Self-organization of Dust Chains in the Presence of Ionization Waves

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(Dated: 2 November 2021)

Recent studies have shown that the positive column of the gas discharge plasma in the Plasmakristall-4 (PK-4) experiment onboard the International Space Station (ISS) supports the presence of fast-moving ionization waves, which lead to variations of plasma parameters, such as the axial electric field, and the electron and ion number densities, temperatures, and drift velocities by up to an order of magnitude from the average background values. This may have interesting implications for the dynamics and self-organization of dust particles in this environment, particularly concerning the formation of dust chains. The electrorheological effect, where clouds of positively charged ions concentrate downstream of the negatively charged dust grain and affect interparticle attractions, is currently considered the most probable mechanism for the formation of structures such as dust strings and crystals. Here we investigate the formation of filamentary dust structures in the PK-4 by employing a molecular dynamics model of the dust and ions with boundary conditions supplied by a Particle-in-Cell with Monte Carlo collisions (PIC-MCC) simulation of the ionization waves. The model is used to examine the effect of plasma conditions at various points in the ionization waves as well as time-averaged plasma conditions. Comparison with experimental data from the PK-4 shows that the simple time average does not accurately reproduce observed results, indicating that more careful treatment of plasma conditions in the presence of ionization waves is required.

I. INTRODUCTION

A complex plasma is comprised of neutral gas atoms, ions, electrons, and micrometer-sized macroparticles, also known as dust. The charged species within the plasma interact with a dust grain leading to an accumulation of charge on the dust grain surface. Due to the high mobility of electrons compared with the more massive ions, the dust quickly reaches a net negative charge.

When an external electric field is applied to a complex plasma, the ions drift relative to the more massive dust grains, with the ion drift velocity \( v_i \) corresponding to the strength of the applied electric field. In some cases, positively charged ions can become trapped in a close orbit around the negatively charged dust grain or even reach the surface of the dust grain where they recombine. However, in the presence of a large external electric field (which results in large ion drift velocities), the ion trajectories are only slightly deflected. The deflected ions form an ion wake, a region where ions build up downstream from the dust grain due to ion focusing. In the case of unidirectional ion flow, the distance of the ion density maximum from the center of the dust grain and the magnitude of the ion density enhancement in the ion wake both increase as the external electric field increases.\(^1\) When the external electric field switches directions (polarity switching) at a frequency that is low enough for the ions to be able to respond, but fast enough that the dust is unaffected, the resulting ion density maxima are stretched symmetrically around the dust grain in the direction parallel to the external electric field (illustrated in Fig. 1). This type of field switching is employed in the PK-4 experiment to keep dust clouds trapped within the field of view of onboard cameras, allowing for prolonged observation periods. The resulting interactions between ion wakes and the charged dust grains are thought to contribute to the stability of liquid-like dust chains,\(^2\) resulting in behavior similar to that which is observed in conventional electrorheological (ER) fluids.\(^3\)

The study of complex plasmas has enjoyed continued scientific interest due to its relevance in many wide-ranging applications, from industrial settings where plasma etching produces microparticles which may contaminate the surface of the materials,\(^4\) astrophysical phenomena such as the formation of planetary rings and comet tails,\(^5\) dust transport and contamination on airless bodies (like the Moon),\(^6\) to the study of fundamental plasma physics where the presence of dust allows for indirect determination of parameters within a plasma which are otherwise difficult to measure.\(^7\) In addition, recent interest has developed in studying the self-organization of dust grains and stability of the resulting dust structures in the presence of non-reciprocal interactions mediated by a flowing plasma environment.\(^8\)
Ground-based experiments have studied the formation of dust structures in the sheath region of a plasma, where a large vertical electric field is required to balance the gravitational force acting on dust particles. In contrast, microgravity dusty plasma experiments performed on parabolic flights or on the International Space Station (currently through the Plasmakristall-4, PK-4, experiment) enable investigations of dust dynamics in the near-abscence of such gravitational influence, where the smaller effects from the dust-dust, dust-ion, and drag forces are the primary drivers of dust motion. In such experiments, the dust cloud can be levitated within the bulk of the discharge plasma where electric fields are weaker, and ion flow speeds are lower, than typically found in a plasma sheath. This allows for a more detailed examination of the interaction between dust grains and the surrounding plasma environment, especially as it relates to the formation of dust particle chains, dust density waves, and other interesting phenomena which have previously been reported.

Recent observations of ionization waves under the conditions present in the PK-4 experiment, and the impact that these observed ionization waves can have upon the plasma parameters of interest for dust chain formation, suggest that further investigation is warranted. The purpose of this work is to quantify the resulting self-organization and stability of the dust chains that form in the environments found at various points within the ionization waves and compare that with the results obtained when using a simple time average of the relevant plasma parameters.

This paper is organized as follows. A description of the PK-4 Experiment and the PIC-MCC model of the PK-4 discharge are given in Section II. A discussion of the results from the PIC-MCC model, and plasma conditions selected for examination in the MD model of the dust and ions are given in Section III. The MD model for dust and ions is described in Section IV and includes details regarding the treatment of ions, dust dynamics, and dust grain charging. Results from the MD model are presented in Section V, with a discussion of the results in Section VI, and concluding remarks in Section VII.

II. BACKGROUND

The Plasmakristall experiments have allowed the study of three-dimensional complex plasmas in microgravity since their first introduction on board the Mir space station in the late 1990s. The most recent iteration, the PK-4, has implemented a long axial DC discharge tube (instead of the compact radio-frequency, RF, plasma used in previous iterations of the Plasmakristall experiments) to further aid investigations of the liquid state of complex plasma. This section will introduce the PK-4 experiment on the ISS and the PIC-MCC model of the PK-4 DC plasma.

