



Inhibited Coagulation of Micron-size Dust Due to the Electrostatic Barrier

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Abstract

The collisional evolution of solid material in protoplanetary disks is a crucial step in the formation of planetesimals, comets, and planets. Although dense protoplanetary environments favor fast dust coagulation, there are several factors that limit the straightforward pathway from interstellar micron-size grains to pebble-size aggregates. Apart from the grain bouncing, fragmentation, and fast drift to the central star, a notable limiting factor is the electrostatic repulsion of like-charged grains. In this study we aim at theoretical modeling of the dust coagulation coupled with the dust charging and disk ionization calculations. We show that the electrostatic barrier is a strong restraining factor to the coagulation of micrometer-size dust in dead zones of the disk (where the turbulence is suppressed). While the sustained turbulence helps to overcome the electrostatic barrier, low fractal dimensions of dust aggregates can potentially block their further coagulation even in this case. Coulomb repulsion may keep a significant fraction of small dust in the disk atmosphere and outer regions.

Key words: accretion, accretion disks – dust, extinction – plasmas – protoplanetary disks

1. Introduction

Grain charge is involved in various aspects of cosmic dust physics. It affects dust drift through ionized gas (Draine & Salpeter 1979; Gail & Sedlmayr 1979; Akimkin et al. 2017; Katushkina et al. 2018), dust interaction with magnetic fields (Scalo 1977; Draine 1980; Lee et al. 2017; Hopkins & Squire 2018), gas ionization-recombination balance and chemistry (Umebayashi & Nakano 1980; Sano et al. 2000; Ilgner & Nelson 2006; Dzyurkevich et al. 2013; Ivlev et al. 2016; Nesterenok 2018; Thi et al. 2019). Particle charge state influences the radiative properties of dust, specifically the interaction of electromagnetic waves with optically small particles (Bohren & Hunt 1977; Kocifaj & Klačka 2012; Kocifaj et al. 2012), and infrared bands of polycyclic aromatic hydrocarbons (DeFrees et al. 1993; Langhoff 1996; Boersma et al. 2018). Coulomb potential also changes the collisional cross section with gas and solids, thus affecting dust evolution due to ion accretion (Mathews 1967; Weingartner & Draine 1999; Zhukovska et al. 2018) and coagulation (Simpson 1978; Simpson et al. 1979; Okuzumi 2009; Mathews et al. 2013; Akimkin 2015). Betatron acceleration of charged grains leads to their sputtering and shuttering in high velocity shock waves (McKee et al. 1987; Tielens et al. 1994; Jones et al. 1996). Moreover, extreme values of charge may lead to the dust destruction via the ion field emission or Coulomb explosions (Draine & Salpeter 1979; Waxman & Draine 2000; Kopnin et al. 2011).

The study of cosmic dust charging has a long history (Jung 1937; Corlin 1938; Spitzer 1941; Watson 1972; Feuerbacher et al. 1973) and resulted in general understanding of main charging mechanisms acting in the interstellar medium (see reviews by Goertz 1989; Mendis & Rosenberg 1994; Fortov et al. 2005; and short summary by Weingartner 2004). These mechanisms include photoelectric effect (Bakes & Tielens 1994; Weingartner & Draine 2001), plasma charging (Draine & Sutin 1987), secondary electron

emission (Draine & Salpeter 1979; Shchekinov 2007), triboelectric charging³ (Desch & Cuzzi 2000; Poppe et al. 2000; Marshall et al. 2005; Harper et al. 2018; Singh & Mazza 2018), and thermionic emission (Lefevre 1975). In varying external conditions the non-equilibrium grain charging should be considered and may affect dust evolution (Corlin 1938; Horanyi & Goertz 1990; Pedersen & Gómez de Castro 2011). However, even in steady-state conditions the grain charge may fluctuate around an average value and an ensemble of equal size grains has non-zero charge dispersion.

The key charging mechanisms in protoplanetary disks are photoelectric, plasma, and triboelectric charging, any of which can dominate depending on disk region or grain size. The charge of small dust is positive in disk atmosphere, due to the photoelectric emission caused by the combined effect of the interstellar UV field and the UV radiation generated locally by the penetrating cosmic-rays (CRs; Ivlev et al. 2015). In disk interiors, the plasma charging dominates and grains are charged predominantly negatively. Grains may exchange their charges in mutual collisions; however, high dust concentration and low ionization degree are needed for triboelectric charging to be dominating over the plasma and photoelectric charging. Unlike the triboelectric charging, which is considered as a minor factor in the growth of dust in protoplanetary disks (Blum 2010), the plasma and photoelectric charging plays a major role in the collisional evolution of $\sim 1 \mu\text{m}$ grains (Okuzumi et al. 2011a, 2011b; Akimkin 2015).

As the grain charge typically scales linearly with the grain size, the electrostatic repulsion of like-charged grains become stronger as dust grows. At the same time, kinetic energy in Brownian motions does not depend on grain mass, so the purely thermal dust coagulation inevitably stops at some point due to increasing Coulomb repulsion. Non-thermal motions, which can be induced by turbulence or differential dust drift, may provide the necessary kinetic energy for dust grains to overcome the electrostatic barrier. Subsonic turbulence present

³ Both plasma charging and triboelectric charging are sometimes referred to as collisional charging.

in dense cores (Barranco & Goodman 1998; Caselli et al. 2002; Pineda et al. 2011; Keto et al. 2015) leads to a weak dependence of dust coagulation on grain charging (Chokshi et al. 1993), as the resulting kinetic energy of colliding grains is typically larger than their repulsion energy. However, the notably weaker turbulence in protoplanetary disks may be insufficient to overcome the electrostatic barrier.

