CHARGING PROCESS OF A NANOPARTICLE IMMERSED INTO PLASMA CONSISTS $(Ar^+, SF_6^-, AND ELECTRONS)$

عملية شحن جسيم نانوي مغمور في بلازما تتضمن (ايونات الأركون الموجبة وايونات سداسي فلوريد الكبريت السالبة والالكترونات)

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Abstract

This research presents a computer study to simulate of charging process for a nanoparticle (radius =50 nm) immersed into plasma contain electrons, positive ions (Ar^+) , and negative ions (SF_6^-) (The mass of negative ion approximately heavier than the mass of the positive ion), and studies statistical fluctuations of a nanoparticle charge with time. The research also appears effect of negative ion density on charge of nanoparticle.

الخلاصة

هذا البحث يمثل محاكات حاسوبية لعمليه شحن جسيم (قطره بحدود 50 نانومتر) مغمور في بلازما تحتوي ايونات الأركون الموجب وايونات فلوريد الكبريت السداسية السالب والالكترونات (كتله الايون السالب تقريبا اثقل من كتله الايون الموجب) لدراسة تغيرات شحنة الجسيم احصائي مع الزمن. هذا البحث أيضا يبين تأثير كثافة الايون السالب على شحنه الجسيم.

I. Introduction

In recent years, computer simulations studies are playing an important role in theoretical investigations in various branches of human activities, the situation is similar in the researches of negative ion plasma and nanotechnology, that is interesting not only for astronomers (interstellar clouds, comet tails etc.), but it found the place also in complicated technological processes like plasma etching of semiconductor devices [1].

Many of experiments and theoretical methods investigations have carried out for understanding the charging of dust particles in a plasma under different conditions [2, 3, 4]. The charge on the dust particle is not a constant, but can fluctuate randomly, or charge fluctuation on dust particle responses to plasma parameters such as the electron density, radius of dust particle, and the presence of negative ion in plasma. There are several experiments and some theoretical models to estimate the charge of a dust particle as well. However, none of them yields a result with perfect precision [3].

Robert L. Merlino and Su-Hyun Kim studied experimentally the effect of negative ions density (SF_6^-) on the charge of dust grains in a plasma in 2006[4], and in the same year, they studied experimentally charge on dust grain in a plasma with negative ion can be reduced in magnitude to zero. When the electrons of plasma are attracted to negative ions [5].

Wong et al. introduced plasma consist argon ions (Ar^+) , electrons and negative ions (SF_6^-) . The plasma with negative ions (SF_6^-) was formed by Electrons attachment to SF_6 molecules when SF gas pumped into an argon discharge. [6].

In this paper, we investigate the charging of nanoparticle in plasma consisting of positive ions (Ar^+) , electrons and negative ions (SF_6^-) .

Here we will consider theoretical model of charging which is known discrete model after it has developed. In general, the model is useful for estimating the charge with an accuracy of about a two factors time and density of negative ion in plasm and also this is useful for gaining a conceptual understanding of how the charge varies with plasma parameters, and how it can fluctuate in time.

II. Orbit Motion Limited (OML)

The Probe theories determined the currents to an electrostatic probe as a function of probe shape and probe potential, The floating potential on probe is derived as the point when ions and electrons currents balance, First probe theories based on orbit motion limited (OML). Later, Probe theories have been applied to compute dust particle charging. Analytic OML model including:

1. The Dust Particle Charge:

The OML model typically assume that the particle is spherical shape, and its surface is an equipotential. In this case, even if the particle is not made of a conductive material, it can be modeled as a capacitor [4, 5]. The charge Q_d is the dust particle's surface potential when a plasma potential is zero, by

$$Q_d = 4\pi \varepsilon \cdot a\phi_s \quad \dots \quad (1)$$

Where ϕ_s is the dust particle surface potential which relates to the plasma potential, and a is the radius of the dust particle. [6].

