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Research Paper

Role of Critical Processing Parameters on Fundamental Phenomena and Characterizations of DC Argon Glow Discharge

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Abstract Given the significance of carefully analyzing the critical range for processing parameters in a sputtering system prior to experiments, as well as their effect on the quality of the deposited thin film, this crucial subject has been simulated and researched in this research. Argon glow discharge conditions were obtained by altering essential processing factors such as electrode spacing, working pressure, and DC voltage delivered to the electrodes. The effect of changing these processing parameters on the potential difference and electric field profiles, ion- and electron-density, ion- and electron-kinetic energy, and cross-section of fundamental processes has been investigated to study the deposition rate and microstructural characteristics of thin films. Furthermore, the cross-section of fundamental ions-and-electron collision processes like ionization, elastic scattering, excitation, and charge exchange has been investigated.

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1. INTRODUCTION

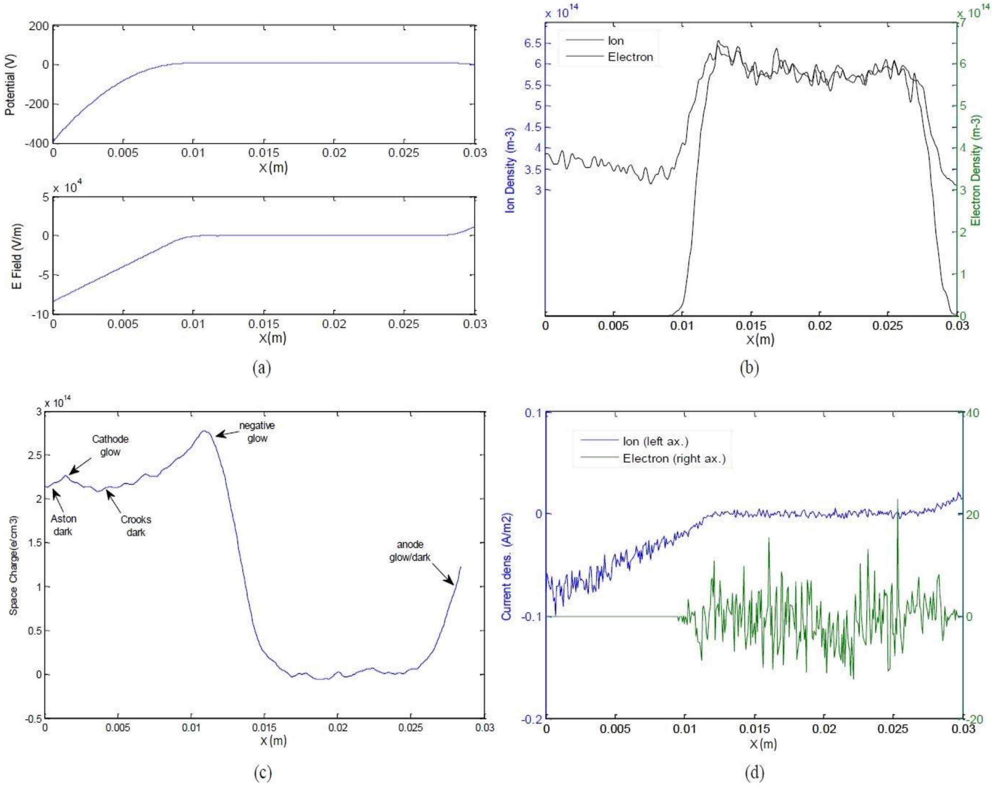
A plasma, often known as the fourth state of matter, is an electrically conducting medium containing about equal numbers of positively and negatively charged particles that form when atoms in a gas get ionized [1-5]. In general, plasmas can be divided into two types: those that are in thermal equilibrium and those that are not [6,7]. Thermal equilibrium indicates that all electrons, ions, and neutral entities have the same temperature. These equilibrium plasmas require high temperatures to create. Thermal non-equilibrium, on the other hand, implies that the temperatures of the various plasma species are not the same; more specifically, that the electrons have substantially greater temperatures than the ions and other substances [8-11]. This subdivision is often related to the plasma pressure, such that, at low gas pressure, only a few collisions occur in the plasma (i.e. a lengthy collision mean free path compared to the discharge length), resulting in distinct plasma species temperatures due to inefficient energy transfer [12]. Plasma is currently utilized as a light source and in the development of new types of television panels. In addition, it forms the foundation of various industrial innovations, enabling applications in microelectronics, packaging, the environment, and medicine. Most economically significant is its use in the material processing of solids and gases [13,14]. Plasmas are industrially useful because they generate active species that are more abundant, diverse in kind, and/or energetic than those generated by chemical reactors. Even in relatively basic circumstances, such as pure argon discharge, which consists of only three primary particles (electrons, neutral particles, and ions), the collisional processes that occur between particles in glow-discharge plasma are complex. In addition, the delicate dependence of plasma characteristics (density profile, temperature, and energy distributions) on the sputtering efficiency and on the fundamental mechanisms leading to excellent film generation in reactive sputtering is a significant area of research. Extensive research has been conducted on the simulation and measurement of sputtering glow-discharges characteristics. Using a particle-in-cell kinetic model, optimal voltage waveforms for capacitive coupled plasma discharges have been explored numerically in [15]. In addition, reference [16] identified VORPAL as a new plasma simulation code with the highest degree of adaptability. [17] Describes the results of simulations that explain many features of ultra-cold neutral plasmas. In [18], the energy distributions of ions striking the cathode in DC glow discharges for argon plasma were measured. In addition, reference [19] published measurements of the ion-energy distributions of ions striking the grounded anode of pulsed argon DC-glow discharge. The research of direct current magnetron argon-nitrogen glow discharge plasma properties is described in reference [20]. Due to the complexity of the discharge behavior of the molecular gases and the complexity generated by the various plasma species under the influence of crossed magnetic and electric fields, it is sometimes necessary to use computer simulation techniques to obtain the required information about plasma properties [21-24]. In this aspect, the vast number of particles in plasma presents the greatest difficulty. Essentially, two computational strategies are employed to address such problems; A approach that models the movement of ions and electrons as a fluid; The Particle-in-Cell (PIC) approach is based on computer particles (super particles) [25-27]. Each of them is a homogenous collection of a large number of real particles with the same mass-to-charge ratio as real particles. Therefore, the second method reduces the number of particles that must be simulated. The Monte Carlo Collision (MCC) algorithm is used to model collisions between distinct particles [28-32].