Okuzumi (2009) showed that the electrostatic repulsion becomes important if the turbulence parameter $\alpha = (v_{\text{turb}}/c_s)^2$ is smaller than $\sim 10^{-2}$, where v_{turb} is the mean turbulent velocity of the gas and c_s is the sound speed. Recent observational efforts to constrain turbulence via CO line profiles in protoplanetary disks put upper limits of $v_{\text{turb}} < 0.05c_s$ and $< 0.08c_s$ for HD 163296 and TW Hya, respectively (Flaherty et al. 2017, 2018), which translates to $\alpha \lesssim 0.003\text{--}0.006$. The effective α -parameter in the dead zones with suppressed magnetorotational instability (MRI) may be even smaller, which poses an important challenge for current understanding of the dust evolution in protoplanetary disks.

Grain charging is still frequently neglected in present theoretical models of dust evolution, even so it may be invoked for the explanation of some observational properties of protoplanetary disks. First, it was shown that unconstrained dust coagulation leads to the depletion of small grains at timescales much shorter than the lifetimes of protoplanetary disks (Dullemond & Dominik 2005). The fast coagulation of small dust would result in a significant drop in near- and mid-IR fluxes, which contradicts observations (Haisch et al. 2001b; Cieza et al. 2007), so there should be a mechanism of either the replenishment of small dust population (e.g., via fragmentation in high-speed collisions) or the slowdown of its coagulation. The electrostatic barrier is a viable mechanism for such a slowdown as it can completely block the coagulation of micron-size dust, especially in the disk atmosphere and outer regions. Second, as the electrostatic barrier is most important for $\sim 0.1\text{--}10\ \mu\text{m}$ grains, it may divide dust population into small and large sub-populations.

In this paper we present numerical simulations of charged dust coagulation for typical protoplanetary disk conditions. These simulations are done in 2D in radial and vertical disk extent, accounting for the co-evolving dead zone with suppressed turbulence and tackles non-compact (fractal) grains. The present model does not consider global dust dynamics as well as fragmentation, as these factors are important for macroscopic dust and are of lesser importance for micron-size grains, for which the electrostatic barrier is crucial.

2. Model Description

To study the grain charge impact on the dust evolution we solve both the coagulation equation and grain charging balance equations. The corresponding model was initially presented in Akimkin (2015, 2017), here we recap its basic features and describe new improvements. The goal of these numerical simulations is to understand at which conditions the electrostatic barrier operates and how it can be overcome.

The electrostatic barrier against dust growth is important for $0.1\text{--}10\ \mu\text{m}$ grains (Okuzumi 2009). Grains of this size range do not experience substantial drift relative to the gas. Hence, in the basic approach, we treat the problem locally, i.e., neglecting the possible influx and outflux of large drifting grains in/from the grid cell. In Section 3 we study how the presence of non-locally grown dust affects the problem.

The background physical conditions during the whole simulation run of 0.9 Myr are assumed to be stationary. This includes stellar parameters, disk density, and temperature distributions, but not the ionization degree as it could have an important feedback loop with the charged dust evolution. The estimates of the protoplanetary disks lifetimes (Haisch et al. 2001a; Sicilia-Aguilar et al. 2006; Pfalzner et al. 2014) are a factor of two to ten longer than our simulation run of 0.9 Myr, so we keep the global disk structure fixed to preserve the clarity in the study. The assumed central star mass, radius, and effective temperature are $M_\star = 0.7 M_\odot$, $R_\star = 2.64 R_\odot$, $T_{\text{eff}} = 4000$ K. The disk is assumed to be azimuthally symmetric with the radial profile of the gas surface density set by the power law tapered at the inner and outer characteristic radii R_c^{inn} and R_c^{out} :

$$\Sigma(R) = \Sigma_0 \left(\frac{R}{1 \text{ au}} \right)^{-\gamma} \exp \left[- \left(\frac{R}{R_c^{\text{out}}} \right)^{2-\gamma} - \left(\frac{R}{R_c^{\text{inn}}} \right)^\delta \right]. \quad (1)$$

While the values of γ and R_c^{out} can be estimated from observations (Williams & Cieza 2011), δ and R_c^{inn} are loosely constrained. We adopt $R_c^{\text{inn}} = 0.5$ au, $R_c^{\text{out}} = 200$ au, $\gamma = 1$, and $\delta = -3$ with the normalization $\Sigma_0 = 300 \text{ g cm}^{-2}$, which results in the total gas mass $\approx 0.02 M_\odot$ within inner 10^3 au and $\Sigma(1 \text{ au}) = 263 \text{ g cm}^{-2}$. The gas mass density ρ_g is calculated from the condition of the vertical hydrostatic equilibrium with (vertically) isothermal gas and dust. For the temperatures we have $T_d(R) = T_g(R) = \varphi^{1/4} T_{\text{eff}} (R/R_\star)^{-1/2}$, with $\varphi = 0.05$ being the grazing angle. This yields the radial scaling of midplane density $\rho_g(R, 0) \propto R^{-9/4}$. The dust-to-gas mass ratio is 0.01 for all disk locations and does not change with dust evolution, the grain solid density $\rho_s = 3 \text{ g cm}^{-3}$ and the initial size distribution follows the power law with boundaries 0.005 and $0.25\ \mu\text{m}$ and power-law slope -3.5 .

The dust coagulation is modeled by the numerical solution of the Smoluchowski equation for charged grains. The coagulation kernel for two colliding grains with radii a_1 , a_2 , and charges $Q_1(a_1)$, $Q_2(a_2)$ can be written as

$$K_{12}(a_1, a_2) = \pi (a_1 + a_2)^2 u_{12} \mathcal{C}_{12}, \quad (2)$$

where

$$\mathcal{C}_{12}(a_1, a_2) = 1 - \frac{2Q_1 Q_2}{(a_1 + a_2) m_{12} u_{12}^2} \quad (3)$$

is the Coulomb factor, m_{12} is the reduced mass of two grains, and u_{12} is their relative velocity. The additional condition on the kernel is $\mathcal{C} \geq 0$. The dominant grain charging mechanisms for the selected physical conditions are plasma and photoelectric charging (Draine & Sutin 1987; Weingartner & Draine 2001). The former leads to the predominantly negative grain charge in the dark midplane, the latter leads to the positive dust grains in the illuminated disk atmosphere. The competition of these two charging mechanisms produces a zero-charge surface somewhere in the disk upper layers. It is important to consider the dispersion of grain charge, so K_{12} should be integrated over the possible charge states of a grain of a given size. We refer the reader to Akimkin (2015) for more information on our approach to the Smoluchowski equation

solution for charged dust. Below we describe the improvements we made in the model in comparison with that work.