2. Currents to the Dust Particle:

For the collection of Maxwellian electron and positive ion currents to the isolated spherical dust grain of radius (a) are calculated from the orbit-limited and given by[8,9]:

$$I_{e} = I_{eo} \times \begin{cases} 1 + \frac{e\phi_{S}}{kT_{e}} & \phi_{s} > 0 \\ e^{e\phi_{S}/kT_{e}} & \phi_{s} < 0 \end{cases} \dots \dots (2)$$

$$I_{+} = I_{+o} \times \begin{cases} e^{e\phi_{S}/kT_{+}} & \phi_{s} > 0 \\ 1 + \frac{e\phi_{S}}{kT_{+}} & \phi_{s} < 0 \end{cases} \dots \dots (3)$$

$$I_{+} = I_{+o} \times \begin{cases} e^{e\phi_{S}/kT_{+}} & \phi_{S} > 0\\ 1 + \frac{e\phi_{S}}{kT_{+}} & \phi_{S} < 0 & \dots \dots \end{cases}$$
(3)

Electrons and ions temperatures are characterized by T_e and T_i respectively. The negative ion current participates in the charging of a dust particle in a plasma with negative ion is [1]:

$$I_{-} = I_{-o} \times \begin{cases} 1 + \frac{e\phi_{S}}{kT_{-}} & \phi_{S} > 0 \\ e^{e\phi_{S}/kT_{-}} & \phi_{S} < 0 \end{cases} \dots \dots (4)$$

The coefficients I_{e0} , I_{-o} and I_{+0} represent the current that is collected for $\phi_s = 0$, and are given by

$$I_{jo} = q_j n_j \left(\frac{kT_j}{m_j}\right)^{1/2} 4\pi a^2 \qquad \dots \dots (5)$$
Where $(j = e, -, or +)$

III. Particle Charging Models

There are some models, often implemented numerically to calculate the charge and potential of particle in a plasma, as described by Discrete Charging Model.

Discrete charging model considers the ion and electron currents collected by the dust grain consist of individual electrons and ions. The charge on the grain is an integer multiple of the electron charge value, $Q_d = Ne$, where N (charge number) changes by +1 when an ion (ion charge+1) is absorbed

And by -1 when an electron is absorbed.

The charge on a particle fluctuates in discrete steps about the steady-state value $\langle Q_d \rangle$ at random times [4, 8].

There are two key aspects of the collection of discrete of plasma particles (we use the term "plasma particle" to refer to either electron or ions).

- First is that the time interval between the absorption of plasma particles (electrons and ions) varies randomly.
- Second is that the electrons and ions arrive at the grain surface is not purely random; but they obey probabilities that depend on the potential of dust grain ϕ_s .

Let us define $p_e(\phi_s)$ and $p_i(\phi_s)$ as the probability per unit time for absorbing an electron or ion, respectively. As the grain potential becomes more positive, more ions will be repelled and more electrons will be attracted to the grain, so p_i should decrease with ϕ_s and p_e should increase. $p_j(\phi_s)$ (j refers to the ions, and electrons) was calculated from the OML currents $I_j(\phi_s)$,

$$p_j = \frac{I_j}{q_j} \qquad \dots \dots \dots (6)$$

This equation is the key to developing the discrete charging model. Basically, it converts the OML currents into probabilities per unit time of collecting particles. This relates the discrete charging model with its probabilities to the continuous charging model with its currents [8].

The total probability per unit time of collecting plasma particle is [8]

$$p_{tot} = \sum p_j \qquad \dots \dots \dots (7)$$

The currents I_j depend on the grain surface potential ϕ_s , so p_{tot} also depends on ϕ_s and hence on charge Q_d .

IV. Development of the Discrete Model

The discrete model was developed to include effect of negative ion density on the charging process of dust grain in a negative ion plasma instead of plasma electron-ion [9]. The model is useful for gaining a conceptual understanding of how the charge varies with plasma negative ion parameters, and how it can vary in time. Which in general is useful for estimating the charge of dust grain.

The model has described the charging process of an isolated dust grain (immersed in a negative ion plasma) and assumed a spherical grain with radius a which initially uncharged under the condition $a \ll \lambda_d \ll \lambda_{mfp}$, where a is the dust particle radius, λ_d is Debye length, and λ_{mfp} is a collisional mean-free-path between neutral gas atoms and either electrons or ions In this case. The charging process is characterized by [9]:

- 1. It is based on the assumption that the plasma particles arrive to dust surface at random time intervals Δt_i , which is not fixed
- 2. The probabilities of arriving electrons or ions (negative or positive) in equations (6) depend on the potential of the dust particle.
- 3. The total probability per unit time of collecting plasma particle is calculated from equation (7)

- 4. The time interval Δt_j depends on the potential of the grain surface ϕ_s and the random number R_I that was generated.
- 5. The discrete model assumes that plasma particles arrive in a random sequence in consistent with the probabilities.
- 6. To recognize the plasma particle type electron or ion (negative or positive), it must compare the probability P_i/P_{tot} with another random number R_2 .
- 7. The charge Q_d of the dust would be changed after each electron or ion (negative or positive) collection, and it is increased or decreased by one charge.

