Charge and Potential Distributions for Particles Approaching Substrates with Regular Structures

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Abstract—The charge and potential distributions for insulating particles approaching a substrate with regular insulating structures are studied by particle-in-cell numerical simulations. An elongated particle and substrate with elongated structures are considered for flowing plasmas. The role of the relative position of the particle and the substrate in their interactions is investigated. It is also demonstrated that the interactions are modified by photoemission due to directed UV light. The simulations are two dimensional with ions and electrons treated as individual particles.

Index Terms—particle deposition, simulation, particle-in-cell, elongated grains, dust, charging, photoemission, UV light.

I. INTRODUCTION

THE plasma aided deposition of particles or grains on substrates allows for the growth of highly ordered structures. Such structures have many applications, including various microelectromechanical systems (MEMS). MEMS components are typically up to hundred micrometer in size, and the size of the whole device can be of the order of millimeter. In the limiting case, structures of nanometer size can be manufactured, examples of which include nanotips, wires, and walls.

The understanding of interactions between small objects and structures is important for controlling the particle deposition. Many experimental and numerical studies have addressed specific problems, but there is still little knowledge on the overall process. In particular, the role of ions and electric fields in the formation of small grain assemblies is not well understood, although the corresponding physics is important. In the studies of charging and interactions of dust grains in a plasma it has been shown that the charge, density and potential distributions depend on grain shapes and material, their relative orientations, and the plasma speed. In the presence of an ion flow, wakes in the ion density and potential as well as a region of enhanced ion density, often referred as the ion focusing, form behind the grain. In other studies, it has been shown that the grain charge can be effectively modified by UV radiation. UV light is often used for cleaning purposes prior to wafer processing or in the photolithography. These processes usually do not include plasma, which can be itself a source of UV radiation.

Studies of interactions between objects in flowing plasmas are also important for controlling the dust grain dynamics in plasma processing devices, where dust can contaminate semiconducting wafers. Various dust cleaning and trapping methods are used during processing, but most methods modify also the conditions of the plasma aided particle deposition. New ways of the dust control can improve the performance of the process.

Small sizes, different shapes, and large numbers of particles and grains embedded in plasma make it difficult to analyze the problem analytically, while the diagnostics in experiments is limited. Numerical simulations allow for studies of such a system with non-invasive diagnostics. With an intention to elucidate the physics of interactions between two insulating objects of complex shapes in flowing plasmas, we present results from numerical simulations on the interactions of an insulating particle (hereafter referred as a grain) approaching an insulating structure with perpendicular rods. We consider a self-consistent charging of the grain and the substrate in the collisionless plasma flow. The charging is by collection of electrons and ions. In addition, we allow for photoionization due to directed UV light. The simulated objects are relatively large, i.e., their dimensions are comparable with the electron Debye length \( \lambda_{De} \). We note that a similar problem can be formulated for studies of the coagulation of two insulating dust grains of different sizes as well as for a spacecraft in the low Earth orbit, which is passing through plasma regions of different densities and temperatures.

II. NUMERICAL CODE

The numerical simulations are carried out with the particle-in-cell (PIC) code. The code was previously described in detail and only some basic features of the numerical environment are provided here. We consider collisionless plasma in a two dimensional system in Cartesian coordinates. Both electrons and ions, which are treated as individual particles, are introduced with Maxwellian velocity distributions within the simulation area of \( 50 \times 50 \) in units of the electron Debye length \( \lambda_{De} \), with the exception of the areas occupied by the simulated objects. Plasma can leave the simulation area and is also injected through the boundaries at each time step \( \Delta t \). The electron to ion temperature ratio is \( T_e/T_i = 100 \), with \( T_e = 0.18 \) eV. We have the ion to electron mass ratio \( m_i/m_e = 120 \). The plasma density is \( n = 10^{10} \text{ m}^{-2} \), and the plasma flow velocity is \( v_d = 1.25 C_s \).
TABLE I
SUMMARY OF THE PLASMA PARAMETERS IN THE SIMULATION.