Determining the effect of important processing parameters of the sputtering system on the plasma conditions of ITO deposition was one of our earliest problems in ITO thin film deposition. The outcomes of our research on ITO thin films are documented in references [7, 21 and 34]. In order to deposit an ITO thin film of sufficient quality and limit the amount of trial and error in our experiments, it was necessary to analyze the plasma characterizations using simulations. As a result, we chose to replicate argon glow discharge prior to conducting additional tests to determine the impact of modifying several crucial processing parameters (including the electrodes distance, working pressure and DC voltage applied to the electrodes). These simulation results were crucial to the advancement of our investigations, but they were not adequately explained in previous articles. As a result, the findings of these research are presented for the first time in this article in order to share them with other specialists in the field.

Simulations were conducted using XPDP1, a well-known open source program created by the Plasma Theory and Simulation Group (PSTG) at the University of California, Berkeley [33-35]. As an open source toolkit, the XPDP1 software is a one-of-a-kind plasma simulation program based on the Monte Carlo algorithm. This study simulates plasma within planar electrodes using a uniformly applied DC magnetic field. In addition, the PIC methodology is utilized to simulate electrons and ions; the leap-frog method is used to solve the motion equations; and the MCC model is used to describe particle collisions [26, 28]. In the PIC scheme, the physical volume is partitioned into grid networks whose crossings are referred to as grid points. This mathematical grid is used to quantify the charge density and the current density J, the electric field E and the magnetic field B, as well as the velocity and location of a charged particle q at a particular place. The whole set of Maxwell's equations is utilized to solve for E and B in electromagnetic simulations. On the other side, the Newton-Lorentz equation of motion is employed to calculate the new locations and velocities of particles. In addition, the MCC technique is implemented because the model is collisional [29-31]. In the second section of this paper, simulations of argon glow discharge patterns in a DC magnetron sputtering system are carried out. In the third section, the effect of crucial processing factors such as electrode distance, working pressure, and DC power on argon glow-discharge characterizations is examined. In the final half of this study, the effects of various processing parameters on deposition rate, microstructural features of films, and the cross-section of fundamental plasma processes are discussed.

2. METHODOLOGY

A conventional dc discharge consists of a negative cathode at one end and a grounded anode at the other, separated by an argon-filled gap and housed within a pair of planar electrodes. A few hundred volts are necessary to maintain the discharge between the cathode and anode. The sort of discharge that forms between two electrodes relies on the working gas's pressure, its composition, the applied voltage, and the geometry of the discharge. This research investigates thermal non-equilibrium DC magnetron glow discharge plasma. While the anode is always grounded in this configuration, the cathode can have any time-varying voltage dependence. In order to get insight into the ion dynamics near the electrodes, a series of simulations of argon DC glow discharges were conducted in this research. The spatial profiles of plasma potential, electric field, ion- and electron-density, space-charge density, and ion and electron current-density are depicted in Fig. 1. The curves derived from a simulation of an argon discharge with a cathode voltage of -400 v and a pressure of 0.5 mbar. The steady-state plasma potential and electric field graph between the cathode (on the left) and the anode are depicted in Fig. 1(a) (at the right side). According to this graph, the entire potential difference between the cathode and the anode is carried by the cathode sheath. Ions entering the sheath are propelled toward the cathode as a result of this potential difference. As we approach the cathode, the ion density within the sheath will gradually decrease. In addition, the anode sheath has a potential differential of only 5 volts. The effect of electric fields is evident in Fig. 1(b), which depicts the graph of ion and electron density. As expected, the average ion and electron densities are roughly equivalent in the bulk plasma region, whereas the sheaths are electron-depleted and ion-rich. When the electron density curve is subtracted from the ion density curve, the net space-charge profile depicted in Fig. 1(c) is obtained. As seen by this graph, it was possible to identify the various dark and glowing sections of the cathode sheath. Fig. 1(d) depicts the graph of electron and ion current densities. According to this graph, the ion current-density attains quite substantial negative values close to the cathode due to the ions' acceleration towards the cathode.



(a) (b)

(c) (d)

Fig. 1. (a) The spatial profile of the plasma potential and electric filed, (b) the spatial profile of the ion- and electron- density, (c) the spatial profile of the space charge, (d) the spatial profile of the ion- and electron-current. Simulated data for a 0.5 mbar, -400v and electrode distance equal to 3cm argon glow discharge.

Also noticeable is the electron depletion in the sheath areas. In contrast, the ion and electron current-densities are in thermal equilibrium in the bulk plasma area. The average kinetic energy of the ions and electrons is given by: Where and represent the masses and velocities of the ions and electrons, respectively.

As demonstrated by simulations, XPDP1 provides insight into fundamental plasma processes. Collisions between ions and electrons and neutral atoms is one of the most essential processes. In glow discharge, the major processes for electron-neutral atom impacts are ionization, scattering, and excitation. In the case of ion-neutral atom collisions, charge exchange and scattering are more prevalent. In the following section of this study, the features of the argon plasma will be investigated by altering the distance between the electrodes, the working pressure, and the applied DC voltage to the electrodes.