A. PK-4 ISS Experiment

The PK-4 experiment on the International Space Station consists of a 30 mm diameter \( \pi \)-shaped cylindrical glass tube, a high voltage power supply, an RF coil which can be moved along the tube axis, dust dispensers, and both manipulation and illumination lasers. The central portion of the main tube is used for imaging by a plasma glow observation camera as well as particle observation cameras. A diagram of the PK-4 experimental setup is included for reference in Figure 2. It is frequently helpful to trap the dust within the field of view of the observation cameras to allow sufficient time to study the complex dust structures that form and evolve. This is accomplished using a polarity switching procedure, where the axial electric field alternates directions with a frequency fast enough that dust grains are unable to respond, which allows the experiment operator to restrict the dust to a desired axial region of the discharge plasma. The high voltage power supply is capable of operating in either a pulse generator mode (which includes the important polarity switching configuration), or in arbitrary generator mode (where output is modulated by one of four digitally tabulated functions). A more detailed description of the PK-4 experiment and capabilities can be found in [23], and details of ground-based and parabolic flight tests performed prior to installation on the ISS can be found in [19].

B. PIC Model of PK-4

Previous theoretical results of dust dynamics have been obtained using the assumption that the positive column of the discharge plasma is homogeneous along the axial direction on timescales relevant to dust dynamics. This assumption has been supported by experimental observations, as in the study of the positive column of the plasma discharge in the PK-4 experiment in [20], which noted that the discharge is...
steady and visually uniform before adding dust, confirmed by a plasma glow observation (PGO) camera with a frame rate of 15 frames per second (fps). Although DC plasma discharges are known to contain self-excited oscillations over a large range of frequencies and varied plasma conditions, the frame rates used to record the PK-4 ISS glow limit observations to those processes which occur on a ms or longer timescale. As a result, the presence of fast-moving ionization waves cannot be excluded even though video data collected from the PK-4 experiment appears to be homogeneous, requiring the use of numerical models or simulations to determine the nature of such ionization waves. The 2D particle-in-cell with Monte Carlo collisions (PIC-MCC) model of the PK-4 revealed the presence of fast-moving ionization waves with a phase velocity in the range of 500 – 1200 m/s, a finding which was experimentally confirmed with high-speed imaging on the PK-4 BU experiment, a ground-based replica.

The PIC-MCC simulation of the DC discharge described in models local plasma parameters in the PK-4 system (a thorough explanation of the uses and applicability of PIC-MCC simulations may be found in ). This model simulates a 400 mm long by 30 mm diameter cylinder with flat metallic disk electrodes at each end. The motions of electrons, ions, and metastable atoms in neon gas are simulated, as well as collisions, secondary electron emission, and charging of the glass wall. Two ground-based experiments were used for validation of the results from the PIC-MCC model, the PK-4BU at Baylor University in Waco, Texas and the BUD-DC in Budapest, Hungary.

The BUD-DC is a ground-based experiment with a straight cylindrical discharge, a design which closely matches the simplified geometry used in the PIC-MCC model while keeping the system as close as possible to the PK-4 in terms of discharge tube diameter, gas type, and range of pressures, among others. The PK-4BU is a ground-based replica of the PK-4 experiment, consisting of a 30 mm diameter π-shaped cylindrical quartz-glass tube, a power supply capable of operation in polarity switching mode with switching frequencies up to

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FIG. 2. Diagram of the PK-4 ISS experimental setup illustrating the π-shaped discharge tube and relative locations of the particle observation cameras (C1 and C2), field of view (FoV), dust dispensers (D1-D6), and the active and passive electrodes.
1000 Hz, and a movable RF coil. The entire experiment is mounted on a movable table, allowing operation with the main discharge tube oriented in either the vertical or horizontal direction.

Experimental data from the BUD-DC with an exposure time of 40 ms shows that global discharge structure and current dependence are properly captured. However, the PIC-MCC simulation also revealed the presence of fast-moving ionization waves which were confirmed by observations in the PK-4 BU. Discharge light emission sequences of the PK-4 BU were obtained using a Photron FASTCAM Mini UX50 high-speed CCD camera with frame rates of 50,000 fps. Experimental data from the PK-4 BU showed that the model accurately represented space-time distributions of light emission from fast-moving ionization waves, including prominent features such as bending, brightness, variation, and bifurcation with only a 15-20% larger spatial distance found in experimental results compared to the model. A comparison of the PIC-MCC simulation results with experimental data obtained from the PK-4 BU is shown in Figure 5, which is reproduced from [30].

C. Results from PIC Model of PK-4

The main feature revealed by the PIC-MCC model is that conditions within the positive column of the PK-4 discharge lead to large, fast-moving ionization waves occurring on timescales on the order of 10 kHz, shown in Fig. 3a. The local plasma parameters within the ionization waves were found to vary by as much as an order of magnitude from the time-averaged values, as shown in Figure 4. Heating of electrons and ions (Fig. 4b) is accompanied by large variations in the axial electric field (Fig. 4c), followed by a depletion of both ions and electrons as the ionization wave passes (Fig. 4d). The delay between peaks in the different plasma parameters is logical, considering that the charge separation provided by the imbalance of electrons and ions produces the large electric field observed in the ionization wave. This time delay between maximum and minimum values in various parameters leads to interesting consequences for the formation of ion wakes and dust structures, and will be discussed below.

III. METHODS

A. Implications of Ionization Waves for String Formation

Previous investigations of dust particle chain formation have focused on time-averaged plasma parameters due to the dust particle’s large inertia and, therefore, large response time compared with other plasma species (with dust typically moving on a millisecond timescale while ions respond on a microsecond timescale). However, as illustrated in Fig. 4, ionization waves in the plasma lead to large oscillations in the axial electric field, plasma number densities, and the electron and ion temperatures (based on the mean kinetic energies) on a microsecond timescale, which in combination impact the formation of ion wakes in complex plasmas. Since the character of the ion wake changes dramatically, further investigation is needed to determine if this is translated into the dust motion.

