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Analogy Computation of Ions Transport and Sputtering Behavior in Coating Process

Hui-xia Pei[a], Yu-mei Wang[b]

[a]Henan Engineering Research Center of Rail Transit Intelligent Security, Zhengzhou 451460, China
[b]Zhengzhou University of Aeronautics, Zhengzhou 450046, China
huixiapei2738@163.com

With radio frequency sputtering as a study case, this paper aims to simulate and analyze the results from analogy computation on the plasma transport and sputtering behavior in the coating process by a computer. The results reveal that, when plasma sheath parameters are equal to pressure strength, the ions are ingested into the target surface at a vertical angle. As the pressure beefs up, the ion density and sputtering yield will gradually grow up, so does the deposition rate. In the end, it is concluded that energy gradient and sputtering behavior of various particles in the coating process correspond to the general law.

1. Introduction

In the coating process, a variety of microprocesses will all interact with each other to play an impact on film properties and growth. Although there are multifarious models for computing coating process, most of them are too ideal or abstract to give a good direction to practical coating since the intermediate parts in the coating process will affect each other. For example, in the study on the simulation of plasma transport in coating process, many simulation models disable survey and analysis on the magnetic fields as applied. However, in the practical coating process, these magnetic fields may have an impact on the plasma transport process. It is found by experiment on plasma that the incident direction, distribution and concentration during the transport of particles all have an effect on the thin film growth, this is the case for substrate surface morphology and temperature, including film properties, film condensation, and continuous film, etc.

In this paper, the existing coating process models that have emerged are taken as references to study some macro parameters such as gas flow, current and working pressure and analyze their impacts possibly caused. Here simulates and discusses ion transport and sputtering behaviors. The results from this experiment recur the movement law of microscopic particles in the coating process.

2. Overview

At present, plasma research generally adopts two basic approximate methods: fluid method and dynamic method. The fluid model is the solution of Poisson's equation and one or more Boltzmann momentum equations, which can obtain the density, momentum and energy of the charged particles. These models can take into account a range of discharge conditions. Some assumptions of fluid approximation limit their application in plasma research. For example, under low pressure conditions, the mean free path of electron and ion collisions is smaller than the electrode spacing. These models are very difficult. However, current research shows that the fluid model can also be applied under low pressure conditions. The fluid model cannot obtain the energy distribution of the electrons. Therefore, the electronic collision rate coefficient and some other transport coefficients must be assumed. It is generally assumed to be E/N (ratio of electric field strength to neutral particle density) or electronic average energy. Assuming that the transport coefficient, such as the ionization coefficient, is a function of the average energy of the electrons, this can be regarded as a major weakness of the fluid model (Anders, 2017).

Dynamical models such as Monte-Carlo Simulation (MCS), Particle-in-Cell (PIC) and convection models, etc., can fully obtain the electronic energy distribution (EED) and the ion energy distribution (IED) and its variation

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with time and space. Through the MCS technology, the collision process in the discharge plasma is processed, or the EED and IED are directly displayed using the results of the convection model. One of the disadvantages of the dynamic model is that it is computationally expensive. However, this has not been a problem in today's society where computer technology is so advanced.

The mixed model is a model that can not only reduce the calculation time but also keep the non-equilibrium characteristics of the EED unchanged. Dai et al. first used this technique for RF discharge, that is, the so-called "beam-bulk" model. The traditional fluid equation is used to describe ions and low-energy electrons, while the electron beam is used to represent secondary electrons emitted from the electrode (Dai et al., 2015). Bleykher et al. combined the MCS and fluid equations to create a hybrid model. They use MCS to deal with the collision of electrons with neutral particles, so as to obtain various transport coefficients. These transport coefficients are used by the fluid equation to process the transport of various particles. It explains the time response of the electron energy distribution in the electric field. However, the electric field and charge density are not self-consistent in this model (Bleykher et al., 2016).