3. RESULTS AND DISCUSSION

A. Role of electrodes distance on argon glow discharge characterization

The electrodes distance is one of the key parameters in deposition process. According to the physical and chemical deposition processes in the sputtering system, the proximity of the target with the substrate, increase the deposition rate and conserve energy of sputter atoms. On the other hand, at electrodes with close distance, etching the substrate and reducing the deposition rate is inevitable. Fig. 2, shows the effect of variation of the electrodes distance from 2 to 5cm on potential difference and electric field profile at 0.5 mbar, -400v, 0.01 T and $\gamma_{se} = 0.2$.

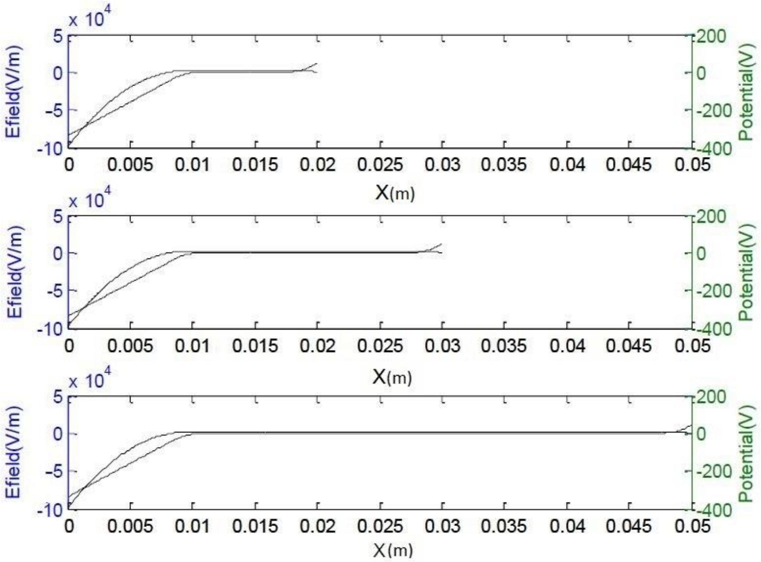


Fig. 2. the effect of variation of the electrodes distance from 2 to 5cm on potential difference and electric field profile at 0.5 mbar, -400v, 0.01 T and $\gamma_{se} = 0.2$ (the potential has been shown with continues line at the right and the electric field has been shown with dash line at the left).

As shown in Fig. 2, the thickness of the cathode sheath is constant by varying the electrodes distance, while the length of the positive column is variable. Fig. 3 shows the variation in the ion- and electron- density by varying the electrodes distance. According to this figure, with the increase of electrodes distance, the ion- and electron-density will decrease.

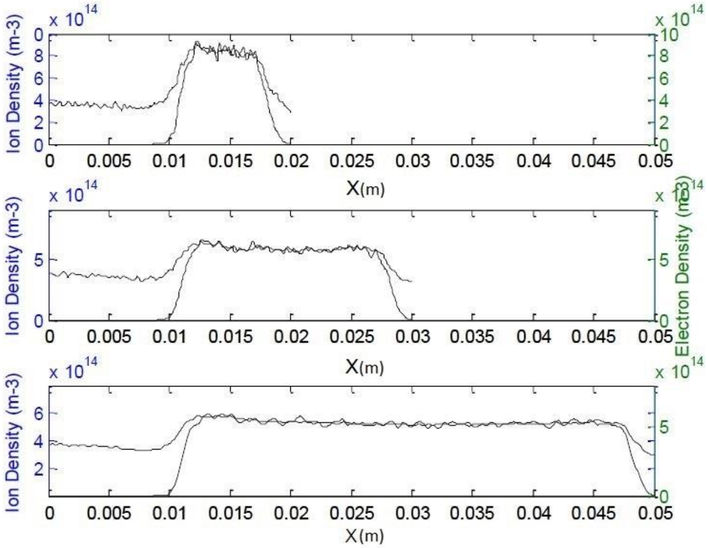
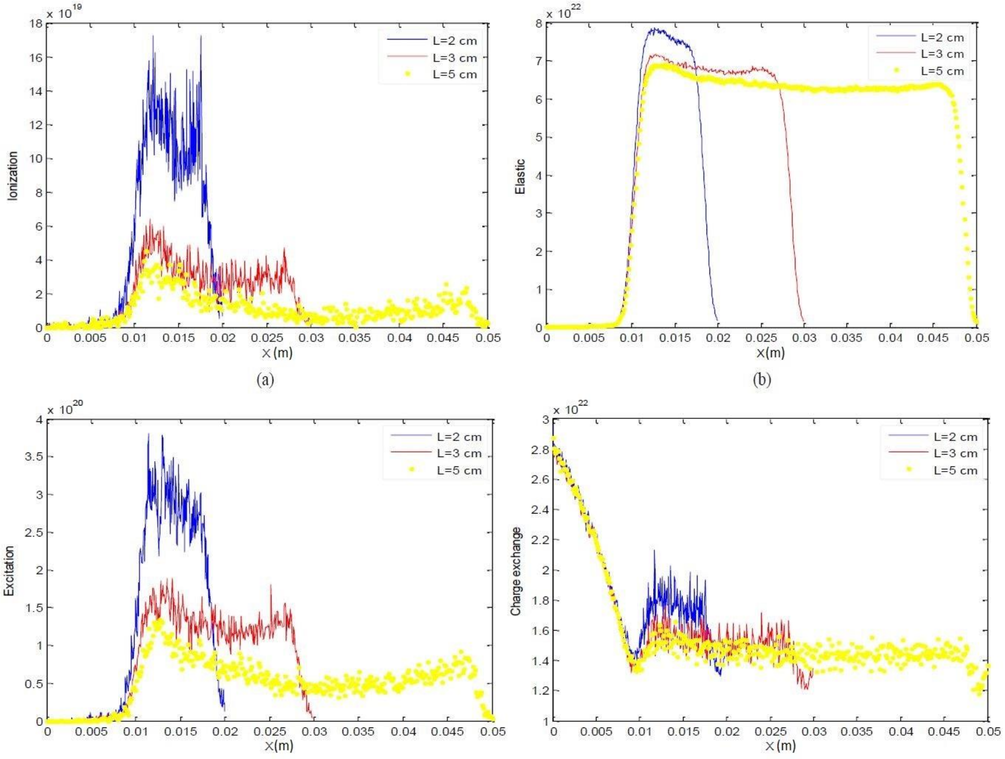


Fig. 3. the effect of variation of the electrodes distance from 2 to 5cm on the ion- and electron-density profile at 0.5 mbar, -400v, 0.01 T and $\gamma_{se} = 0.2$ (the electron-density has been shown with continues line at the right and the ion-density has been shown with dash line at the left).