Interactions between dust grains and a flowing plasma have been characterized using the Mach number, $M = v_i/c_s$, where $v_i$ is the ion drift velocity and $c_s = \sqrt{k_B T_e/m_i}$ is the ion sound speed (as in [35]). The Mach number (representing the ion flow speed) is shown in Fig. 4e. Previous investigation of intergranular forces in low-Mach plasma wakes using a particle-in-cell code [36] found that wake enhancements were not present when the flow velocity is less than $0.3c_s$, given $T_e/T_i = 100$ (as is the case in the current investigation, shown in Fig. 4d). Moreover, it was noted that grain-aligning forces would be negligible and likely would not be responsible for the formation of dust chains at low Mach numbers. As shown in Fig. 4f, the range of ion flow speeds found are all much less than this threshold value suggesting that, in this case, the dust should be unlikely to form strings. However, results from PK-4 experiments show that the modeled conditions do lead to the formation of long (tens of particles) and stable dust strings.

B. Data Selection

In a previous paper [37], the impact of ionization wave conditions on dust chain formation was considered, with a focus on the effect of increasing electric fields and ion drift velocities. The current investigation seeks to isolate the influence that all of the changing plasma conditions within the ionization waves have on the formation and stability of dust particle chains, which includes the electron and ion temperature, electron number density, and magnitude of the axial electric field, and ion velocity. The electron and ion temperatures, which in combination with the plasma densities influence dust grain charging, reach values within ionization waves that are two to six times the background values (see Fig. 4a and c). The plasma densities also impact the formation of wake structures around the charged dust grains, which in turn influences both the formation and the stability of the dust chain. The axial electric field (Fig. 4b) which drives the ion flow, leading to wake formation and dust chain stability, reaches peak values in ionization waves as large as 20 times the value between peaks. Specific conditions from the time history are used in the MD simulation to investigate their effect on string formation, and results are subsequently compared to dust dynamics where the full time-averaged plasma conditions are used. Since the axial electric field drives the ion flow, specific time frames for averaging are chosen based on the behavior of the electric field. The different plasma conditions are: Case (1) Full Time Average, where the values of each parameter averaged over a time span (440 μs) covering several ionization waves are considered; Case (2) Between $E_z$ Peaks, where only data between the large peaks in the axial electric field are considered, representing a region of minimum ion flow and a steady, constant plasma column; Case (3) Rising $E_z$ and Minimum $n_i$, where data within the rise of the axial electric field are considered, corresponding to a time when electron and ion number densities are depleted; Case (4) Full-Width
FIG. 3. Space-time distribution of the computed excitation source (a) and the measured light intensity distribution (b) along the symmetry axis in the positive column region illustrating the presence of fast-moving ionization waves. The vertical x-axis here represents the axis of symmetry along the cylindrical plasma discharge. The experimental data in panel (b) was measured on the PK-4BU system by means of high-speed video imaging. Reproduced from Figure 4 of [30]

*Half-Maximum $E_z$ Peaks*, where the data is averaged over the FWHM of peaks in the axial electric field, representing the maximum ion flow. A representative time interval indicating the data selected for each of the averaging cases is illustrated in Figure 5 and the resulting averaged plasma parameters for each case are listed in Table 1.

IV. NUMERICAL MODEL

The numerical model used for the current investigation is DRIAD (Dynamic Response of Ions And Dust). This model is described in detail in [1], and here we provide only a brief overview of relevant components. DRIAD is a molecular dynamics simulation which resolves dust and ion motion each at their own relevant timescales using a timestep of $\Delta t_d = 10^{-4}$ seconds for the dust and $\Delta t_i = 10^{-9}$ seconds for the ions. The treatment of ion-dust and ion-ion forces follows the Molecular Asymmetric Dynamics (MAD) code developed by Piel[39] and has previously been shown to yield reasonable results for potential distributions and interparticle forces when compared to PIC simulation[36]. In the asymmetric treatment of dust and ions, the forces ($\vec{F}_{id}$) on the ions by the charged dust are calculated with the "naked" Coulomb potential given in equation 3, but the force on the dust by the ions is calculated using a shielded Yukawa interaction. This method is used to bridge the limiting cases to determine a satisfactory approximation for the equations of motion close to a dust grain where $|e\Phi| \gg k_B T_e$ (and electrons are depleted), and sufficiently far from the dust grain that $|e\Phi| \ll k_B T_e$.

The motion of ions and dust grains are governed by their respective equations of motion. For an ion of mass $m_i$, the equation of motion is given by

$$m_i \ddot{r} = \vec{F}_{ij} + \vec{F}_{ID} + \vec{F}_E(z) + \vec{F}_{\text{bound}}(r,z) + \vec{F}_{\text{in}}.$$  \hspace{1cm} (1)
TABLE I. Plasma parameters used for each the four averaging cases. Note that $+(-)$ values for $E_z$ and $v_{z,i}$ indicate parallel (anti-parallel) orientation relative to the tube axis.

| Averaging Case        | $E_z$ [V/m] | $n_{e0}$ [m$^{-3}$] | $n_{i0}$ [m$^{-3}$] | $T_e$ [K] | $T_i$ [K] | $v_{z,i}$ [m/s] |
|-----------------------|-------------|---------------------|---------------------|----------|----------|----------------|
| 1. Full Time Average  | 211.1       | 1.17e15             | 1.18e15             | 50107    | 466      | 111.5         | 0.022 |
| 2. Between $E_z$ Peaks| -45.2       | 1.58e15             | 1.59e15             | 37549    | 425      | -29.8         | 0.008 |
| 3. Rising $E_z$ and Min. $n_i$ | 474.3       | 4.32e14             | 4.43e14             | 65330    | 509      | 231.7         | 0.043 |
| 4. FWHM $E_z$ Peaks   | 814.8       | 6.29e14             | 6.48e14             | 69767    | 565      | 377.3         | 0.070 |