In the study, Jin et al. pointed out the real mixed model of discharge plasma simulation. In their model, the MCS obtains various collision coefficients. Then, they are used in the fluid equation. In their fluid equation, Poisson's equation is added. It can obtain charge density distribution, different electric field and potential distribution. These parameters are then used in the MCS of the next cycle, which repeats until steady state (Jin et al., 2014).

None of the above-mentioned work has considered the effect of external magnetic fields on the plasma transport process. In the actual plasma application, outside the plasma, a magnetic field is used to change the plasma transport process. It is a commonly used technique. Therefore, the plasma transport in the magnetic field has its special significance. Porteous and Graves established a hybrid model for magnetically confined plasmas such as electron cyclotron resonance-ECR discharge plasmas. Fluid simulation electronics are used in the model. Particles simulate the transport of ions. In ECR, electrons are magnetized. The mobility is lower than that of ions, and the average free path of ions is equivalent to the reaction chamber. In addition, the density of electrons in this plasma is 50,100 times that of other conventional plasmas. The behavior of electrons and ions can be calculated separately. Ostadhossein et al. used the same method to simulate EED in ECR. Electrons are seen as particles and ions are seen as fluids (Ostadhossein et al., 2016). Popa et al. also simulated plasma in ECR (Pop et al., 2016).

Talin et al. have done a lot of work in plasma transport in recent years, especially in the study of plasma transport in magnetic fields. In these works, the MCS model was used to study the changes of plasma density, plasma temperature, distribution of electron and ion parameters (velocity, energy, etc.) and various collision processes in plasma in the presence of a magnetic field. The theoretical calculation results agree well with the experimental results (Talin et al., 2016). Through these studies, the energy distribution and the kinematic behaviour of ions in the near-surface plasma have been discovered. This will be the basis for the study of plasma deposition thin film growth. Software MARLOWE is simulated using molecular dynamics methods. When solving the particle equation of motion, the integration step over time must be carefully chosen. The smaller the integration step of time, the more accurate the solution will be. However, the amount of calculation is increased. In addition, the interaction potential between particles, boundary conditions, and initial conditions are all factors that must be considered. This takes into account the lattice structure of the target and stores it in a computer.

Sputtering is the action of incident ions on target atoms. They exchange energy between them. The target atoms leave the target surface. It is a physical phenomenon of sputtering and a physical process away from thermal equilibrium. The physical quantities such as sputtering yield and sputtering threshold are important parameters to describe the sputtering phenomenon. They have been extensively studied both experimentally and theoretically. The understanding of the sputtering mechanism first broke through theoretical research. It is an interdisciplinary discipline combining low-energy nuclear physics with solid physics. The movement of ions in solids and the mechanism of energy loss are the key to the sputtering process. The sputtering process was also studied using computer simulations. Existing ready-made simulation software is widely used. You et al. used SRIM 2003 (the Stopping and Rang of Ions in Matter) to simulate target sputtering. The emission energy and angle of sputtered atoms are the physical quantities for studying the sputter phenomenon and are also the initial state of sputter atom transport. Computer simulations of the sputtering process can also be divided into molecular dynamics methods and Monte Carlo methods. When modeling with molecular dynamics, particle systems are usually described using Newtonian mechanics. According to the force of the particles, the equation of motion of the particles is established. The change of the particle system's motion state with time is obtained by solving the particle's equation of motion. The force acting on a particle is generally determined by the potential energy of the interaction between the particles (You et al., 2016).

In summary, previous studies have focused on near surface plasma transport. The results of these studies are very helpful for the later research on the movement of deposited particles on the surface. Therefore, based on the above research status, the simulation and calculation of ion transport and sputtering behavior in the coating process are mainly studied. In the simulation, an energy threshold Vmin is generally set. When calculating the force on particle i, only those particles with potential energy greater than Vmin are considered. When the force on the particle is determined, the particle motion equation can be solved to determine the particle velocity and position change process. The molecular dynamics method can not only simulate the sputtering process, but also can solve the slowing process and range distribution of ions in the target.