In dense dark conditions the number density of dust grains becomes sufficiently high to affect the overall charge balance, leading to significant electron depletion onto grains (Umebayashi & Nakano 1980; Okuzumi 2009), so that electron and ion number densities are no longer equal and $n_e \ll n_i$. This effect was not considered in Akimkin (2015), so we added it following Ivlev et al. (2016), where we studied the transition between the electron–ion, dust–ion, and dust–dust plasma regimes. To find the local charge structure (distribution of dust charges and abundance of free electrons and ions) one should solve the equations on overall charge neutrality and ionization–recombination balance (see Equations (11)–(12) in Ivlev et al. 2016). Input parameters for these calculations were the dominant ion mass and the distribution of the total ionization rate $\zeta(R, z)$. The grain charge acquired due to collisions with plasma particles weakly depends on the ion mass. Heavy ions with $m_i \gtrsim 20 m_H$ are typically expected in the warm midplane regions, while lighter H_3^+ ions dominate in the colder outer parts (Semenov et al. 2004). We adopt $m_i = 29 m_H$, which corresponds to either HCO^+ or N_2H^+ ions, as the representative value for this paper.

CRs, X-rays, and radioactive elements are considered as main ionization sources. For CR ionization we use the approach presented in Padovani et al. (2018; see their Equation (46) and appendix F for model \mathcal{H}). As described in Padovani et al. (2018), for the effective gas surface densities Σ_{eff} below the transition surface density, $\Sigma_{\text{tr}} \approx 130 \text{ g cm}^{-2}$, the ionization occurs mainly due to CR protons. Effective surface density, which accounts for non-vertical magnetic field morphology, is taken to be 3.3 times the actual gas surface density (see Section 7.1 in Padovani et al. 2018).⁴ For regions with high surface densities, $\Sigma_{\text{eff}} \gtrsim \Sigma_{\text{tr}}$, the ionization is dominated by secondary gamma-rays (produced by CRs) and, thus, the magnetic fields do not affect the results in this case. In this case, the CR ionization rate should be calculated by the averaging over all directions to the transition surface; in this work we do averaging only in the z -direction for simplicity.

For the X-ray ionization rate we adopt the approach from Bai & Goodman (2009; see their Equation (21)) assuming stellar X-ray luminosity $10^{30} \text{ erg s}^{-1}$ and $T_X = 3 \text{ keV}$. The lowest total ionization rate is limited by the contribution of radioactive decay, which we set to $1.4 \times 10^{-22} \text{ s}^{-1}$ (Umebayashi & Nakano 2009).

The key part of any dust evolution model is the source of collisional velocities. The relative velocities due to the Brownian motion u_{Br} of dust grains with the same size a decrease with a . However the grain charge Q typically scales linearly with a , so the Coulomb factor in Equation 2 inevitably becomes zero for sufficiently large a . Thus, the purely Brownian motion, although being the the main driver of early dust coagulation, can not be responsible for the overcoming of the electrostatic barrier. However, it defines the critical grain size $\sim 1 \mu\text{m}$, where dust coagulation starts to be strongly affected by the charge, which we studied in Akimkin (2015) and Ivlev et al. (2016). In this paper we also included the turbulence-induced collisional velocities using closed form expressions from Ormel & Cuzzi (2007) using a procedure

implemented by Birnstiel et al. (2010). The stopping time of a compact grain $t_s = \rho_s a / (v_{\text{th}} \rho_g)$ (Armitage 2018) can be rewritten as $t_s = 3m(a) / (4v_{\text{th}} \rho_g \pi a^2)$ in the general case of fractal dust. Here, $m(a)$ is the mass of the aggregate of size a (consisting of monomers with material density ρ_s) and v_{th} is the thermal speed of molecules. The total collision velocity is $u_{12} = \sqrt{u_{\text{Br}}^2 + u_{\text{turb}}^2}$. In our simulations we account for the presence of a dead zone with suppressed turbulence and define it as a region with sufficiently low ionization degree $x_e < x_{\text{cr}} = 10^{-13}$ (Dudorov & Khaibrakhmanov 2014). We adopt the turbulence parameter $\alpha_{\text{active}} = 10^{-3}$ for the MRI active region and $\alpha_{\text{dead}} = 10^{-6}$ for the dead zone. The value of α_{active} is taken according to the available observational constraints (Flaherty et al. 2017, 2018). As the gas ionization degree in dense regions depends on the current dust size distribution, we recalculate the position of the dead zone consistently with the dust evolution.

Okuzumi (2009) pointed out the importance of dust fluffiness in the evolution of charged dust. In our modeling we consider several choices for the fractal dimension D of dust aggregates. Fractal dimension D is defined via a scaling relation between aggregate mass m and its characteristic size a ,

$$m(a) = m_0 \left(\frac{a}{a_0} \right)^D, \quad (4)$$

where $m_0 = (4\pi/3)\rho_s a_0^3$ is the mass of a compact monomer having radius a_0 . For any choice of D we assume that initially all particles are compact, while all grown particles are made of monomers with the size equal to the largest one in the initial distribution, i.e., $a_0 = 0.25 \mu\text{m}$. To compare different cases of the fractal dimension D , we introduce an equivalent radius a_c equal to the radius of a compact grain of the same mass

$$a_c^3 = 3m / (4\pi\rho_s) = a_0^{3-D} a^D. \quad (5)$$

The charging of fractal dust aggregates is a complicated and poorly studied topic, as dipole interactions and stochastic nature of interactions of free charge with asymmetrically charged aggregate are important factors. We neglect these effects in the current study and assume that the cross section of a grain with mass m is equal to πa^2 , where a is defined from Equation 4. This expression for the cross section is used in both coagulation and charging equations. The consideration of fractal dust is our third and last major improvement to the model by Akimkin (2015; with electron depletion and turbulence-induced velocities being the other two ones).

