Chapter 5

Study of effects of attractive potentials on Coulomb crystal formation

In this chapter, a comparative study between the effect of coupled Yukawa-Shadowing potential and Overlapping Debye Sphere (ODS) potential on 2D dust crystal formation has been done by using MD simulation. The structure of the system is investigated by calculating Radial Distribution Function \( g(r) \) for different values of \( \Gamma, \kappa \) and dust number densities \( n_d \). The results for Yukawa-Shadowing and ODS potential are compared with experimental results and a close agreement is obtained for attractive Shadowing force.

5.1 Introduction:

The formation of dust crystal is a wellknown phenomenon in dusty plasma physics. Due to large negative charge, dust particles immersed in plasma can turn plasma into a strongly coupled system. Dusty plasma exhibits interesting phenomena such as the formation of a liquid or solid structure when the coupling is sufficiently strong\(^{121,189}\). Dust crystals have been produced experimentally and their structural and dynamical
behaviours are studied in many laboratories\textsuperscript{120,122,123,190,191}. The discovery of plasma crystals has encouraged the plasma physics community to work in this area. Dusty plasmas provide a model system for crystalline structures to study phase transitions, melting process etc. in condensed matter. Plasma crystal offers ideal tool to observe phase transition at kinetic level due to two factors; direct visualization of individual particles and short restoring time that offers the particles required to reach equilibrium after a perturbation.

One outstanding problem of dust crystal is that the average interaction potential between two dust particles is not known precisely. Shielding of dust particle and resulting interaction potential are not explored properly. It is usually assumed that the average interaction potential between two dust particles is of the Debye-Hückel or Yukawa type. It is now well established that dust particles form Coulomb crystal in presence of strong repulsive forces\textsuperscript{134,192}. However, a question generally arises regarding existence of any attractive force between the grains. The mechanism of interaction among grains in plasma is a complex phenomenon and it needs substantial amount of research both at theoretical and experimental levels to understand it. For system where inter-particle distance is larger than Debye length, it may not be sufficient to consider Debye-Hückel potential as the interaction potential among the dust grains. The effect of attractive force like Shadowing force or overlapping Debye sphere can not be ignored in such cases.

In dusty plasma, the overlapping Debye spheres around dust grains produce an attractive force\textsuperscript{149,193,194}. The interaction energy of the sheath of one grain with the bare charge of the other grain can be expressed as

\begin{equation}
\phi_{ODS}(r_{ij}) = -\frac{Q^2_d}{4\pi\varepsilon_02\lambda_D} \exp\left(-r_{ij}/\lambda_D\right) \tag{5.1.1}
\end{equation}

where \(\lambda_D\) represents the Debye length of the background plasma. Here, the grains are assumed to have identical charges. The result of this potential is a weak attraction
at larger distances (beyond a critical radius $r_c = 2.73\lambda_D$). Very recently Hou et al.\textsuperscript{149} have used molecular dynamics simulation to study the effect of overlapping Debye sphere on structure of 2D dusty plasma. For this, they have made a comparison between the normal Yukawa potential and potential due to overlapping Debye spheres. Their results show a clear difference between the two potentials for large screening parameter $\kappa$ or at low dust density.

Shadowing force is exerted between neighboring particles due to mutual distortion of ion or neutral flux to the particles, detail of which is discussed in Chapter 4. The existence of an attractive component in the force between dust particles was experimentally studied and verified by several methods\textsuperscript{174,195,196}. It was suggested by Tsytovich et al.\textsuperscript{167} that the grains create flux of plasma particles towards their surface and the shadow of the plasma flux to one of the interacting grains by another grain creates an attractive force. Since these forces are not screened, they can dominate Coulomb repulsion force at distances larger than the ion Debye screening length. This attractive force may play a major role in the formation of dust crystal. Ramazanov et al.\textsuperscript{197} investigated the interaction between dust particles in a plasma on the basis of experimental pair correlation function. They confirmed existence of an attractive component in the interaction potential of dust particles.