The effect of electrodes distance on the cross-section of fundamental processes including as ionization, elastic scattering, excitation and charge exchange are shown in Fig. 4. According to the Fig. 4(a), for the different values of the electrodes distance, the maximum ionization occurs in the bulk plasma region. Similarly, by reducing the electrodes distance up to L=2cm, the probability of ionization process is greatly increase. According to the Fig. 4(b), the elastic scattering related to neutral electron-atom collisions in the sheath region is negligible and decrease slightly in the bulk plasma region by increasing the electrodes distance. Also, as shown in Fig. 4(c), the probability of excitation process in electron-neutral atom collisions in the sheath region is very small and decreases in the bulk plasma by decreasing the electrodes distance. In addition, as shown in Fig. 4(d), due to the high ion-density compared to the electron-density in sheath region at the near the target (cathode), the probability of charge exchange processes during ion-neutral atom collisions, is independent of variation of the electrodes distance and has a large amount.



(a) (b)

(c) (d)

Fig. 4. The effects of variation of electrodes distance on fundamental processes. (a) the ionization process, (b) the elastic scattering process, (c) the excitation process and (d) the charge exchange process in electron-neutral atom collisions. Simulated data for a 0.5 mbar, -400v and electrode distance change from 2 to 5cm.

As shown in Fig. 5, as the electrodes distance increases the kinetic energy of the ions and electrons decreases. Also, considering of little mass of electrons than ions, the average kinetic energy of electrons is more.

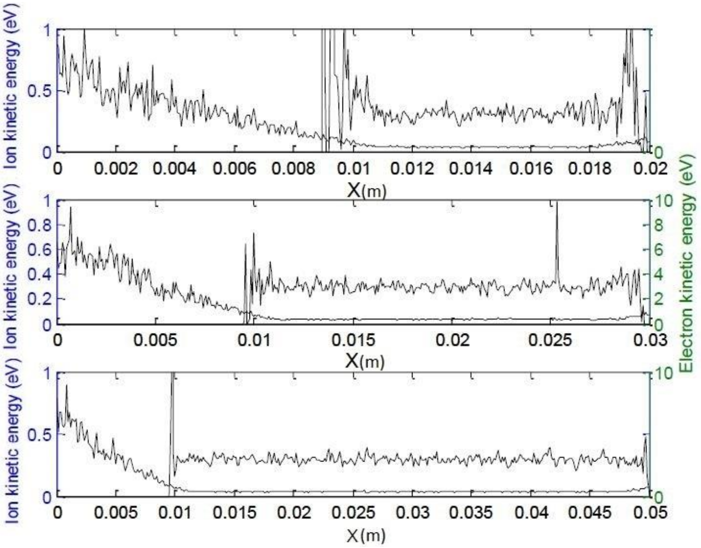
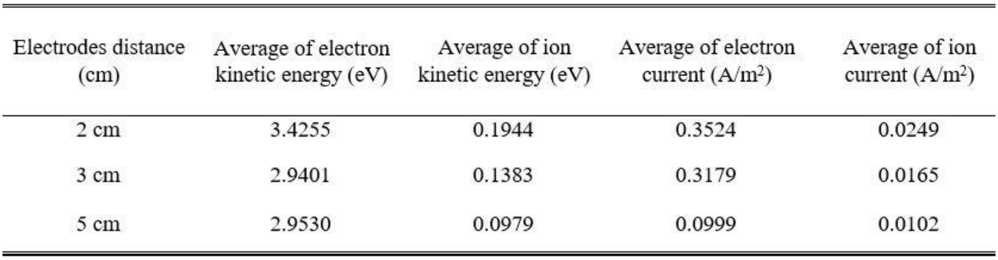


Fig. 5. the effect of variation of the electrodes distance from 2 to 5cm on the ion- and electron-kinetic energy at 0.5 mbar, -400v, 0.01 T and $\gamma_{se} = 0.2$ (the electron-kinetic energy has been shown with continues line at the right and the ion-kinetic energy has been shown with dash line at the left).

The effect of variation of the electrodes distance from 2 to 5cm on the average kinetic energy and average current of electrons and ions are shown in the Table1. As shown in this table, by reducing the electrodes distance, the average kinetic energy and current of ions increase, whereupon the deposition rates and energy conservation of sputtered atoms increase too.

TABLE 1
THE EFFECT OF ELECTRODES DISTANCE VARIATIONS ON THE AVERAGE OF ION/ELECTRON KINETIC ENERGY AND CUTTENT AT 0.5 MBAR, -400V, 0.01 T AND $\gamma_{se} = 0.2$



Electrodes distance (cm)	Average of electron kinetic energy (eV)	Average of ion kinetic energy (eV)	Average of electron current (A/m^2)	Average of ion current (A/m^2)
2 cm	3.4255	0.1944	0.3524	0.0249
3 cm	2.9401	0.1383	0.3179	0.0165
5 cm	2.9530	0.0979	0.0999	0.0102