3. Results

3.1. Coagulation of Charged Grains

The numerical simulations of charged dust coagulation provides us with the evolution of the dust size distribution at a given disk location. To show the broad picture of the grain charge impact on the dust growth, we compute the average grain radius in different locations of a 2D vertical cut of the disk and use it as a measure for the severity of the electrostatic barrier. Then we analyze the size distribution at some selected locations in more detail. The neglect of dust drift in our modeling does not allow us to rely on the macroscopic tail of the grain size distribution ($\sim 1 \text{ mm}$) on a par with the current state of the art dust evolution models. But for the goals of the paper we need the fact that grains are able to

⁴ In many studies, the fact that CRs propagate along the magnetic field is completely ignored. This generally leads to underestimated column density traversed by CRs and, hence, to overestimated ionization.

overcome $\sim 10 \mu\text{m}$ size at some disk locations. This would mean the insignificance of the electrostatic barrier there.

The average grain mass at every disk location is defined as

$$\bar{m} = \int mf(m)dm / \int f(m)dm, \quad (6)$$

where $f(m)$ is the grain mass distribution. In Figure 1 we show the radial and vertical distribution of an equivalent average grain radius (i.e., of an equivalent radius of a grain with the average mass \bar{m}) after 0.9 Myr since the start of dust coagulation for six cases:

- (a) purely Brownian coagulation of neutral dust (panel (a));
- (b) purely Brownian coagulation of compact charged dust (panel (b));
- (c) Brownian plus turbulence-induced coagulation of dust aggregates with fractal dimensions $D = 3.0$ (panel (c)), 2.5 (panel (d)) and 2.1 (panel (e));
- (d) case from panel (e) for $D = 2.1$, but with artificial presence of large $\approx 50 \mu\text{m}$ grains to simulate dust drift (panel (f)).

As noted above, the ratio of electrostatic-to-kinetic energy in Equation (3) generally increases with the grain size for Brownian motion, so the purely thermal coagulation of charged grains is inevitably stopped by the electrostatic barrier at some limit size. We demonstrate this in panels (a) and (b) of Figure 1. It is seen from the panel (b) that the Coulomb repulsion stops thermal dust coagulation at $\sim 1 \mu\text{m}$ throughout the whole disk volume. Such small size limit is crucial for the subsequent dust growth as other sources of grain relative velocities are not strong enough at this stage. The grain size on panel (a) of Figure 1 may be overestimated as artificial growth is possible if the number of size bins is not large enough (we divide the size range from 5×10^{-7} to 1 cm into 128 bins). However, for dust trapped behind the electrostatic barrier, this numerical effect is less important as there is a physical mechanism blocking the growth of particles with sizes close to the initial ones. The fingerprint of the zero charge surface, where the photoelectric and plasma charging are balanced, is seen in panel (b) as a faint rim in the disk upper layers. In this region, dust growth is almost not affected by the charging effects.

The consideration of turbulence-induced velocities solves the problem of electrostatic barrier for compact grains ($D = 3.0$; panel (c)) everywhere in the disk except for the dead zone. The dead zone boundary at the moment $t = 0.9 \text{ Myr}$ is shown with the long dashed line, while the short dashed line corresponds to the initial location of the dead zone. The dead zone shrinks with the start of dust coagulation as the electron depletion onto dust grains become less important. This leads to the increase in the ionization degree, which can exceed the critical value of 10^{-13} for the MRI development. Such behavior is strongly affected by dust fragmentation as well as active and dead zone physics, which is surely quite simplistic in our model. This stresses the need for separate study of self-consistent treatment of dust evolution and MRI development.

The macroscopic grain sizes denoted by the reddish color in Figure 1 are not necessary attainable at a given location due to several effects not considered in the presented modeling. They include the radial and vertical dust drift, as well as fragmentation and compaction of the aggregates. Instead, the reddish color traces the disk regions where the electrostatic

barrier can be overcome and dust evolution is a charge-independent phenomenon.

The grain fractality ($D < 3$) may play a double role in charged dust coagulation. First, it increases the collisional cross section for a dust grain of given mass, thus boosting the coagulation rates. Second, it suppresses the turbulence-induced dust velocities as they scale as $a^{(D-2)/2}$. Low values of D may move forward the threshold grain size where turbulence starts to dominate over the Brownian velocities. To explore the dependence of the dust coagulation on dust fractality we considered two additional choices of $D = 2.5$ and 2.1.

One can see that the moderate fractality ($D = 2.5$; Figure 1(d)) allows easier, charge-independent grain growth outside the dead zone. This can not be said about the dead zone where almost all dust population is still locked behind the electrostatic barrier. More fluffier aggregates ($D = 2.1$, Figure 1(e)) are electrostatically blocked from coagulation not only in the dead zone but almost everywhere in the disk, which is consistent with previous studies (Okuzumi 2009). Such a severe barrier arose due to the fact that the electrostatic-to-kinetic energy ratio is larger than unity at grain sizes smaller than those affected by the turbulence.

To check the dependence of our results on the improperly considered effects (radial and vertical drift of grown dust), we artificially added grown aggregates with sizes $\approx 50 \mu\text{m}$ to the initial grain size distribution. Their mass fraction is $\sim 10\%$ of the initial dust mass. This may simulate the charge-independent grain growth outside the dead zone and subsequent inward drift. The results for $D = 2.1$ are shown in Figure 1(f). One can see that this helps to overcome the electrostatic barrier just outside the outer dead zone boundary, but again not in the dead zone itself.

To have a closer look at the possibilities to overcome the electrostatic barrier we plotted in Figure 2 the value of the Coulomb factor integrated over the grain charge states (coagulation efficiency),

$$\bar{c}(a_1, a_2) = \iint c_{12} G_1 G_2 dQ_1 dQ_2, \quad (7)$$

where $G_i \equiv G(a_i, Q_i)$ is the Gaussian charge distribution of grains having the radius a_i . The corresponding values of average grain charge and its dispersion are calculated similar to Akimkin (2015). We show the results for three choices of fractal dimension $D = 3.0, 2.5$, and 2.1 as well as three radial locations at 1, 11, and 46 au lying well inside the dead zone, just outside it and at the disk periphery, respectively.

