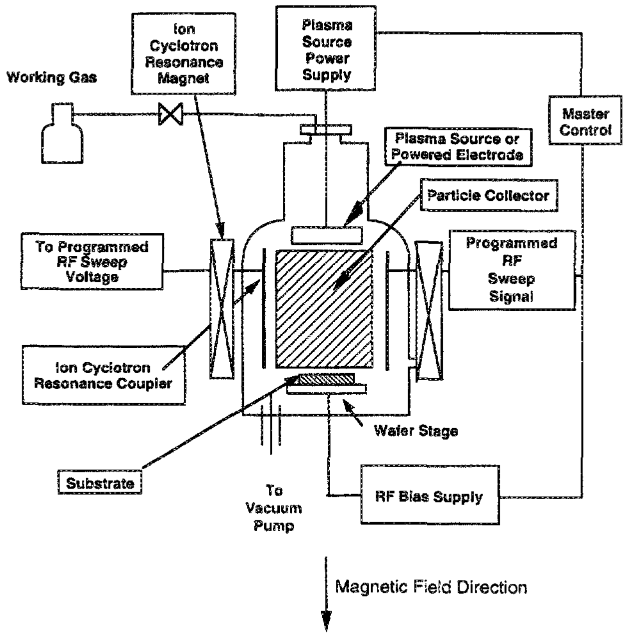

FIG. 1. A PSII system with an incorporated FTMS system.

lend themselves readily to the ICR/FTMS filtering techniques.

The use of ICR/FTMS in the system is based on the property that in a dc magnetic field, ions orbit about the magnetic field lines with a well-defined cyclotron frequency that is directly proportional to the magnetic field strength, and the ion's charge-to-mass ratio. An oscillating electric field whose frequency is equal to the ion cyclotron frequency will accelerate the ions and cause their orbits around the magnetic field line to increase in radius. If the radius of the orbit is sufficiently large, the ions can be expelled from the cell. Radiofrequency signals that contain frequency components that are the same as the cyclotron frequencies of those ions desired to be expelled may be imposed across the cell by a suitable rf coupling mechanism. This technique can be used to obtain a programmed expulsion of selected masses.

When cyclotron resonance is achieved, the radius of gyration of a charged particle in a dc magnetic field increases linearly with time according to the expression $r=(E/B)t$, where E is the rf electric field magnitude, B is the magnitude of the magnetic field, and t is time. Note that the radius is independent of the mass.

Nonresonant ions may initially gain energy, but then will experience a loss of energy, as their velocities become out of phase with the applied rf electric field. Thus, by appropriately programming a frequency sweep into the rf excitation field, ions of a particular charge-to-mass ratio my be expelled from the plasma and collected, as long as the pressure is low enough so that the ion trajectories are not perturbed by collisions.

A diagram of a typical FTMS cell is shown in Fig. 2. Note that the direction of the magnetic field is perpendicular to the direction of the rf electric field. In the absence of collisions, the ion spirals out to the walls of the cell, where it can be collected. Collisions with neutrals, in which all ordered orbital momentum is lost, can have a detrimental effect on efficient ICR expulsion.

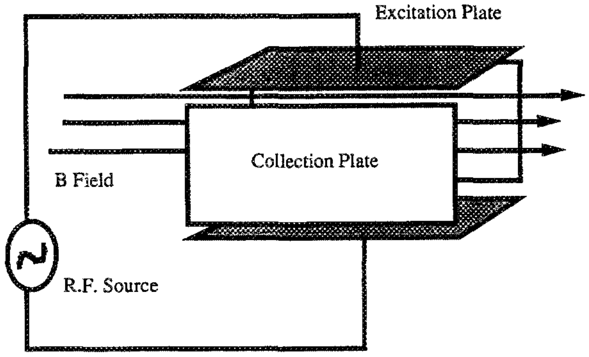

FIG. 2. A typical FTMS cell.

The PSII process is typically pulsed. That is, acceleration of ions toward the target takes place only during the time that the high voltage is applied through the pulse modulators. During the time that the acceleration pulse is off, the programmed rf excitation pulse is applied to the FTMS cell. In our numerical work, rather than employing a parallel plate excitation, which would be subject to significant plasma shielding of applied potentials across the sheath, we will model an inductively coupled (antenna launched) electromagnetic wave as our rf driving potential. This scheme allows stronger electric fields to permeate the bulk region of the plasma.