B. Role of working pressure on argon glow discharge characteristics

Increasing the working pressure at a certain given power, causes to be increased the discharge current density and subsequently, increased the deposition rate. On the other hand, this occurrence prevents further increase of pressure. At high pressures (more than 7Pa), ions, via successive collisions to neutral atoms, reach the target with less energy than at optimal pressure. In these conditions, the sputtering efficiency and also deposition rate are reduced. Because of the number of collisions that lead to the loss of particle energy are inversely proportional to mean free path. On the other hand, stress in thin films is considered as one of the most important technological issues in terms of efficiency and reliability in the integrated circuit manufacturing industry. High levels of stress in the deposited film structure will result in a lot of porosity. Practically, all deposited films in the sputtering system are subject to stress. In fact, this stress relies on the microstructure of the film and kinetic energy of particles on the film surface during the deposition process. So far, many studies have been done on the role of working pressure on the stress created in the film. Considering to high mean free path at low pressures, argon ions and sputtered atoms reach the substrate with less collision. In these conditions, these particles have more momentum and bombard the substrate at an angle close to the normal surface vector. These conditions will be effective in more surface adhesion and conductance of the film. At higher pressures, due to the large collision, the sputtered argon atoms with smaller momentum bombard the substrate with angles away from the substrate normal vector. Such conditions reduce the particle mobility during the deposition process, and causing the atomic shadowing, and stress in the film. In this paper to investigate the effect of working pressure on the deposition process, the argon glow discharge characterizations under different pressures have been studied. Fig. 6, shows the effect of variation of pressure from 3 to 10mbar on potential difference and electric field profile at 3cm, -400v, 0.01 T and $\gamma_{se} = 0.2$.

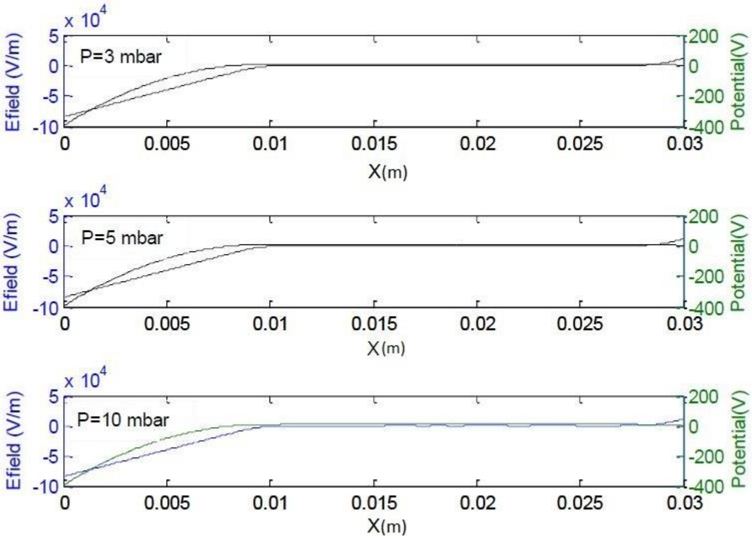


Fig. 6. the effect of working pressure variations from 3 to 10mbar on potential difference and electric field profile at 3cm, -400v, 0.01 T and $\gamma_{se} = 0.2$ (the potential difference has been shown with continues line at the right and the electric field has been shown with dash line at the left).

As shown in Fig. 6, the variation of pressure is not affect the thickness of the cathode sheath region. Also, at 3mbar pressure, the electric field at the edge of the sheath region slightly decreases compared to higher pressures. It reduces the ion-concentration in the sheath region, at lower pressures. Fig. 7 shows the effect of pressure on the ion- and electron-density. As shown in this figure, great reduction of ion densities at the cathode sheath region occurs in 3mbar. In these conditions, despite of increasing the ion- and electron-density in bulk plasma duo to increase of ionization, decreasing of the ion current in cathode sheath region is unavoidable duo to reduce the electric field. On the other hand, at higher pressure, the difference of ion- and electron-density in sheath region and bulk plasma is minimized. Considering to strong electric field in cathode sheath region, an increase of the ion current at 5mbar and higher pressures would be unavoidable. Increasing the ion current in cathode sheath region is one of the most important issues in terms of deposition rate. Also reducing the ion- and electron-density in bulk plasma by increasing of working pressure is due to increase of recombination.

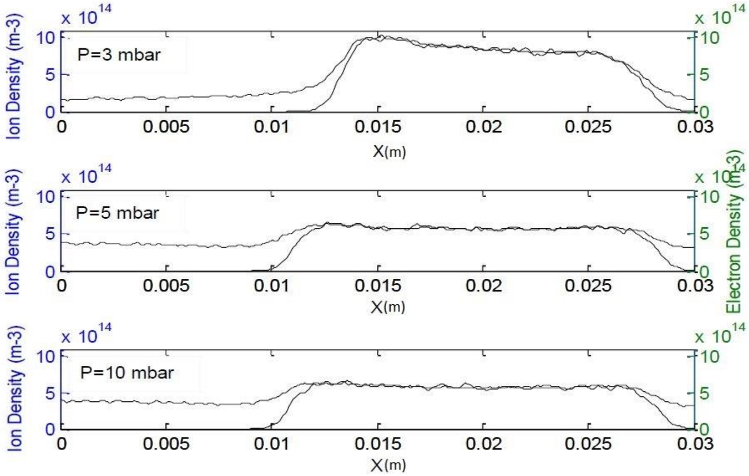


Fig. 7. The effect of working pressure variations from 3 to 10mbar on the ion- and electron-density profile at 3cm, -400v, 0.01 T and $\gamma_{se} = 0.2$ (the electron-density has been shown with continues line at the right and the ion-density has been shown with dash line at the left).

The effect of working pressure on the cross-section of fundamental processes including as ionization, elastic scattering, excitation and charge exchange are shown in Fig. 8.