Figure 2 shows that the electrostatic barrier plays almost no role for coagulation of grains with $a \gtrsim 100 \mu\text{m}$ (except for very fractal grains with $D = 2.1$, located in the dead zone). This means that if large “seed particles” can be transported into the dead zones for cases $D = 2.5$ and 3.0, this should trigger the dust growth. A similar effect should occur outside the dead zone at 11 au for $D = 2.1$ (see middle panel in the last row of Figure 2). At that location, the coagulation within the ensemble of small dust is inhibited, but the coagulation with larger particles is barrier-free. Seed particles added to that location absorb the small grains, which are otherwise electrostatically “locked” (compare black and red dashed lines in the middle panel of the first row of Figure 2).

In the vicinity of the zero-charge layer, dust grains can freely coagulate. The sustained turbulence ensures repetitive passage of aerodynamically small grains through this zone, which

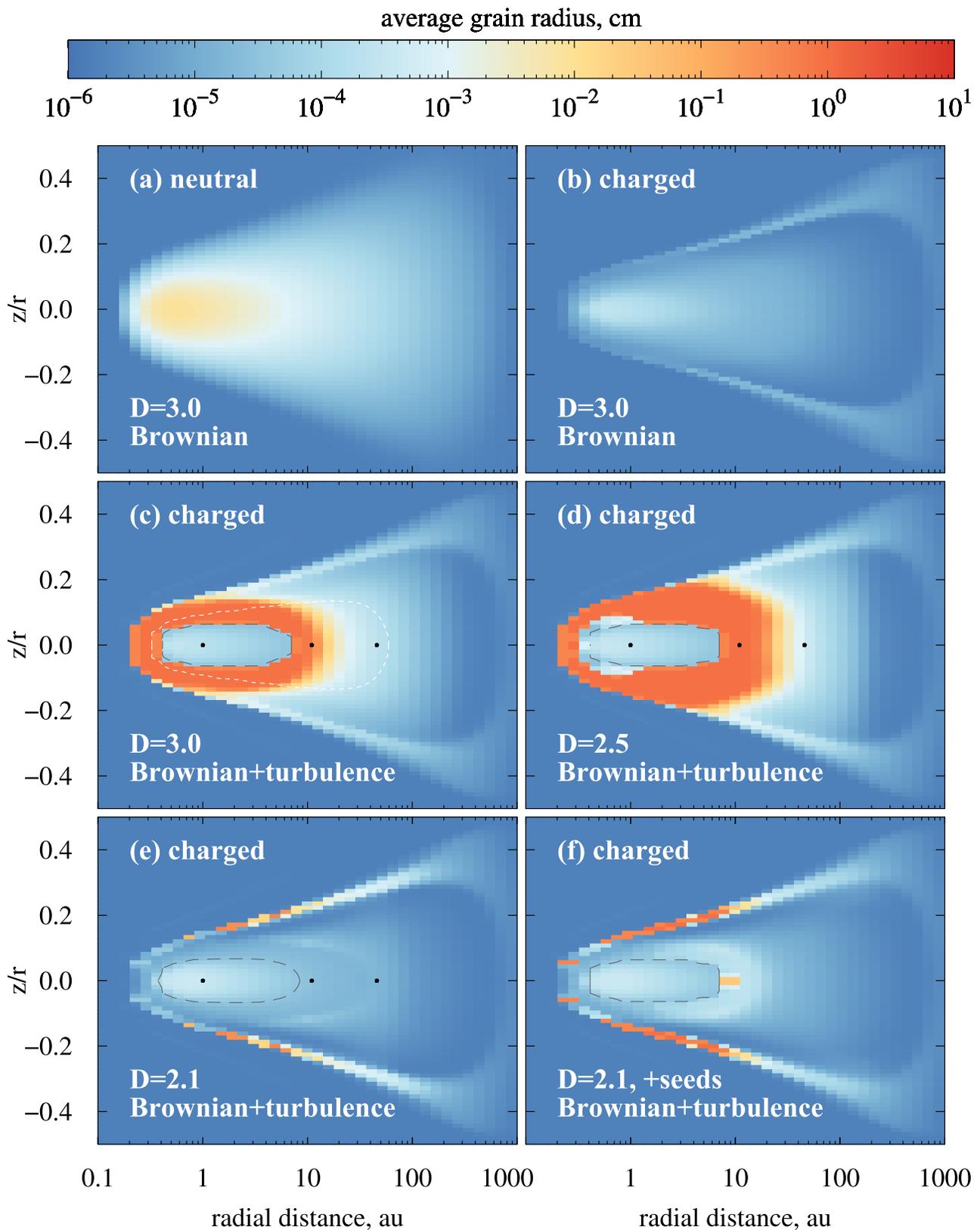


Figure 1. Equivalent average grain radius in different disk locations after 0.9 Myr of in situ coagulation. Panels (a) and (b) show purely Brownian coagulation of neutral (a) and charged (b) grains. For other panels the turbulence-induced velocities are also included. Panels (c)–(e) present the results for different values of the fractal dimension of dust aggregates, $D = 3.0, 2.5,$ and 2.1 . Panel (f) represents the case from panel (e), but with initial size distribution contaminated by the artificially large $\approx 50 \mu\text{m}$ seed particles. The long dashed lines show the location of a dead zone for $t = 0.9 \text{ Myr}$ ($\alpha_{\text{active}} = 10^{-3}$, $\alpha_{\text{dead}} = 10^{-6}$), the short dashed line in panel (c) shows the location of the dead zone at $t = 0$ (which is the same for panels (d)–(f), but not shown on them). The black bullets indicate the locations for which the data in Figure 2 are presented.