The electrostatic force between ions $i$ and $j$, $\vec{F}_{ij}$, is derived from a Yukawa potential, where the electrons provide shielding, resulting in the expression

$$\vec{F}_{ij} = \sum_{i\neq j} \frac{q_i q_j}{4 \pi \varepsilon_0 r_{ij}^3} \left(1 + \frac{r_{ij}}{\lambda_{De}}\right) \exp\left(-\frac{r_{ij}}{\lambda_{De}}\right) \vec{r}_{ij},$$

(2)

where $q_i$ ($q_j$) denotes the charge of ion $i$ ($j$), $r_{ij}$ denotes the distance between ions $i$ and $j$, $\lambda_{De} = \sqrt{\varepsilon_0 k_B T_e / (n_e e^2)}$ is the electron Debye length with $T_e$, $n_e$, and $e$ representing the temperature, number density, and charge of electrons, respectively. The force on the ions due to dust grains, $\vec{F}_{id}$, is derived from a Coulomb potential (as the electrons are depleted in the vicinity of the negatively charged dust)

$$\vec{F}_{id} = \sum_d \frac{q_i Q_d}{4 \pi \varepsilon_0 r_{id}^3} \vec{r}_{id},$$

(3)

FIG. 4. Results from the PIC-MCC model illustrating time-varying (a) electron and ion temperatures, $T_e$ and $T_i$, (b) axial electric field, $E_z$, (c) electron and ion number densities, $n_e$ and $n_i$, (d) the ratio of $n_i$ to $n_e$, and (e) the Mach number, $M$. The associated time-averaged value of the parameters are indicated by a dashed line corresponding to the values ($\langle T_e \rangle = 50107$ K, $\langle E_z \rangle = 211.1$ V/m, $\langle n_e \rangle = 1.18 \times 10^{15}$ m$^{-3}$, and $\langle M \rangle = 0.022$, respectively. The dot-dashed line in (d) corresponds to $n_i/n_e = 1$. The vertical red line in each panel marks the time of the first peak in temperature. Discharge parameters are: neon gas, pressure = 60 Pa, current = 2 mA.

FIG. 5. Results of the PIC-MCC model showing (as a solid line) the time-varying (a) electron temperature, $T_e$, (b) axial electric field, $E_z$, and (c) electron number density, $n_e$. The data points selected for the various averaging schemes are denoted by: Between $E_z$ Peaks (blue circles), Rising $E_z$ and Minimum $n_i$ (dark blue squares), and FWHM $E_z$ Peaks (red crosses). For comparison, the Full Time Average value of each variable is shown as a dashed horizontal line extending over the full extent in each plot.
where the sum is taken over the \( d \) dust grains, \( Q_d \) represents the charge on the dust grain, and \( \bar{r}_{id} \) is the distance between an ion \((i)\) and dust grain \((d)\). The force on the ions due to the external axial electric field, \( \bar{E}(z) \), which switches directions at the polarity switching frequency of 500 Hz, is \( \bar{F}_E(z) = q_i \bar{E}(z) \). The ions outside the simulation region exert a force on ions within the simulation through \( \bar{F}_{bound}(r,z) = q_i \bar{E}_{bound}(r,z) \). The electric field due to ions outside the simulation region, \( \bar{E}_{bound}(r,z) \), is calculated as the negative gradient of the potential in a cylindrical cavity, found by numerical calculation of the potential of uniformly distributed ions within a cylinder, which is then subtracted from a constant potential. The ion-neutral collisions \( \bar{F}_{n} \) are treated using the null-collision method, with the isotropic and backscattering cross section collision data taken from the Phelps database (hosted by LXCat project).

The equation of motion for a dust grain with mass \( m_d \) is given by
\[
m_d \ddot{\mathbf{r}} = \bar{F}_{di} + \bar{F}_{dd} + \bar{F}_C + \bar{F}_E(z) + \bar{F}_{drag} + \bar{F}_B.
\]
(4)

The force of ions on the dust grains, \( \bar{F}_{di} \), is calculated from a Yukawa interaction,
\[
\bar{F}_{di} = \sum_i q_i Q_d \left( 1 + \frac{r_{di}}{\lambda_{De}} \right) \exp \left( -\frac{r_{di}}{\lambda_{De}} \right) \bar{r}_{di},
\]
(5)

where \( r_{di} \) represents the distance between the ion \((i)\) and dust grain \((d)\). At each dust timestep, the cumulative force of ions acting on a dust grain is averaged over the elapsed ion timesteps. The force between dust grains, \( \bar{F}_{dd} \), is a Coulomb interaction, as the screening by ions is included in the expression for \( \bar{F}_{di} \).

The confinement force, \( \bar{F}_C \), simulates the effect of neighboring dust chains outside the simulation region. The confinement is included using the expression
\[
\bar{F}_C = \omega^2 \bar{Q} Q_d \bar{r},
\]
(6)

where the confining strength, \( \omega^2 \), is proportional to
\[
\omega^2 \propto \frac{C \bar{Q}}{4 \pi \varepsilon_0 \Delta^2} \left( 1 + \frac{\Delta}{\lambda_{De}} \right) \exp \left( -\frac{\Delta}{\lambda_{De}} \right),
\]
(7)

with \( \bar{Q} \) and \( \Delta \) representing the expected average dust charge and inter-grain separation. The constant \( C \) is used to scale the confining force provided by surrounding chains, and is based on the expected inter-chain spacing and average dust grain charge (here \( C \approx 12 \)). The axial electric field provides a force \( \bar{F}_E(z) = Q_d \bar{E}(z) \). The drag force, \( \bar{F}_{drag} = -\beta \bar{v} \), is the neutral gas drag acting on a dust grain with velocity \( \bar{v} \), and drag coefficient
\[
\beta = \frac{4 \delta a^2 p}{3} \sqrt{\frac{8 \pi m_i}{k_B T_n}},
\]
(8)

where \( \delta \) is a material-dependent constant (set to a value of 1.44, measured for melamine formaldehyde in argon and assumed to be similar in neon), \( a \) is the radius of a dust grain, and \( p \) and \( T_n \) are the neutral gas pressure and temperature, respectively. The dust is immersed in a thermal bath which is implemented using the force \( \bar{F}_B = \tau \zeta(t) \), where \( \tau \) is a random number generated from a normal distribution and
\[
\zeta = \sqrt{\frac{2 \beta k_B T_n}{m_d \Delta t}}
\]
(9)

is the maximum acceleration imparted due to a kick.