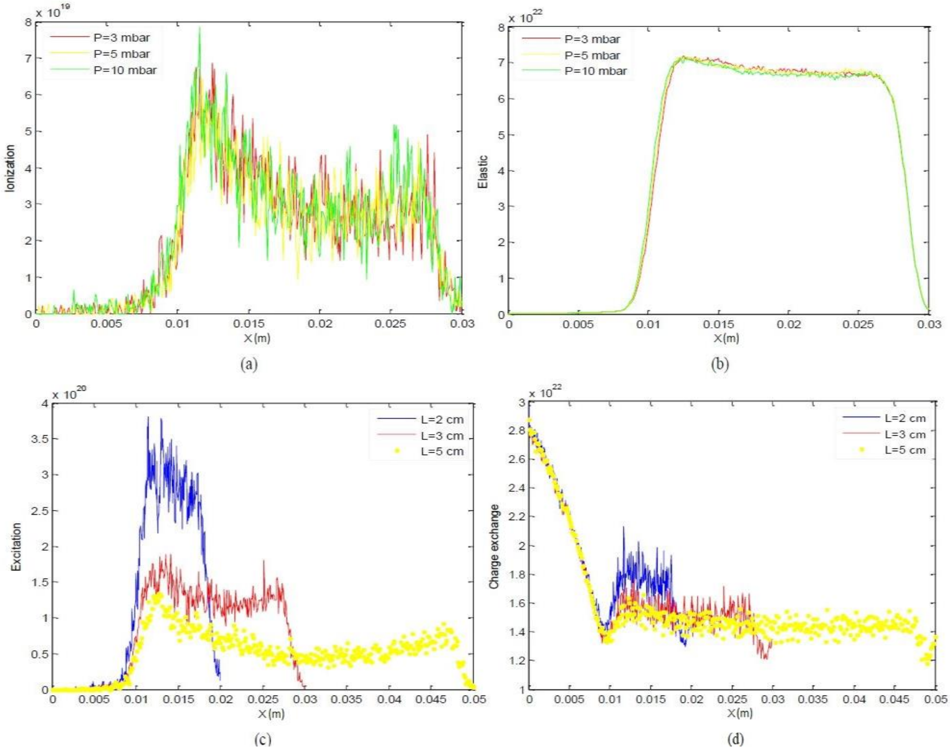


Fig. 8. The effects of working pressure on fundamental processes. (a) the ionization process (b) the elastic scattering process, (c) the excitation process and (d) the charge exchange process in electron-neutral atom collisions. Simulated data for a 3cm, -400v and pressure change from 3 to 10mbar.

According to Fig. 8(a), due to the more electrons-density in bulk plasma compared to sheath region, the most probability of ionization process occurrences in bulk region and it would be increased slightly by increasing pressure. Also, at Fig. 8(b), the probability of elastic scattering process via electron-neutral atom collisions is nearly independent of pressure variations. On the other hand, according to Fig. 8(c), pressure variations affect ion-neutral atom collision processes. So that with increasing pressure, as shown in Fig. 8(d), the probability of a charge exchange processes would be increased.

The effect of working pressure from 3 to 10mbar on the ion- and electron-kinetic energy is shown in Fig. 9. The average kinetic energy and ion/electron current influenced of pressure variations are presented in Table 2.

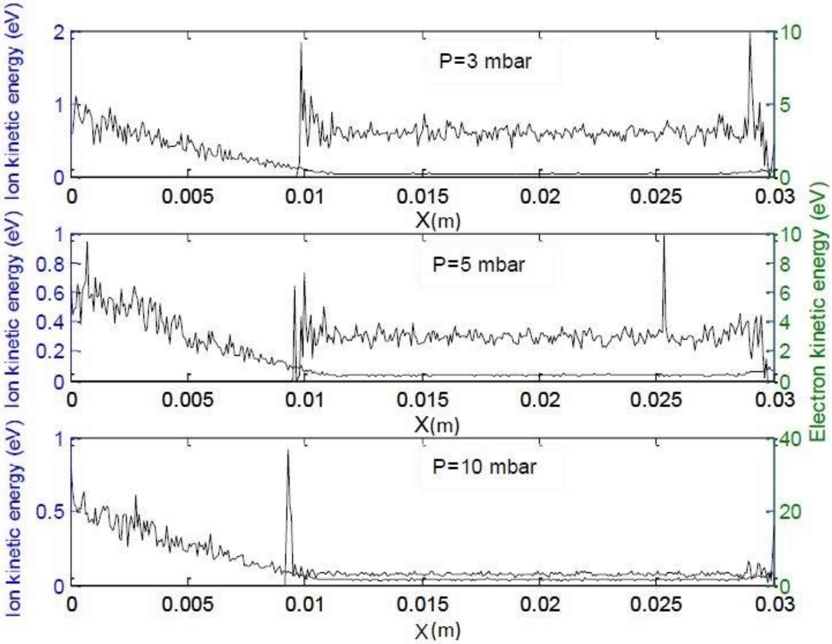


Fig. 9. The effect of working pressure variations from 3 to 10mbar on the ion- and electron-kinetic energy at 3cm, -400v, 0.01 T and $\gamma_{se} = 0.2$ (the electron-kinetic energy has been shown with continues line at the right and the ion-kinetic energy has been shown with dash line at the left).

TABLE 2
THE EFFECT OF WORKING PRESSURE VARIATIONS ON THE AVERAGE OF ION/ELECTRON KINETIC ENERGY AND CUTTENT AT 3 CM, -400V, 0.01 T AND $\gamma_{se} = 0.2$

Working pressure (mbar)	Average of electron kinetic energy (eV)	Average of ion kinetic energy (eV)	Average of electron current (A/m^2)	Average of ion current (A/m^2)
3 mbar	2.9812	0.1725	0.2616	0.0184
5 mbar	2.9401	0.1383	0.3179	0.0165
10 mbar	3.2236	0.1220	0.2034	0.0158

According to Fig. 9 and Table2, ion kinetic energy would be decreased influenced of increasing the working pressure due to increase of ion inelastic collisions. Also, at lower pressures the average of ion kinetic energy and current increase due to reduce collisions and less energy waste. It increases the sputtering yield. On the other hand, the thin film would be deposited with the least structural stress due to increase the mean free path.