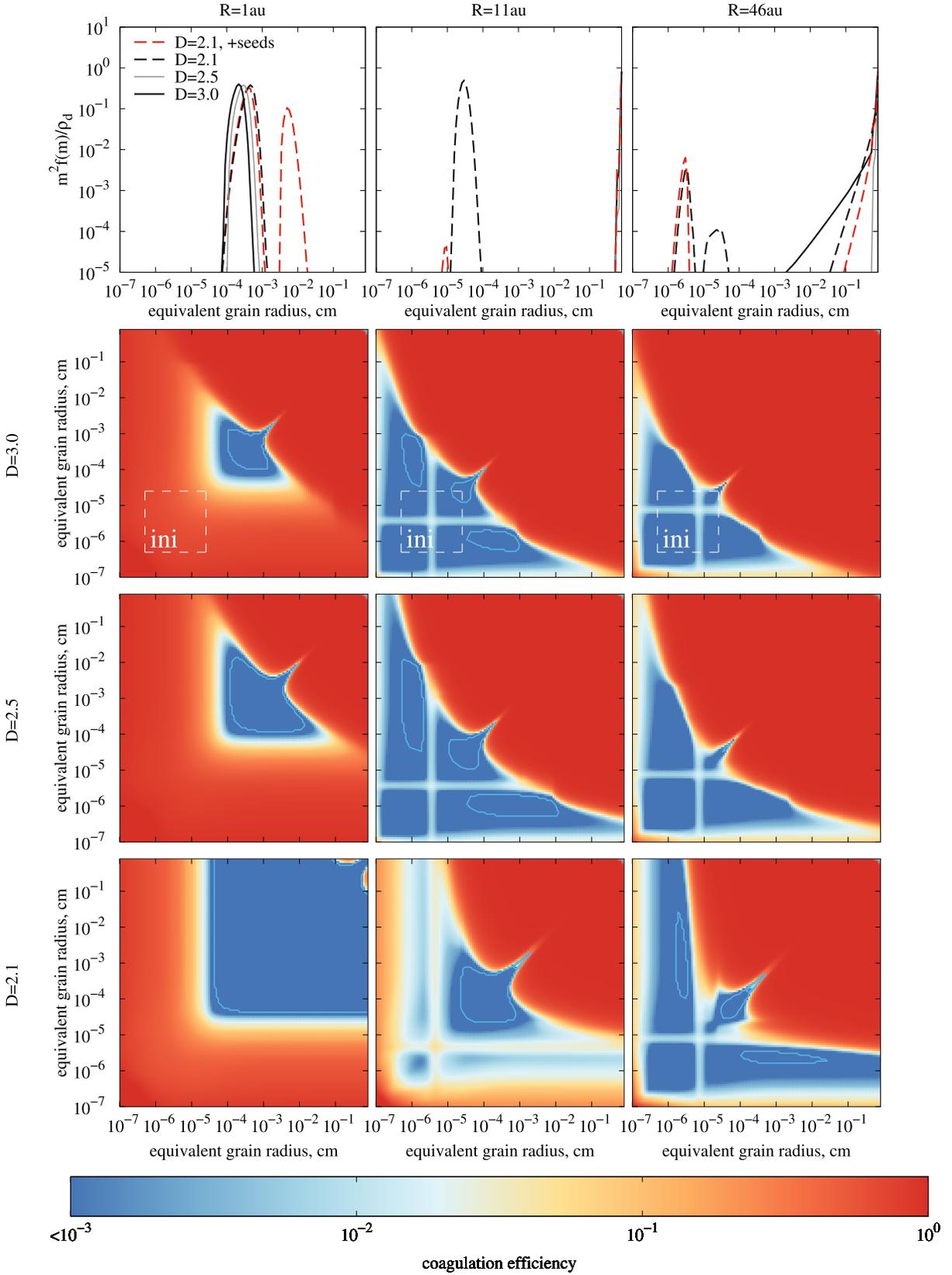


Figure 2. Grain size distribution at $t = 0.9$ Myr (upper row) and the charge-averaged Coulomb factor $\bar{C}(a_1, a_2)$ (coagulation efficiency) as a function of equivalent radius of colliding grains for fractal dimension $D = 3.0$ (second row), $D = 2.5$ (third row), $D = 2.1$ (bottom row). The columns correspond to different radial positions: dead zone (1 au; left column); active region near outside boundary of the dead zone (11 au; middle column); and disk periphery (46 au; right column). The dashed squares marked with “ini” indicate the size range of the initial distribution (grains in the initial distribution are assumed to be compact for all D). Blue contour lines confine the size domains with the coagulation efficiency of $\leq 10^{-10}$.

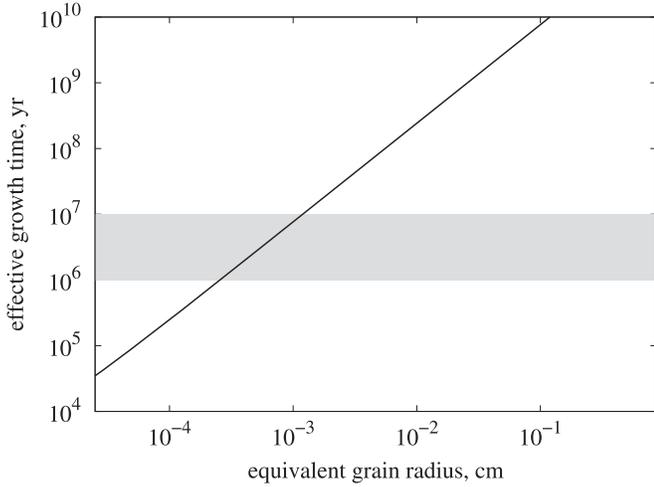


Figure 3. Effective timescale of dust coagulation due to turbulence-induced crossing of the zero-charge layer, plotted versus the equivalent grain radius. The horizontal gray stripe shows the range of typical lifetimes of protoplanetary disks.