The simulation converts the physical discrete charging model after add negative ions current to program which simulates the charging process of a dust grain immersed in plasma with negative ion.

At first the dust grain would be uncharged so the computer experiment starts with a zero charge $Q_j = 0$ at a time step equal zero $t_j = 0$ where j refers to plasma particle electron, negative ion or positive ion, then two steps will be repeated for plasma particles which will fall on the dust.

A. First Step: The Random Time Intervals

This step is based on the physical discrete charging model, which assumes that the plasma particles arrive at random time intervals, there will be one time step per particle that is collected and it corresponds to:

$$\Delta t_i = t_i - t_{i-1} \qquad \dots (8)$$

The currents I_e , I_- and I_+ must calculated from equations (2, 3, and 4) there are predicted by the OML theory to find the probabilities.

The random time step Δt_j depends on the probability per unit time of collecting a plasma particle $P_e(\phi_s), P_-(\phi_s), P_+(\phi_s)$ and the total probability is given in equation (7)

The probability of collecting a plasma particle is [8]:

$$P = 1 - exp(-\Delta t_i.P_{tot}) \qquad \dots (9)$$

To calculate the random time interval one must generate a random number R_I where $0 \le R_1 \le 1$ and equate it to the previous equation of probability to yield [8]:

$$\Delta t_j = -\ln(1 - R_1)/P_{tot} \qquad \dots (10)$$

B. Second Step: The type of plasma particle

The plasma particle arrives in a random sequence. Generate a random number R_2 to determine whether the next collected particle is an electron or an ion (negative or positive), where $0 < R_2 < 1$. Probability of the next particle (electron, negative ion or positive ion) equals to $= P_j/P_{tot}$ and compares with R_2 as follows [10]:

- i. If $R_2 < P_e/P_{tot}$ then the charge will be $Q_j = Q_{j-1} e$ that means the process is electron collection. However, at state $R_2 > P_e/P_{tot}$ that means the process isn't electron collection. The probability of other particle must examined.
- ii. If $R_2 < P_-/P_{tot}$ then the charge will be $Q_j = Q_{j-1} e z_{ni}$ that means the process is negative ion collection.
- iii. If $R_2 > P_-/P_{tot}$ then the charge will be $Q_j = Q_{j-1} + e z_{pi}$ that means the process is positive ion collection.

V. Programing of The model

After the discrete charging model was developed, that was translated to numerical calculations using computer program. The program was written in MATLAB to simulate a computer experiment of the charging process for a dust grain in negative ion plasma. The program computed statistical calculations such as the time distribution of a dust charge, equilibrium charge and charging time for different value of η_e (ratio of number density of electron to number density of positive ion)[10]. In this research, we can apply this model on nanoparticle that immersed into plasma. This plasma contains electrons, positive ions (Ar^+) , and negative ions (SF_6^-) (The negative ions have a mass approximately heavier than the mass of a positive ion). the positive ion, negative ion and electron have equal temperatures $T^+ = T^- = T_e = 0.2$ eV.

VI. Results and Discussion

The results of program are a sequence of the calculations process, which is done as the following steps:

1. The charge fluctuations on nanoparticle

The first, we will study charging process of nanoparticle (with radius=50nm) immersed into plasma consists electrons and argon ions Ar^+ only (For comparison purpose). That leads to charging the particle negatively because the mobility of electrons larger than mobility of ions. The ions and electrons have equal temperatures $T^+ = Te = 0.2$ eV.

The charge on the grain will reach the equilibrium state in which the charge Q will fluctuate around the equilibrium charge<Q>. Figure(1) shows the chraging process for a nanoparticle by collecting electrons, and positive ions from plasma with out negative ion, notes that the range of the charg fluctutions between -31 and-42.