The dust grains charge in response to electron and ion currents; as the electrons are not modeled directly, they are assumed to be Boltzmann-distributed, and the electron current, \( I_e \), is calculated using orbital motion limited (OML) theory:
\[
I_e = 4 \pi a^2 n_e \left( \frac{k_B T_e}{2 \pi m_e} \right)^{1/2} \exp \left( \frac{e \phi_d}{k_B T_e} \right),
\]
(10)

where \( n_e \), \( m_e \), and \( T_e \) are the electron density, mass, and temperature, respectively, \( k_B \) is the Boltzmann constant, and \( \phi_d = Q_d / (4 \pi \varepsilon_0 a) \) is the surface potential of the dust grain. The ion current is comprised of ions which cross the ion collection radius, \( b_c \),
\[
b_c = a \left( 1 - \frac{2 q_i \phi_d}{m_i V_i^2} \right)^{1/2},
\]
(11)

\( V_i \) is the characteristic velocity of the ions
\[
V_i = \left( \frac{8 k_B T_i}{\pi m_i} + v_i^2 \right)^{1/2},
\]
(12)

and \( v_i \) is the drift speed of an ion, which may conveniently be reported as a fraction of the sound speed \( v_i = M_i c_s \).

Dust charging and dynamics were simulated using the plasma conditions shown in Table 1 for each case. The other simulation parameters are: neon gas with neutral gas pressure \( p = 60 \text{ Pa} \), neutral gas temperature \( T = 295 \text{ K} \), frequency of the electric field polarity switching 500 Hz, dust radius \( a = 1.69 \mu m \), and dust mass density corresponding to that of melamine formaldehyde \( (1.510 \text{ g/cm}^3) \). The simulation region is a cylinder of radius \( 840 \mu m \) and length \( 8050 \mu m \), which provides enough space for the dust grains to reach the expected average interparticle spacing determined from the PK-4 experiment with at least one electron Debye length between the axial ends of the simulation and the outermost dust grain. The dust was initially placed in a region roughly \( 450 \mu m \) in diameter near the center of the simulation region. The dust cloud expanded, and was allowed to evolve for 1.2 seconds, with the dust in each case reaching equilibrium after approximately 1.0 seconds. Data collected during the final 200 ms, which is equivalent to approximately 2 dust plasma periods \( (\tau_d) \), where \( \tau_d = 2 \pi \sqrt{\varepsilon_0 m_i / (n_d Q_d^2)} \) and dust number density \( n_d \approx 1.1 \times 10^{10} \text{ m}^{-3} \), was used for the results presented below.

V. RESULTS

The ion densities averaged over the final 0.1 seconds are shown for each simulation case in Figure 6. Note that the
TABLE II. Size of the cylindrical simulation region expressed in Debye lengths for each case.

| Case                        | Debye Length $\lambda_{De}$ [\(\mu m\)] | Radius (838.5\(\mu m\)) [\(\lambda_{De}\)] | Length (8050\(\mu m\)) [\(\lambda_{De}\)] |
|-----------------------------|----------------------------------------|----------------------------------------|----------------------------------------|
| 1. Full Time Average        | 450.3                                  | 1.9                                    | 17.9                                   |
| 2. Between $E_z$ Peaks      | 335.5                                  | 2.5                                    | 23.8                                   |
| 3. Rising $E_z$ and Min. $n_i$ | 838.5                                  | 1.0                                    | 9.6                                    |
| 4. FWHM $E_z$ Peaks         | 715.8                                  | 1.2                                    | 11.3                                   |

$\lambda_{De}$ is the Debye length of the ion. $n_i$ and $n_{i0}$ are the ion density inside and outside the dust chain, respectively. $\phi$ indicates the position along the chain. $\lambda_{De}$ is the Debye length of the ion.

FIG. 6. Plot of ion density for (a) Case 1: Full Time Average, $n_{i0} = 1.18 \times 10^{15} m^{-3}$. (b) Case 2: Between $E_z$ Peaks, $n_{i0} = 1.58 \times 10^{15} m^{-3}$. (c) Case 3: Rising $E_z$ and Minimum $n_i$, $n_{i0} = 4.32 \times 10^{14} m^{-3}$. (d) Case 4: FWHM $E_z$ Peaks, $n_{i0} = 6.29 \times 10^{14} m^{-3}$, averaging cases. The colorbar corresponds to the ion density normalized to the background ion density far from the dust, $n_i/n_{i0}$. The shade of the dust grain indicates distance along the $y$ axis (in or out of the page), with black indicating dust grains positioned on the xz-plane and white indicating dust grains 0.25 $\lambda_{De}$ from the xz-plane.

The resulting maps for the electric potential of the negatively charged dust and positive ion wakes, $\phi = \phi_{ion} + \phi_{dust}$, averaged over the final 0.1 seconds are shown in Figure 8 for each of the four cases. As in Figure 6, the view is zoomed in on the central part of each chain so that the details in the radial direction are visible. The dust grains are shown as grayscale dots, where the color of the dot indicates the magnitude of the distance from the xz-plane (out-of-plane direction), with black indicating dust grains positioned in the xz-plane and white indicating a displacement of 0.25 $\lambda_{De}$, the maximum out-of-plane distance found at equilibrium. The colorbar indicates the ion density normalized to the background ion density far from the dust, $n_i/n_{i0}$, where values for $n_{i0}$ for each case are given in Table I. From the data shown in Figure 8, it is clear that the different cases lead to different ion wake structures, as expected since the extent and location of an ion wake formed in the presence of a charged dust grain depends on the external electric field and resultant ion drift velocities.