III. NUMERICAL SIMULATION CODE

We have developed a two and one-half-dimensional (three velocity components, two spatial components) Monte Carlo simulation (MCS) to investigate reactor conditions for which this ICR/FTMS technique may be used to expel selected ions from the plasma for PSII. The MCS integrates the equations of motion of ion pseudoparticles in time-varying electric and spatially varying magnetic fields; and collects statistics on the times and locations at which ions are collected at the boundaries of the plasma. The purpose of the MCS is to demonstrate a proof of principle of the method; and the assumed plasma conditions have therefore been greatly simplified. No attempt has been made in the work presented here to self-consistently calculate plasma conditions, such as the location and magnitude of the ion sources and the complete details of the electrostatic potentials.

The MCS begins by calculating the static magnetic field as a function of (r,z) based on specified reactor dimensions, locations of coils and distribution of current through those coils. The magnetic field is stored on an (r,z) mesh whose values are interpolated during the MCS. The incident rf electric field is assumed to uniformly propagate parallel to the z axis with a circular polarization. The amplitude and frequency chirp of the rf field are also specified as input,

$$E(z,t)=E_0 \sin[\omega(t)t+\varphi].$$

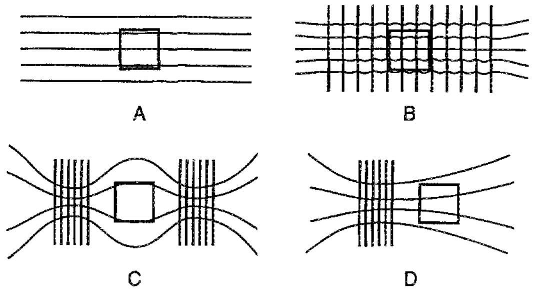

FIG. 3. Simulation geometries—(A) A uniform, arbitrarily imposed field. (B) A solenoidal arrangement of 104, uniformly spaced coils. (C) A magnetic mirror type arrangement. (D) A diverging field.

Here $\omega(t)$ is the chirp (sweep) function and φ is an arbitrary phase. Pseudoparticles representing a user-specified variety of ions are initially randomly distributed within a subvolume of the reactor. The equations of motion of the ions in the electric and magnetic fields are integrated using a second-order Runge–Kutta technique. Time steps are chosen to be the minimum of 0.01 of the instantaneous rf period, 0.01 of the local ion cyclotron resonance period, or 0.5 of the time required to cross the local computational cell. Ions striking the radial walls or axial endplates are assumed to be collected with unit efficiency. The trajectory of each individual ion pseudoparticle is followed until it strikes a surface or a specified time elapses.

Collisions of the ions are included using standard Monte Carlo techniques.[8] Based on the gas pressure, and specified charge exchange and elastic collision cross sections, a mean time between collisions for each ion species is obtained, $t(i)$. The randomly selected collision for ion i then occurs at

$$t(c)=t(\mathrm{co})-t(i)\ln(r),$$

where t(co) is the time of the last collision and r is a random number distributed on (0,1). The collision is elastic if

$$r<\sigma(\mathrm{elastic})/[\sigma(\mathrm{elastic})+\sigma(\mathrm{charge\ exchange})],$$

where σ is the cross section and r is another random number (0,1). Otherwise it is a charge-exchange collision. All collisions are isotropic. The product ion of charge-exchange collisions is assumed to have a Maxwellian velocity distribution at the gas temperature.

IV. SIMULATIONS OF PSII/FTMS

The model system has a 15 cm×15 cm×15 cm region of plasma with parameters chosen to approximate a PSII chamber. The ions and neutrals initially have a Maxwellian velocity distribution with a temperature of 300 K. The gas pressure is 0.1 mTorr.

Two methods were used to model the magnetic field. The first used a uniform 876.5 G field parallel to the axis of the cell. The second explicitly calculated $B(r,z)$ based on specified magnetic coil configurations. Three separate coil arrangements were used (see Fig. 3). The first was a uniform set of 104 coils, each 30 cm in radius and carrying equal current. The coils were spaced to produce a nearly solenoidal magnetic field.