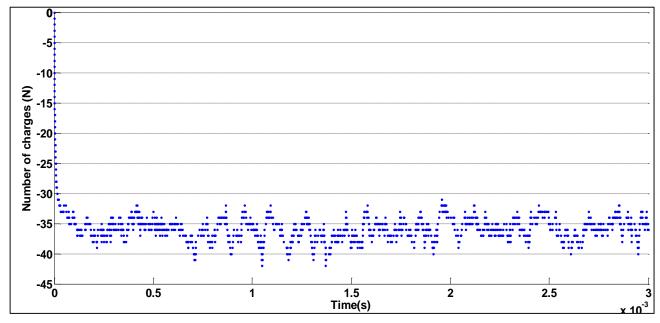


Figure (1): Charges number on surface of nanoparticle as a function time when radius of particle=50nm, $\eta e = 1$ (no negative ion)

The second, a nanoparticle (with radius = 50nm) is immersed in plasma Ar^+ after add SF_6 , a fraction of the electrons are attracted with SF_6 . This process can be described as

$$SF_6 + e \rightarrow SF_6^-$$

When the SF_6^- density is created in Ar^+ plasma, the electrons current will reduced due to some electrons become attached to form SF_6^- ions, as Figure (2) shows that the range of the charge fluctutions is between -28 and -18 and the renge drifts toward positive compare with Figure (1).

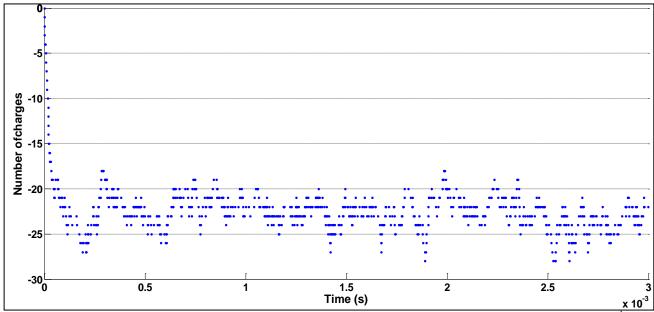


Figure (2): Charges number on surface of nanoparticle as a function time when radius of particle =50nm, η_e =10⁻¹.

When the SF_6 density is increased in argon plasma, more electrons become attached to form SF_6^- ions. Therefore, the negativity of charge number on nanoparticle decreases gradually. Figures (3), and (4) show that the ranges of the charge fluctuations are about (-15, -7), and (-5, 3) respectively.

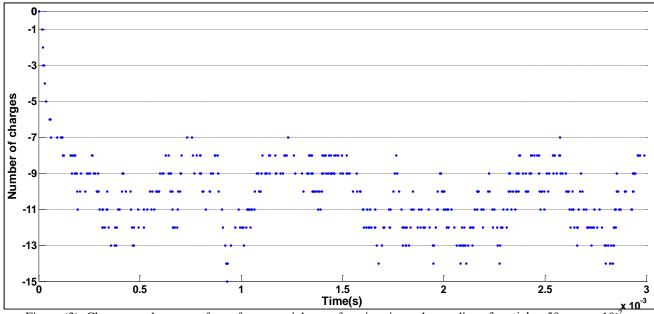


Figure (3): Charge number on surface of nanoparticle as a function time when radius of particle =50nm, η_e =10⁻²

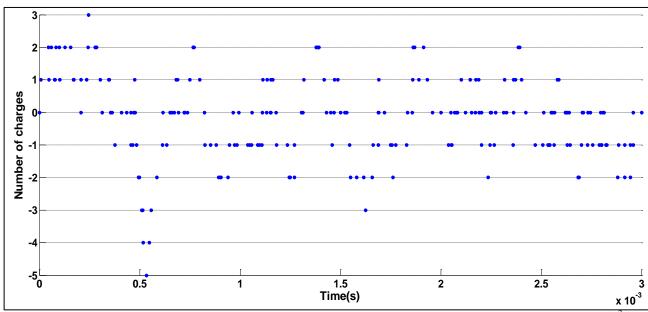


Figure (4): Charge number on surface of nanoparticle as a function time when radius of particle =50nm, η_e =10⁻³

In figure (5) the fluctuation of charge on nanoparticle become positive between 8 and 13 which means dominate argon ions on the charging process