In Case 1 (which uses the full time average of plasma parameters, Fig. 6a) and in Case 2 (which is averaged over the minimal external electric field between ionization wavefronts, Fig. 6b), the dust forms a somewhat aligned chain with most of the disorder seen in the out-of-plane direction, and the large ion density maxima centered around the dust grains. In Case 3 (averaged over the rise in external electric field, Fig. 6c), the ion density maxima are less intense and are elongated between the dust grains, and the chain structure shows considerably less displacement out-of-plane. Case 4 (averaged over the FWHM peaks of the external electric field), Fig. 6d, shows results similar to that of Case 3, with even greater enhancement of ion density between grains. The maximum displacement out-of-plane in this case is slightly larger than in Case 3, due to the greater charge on the dust grains. The results shown in Fig. 6 lead to two broad classifications of the four averaging cases: low ion flow with distinct ion clouds collected around each dust grain (as in Cases 1 and 2), and high ion flow resulting in elongation and merging of the ion clouds (as in Cases 3 and 4).

The simulation results for the electric potential have a large variation in the background potential along the $z$-axis due to the enhanced accumulation of ions near the dust chain, illustrated in Figure 7. This overall variation in the background potential can be eliminated by subtracting a fit to the potential along a line parallel to the $z$-axis at a radial distance of $\lambda_{De}/3$. The total potential of the ions and dust (indicated by a solid line) and the fit to the background potential (indicated by a dot-dashed line) are shown in Fig. 7. This fit to the potential is subtracted from the total potential to yield a background potential that is more uniform along the $z$-axis. Then, to compare the variations in the potential due to the ion wakefield, a constant value is subtracted from each of the potentials so that the midpoint between two dust grains near the end of the chain is at $\phi = 0$ V. The location within the chain used to calculate this constant value is shown by the red box in Fig. 7. The asterisks in Fig. 7 indicate the specific point selected for each case.

The resulting maps for the electric potential of the negatively charged dust and positive ion wakes, $\phi = \phi_{ion} + \phi_{dust}$, averaged over the final 0.1 seconds are shown in Figure 8 for each of the four cases. As in Figure 6, the view is zoomed...
FIG. 7. Plots showing relevant data used for processing the electric potential. (a) The total electric potential of dust and ions (solid line) and fit to the background potential at the radial distance \( x = \frac{\lambda_{de}}{3} \) (dot-dashed line) for all four cases are shown. The region selected for calculating the zero-point adjustment is indicated by a red box. The electric potential after subtracting the fit to the background potential is shown in (b), with the asterisk indicating the point midway between two grains selected for the zero-point adjustment.

in on the central portion of the chain to show the detail in the radial direction. The dust grains are shown as grayscale dots, where the color of the dot indicates the distance from the xz-plane (out of the page). Each case shows a general decrease in potential moving outward in the radial direction, with the extent and depth of the negative potential well correlated to the magnitude of the charge on the dust grain, which increases with ion flow speed. The positive potential associated with the focused ions is centered along the dust chain, with the potential decreasing in the radial direction. Along the axis of the dust chain, the magnitude of the positive potential peaks increases with increased ion flow speed.

To further characterize the order seen in the dust chains in each case, the pair correlation function, \( g(r) = \frac{\langle \sum_{i \neq 0} \delta(\vec{r} - \vec{r}_i) \rangle}{\rho} \), where \( \rho = \) (number of particles)/(volume), was calculated for each averaging case, shown in Figure 9. Order is indicated by well-defined, sharp peaks in the \( g(r) \) function at distances corresponding to integer multiples of the average interparticle spacing. As shown in Fig. 9 the greatest correlation is seen for Cases 3 and 4. Cases 1 and 2 show the least order in the \( g(r) \) function due to the increased disorder in the out-of-plane direction, which also causes increased variation of the spacing in the z-direction.

The pair correlation functions also allow for comparison between the DRIAD simulation results and results obtained from microgravity experiments. Parameters used for the current simulation closely match experimental conditions during Campaign 7 of the PK-4 experiment, which were: 70 Pa neon gas, 0.7 mA current, 500 Hz electric field switching frequency, and 1.69 \( \mu \)m radius dust grains. Video data were collected at 71.4 fps, from which 2D images of the dust cloud were analyzed using particle tracking over 90 frames, and three chains were then selected for analysis (highlighted in the top pane of Fig. 10). The pair correlation functions for the three selected
TABLE III. Average final interparticle spacing and final charge on dust grains for each case.

| Case                          | Charge | $d$ [µm] | $[\lambda_{De}]$ | $[\lambda_{Di}]$ |
|-------------------------------|--------|----------|-------------------|-------------------|
| 1. Full Time Average          | 2260   | 345      | 0.77              | 7.9               |
| 2. Between $E_z$ Peaks        | 2040   | 246      | 0.73              | 6.9               |
| 3. Rising $E_z$ and Min. $n_i$ | 2270   | 363      | 0.43              | 5.9               |
| 4. FWHM $E_z$ Peaks           | 2630   | 370      | 0.52              | 5.7               |

FIG. 8. Plots showing electric potential for (a) Case 1: Full Time Average, (b) Case 2: Between $E_z$ Peaks, (c) Case 3: Rising $E_z$ and Minimum $n_i$, (d) Case 4: FWHM $E_z$ Peaks averaging cases. The shade of the dust grain indicates distance from the y-axis (out of the page), with black indicating dust grains positioned on the xz-plane and white indicating dust grains farther from the xz-plane.