| Parameter                              | Value                        |
|----------------------------------------|------------------------------|
| Simulation area length, \( L_x = L_y \) | \( 5 \times 10^{-4} \) m     |
| Electron Debye length, \( \lambda_{De} \) | \( 10^{-4} \) m              |
| Electron temperature, \( T_e \)         | 0.18 eV                      |
| Temperature ratio, \( T_e/T_i \)        | 100                          |
| Ion to electron mass ratio, \( m_i/m_e \) | 120                          |
| Electron plasma frequency, \( \omega_{pe} \) | 1.79 \times 10^9 s^{-1}      |
| Ion plasma frequency, \( \omega_{pi} \)  | 1.63 \times 10^8 s^{-1}       |
| Plasma density, \( n \)                | \( 10^{19} \) m^{-2}          |
| Plasma drift speed, \( v_d \)           | 1.25 \( C_s \)               |

with \( C_s \) denoting the speed of sound. Because of the large electron thermal velocity, the plasma flow is represented by the ion drift. The plasma parameters are typical for rf and dc discharge plasma, and are summarized in Table I.

The deposited grain and the substrate are placed within the simulation area, far away from the boundaries. The substrate consists of three elongated structures oriented parallel to the flow, and an orthogonal plate. The grain is elongated and aligned with the flow. The grain dimensions are \( \approx 3.6 \) and \( y \approx 0.75 \) measured in units of \( \lambda_{De} \). We consider grains with different distances \( d \) and different offsets from the symmetry line \( p \) with respect to the substrate: \( d = \{1, 5, 10\} \), \( p = \{0, 0.5, 1, 2\} \) both measured in units of \( \lambda_{De} \). The schematics of the arrangement is shown in Fig. 1. The deposited grain and substrate are both massive and immobile during the simulation. They are initially not charged. Since we consider insulating objects, the plasma particle hitting the surface of the object remains there for all later times contributing to the local charge density.

When the photoemission is considered [14], a pulse of a directed light is switched on at approximately 35 ion plasma periods \( \tau_i \) . At this time, we can assume that the surface charge modification on the objects has reached a stationary level. The pulse duration is approximately \( 3\tau_i \). The code is run typically up to \( 50\tau_i \). The angle between the incident photons and the plasma flow direction is \( \alpha = 45^\circ \), and the photon flux is \( \Psi_{he} = 2.5 \times 10^{11} \) m\(^{-2}\)s\(^{-1}\). When a photon hits the dust, a photoelectron is produced at distance \( l = s v \Delta t \) from the dust surface, where \( s \) is a uniform random number \( s \in (0, 1) \), and \( v \) is the photoelectron speed. Photoelectron velocity vectors are uniformly distributed over an angle of \( \pi \) and directed away from the dust surface. We consider monoenergetic photoelectrons with the energy \( E = 0.5 \) eV.

III. NUMERICAL RESULTS

An insulating grain approaching a substrate is charged by the surrounding plasma, with the total charge on the grain being negative. We observe positive and negative maxima in the charge and potential distributions on the grain surface. The maxima are due to the ion dynamics around a perfectly insulating object. Behind the grain, the wakes in the plasma potential and density are formed, together with the region of an enhanced ion density, which is due to the bending of ion trajectories by strong electric fields in the vicinity of grain. The charging of an insulating, elongated grain has been studied in more detail elsewhere [20].

The wake behind the grain modifies the plasma density and potential distributions in the vicinity of a substrate, see Fig. 2. The plasma density is reduced close to the substrate, with the strongest reduction between the rods. With decreasing distance \( d \) between the grain and a substrate, the ion focusing region is located closer to the rods on the substrate. For small \( d \), the end of the rod placed behind the grain can be exposed to ion fluxes higher than rods located further in the wake of the grain or even in an undisturbed plasma. On the other hand, rods located far from the grain in the direction perpendicular to the flow, can have their ends outside the ion wake for small \( d \). In both cases the charges on the rod ends become more positive due to a directed ion flow, and the rod that is closest to the ion focusing region experiences the highest flux. The end of the grain in the shadow of the flow is negatively charged. This can accelerate the grain towards the rods at smaller distances \( d \).