Two nonuniform field configurations were also used: (1) a mirror system and (2) a nonsymmetric diverging field. The mirror used the same 104 coils and currents, but half of the coils were centered at $z=-30$ cm and half at $z=30$ cm. The nonsymmetric diverging field configuration had all 104 coils centered at $z=-30$ cm. These arrangements allowed us to characterize the effects of nonuniform magnetic fields. All the fields were scaled to have a value of 876.5 G in the center of the cell in order to emphasize the effects of the nonuniformity of the fields, rather than the effects of the varying magnitudes of the fields.

The modeled rf electric field strength was 1 V/cm, which is sustainable in the low-density plasmas used in PSII. An inductively coupled rf coil, or another antenna structure

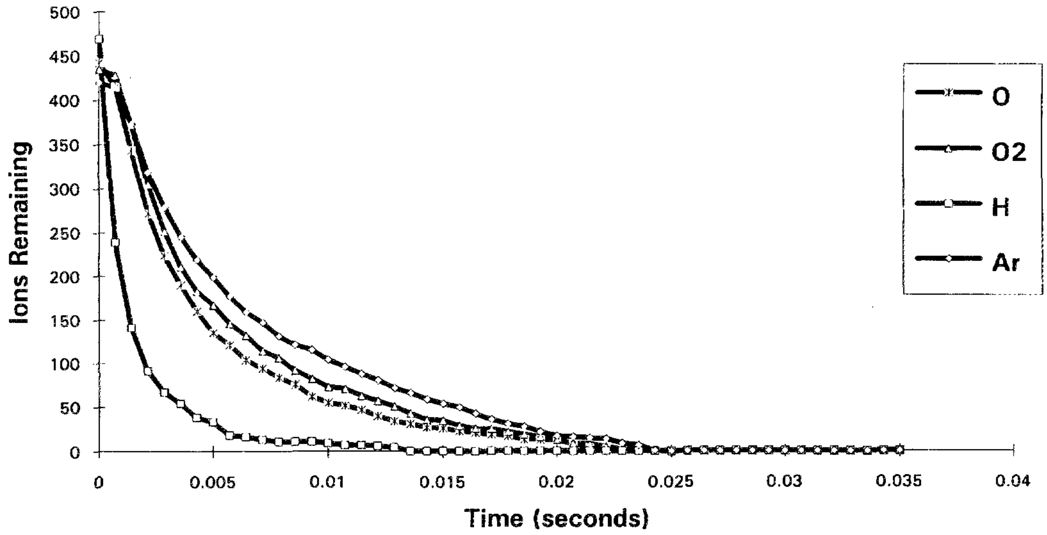

FIG. 4. Diffusion from the cell of various ions for a uniform 876.5 G magnetic field with no rf applied. Particles escaped almost exclusively to the front and back endplates of the cell.

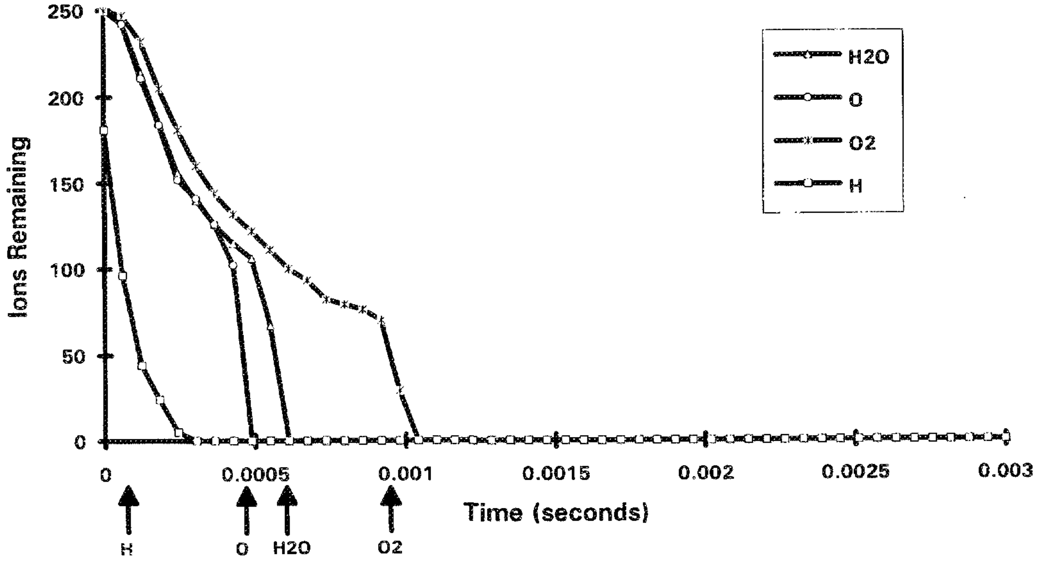

FIG. 5. Ions remaining in the cell as a function of time. 250 of each species were in the cell initially. Magnetic field was a uniform 876.5 G. Frequency ramped from 1.5 MHz to 0 Hz in a piecewise linear fashion. Times at which excitation was at resonance of a particular species are denoted by arrows.