3. Method

3.1 Simulation of ion transport during coating

Plasma is a state of gaseous substance, under which, the gas consists of ions, electrons, and neutral atoms and is electrically neutral on a macro level. When an electric field is applied to the gas in a low-pressure vessel, a few electrons in the gas will be accelerated by the electric field and easily to the peak due to the low pressure and the high mean free path of the gas. If the collision is purely elastic, the kinetic energy of the atom or molecule increases and the gas temperature jumps up; if it is inelastic, the atom or molecule undergoes excitation and ionization, resulting in many different ions and radicals. These ions are all chemically active particles. They can generate new particles and involve in chemical reactions; newly generated electrons are accelerated by the electric field to collide with other atoms or molecules. The above process is repeated to make the gas rapidly ionized so that an ion state is formed. (The plasma energy exchange is shown in Figure 1 below.) The space size for generating this discharge should be given as follows:

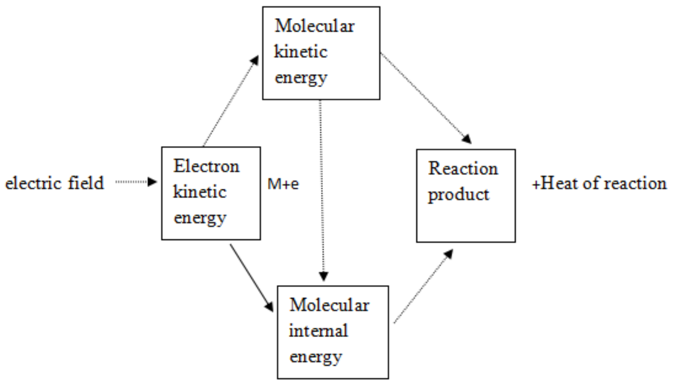

Figure 1: plasma energy exchange

Table 1: changes of particle temperature at different pressures with rf power

Temperature K	The pressure Pa	0.1	0.3	0.3	0.5
Power W					
15		---	---	60	---
20		---	300	70	140
25		---	320	---	159
30		160	358	90	177
35		190	389	100	192
40		207	420	124	210
45		228	457	140	225
50		240	486	159	240
55		255	---	165	253
60		268	521	173	---
70		280	565	195	---
80		300	600	215	---
90		320	630	238	---
100		338	660	269	---

In the RF magnetron sputtering coating, the target base distance, working gas pressure, gas flow, sputtering power, self-bias, etc. are important process parameters. The purpose of most experiments is to seek how the above process parameters affect coating and film properties. As a result, except for the RF power and gas flow, the above parameters are all initial input parameters. There are also other parameters such as temperature and target radius of the neutral particles and ions in the vacuum chamber. RF power mainly consumes away by several processes such as glow discharge, ion transport, and target sputtering, etc., which are quite complicated, for example, glow discharge power will be consumed via ionization collision, excitation, and radiation, etc. Therefore, it is difficult to reveal how correlated the power consumption behaves; additionally, as the ion transport is mainly determined by sheath parameters, the glow discharge power is not regarded as an input parameter. The RF voltage (Upp) target surface self-bias (Ub) and target surface current are chosen as input parameters instead. In the plasma, since the electric field is zero, the ion and neutral particle masses are equivalent, so that it is considered that both are at equal temp and perform thermal motions. The particle temperature can be directly measured. (the measured particle temperature under different conditions is shown in Table 1).

After the initial coordinate and velocity of the ion are determined, the transport process of the ions in the sheath will be simulated. The first step is to determine the sheath parameters, then distance and the stress of the ion transport. It is required to define the sheath width and the electric field distribution. For most sputter coatings, the pressure in the vacuum chamber gets very low, so that the ion free path presents relatively high, and the sheath is generally narrow. When the ions are transported in the sheath, almost no collision with other particles occurs. It is the reason why the Lnagmiur-Chidl theory will be used to describe the sheath. Determine the sheath width and the electric field distribution therein by the formula, the ion current density on the target surface can be calculated by dividing the target surface current density calculated by the target surface current and the target area by 2.