An offset \( p \) of the grain from the symmetry axis leads to asymmetric charging of the rods on the substrate. The asymmetry is stronger for distances \( d = 1\lambda_{De} \), when the ion focusing region is close to the rods, see Fig. 2(c)-e). For grains located near to one of the rods, most of the ion flux from the ion focus will positively charge the end of this rod. For the grain located between two rods, both rods can receive significant ion flux, which results in both rods having positively charged ends. The charge modification on the rod ends for small \( d \) is manifested by variations in the potential distribution on a substrate. Weaker variations are present also for larger \( d \).

The average ion flux density \( \psi_i = \pi_\lambda v \) to the rods on the substrate is shown in Fig. 3 for different \( d \) and \( p \). The average is taken over a time interval of seven ion plasma periods and over the area of each grid cell. We observe an enhancement in the flux for the ion focusing regions. For \( d = 5\lambda_{De} \) and \( p = 2\lambda_{De} \), the ion flux density is reduced in the wake and a weak asymmetry is observed. For \( d = 1\lambda_{De} \) and \( p = 1\lambda_{De} \), the fluxes to the ends of the two nearest rods are enhanced, but the flux reduction is observed between these rods closer to the substrate. The asymmetry in the flux between the rods closest to the grain is pronounced, while only weak asymmetries are observed between other rods. Some of the ions behind the grain can be lost to the rod surface before reaching the substrate, and thus the wake of a charged insulating grain
Fig. 2. Ion density (left) and potential (right) distributions for different distances \(d\) and offsets \(p\): (a) \(d = 10 \lambda_{De}\), \(p = 0\); (b) \(d = 5 \lambda_{De}\), \(p = 2 \lambda_{De}\); (c) \(d = 1 \lambda_{De}\), \(p = 0 \lambda_{De}\); (b) \(d = 1 \lambda_{De}\), \(p = 1 \lambda_{De}\); (b) \(d = 1 \lambda_{De}\), \(p = 2 \lambda_{De}\). The data are averaged over seven ion plasma periods at the end of simulation. Note different scales on \(x\) and \(y\) axes for (a)-(b) and (c)-(e). Potentials are normalized with \(kT_e/e\), where \(e > 0\). The plasma flows in the positive \(x\) direction.

Fig. 3. The averaged ion flux density for (a) \(d = 5 \lambda_{De}\) and \(p = 2 \lambda_{De}\) and for (b) \(d = 1 \lambda_{De}\) and \(p = 1 \lambda_{De}\). The data are averaged over a time interval of seven ion plasma periods at the end of simulation and over each grid cell by weighting the ion velocities to the nearest grid points. The ion flux densities are shown for a reduced number of grid points. The areas occupied by the grain and the substrate are marked grey.

The surface charge distributions on the grain and a substrate are modified by the photoemission due to the pulse of UV light. The grain and substrate become more positively charged during the illumination on the side of the photon incidence. The region of enhanced ion density moves away from the grain and the wake is distorted. The light shadowing by the rods lead to a complicated surface charge distribution. After the pulse, the total charge on each object recovers to the previous value, but the remaining complicated charge distribution due to the photoemission can modify the plasma dynamics, see Fig. 4. As a result, the inner sides of the nearest rods can be effectively shields the microchannel formed by two rods from a plasma.
positively charged: one by photoemission, and the other by
the ion focusing. The grain between such rods can be drawn
towards the substrate. Different angles of the photon incidence
can lead to different surface charge distributions and scenarios
for the grain deposition.