could be used to launch an electromagnetic wave of such a strength into the plasma. This field would be more spatially uniform than that produced by a parallel plate excitation.

A primary concern in the practical application of the FTMS technique as it relates to PSII is the rate of diffusion of ionized impurities. Expelled species must remain outside the implantation region for at least the duration of the applied high voltage in order for the implantation to be effectively purified. Since the MCS code considers only the initial set of particles within the cell, and eliminates them when they hit the boundary of the cell, it allows us to estimate the rates of diffusion of ionized species out of the cell in the specified magnetic fields. With the rf frequency sweep turned off, the ions are free to diffuse, subject only to random thermal collisions and the confining effect of the imposed magnetic field. A measure of the ions remaining in the cell as a function of time provides an estimate of the diffusion rates.

The results of the simulation, as shown in Fig. 4 show that the heavier ions diffuse out of the cell slower than the lighter species, which is to be expected from classical diffusion theory. For the field configurations that are used in this work, diffusion out of the cell occurred almost exclusively along the Z axis, due to the radial confinement along magnetic field lines. Under these conditions, the MCS code showed that a majority of the particles was collected on the axial endplates

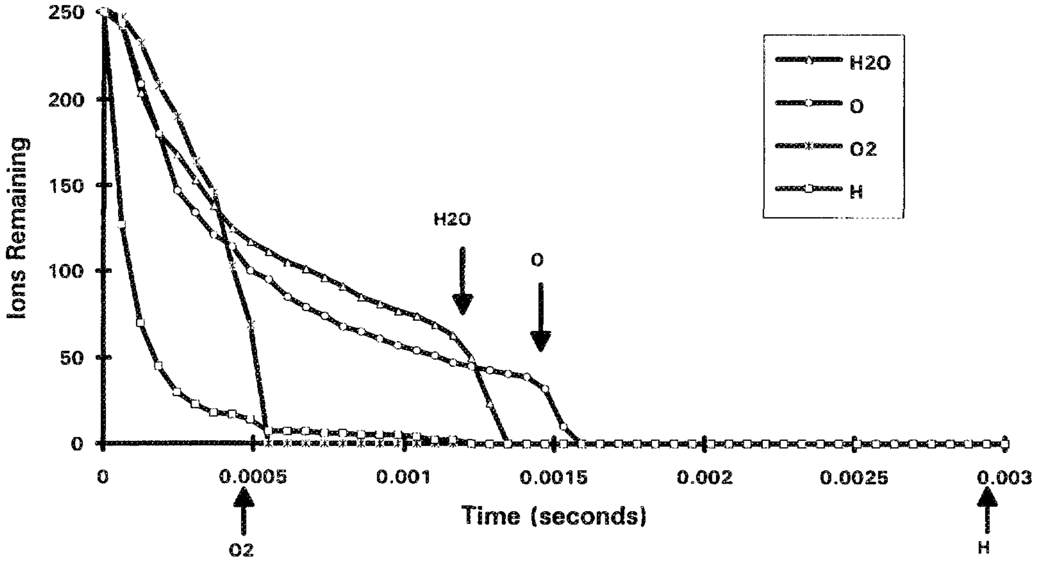

FIG. 6. Ions remaining in the cell as a function of time. 250 of each species were in the cell initially. Magnetic field was a uniform 876.5 G. Frequency ramped from 20 kHz to 1.5 MHz in a piecewise linear fashion. Times at which excitation was at resonance of a particular species are denoted by arrows.