provides a potential mechanism to overcome the electrostatic barrier even for low fractality of $D = 2.1$ (where the addition of $\sim 50 \mu\text{m}$ seed particles is not efficient). To evaluate the significance of this mechanism, we notice that the size growth rate (see, e.g., Birnstiel et al. 2016, Section 3.3) can be straightforwardly generalized for fractal grains,

$$\dot{a} = u_{12} \frac{\rho_d}{\rho_s} \frac{3}{D} \left(\frac{a}{a_0} \right)^{3-D}, \quad (8)$$

where ρ_d is the volume density of dust in the disk. The resulting charge-free coagulation timescale, $t_{\text{coag}}^0 = a/\dot{a}$, should be modified to account for limited time grains staying in the zero-charge layer. With the vertical thickness Δz_0 of the layer at the vertical position z_0 , the ratio $\Delta z_0/z_0$ is an order-of-magnitude estimate of the time fraction the grains are spending in the layer. We define $\Delta z_0(a)$ as the height difference where the average charge number of a grain changes from $+1$ to -1 . The layer thickness shrinks for larger grains as the vertical charge gradient increases with their size. In Figure 3, we plot the effective growth timescale, $(z_0/\Delta z_0)t_{\text{coag}}^0$, as a function of the equivalent grain radius. We see that for $a > 10 \mu\text{m}$ the timescale becomes larger than the typical protoplanetary disk lifetime of $\sim 10^7$ yr. Thus, even for $D = 2.1$ the turbulent vertical stirring of dust appears to be inefficient in overcoming the electrostatic barrier.

To understand the shape of the “inhibited zones” (blue regions) in Figure 2, let us evaluate the ratio of the contact energy of the electrostatic repulsion between two grains to the kinetic energy of their relative motion—according to Equation (3), this value determines the deviation of $\bar{C}(a_1, a_2)$ from unity. Given a Gaussian charge distribution, we expect the average coagulation rate to be drastically reduced when this ratio (calculated for the average charge) is of the order of unity or larger. Considering a pair of grains with radii $a_1 > a_2$, this condition can be approximately presented in the following

form:

$$\frac{\tilde{\varphi}_0 |Z_1 Z_2| / \tilde{a}_1}{1 + c \alpha \text{St}_0 (m_0/m_g) \tilde{a}_1^{D-2} \tilde{a}_2^D} \gtrsim 1. \quad (9)$$

Here, $\tilde{a}_{1,2} = a_{1,2}/a_0$ are the grain radii normalized by the radius of a monomer, $\text{St}_0 = \Omega_K t_{s0} (\ll 1)$ is the monomer Stokes number (expressed via the local Keplerian frequency $\Omega_K \propto R^{-3/2}$ and the local stopping time of the monomer $t_{s0} \propto a_0 \rho_g^{-1} T^{-1/2}$), and c is a constant of the order of unity. The relative magnitude of the repulsion barrier is given by the product of charge numbers, $Z_{1,2} = Q_{1,2}/e$, multiplied with the unit-charge electrostatic energy at the monomer surface (normalized to the thermal energy), $\tilde{\varphi}_0 = e^2/(a_0 k_B T)$.

As long as grains are small enough, $\tilde{\varphi}_0/\tilde{a}_i \gg 1$, they are (typically) singly charged ($Z_i = -1$) due to the induced-dipole attraction of plasma charges. Furthermore, for small grains the term in the denominator of Equation (9) is negligible. Therefore, the left-hand side is simply $\tilde{\varphi}_0/\tilde{a}_1 \gg 1$, hence the coagulation of such grains is completely inhibited. Of course, reducing the grain size further makes the grains neutral, but this transition typically occurs when the size is about a nanometer, as one can see in the middle and right columns of Figure 2. On the other hand, the left column represents the plasma regime with a strongly depleted electron density (see Section 3.2), and therefore grains of the initial size distribution remain neutral in this case.

The transition to multiply charged grains at a given location occurs where $\tilde{\varphi}_0/\tilde{a}_i \simeq 1$ (assuming the electron depletion is not strong), which is revealed in Figure 2 by the crossing lines in the inhibited zone. The origin of these lines is obvious—Equation (9) in this case is marginally satisfied, and therefore the coagulation rate is only moderately reduced. The further increase of the grain sizes leads to the average charges such that the product $\tilde{\varphi}_0 |Z_i|/\tilde{a}_i$ is a constant of the order of a few (its value is determined by the local plasma regime). Hence, the numerator of Equation (9) becomes proportional to $a_2 T$. For sufficiently large grains the second term in the denominator is dominant, and then the left-hand side starts rapidly decreasing. Taking into account the scaling dependence of St_0 on the radial position, we conclude that the electrostatic barrier is unimportant if the sizes exceed a threshold determined from the relation $\alpha R^{3/2} \tilde{a}_1^{D-2} \tilde{a}_2^{D-1} = \text{const}$. Except for the proximity of the diagonal line $a_1 = a_2$, where more detailed analysis is required, this relation well describes the “outer” boundaries of the inhibited zones in Figure 2.

3.2. Dusty Plasma Regimes

Generally, the coagulation may be stopped by the electrostatic barrier at either dust–ion or electron–ion state depending on the underlying grain–grain relative velocities. The wealth of free electrons in the electron–ion plasma allows the most negative grain charges (for given plasma temperature and ion mass) and, consequently, the hardest conditions for the grain growth. In high-density low-ionization regions, where the ionization degree is comparable with the dust abundance, the plasma state shifts to the dust–ion regime and grains become less charged as fewer electrons hit the dust. In the limit of dust–dust plasma, where both electrons and ions are severely depleted from gas, the average grain charge is near zero and the electrostatic barrier disappears (Ivlev et al. 2016). The largest