3.2 Simulation of sputtering behavior in the coating process

Sputtering is a physical phenomenon where an incident ion acts on a target atom to mutually exchange energies in this way the target atom detaches from the target surface. The sputtering is a physical process far away from thermal equilibrium. Ion sputtering on a solid surface is a form of interaction between particle and solid, in fact, it is an interaction between the atoms in the particle and solid, as well as the resultant energy exchange process between the two, namely a process of energy loss from particles in solids. (The energy loss mechanism of the particles in the solid is shown in Table 2) The energy loss of the ions in the sputtering process is mainly aroused by the electron and nuclear stoppings. If the energy loss of the incident ions attributes to electron stopping, the velocity must be greater than that of target electron, so that the target electrons can be deemed as stationary. If the incident ions move too slow, all the electrons have time to adjust their motion orbits to fit their instantaneous position. Then energy absorbed by the electrons is less, while the ion mass is high! When the incident speed is low, the energy loss caused by the electron stopping is low. The energy loss is attributed to the blockage of the atomic nucleus.

Table 2: Energy loss of ions in solids

Electronic stop	Nuclear deterrent	bremsstrahlung	The nuclear reaction
Ionized ions transfer energy to electrons, which excite or ionize the target atoms. The energy excited or ionized is called electron energy loss or inelastic energy loss. This is the main mechanism of energy loss of high - speed incident.	The incident particle passes energy to the target nucleus through the elastic collision, which causes the target atom to vibrate or recoil. The energy of the particle loss is called the elastic energy loss. This is the main mechanism of energy loss of low - speed incident particle.	At relativistic speeds, the incident ions emit photons in the target due to changes in momentum.	Nuclear reaction occurs when the incident ion and target atom nuclear energy meet the combination rules of the nuclear reaction and reach the energy threshold of the reaction.

SRIM builds a model based on the cascade collision theory. It treats the target material as an amorphous structure. The target atom is positioned randomly. During the simulation, the S class M traces to the motion trails of each incident ion and recoil atom until their kinetic energy gets lower than specific value or exceeds the target's volume range; a two-body collision approximation is performed when dealing with collision between the treatment ion and the target atom. In this sense, a quantum mechanics and a statistical method are used to measure the distance migrated between two collisions, that is, allow ion randomly jump between two collisions. The jump distance depends on the mean free path of ions that move in the target; the potential energy of the interaction between ions and atoms takes from the shielding Coulomb (such as ZBL interaction potential); the charge state of the ions in the solid adopts an effective charge approximation, while the effective charge matters the speed of ions, such as the Pohl effective charge approximation:

$$z^* = z \frac{\upsilon}{e^2 / h}$$

4. Results and discussion

4.1 Discussion of ion motion simulation results

With reference to the simulation conditions, the results from simulation are verified using the existing sputter coating equipment in the lab. A radio frequency sputtering target is used and pure Ar gas as a sputtering gas to sputter the copper target. The working pressure for controlling pure hydrogen falls around 3.IPa, the gas flow changes. The deposition rate measures up by the film thickness to obtain the relationship between the working gas flow and the deposition rate, as shown in Figure 2. As can be seen from the Figure, the deposition rate is almost insignificant when the working gas flow builds up by three times.