FIG. 9. Plot of $g(r)$ pair correlation functions for (a) Case 1: Full Time Average, (b) Case 2: Between $E_z$ Peaks, (c) Case 3: Rising $E_z$ and Minimum $n_i$, (d) Case 4: FWHM $E_z$ Peaks averaging cases.

VI. DISCUSSION

The structure of the ion wake around dust grains has been shown to impact the formation and stability of dust chains in a complex plasma. The plasma conditions in Cases 3 and 4, with large axial electric field driving ion flow, yielded the largest region of enhanced ion density between the dust grains (Fig. 6c-d), as well as resulting in the most ordered final chain structures as seen in the pair correlation functions (Fig. 9c-d). In contrast, the dust chains that formed in Cases 1 and 2, with small ion flow, displayed the least order (Fig. 9a-b), and lacked the region of enhanced ion densities between dust grains (Fig. 6a-b).

The increased interparticle spacing in the simulated results...
ever, even with this limitation, the qualitative behavior of the grains in the simulation conditions would be reduced. How-the electrons were taken into account, the charge on the dust unaccounted for in the current simulation. If this depletion of dust cloud (dependent on the number density of dust) that is experiment lead to a decrease in the electron density within the cloud reside on the dust grain surface. It is therefore logical that as much as 50% of the electrons present in the dust charge on dust grains in microgravity conditions at 60 Pa are \( \approx 10^{10} \times 10^{-20} \) m\(^{-3}\), while Lang-muir probe measurements in the dust-free discharge show an electron density on the order of \( n_e \approx 4 \times 10^{14} \) m\(^{-3}\). The charge on dust grains in microgravity conditions at 60 Pa are theoretically estimated in [43] to be \( Q_d \approx 2 \times 10^5 \) e\(^-\), indicating that as much as 50% of the electrons present in the dust cloud reside on the dust grain surface. It is therefore logical to conclude that the neighboring dust chains present in the experiment lead to a decrease in the electron density within the dust cloud (dependent on the number density of dust) that is unaccounted for in the current simulation. If this depletion of the electrons were taken into account, the charge on the dust grains in the simulation conditions would be reduced. However, even with this limitation, the qualitative behavior of the pair correlation function seen in the experiment most closely matches the simulation results in Cases 3 and 4.

Results from this simulation also allow for the comparison of the resulting total electric potential with commonly used analytic forms of the electric potential. The simplest model for the electric potential surrounding a point charge is the Coulomb potential (Eq. [9]). This form of potential is only dependent on the distance \( r \) from the point charge, and therefore fails to capture any effects resulting from local non-neutrality of the charge distribution close to a dust grain. To account for the changes in charge distribution near a dust grain, it is necessary to use the slightly more complex form of electric potential developed by H. Yukawa [44] which is typically adapted for use in the field of complex plasmas as the Yukawa potential (Eq. [10]). The Yukawa potential (also sometimes referred to as a Debye-Hückel potential) is dependent not only on the distance from the point charge, but also on the temperature and number density of the charged species within the plasma through the \( \lambda_D \) term in the exponent. While the Yukawa potential does improve upon the Coulomb potential by taking into account the shielding provided by mobile charges in the plasma, it fails to account for the changes in potential structure that arise from a flowing plasma. A potential model based upon the Bhatnagar-Gross-Krook collision operator has been developed by R. Kompaneets [45] which has the form

\[
\phi(\vec{r}) = \frac{Q}{|\vec{r}|} F_{BGK}(\theta) + o\left(\frac{1}{|\vec{r}|^3}\right),
\]

with

\[
F_{BGK}(\theta) = -\frac{8}{\pi} \frac{u \lambda_D^2 T_e}{v_{Te}} \cos \theta + \left(2 - \frac{\pi}{2}\right) \frac{u^2 \lambda_D^2 T_e}{v_{Te}^2} \left(1 - 3 \cos^2 \theta\right) + o(u^2),
\]

where \( \lambda_D = \sqrt{T_e/(4\pi n_e e^2)} \), \( u \) represents the drift velocity, \( v_{Te} = \sqrt{T_e/m_e} \), and \( \theta \) represents the angle between \( \vec{r} \) and the ion drift. This form has been adapted to account for the symmetric ion wake present in a plasma subjected to an alternating external electric field (as in [46]), yielding the form referred to here as the Multipole Expansion Potential:

\[
V(r, \theta) = Q \left[ e^{-r/\lambda_D} - 0.43 \frac{M_T^2 \lambda_D^2}{r^3} \left(3 \cos^2 \theta - 1\right) \right],
\]

where \( M_T = u_i/v_{Te} \) is defined as the “thermal” Mach number, and \( \theta \) represents the angle between the external electric field and \( \vec{r} \).

Contour plots showing comparisons between the potential forms and results from each of the four averaging cases analyzed using the DRIAD simulation are shown in Figure 11. The region \( r < \lambda_D/5 \) (approximately equal to \( r < 2\lambda_D \)) around each dust grain in the bottom row of Figure 11 is replaced with the Yukawa form of the potential. The Multipole Expansion potential for each case is adjusted to match that of the Yukawa potential at \( r = 2\lambda_D \) at the angle \( \theta = \pi/2 \) (in the radial direction). The Yukawa and Multipole Expansion potentials in each of the four cases are then adjusted by a
constant value to match the maximum positive electric potential found in the simulation results at a point midway between the two dust grains.