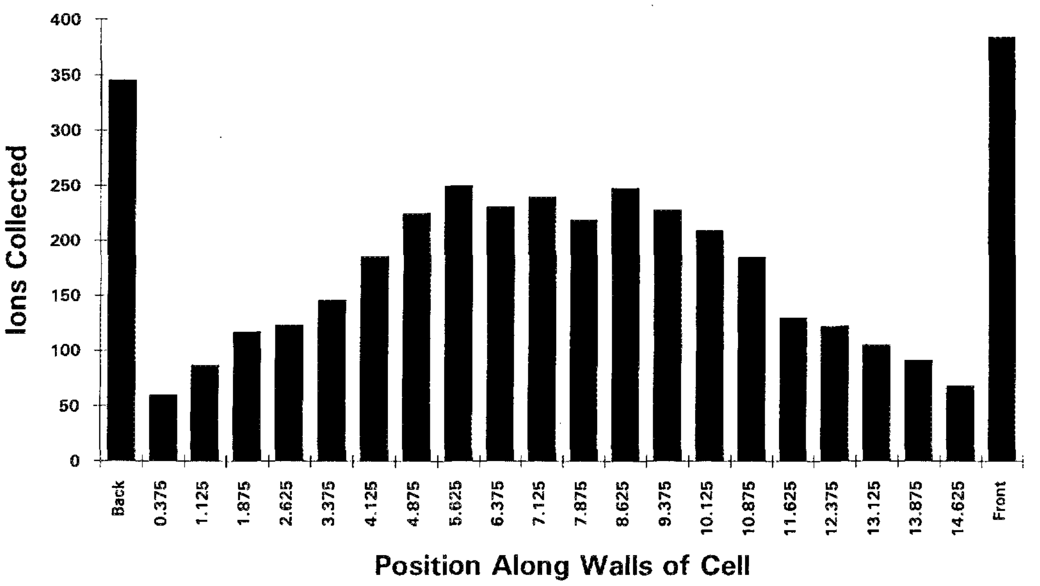

FIG. 7. Plot of O_2 ions collected on sidewalls during an rf excitation similar to that of Fig. 6. About 20% of the ions still escaped to the axial endplates, but the remainder of the original 3000 ions modeled in this run gained enough energy to travel to the sidewalls, as indicated.

of the cell, and the particular geometry of the field had little effect upon the rate of escape of the ions.

These results have important implications for PSII. If impurity ions are expelled from a region of plasma by a chirped frequency pulse, there is a finite amount of time for the high voltage implantation pulse to be applied and to have a pure implantation prior to impurities diffusion from outside the FTMS region. After this time, the high voltage pulse must be switched off, and the rf ICR/FTMS excitation must be applied again. While implantation parameters will determine the actual duty cycle of the implantation pulse, the diffusion and production rates of the impurities will determine the duty cycle of the rf chirped pulse.

Ion expulsion from the cell was observed in our model when the ICR electric field was 1 V/cm. Although diffusion still played a role, the ions were driven to the walls of the cell much faster when excited by the rf field at their cyclotron resonance. The rf excitation was modeled as having a time-ramped frequency. A plot of ions remaining in the cell as a function of time in the uniform magnetic field case appears in Fig. 5. We began with 250 ions each of H_2O, O, H, and O_2, all of which are typical impurities in PSII systems. A