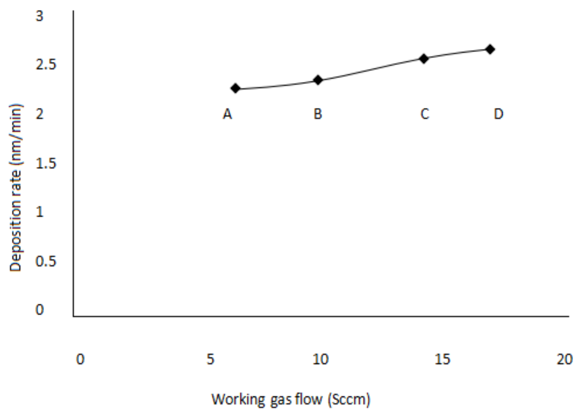

Figure 2: relation curve of working gas flow rate and deposition rate

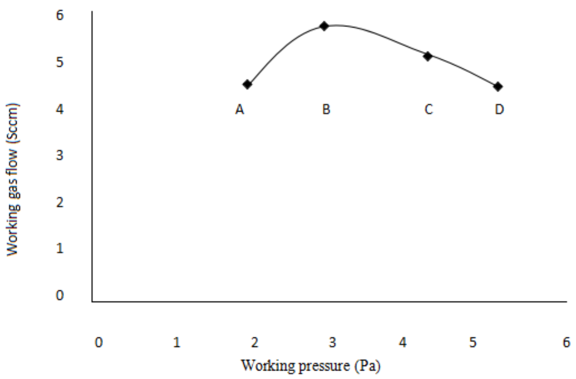

Figure 3: relation curve of working pressure and deposition rate

The deposition rate shows a peak around point B. In the AB section, the deposition rate jumps up as the pressure increases, while in the BD section, the relationship between the deposition rate and the pressure presents an opposite trend. We believe that with the increase of pressure in the AB section, the ionization dominates, thus contributing to a rising trend in deposition rate; while in the BD section the pressure continues to increase, the disorder of the ions and collision probability hike up sharply to be the dominant factors that lead to the change of deposition rate, instead of the ionization, showing a decline. This experimental phenomenon consistent with the simulation results proves the correctness of the simulation results. (the curve of relationship between working pressure and deposition rate is shown in Figure 3)

4.2 Discussion of sputtering behavior simulation calculation results

As the incident ion energy increases, the sputtering yield grows, rapidly in the low-energy zone, but gradually slows down in the high-energy zone. When the energy is high, the sputtering yield will somewhat decrease, as shown in Figure 4. This is due to the fact: when the range of the ions in the target waxes when the energy is very high, the ions are injected into the target deeply, the cascade collision expands into the target, most of the ion energy is consumed in the target body and less on the target surface.

The sputtering yield subject to the change law of incident angle has a stake in the extended area of the cascade collision. When the incident angle is small, the cascade expansion marches toward the target longitudinally. When the incident angle gets wider, it tends to be parallel to the target surface transversely. The sputtering yield increases with the number of cascade collisions within a certain depth near the target surface, and the sputter yield enlarges. When the incident angle is wider, the cascade collision is too close to the target surface to limit the further expansion of the collision. The ion reflection also increases when the incident angle is too wide, so that the sputtering yield swoops.

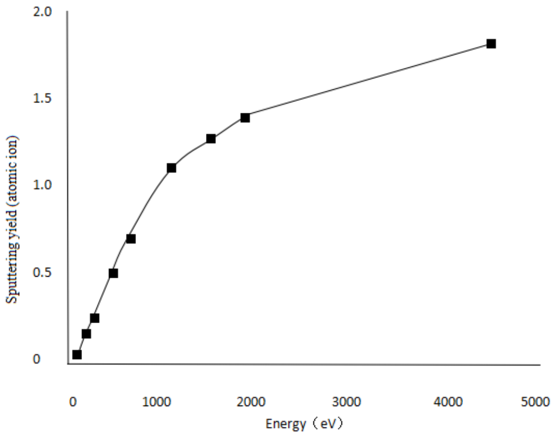

Figure 4: the change of the sputtering yield of the Cu with the incident energy during the vertical incident

5. Conclusion

This paper simulates the ion transport and sputtering behaviors in the coating process with the simulation software SFD and SRIM, and then combine with replication experiments to determine whether the results of this study comply with the general laws. Study finds that during the ion transport process, the deposition rate and working gas flow stay intimate with the working pressure. When the working pressure gradually builds up, the sputtering yield and deposition rate will gradually increase. The ion energy will be subjected to a collision occurred within the sheath. When the gas pressure jacks up, the number of high-energy ions will gradually decrease.

In the course of this study, due to limited space, the incidence direction, pressure conditions and deposition rate in the coating process are focused on here. Although the present study finds that various ions in the coating process will have a bearing on the growth of the film subject to the universal law, it is still required to demonstrate this by practice test whether it is available and operable. This is the keystone of the author's study in the future.

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