Careful consideration of the results shown in Figure 11 makes it evident that the simulation results are not adequately described by the expressions for dust potential using the Yukawa potential or equation 15. A comparison between a 3D PIC simulation and the numerical solution of linearized electrostatic potential was carried out in 48. This study showed that the charge and potential of the downstream grains can be significantly modified by wake effects in a system of several grains, and the wake pattern can show significant deviations from the potential determined from a linear combination of a wake behind a single grain in subsonic flows. These findings correlate with the comparison shown in Fig. 11 where it is seen that the potential for the dust strings is not well represented by the models developed for isolated grains. PIC models also typically consider dust grains with a larger radius relative to the electron Debye length (for example, 48 considers grains with a radius $a = 0.185 \lambda_D$), while the present study uses dust grains with a radius on the order of $10^{-3} \lambda_D$. Further investigation of the electric potential structure is needed, given that the dynamics of charged species within a complex plasma and the form of electric potential are inextricably linked, and will be the focus of a forthcoming study.

VII. CONCLUSION

Varying conditions within the ionization waves present in the PIC-MCC simulation of conditions within the PK-4 ISS have a significant impact on the formation of dust chains. The effect of fast-moving ionization waves on the formation of ordered dust particle chains has been investigated by first identifying regions of interest within the time evolving plasma conditions (shown in Figure 5), labeled as the four cases: (1) Full Time Average, where the values of each parameter are averaged over a time span (440 $\mu$s) encompassing several complete ionization waves; (2) Between $E_z$ Peaks, where only the data in the interval between the large peaks in the axial electric field are considered, representing a region of minimum ion flow and a steady, constant plasma column; (3) Rising $E_z$ and Minimum $n_i$, where the data within the rise of the axial electric field are considered, corresponding to an interval where electron and ion number densities are depleted; and (4) Full-Width Half-Maximum $E_z$ Peaks, where the data is averaged over the FWHM of peaks in the axial electric field, representing the maximum ion flow. The specific plasma parameters identified for each case (listed in Table I) were then modeled using DRIAD, a molecular dynamics simulation capable of resolving dust and ion motions on each of their respective timescales, and results for the ion density (Figure 9), electric potential (Figure 8), and analysis of the final dust structure (Figure 9) have been presented for each of the four cases.

Although considered separately in this investigation, it is important to recall that the conditions of Cases 2, 3, and 4 represent different features within the ionization waves, with each case describing an interval of 10-20 $\mu$s within a full ionization wave (with peak-to-peak interval of $\approx 40 \mu$s), while the relevant dust dynamics occur on a timescale of 100 $\mu$s. As such, in the time-evolving experimental system, the decreased ion wake structure and diminished order for Case 2 (Figures 6 and 9) is immediately followed by the enhanced wake and order found in Case 3 (Figures 6 and 9). As the ionization wave moves past a dust chain, conditions between ionization wave peaks (minimum ion velocities and maximum ion density) lead to an increase in ion current and subsequent decrease in the magnitude of charge on the dust grains, which allows dust grains to move closer together. As the wave continues past the dust grains (with increased ion velocities and minimum ion density), the magnitude of the charge on the dust grains and interparticle separation increases, and the region of positive potential between dust grains is the largest. Even though the average charge on dust grains increases during this phase, the large positive potential in the strongly focused ion wake allows for smaller interparticle spacing, as well as increasing the grain alignment. As shown in Figure 9c-d, this leads to the largest order in the resulting dust chain.

Due to the nature of the plasma currents, dust grains undergo stochastic charging and discharging, where the charge on a dust grain fluctuates with the addition of discrete amounts of charge due to individual ions and electrons reaching the grain surface at different times. Additionally, the discharging time is found in 50 to be longer than the charging time, which would allow the dust grains to retain larger negative charges obtained during the phases of ionization waves with enhanced axial electric field. Since the time a dust grain takes to reach equilibrium charge could be longer than the time it takes for an ionization wave to pass, the actual dust charges may differ from those shown in Table III. The plasma parameters used in the current model are chosen at specific points in time to give a snapshot of dust dynamics calculated using these specific parameters. However, in light of the impact fluctuating charges will have on the formation and stability of dust structures, future investigation utilizing time varying plasma parameters is needed to further quantify the impact ionization waves have on dust dynamics in the PK-4 environment. The balance between the various parameters is not captured by the full time average (Case 1), and as such, it is likely that the full time average does not provide an accurate representation of the conditions to be used to model dust dynamics. Additionally, further work is needed in modeling the effect of ions through a modification of the potential of charged dust grains, as the current models do not match the ion behavior.

ACKNOWLEDGMENTS

Support for this work from NSF grant number 1740203, NASA grant number 1571701, and the U.S. Department of Energy, Office of Science, Office of Fusion Energy Sciences under award number DE-SC-0021334, and by the National Office for Research, Development, and Innovation of Hungary (NKFIH) via grant 134462 is gratefully acknowledged. All authors gratefully acknowledge the joint ESA - Roscosmos "Experiment Plasmakristall-4” on-board the Inter-
national Space Station. The microgravity research is funded by the space administration of the Deutsches Zentrum für Luft- und Raumfahrt eV with funds from the federal ministry for economy and technology according to a resolution of the Deutscher Bundestag under Grants No. 50WM1441 and No. 50WM2044. A. M. Lipaev and A. D. Usachev were supported by the Russian Science Foundation Grant No. 20-12-00365 and participated in preparation of this experiment and its execution on board the ISS.

DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.

FIG. 11. Comparison of electric potential from the simulation with the analytic potential forms discussed in Section VI. The simulation results are shown in the top row (a-d), the Yukawa Potential is shown in the middle row (e-h), and the Multipole Expansion Potential is shown in the bottom row (i-l), with the colorbar corresponding to each row shown on the right (note that each colorbar has a different minimum and maximum value). The first column on the left (a, e, and i) shows Case 1 (Full Time Average), the second column (b, f, and j) shows Case 2 (Between $E_i$, Peaks), the third column (c, g, and k) shows Case 3 (Rising $E_i$, and Minimum $n_i$), and the fourth column (d, h, and l) shows Case 4 (FWHM $E_i$, Peaks). Positions of dust grains are marked with a white cross (+).

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