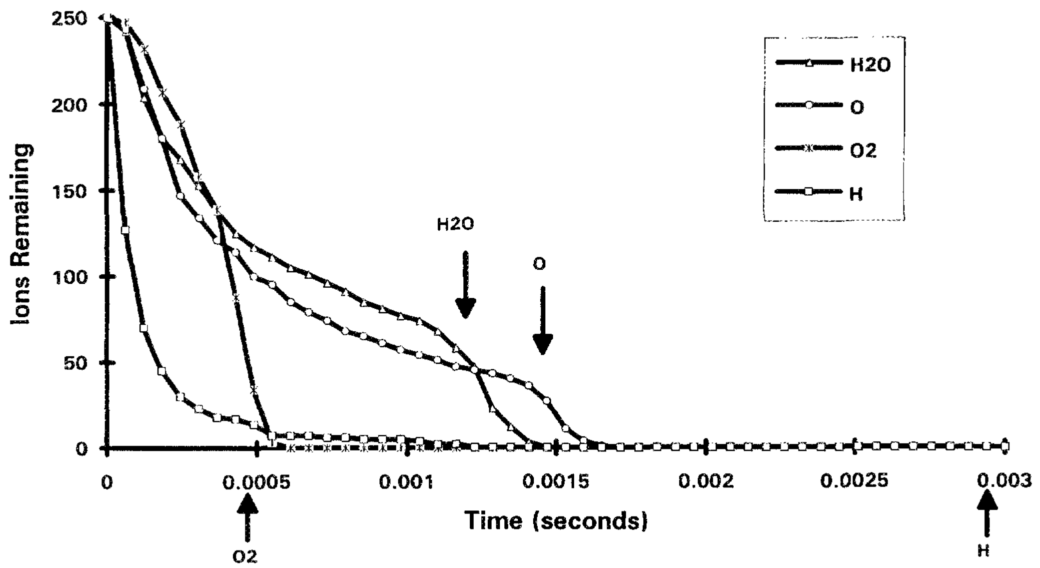

FIG. 8. The same conditions as in Fig. 6, except the mirror magnetic field was used. Expulsion rates near ion resonances are slightly slower than in the case of the uniform field, but overall expulsion was equivalent.

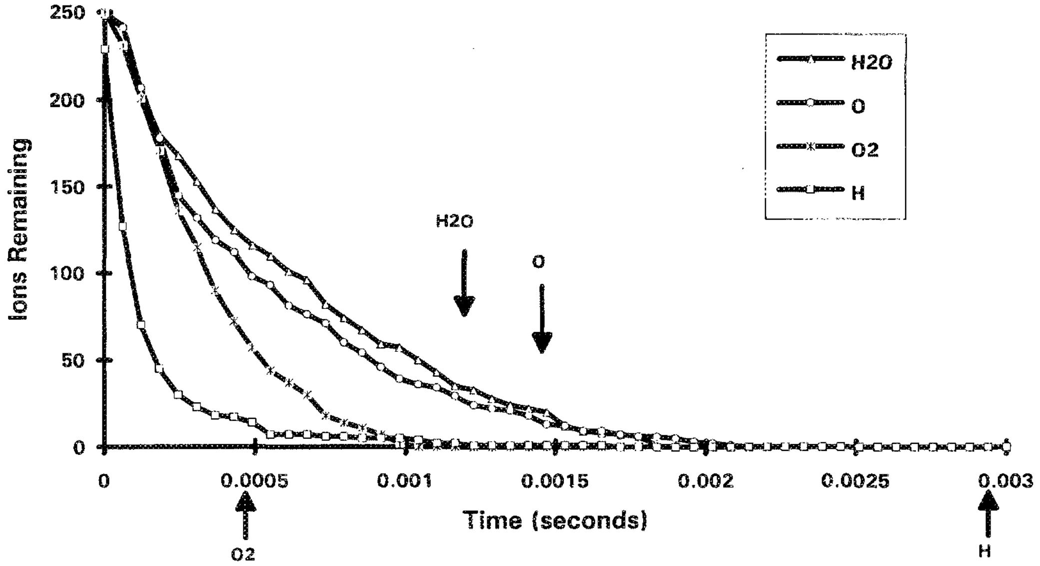

FIG. 9. The same conditions as in Fig. 6, except the diverging magnetic field was used. The resonance expulsion effects are barely observable due to the wide variation of field strength across the cell.

swept pulse of 3 ms duration was used. The frequency was ramped linearly from 1.5 MHz to 100 kHz in the first 0.25 ms, and then ramped linearly to 0 Hz for the remaining 2.75 ms. When the excitation frequency equaled the resonance frequency of the particular species, expulsion was more rapid. Ions were observed to leave the cell in less than 50 μs when their resonance frequency was reached. O_2 was the last species to be expelled. If it is desired to implant O_2, for instance, then the high voltage implantation pulse should be applied between ~0.65 and ~1.0 ms, since at that time the plasma will consist of almost pure O_2, with few impurities.

In a second trial, the rf excitation frequency started at 20 kHz and was ramped to 100 kHz in 2 ms; and then ramped from 100 kHz to 1.5 MHz for an additional millisecond. This frequency sweep scanned slowly through the resonances of the heavier species (O_2, H_2O, O), and then quickly ramped up to the ion cyclotron resonance frequency of hydrogen. Ions started gaining energy from the field at frequencies slightly lower than their predicted resonances in the uniform 876.5 G field, as shown in Fig. 6, since expulsion rates increased rapidly at times just slightly before the rf excitation reached the exact resonance.