C. Role of DC power on argon glow discharge characterizations

Fig. 10 shows the effect of DC voltage variations applied to the cathode on potential difference and electric field profiles. According to this figure, cathode sheath thickness and electric field in this region increase by increasing the DC voltage. Also, Fig. 11 shows the effect of DC voltage applied to cathode on ion- and electron-density. As this figure shows, ion- and electron-density slightly increase by increasing the DC voltage (the anode is connected to the ground).

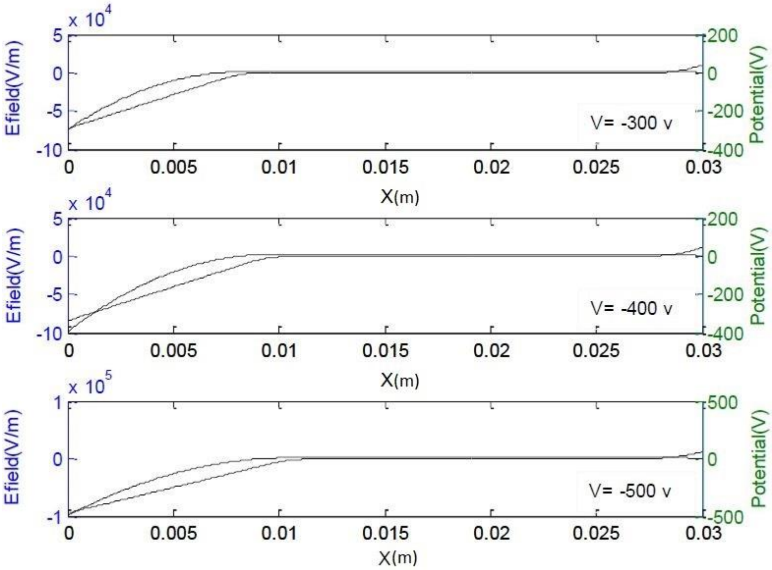


Fig. 10. the effect of DC voltage variations applied to the cathode from -300 to -500 v on potential difference and electric field profile at 3cm, 0.5 mbar, 0.01 T and $\gamma_{se} = 0.2$ (the potential difference has been shown with continues line at the right and the electric field has been shown with dash line at the left).

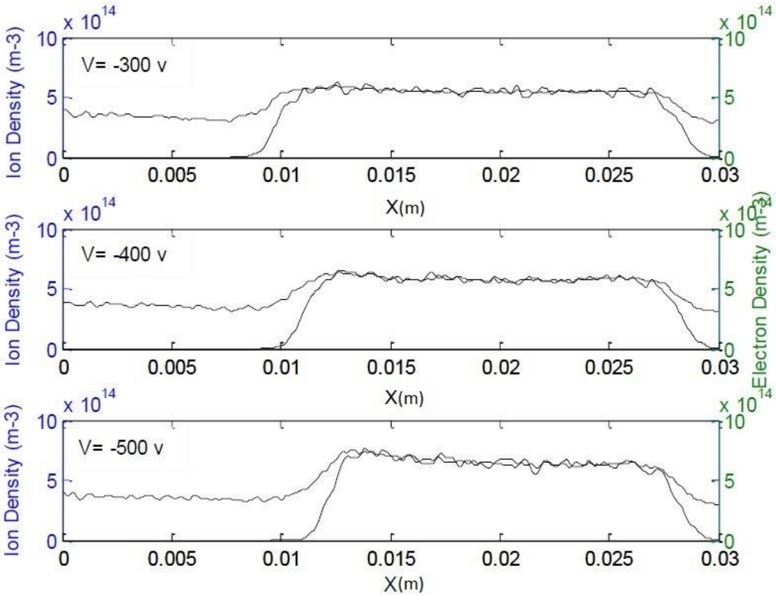
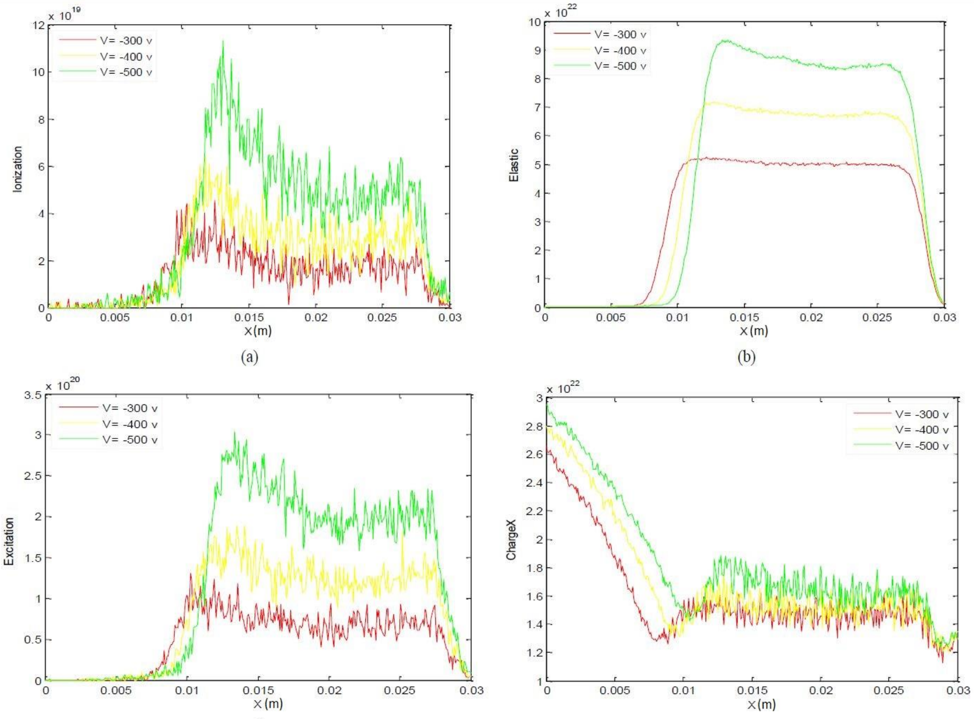


Fig. 11. the effect of DC voltage variations applied to the cathode from -300 to -500 v on the ion- and electron-density profile at 3cm, 0.5 mbar, 0.01 T and $\gamma_{se} = 0.2$ (the electron-density has been shown with continues line at the right and the ion-density has been shown with dash line at the left).