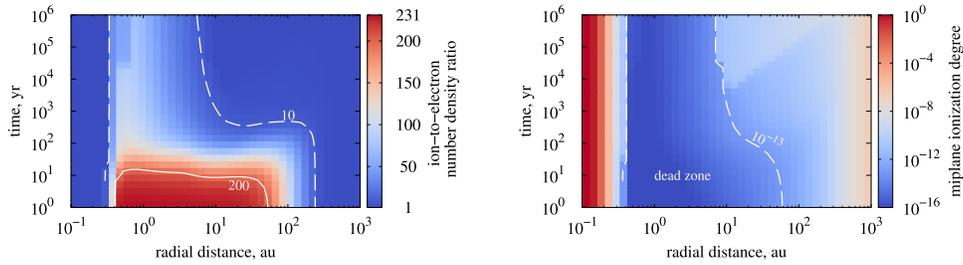


Figure 4. Left panel: the evolution of the ion-to-electron ratio n_i/n_e in the disk midplane for the case of non-fractal dust ($D = 3.0$; corresponds to panel (c) in Figure 1). Right panel: the evolution of the ionization degree $x_e = n_e/n_{\text{gas}}$ in the disk midplane for the same case. The dead zone with suppressed turbulence ($\alpha_{\text{dead}} = 10^{-6}$) is defined as a region with $x_e < 10^{-13}$. Its size shrinks with dust evolution.

disproportion in abundances of ions and electrons,

$$\left(\frac{n_i}{n_e}\right)_{\text{max}} = \frac{s_e}{s_i} \sqrt{\frac{m_i}{m_e}}, \quad (10)$$

is achieved in dust–dust plasma. In the case of perfect electron and ion sticking ($s_e = s_i = 1$) and N_2H^+ or HCO^+ being the dominant ion ($m_i = 29m_{\text{H}}$), the maximum ion-to-electron number density ratio is $(n_i/n_e)_{\text{max}} = 231$. The grain growth in absence of fragmentation changes the plasma state in the direction from dust–dust state to dust–ion and then to electron–ion state. This also leads to the decrease of n_i/n_e down to unity and to the increase in the ionization degree.

In the left panel of Figure 4, we show the evolution of the ion-to-electron ratio n_i/n_e in the disk midplane for the case of non-fractal dust (corresponding to the case (c) in Figure 1). At the very beginning of simulations the plasma is in the dust–dust state within 0.4–50 au and $n_i/n_e > 200$. However, it quickly switches to the dust–ion and electron–ion state. In the right panel of Figure 4, we show the corresponding ionization degree. The dashed isoline for $x_e = 10^{-13}$ demonstrates the evolution of the dead zone due to the dust coagulation. By the end of simulations at 0.9 Myr the dead zone shrinks from 0.3–60 au to 0.4–7 au and coincides with the electrostatic barrier region. While the electrostatic barrier may occur in both dust–ion and electron–ion plasma, for non-fractal dust ($D = 3.0$) and chosen disk parameters it happened in the dust–ion regime (see also Ilgner 2012).

4. Discussion

While protoplanetary disks are likely to have favorable conditions for coagulation of micrometer-size particles into macroscopic pebbles, we still lack the clear understanding of this pathway. Dense midplane regions with mild sources of relative grain velocities are thought to foster the rapid dust coagulation up to the sizes at which grains start to experience the notable drag relative to the gas. This allows the grains to concentrate in dust traps and trigger the subsequent formation of planetesimals and, eventually, planets. At the same time, small micrometer-size dust is persistent along the entire protoplanetary disk evolution. It provides the key source of disk opacity in ultraviolet and optical range and shields molecules in disk interiors from dissociation. The presence of small dust can be inferred from near-IR spectral energy distributions (Haisch et al. 2001b; Cieza et al. 2007) and imaging (Avenhaus et al. 2018).

Sustaining large amounts of small dust can be explained by the replenishment of its population from larger grains due to the fragmentation (Dullemond & Dominik 2005), or/and by

extremely inefficient coagulation in micrometer-size range due to the Coulomb repulsion. The important difference between these two alternatives is the role of turbulence. If the fragmentation is the dominant mechanism of small dust replenishment, one may expect larger amounts of micron-size dust in disks with stronger turbulence. On the other hand, strong turbulence makes the electrostatic barrier less effective in maintaining small dust population. Thus, future measurements of non-thermal line widths may be crucial for our understanding of dust evolution in protoplanetary disks (Flaherty et al. 2017, 2018).

5. Conclusions

Coagulation of small particles is a key process in protoplanetary disk evolution and formation of planets. This process is controlled by a number of microphysical factors like sticking, bouncing, sintering and fragmentation as well as global dust dynamics. In this paper we study the coagulation of grains charged due to photoelectric effect and the collection of free electrons and ions. We solve the Smoluchowski equation coupled with grain charging and gas ionization equations to study the conditions where the electrostatic barrier between like-charged grains can play an important role. As the Coulomb repulsion is typically important for small 0.1–10 μm grains, which are not large enough to drift relative to the gas, we neglect global dust dynamics. The simulations are done in the 2D vertical and radial extent of a typical protoplanetary disk and account for the simple self-consistent co-evolution of the dead zone and dust inside it. We consider three characteristic values of the fractal dimension of dust aggregates, $D = 3.0, 2.5$, and 2.1, defining a dependence of the grain mass on the size, $m \propto a^D$. Our conclusions can be summarized as follows:

1. Small 0.1–10 μm grains in protoplanetary disk interiors are sufficiently negatively charged to inhibit their mutual collisions.
2. Sustained turbulence with $\alpha \gtrsim 10^{-3}$ is necessary, but not sufficient, to overcome the electrostatic barrier between small grains, which makes the initial dust growth blocked in dead zones.
3. Although the *mutual* coagulation of small particles in the dead zone is inhibited, their collisions with large grains ($>100 \mu\text{m}$) having $D = 2.5$ or 3.0 are possible. Thus, large particles (drifting, e.g., from the outer disk) may serve as seeds for barrier-free coagulation in the dead zone.

4. The coagulation of highly fractal dust with $D = 2.1$ is blocked not only in the dead zone, but almost in the entire disk.

Thus, the mutual electrostatic repulsion of small, μm -size grains can efficiently prevent their coagulation in regions where large dust is absent. This can serve as an alternative (to fragmentation) mechanism explaining the presence of small dust in disk atmosphere and outer regions.

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