IV. DISCUSSION AND CONCLUSION

Interactions between an insulating grain and a substrate
with insulating structures in a flowing plasma depend on their
relative positions. The charge and potential distributions on
the substrate are modified by the wake originating from the
plasma flowing around the grain. Without photoemission, the
electrons are Boltzmann distributed, while ions trajectories are
bent by strong electric fields in the vicinity of the grain. As a
result, the region of an enhanced ion density forms in the wake
of the grain. This effect is similar to the electrostatic lensing,
and it will also be present for smaller grains [5], [21]. The ion
focusing is stronger for smaller grains, and weaker focusing is
observed also for subsonic ion velocities [12].

The ion focusing in the wake of the grain has implications
for the control of the plasma enhanced chemical vapor deposi-
tion (PECVD). The grain above the surface of the substrate
electrostatically focuses the ion flux, making it possible to
converge the deposited material on a substrate. For elongated
grains tilted with respect to the average ion flow, the ion
dynamics can be asymmetric behind the grain [20]. Therefore,
by manipulating the position and orientation of the grain by
external forces (e.g., laser and/or electric field), it is possible
to control the growth of microstructures on the substrate by
changing the PECVD flux locally.

Except for the region of ion focusing, the wake behind
the grain is characterized by the reduction in the plasma density.
This reduction is observed already at a distance $d = 10\lambda_D$.
Hence, when a few grains are present close to the substrate,
the grain with larger $d$ can influence the dynamics of the grain
located closer to the substrate.

The wake structure causes the charge on individual rods on
the substrate to be a function of the position of the grain. In
particular, the ions streaming out of the ion focusing region
contribute to the positive charging of the structures on the
substrate. This will lead to attraction of the grain, which is
negatively charged on the wake side, by the positively
charged ends of the structures. Furthermore, complicated sur-
face charge distributions on the grain and substrate will lead
to a torque on the grain. The torque will originate not only
from the electrostatic potential distribution in the vicinity
of the grain, but it is also due to the momentum transfer from
incoming ions. By controlling the position of the grain above
the substrate, the grain deposition angle can also be controlled.
The elongated grain can be, for example, deposited on the
structure perpendicular to the flow to further reduce the ion
density between the rods.

Photoemission due to the pulse of UV light modifies the
charge distribution on the grain and substrate and provides
yet another mean of controlling the PECVD process. Af-
after the pulse, the surface charge distribution remains to be
complicated, and it influences the ion dynamics close to
the objects. Different scenarios for the grain deposition are
possible, depending on the angle of the photon incidence. For
instance, the grain can be drawn towards the surface of the
substrate between the rods, which can be achieved by the
illumination of the substrate from both sides.

We considered pulsed radiation because the charge satura-
tion is not always the case for insulating grains exposed to
continuous radiation. This due to the development of a strong
electric dipole moment on such grains. The charge saturates,
however, for conducting grains charged by photoemission [14].
For usual conditions we have the work function for insulators
between five and ten electronvolts. If the work function of
a grain is lower from the substrate, or if the the substrate
is biased, the photoemission due to directed light allows to
modify the grain potential and wake without changing the charge distribution on the substrate for $d > 1\lambda_D e$ (when the ion focusing does not modify much the surface charge distribution on the substrate). In particular, our results for photoemission can also be applied for insulating spacecraft components interacting with other objects in space.

Two dimensionality of the model implies that the rods on the substrate can be interpreted as elongated structures forming walls or trenches. The sizes of the simulated objects are comparable with the electron Debye length, thus corresponding to structures of the sizes of MEMS components or larger grains in processing devices. In the limiting case of nanotechnology, most of the processes happen in the sheath region, and the size of the structures is usually much smaller than the Debye length. The physics can be different there due to lack of effective shielding of closely spaced objects. Nevertheless, the characteristic features of the plasma flowing around an object, such as the potential enhancement corresponding to the ion focusing region, will be still present around objects much smaller than the Debye length \[11, 22\].

To summarize, we have shown that for an insulating grain and insulating substrates, the ion dynamics around the grain will effectively modify the charge on the rods on a substrate and lead to attraction between the rod end and the grain. Photoemission changes the charge and potential distributions on the grain, and it can provide a method for controlling the dynamics of small grains above substrates.

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