The effect of DC voltage on the cross-section of fundamental processes including as ionization, elastic scattering, excitation and charge exchange are shown in Fig. 12. According to this figure, the cathode sheath is widening with increasing the DC voltage applied to the cathode. Also, increasing the DC voltage has a significant increment on electron- and ion-neutral atom collisions in bulk plasma.

The effect of DC voltage from -300 to -500v on the ion- and electron-kinetic energy is shown in Fig. 13. The average kinetic energy and ion/electron current influenced of DC voltage variations are present in Table 3.



(a) (b)

(c) (d)

Fig. 12. The effects of DC voltage applied to the cathode on fundamental processes. The top left is the ionization process, the top right is the elastic scattering process, the bottom left is the excitation process and the bottom right is the charge exchange process in electron-neutral atom collisions. Simulated data for a 3cm, 0.5mbar and DC voltage applied to the cathode varies from -300 to -500v.

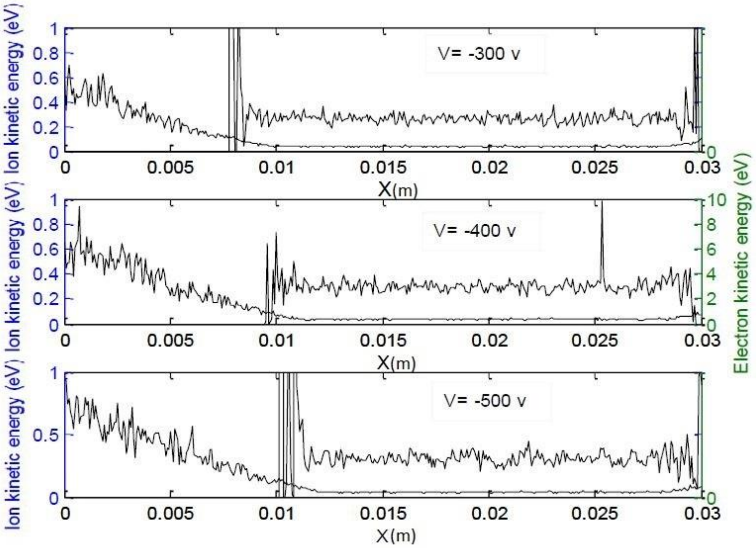


Fig. 13. The effect of DC voltage variations applied to the cathode from -300 to -500 v on the ion- and electron-kinetic energy at 3cm, 0.5 mbar, 0.01 T and $\gamma_{se} = 0.2$ (the electron-kinetic energy has been shown with continues line at the right and the ion-kinetic energy has been shown with dash line at the left).

TABLE 3
THE EFFECT OF DC VOLTAGE VARIATIONS ON THE AVERAGE OF ION/ELECTRON KINETIC ENERGY AND CUTTENT AT 3 CM, 0.5 MBAR, 0.01 T AND $\gamma_{se} = 0.2$

DC voltage applied to the cathode (v)	Average of electron kinetic energy (eV)	Average of ion kinetic energy (eV)	Average of electron current (A/m^2)	Average of ion current (A/m^2)
-300 v	2.6567	0.1097	0.2616	0.0123
-400 v	2.9401	0.1383	0.3179	0.0165
-500 v	3.3638	0.1678	0.2826	0.0203

DC voltage applied to the cathode has to have minimum amount required for glow discharge plasma based on pachen's low. So, according to Fig. 13, by adjusting the voltage, it is possible to obtain maximum average of ion- and electron-current and kinetic energy at the minimum working pressure. According to Table 3 it is obtained at a voltage of -500 volts.

4. CONCLUSIONS

The objective and approach of this work was to optimize the plasma conditions for ITO deposition in order to increase the quality of the ITO thin film. Therefore, utilizing XPDP1 software, theoretical investigations have been conducted in order to eliminate trial and error in our experiments and reduce the search space in order to attain the desired ITO thin film characterization. We opted to simulate argon glow discharge before doing additional tests to establish the effect of varying key critical processing factors, such as the electrodes' distance, working pressure, and applied DC voltage. In this study, the distance between the electrodes was varied from 2 to 5 cm, the working pressure was varied from 3 to 10 mbar, and the absolute voltage applied to the cathode was varied from 300 to 500 v in order to characterize microstructural thin films deposited using a DC magnetron sputtering system. These processing parameters have a substantial effect on the potential difference and electric field profiles, ion- and electron-density, ion- and electron-kinetic energy, and fundamental plasma processes, resulting in variations in the deposition rate and microstructural characteristics of the films. By decreasing the distance between the electrodes, the average ion- and electron-density and kinetics rise, leading to an increase in deposition rate and energy conservation of sputtered atoms. Also, at very close distances between the anode and cathode, substrate surface etching is inevitable, resulting in a decrease in deposition rate. Simulations of working pressure impacts on plasma characterizations, on the other hand, reveal that at lower pressure, the average ion energy rises due to fewer inelastic collisions and less energy loss. This action increases the sputtering of target atoms, hence increasing the deposition rate. In addition, studies of fundamental processes indicate that at higher pressure, inelastic scattering inhibits electron energy from achieving ionization. In reality, at reduced pressure, the mean free path has been widened to create optimal conditions for the deposition of thin films with less microstructural stress. Investigation of the influence of DC power on plasma characterizations reveals that by modifying the cathode voltage, the maximum average ion-density and energy may be attained with the least amount of sustainable working pressure for the deposition process. Due to an excessive increase in ion- and electron-kinetic energy, an excessive increase in applied cathode voltage will result in microstructural damage to the target material and substrate.

CONFLICT OF INTEREST

The authors state that publication of this manuscript does not involve any conflicts of interest.

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