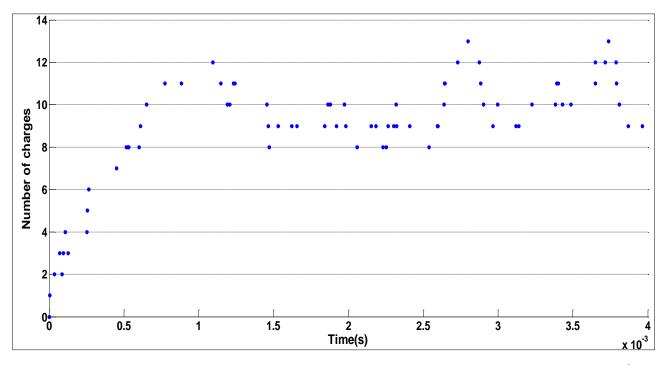


Figure (5): Charge number on surface of nanoparticle as a function time when radius of particle =50nm, η_e =10⁻⁴

2. The Time Distribution of The grain Charge

After the collection of charges by nanoparticle, these charges will approach the equilibrium value $\langle Q \rangle$ and the probabilities for collecting electrons, negative ions (SF_6^-) , and positive ions (Ar^+) are unequal so the charge will always fluctuate around the equilibrium value. The charge distributions are determined from the time series by making histogram each charge level to calculate charge equilibrium value, the equilibrium charge number takes larger time from computer experiment time. Figures (6), (7), (8), (9) and (10) show distribution functions for each case in the previous section.

In figure (6) the chraging process for a nanoparticle by collecting electrons and positive ions (Ar^+) from plasma. Positive ions (Ar^+) are much heavier than electrons therefor the nanoparticle becomes negatively charged. The equilibrium charge number is -36 because this level takes longer time in comprison with other levels.

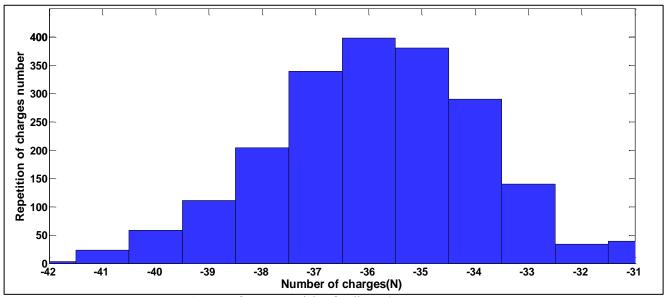


Figure (6): Charge distribution function for nanoparticle of radius=50nm, η_e =1 (no negative ion) The equilibrium charge number is=-36

When the SF_6 density is pumped in Ar^+ plasma, some electrons become attached to form SF_6^- .if η_e =10⁻¹, the negativity of charge number on nanoparticle decreases and the equilibrium charge number becomes -23. Figure (7) shows that.

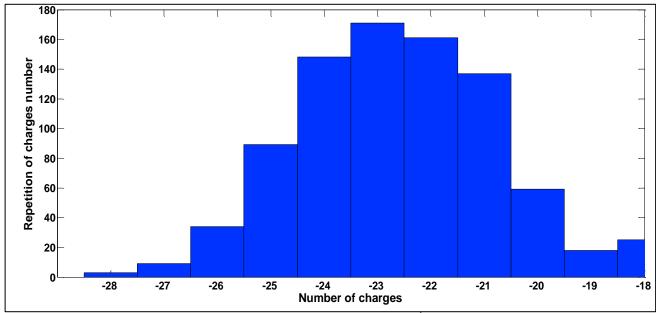


Figure (7): Charge distribution function for nanoparticle of radius=50nm, $\eta_e=10^{-1}$. The equilibrium charge number is= -23

If the SF_6^- density is increased in argon plasma so as to $\eta_e=10^{-2}$, the equilibrium charge number becomes -10 as in the figure (8).