It is also important to note where on the cell boundaries the ions were collected. Hydrogen ions were collected only on the axial endplates of the cell, in a pattern that was similar to the previously mentioned magnetically confined diffusion.

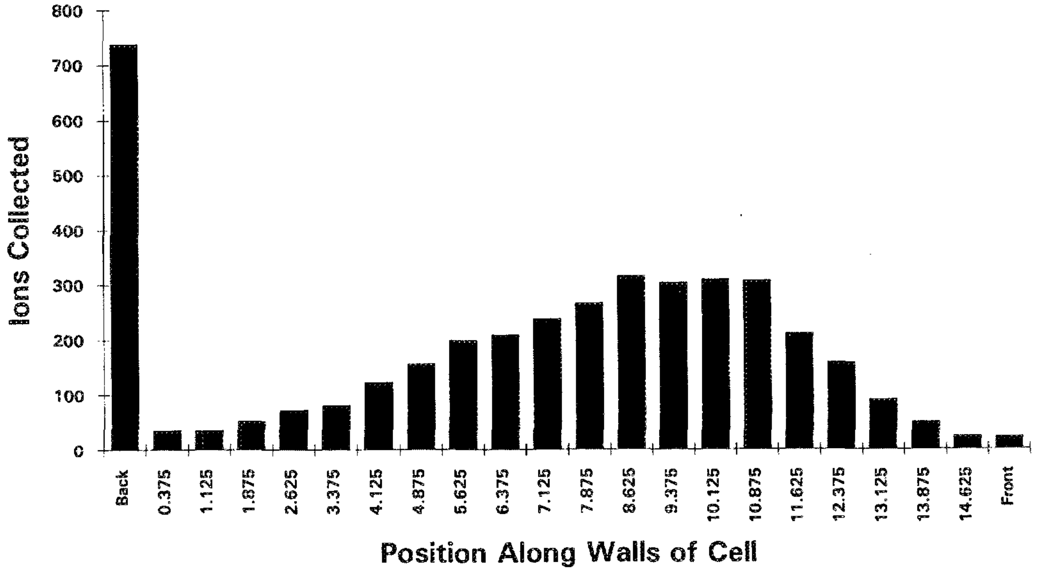

FIG. 10. Plot of O_2 collected on the sidewalls of the cell during a run similar to that of Fig. 9. Of the 3000 ions modeled in this simulation, 738 escaped to the endplate at 0 cm and 23 escaped to the endplate at 30 cm. The rest were collected on the sidewalls, as indicated.

This is because the hydrogen ions diffused to the axial endplates before the rf frequency sweep had reached their relatively high resonance frequency. Heavier ion species are collected at the sidewalls, since the rf field imparts energy into the cyclotron orbits of these species, increasing their radii, even though most still escaped to the axial endplates. The spatial distribution of O_2 ions that were collected on the sidewalls is shown in Fig. 7.

The same frequency sweep was examined using the nonuniform magnetic fields to determine their effects. These results are in Figs. 8 and 9. With the magnetic mirror arrangement, the overall time for complete impurity expulsion was nearly the same as for the uniform field of Fig. 6. Due to the variation of the magnetic field strength across the cell, however, there was a broader range of frequencies that caused expulsion. A similar phenomena was observed for the diverging field arrangement. Due to the large variation of magnetic field strength across the cell, there was a large range of frequencies that could be resonant for a particular ion, but there was indeed evidence of rf-induced expulsion, as evidenced by the spatial escape profile plotted in Fig. 10. Ions were able to be accelerated enough to escape to the radial sidewalls. Notice that more ions travel to the sidewalls in the region of the cell where the magnetic field is weaker.

V. SUMMARY

We have performed proof-of-principle modeling for using an ICR/FTMS mass filtering technique for PSII. A frequency ramped rf excitation scheme was shown to be effective in expelling impurities from low-pressure (0.1 mTorr) plasmas permeated by nonuniform magnetic fields. Nonuniformities in the resulting resonances across the cell are largely compensated for by the linear ramp of frequencies surrounding the ideal resonance frequency. A programmed rf pulse composed of frequencies that are the resonances of the impurities in the plasma might be less effective due to the resonance-broadening effects of the nonuniform magnetic fields. However, the fact that ions absorb energy from the field at frequencies slightly below resonance allows one more flexibility in designing mass filters when the magnetic field is nonuniform.

ACKNOWLEDGMENT

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