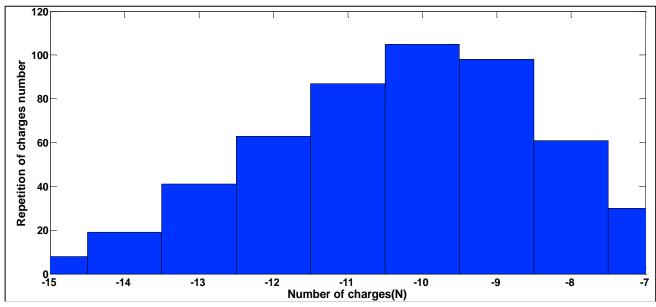


Figure (8): Charge distribution function for nanoparticle of radius=50nm, η_e =10⁻². The equilibrium charge number is= -10

In figure (9) the number of charges equals zero because number of positive charges equals number negative charges on nanoparticle (the nanoparticle is neutral)

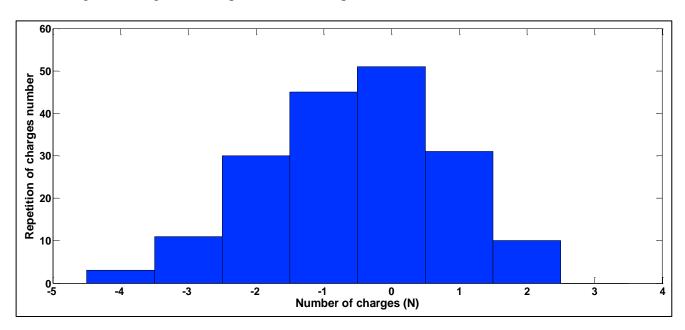


Figure (9): Charge distribution function for nanoparticle of radius=50nm, $\eta_e=10^{-3}$. The equilibrium charge number is= zero

When the ratio of number density of electrons to number density of positive ions equals 10^{-4} . The charge number on nanoparticle becomes positive and equals nine that means the positive ions current dominates on charging process of nanoparticle and probability of positive ions to arrive nanoparticle's surface larger than probability of electrons. Because, the negative ions have a mass approximately heavier than the mass of the positive ion and number density of electrons is sufficiently small. Figure (10) shows that.

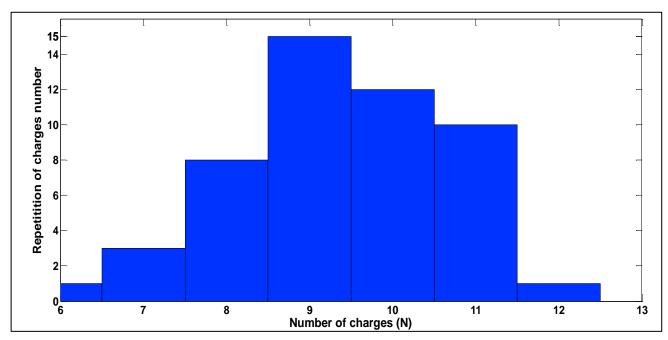


Figure (10): Charge distribution function for nanoparticle of radius=50nm, $\eta_e=10^{-4}$. The equilibrium charge number is= 9

VII. Conclusions

The charging of nanoparticle in plasma contains electrons, positive ions (Ar^+) , and negative ions (SF_6^-) (The negative ions has a mass heavier than the mass of the positive ion) can be controlled by changing density of negative ions in the plasma. When the negative ion density increases, the relatively mobile electrons are attracted to create negative ions therefor, the magnitude of the negative nanoparticle charge is reduced and became positive.

The charge equilibrium value calculates from the time series by making histogram of time spent at each charge level. Where, the charge distribution function has peak at the equilibrium charge value.

VIII. Reference

- 1. A. A. Mamun and P. K. Shukla, Phys. Plasmas, Vol. 10, No. 5, (2003).
- 2. A. Melzer, and J. Goree, "6 Fundamentals of Dusty Plasmas", WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany (2008).
- 3. M. Schwabe, "Microparticles as Probes in a Highly Magnetized Dusty Plasma", Thesis in Technische Universität München (2006).
- 4. S.-H. Kim and R. L. Merlino, Phys. Plasmas, Vol. 13, No. 052118 (2006).
- 5. R. L. Merlinoa, and S. -H. Kim, Appl. Phys. Lett., Vol. 89, No. 091501 (2006).
- 6. B. Song, N. D'Angelo, and R. L. Merlino, Phys. Fluids B, Vol. 3, No. 2,(1991).
- 7. C. Cui and J. Goree, IEEE Transactions on plasma science, vol.22, no.2, pp. 151-158 (1994).
- 8. S. J. Choi, and m. j. Kushner, IEEE Transactions on plasma science, vol.22, no.2,pp.138-150, (1994).
- **9.** Z.A.Mankhi,"Dust Grain Charge process in Negative Ion Plasma", M.Sc. thesis, Baghdad University (2012).