Shukla and Rao\textsuperscript{148} have discussed the possibility of Coulomb crystallization under an attractive force between charged dust grains in a multi-component dusty plasma whose constituents are tenuous electrons, streaming ions and negatively charged dust grains. They have shown that these could be a far-field non-Coulombian potential that may be responsible for bringing the like particulates together that leads to microscopic Coulomb crystallization in dusty plasma. Quasi-lattice structures may be formed under such attractive forces between like polarity dust grains. Resendes et al.\textsuperscript{193} have suggested a static screening mechanism for the formation of plasma molecules in the bulk plasma and in the plasma sheath. They identified correlation
Coulomb energy as the mechanism responsible for plasma crystals. They suggested that each grain is correlated with its own Debye sheath and the interaction takes place between the dressed grains.

Tsytovich pointed out that the observed values of the critical coupling constant in most of the experiments are not consistent with the physical and theoretical estimates of this quantity. He suggested a new physical model for phase transition in a dusty plasma. He has shown that the balance between nonlinear screening at short distances and collective attraction at large distances determines the mean interparticle distances corresponding to the values observed in the transition to the crystalline state. Ishihara et al. have shown that a like-charge attraction could align dust particles along the equipotential line on a void boundary perpendicular to the ion flow in the complex plasma. Tsytovich et al. have reported about some of their interesting results regarding helical dust structures. They have performed molecular dynamics (MD) simulations to demonstrate that a random distribution of grains, interacting via a potential with shallow attractive well and experiencing background friction and stochastic kicks, forms spherical grain crystals.

Although there exist different theories about attractive interactions among dust grains in plasma, a clear understanding of the mechanism is still lacking. There are few experimental studies that investigate about the interactions among the particles. Melzer et al. performed an experiment where they had demonstrated that attractive binding forces between the negatively charged dust exist. They found by laser manipulation of dust particles that net forces between the particles can be reversibly changed between attraction and repulsion.

Here in this chapter, a molecular dynamics code is developed to study phase transition of 2D Coulomb crystals in presence of Shadowing and Overlapping Debye sphere (ODS) potentials. The study has shown some interesting results. Both shadowing and ODS potential have distinct roles to play for different parameter regimes of the
dusty system. In section 5.2 of this Chapter, the theoretical and simulational model used to study this problem have been discussed. Results are discussed in section 5.3. Section 5.4 deals with the concluding remarks of the present investigation.

5.2 Theoretical modelling and simulation

Here, a 2D dusty plasma system is considered consisting of identical, spherical particles of mass $m_d$ and charge $Q_d$ immersed in a neutralizing background plasma. It is assumed that the average interparticle potential between two dust particles separated by a distance $r_{ij}$ is of Debye-Hückel or Yukawa type, given by Eq.(3.3.2) in 3rd chapter. It is well known that because of large charge on dust particles, dusty plasma easily attains strongly coupled regime and when the value of the Coulomb coupling parameter $\Gamma$ exceeds a certain critical value, the dust pericles may crystalline into solid-like structure. The phase transition of such a system are determined by two basic parameters $\Gamma$ and screening parameter $\kappa = a/\lambda_D$. Here, $a$ represents the mean-interparticle distance.

It has been already discussed that role of attractive force in forming plasma crystal cannot be ignored. In this Chapter, we intend to have a comparative study between effects of Shadowing potential and ODS potential on Coulomb crystal formation. It is interesting to find out regimes of dominance of the two attractive potentials.

We examine the effect of coupled Debye-Hückel and Shadowing potential

$$\phi(r_{ij}) = \frac{Q_d^2}{4\pi \varepsilon_0 r_{ij}} \exp \left( -\frac{r_{ij}}{\lambda_D} \right) - \frac{3}{8} \frac{r_d^2}{\lambda_D^2} \frac{Q_d^2}{r_{ij}}$$

and Yukawa potential combined with ODS potential

$$\phi_{Yu,ODS}(r_{ij}) = \frac{Q_d^2}{4\pi \varepsilon_0 r_{ij}} \exp \left( -r_{ij}/\lambda_D \right) - \frac{Q_d^2}{4\pi \varepsilon_0 2 \lambda_D} \exp \left( -r_{ij}/\lambda_D \right)$$
on pair correlation function of the dusty system. The first term of both the above expressions represents Debye-Hückel potential, whereas the second term of equation (5.2.1) is due to the Shadowing potential. In equation (5.2.2) the second term arises due to interaction of sheath of one grain with the bare charge of the other grain.

Here the already developed MD code is implemented to study 2D crystal formation. The combined potentials: Yukawa-ODS and Yukawa-Shadowing have been incorporated to derive the interacting force among the particles. Simulations have been performed for wide-range of the parameters such as Coulomb coupling parameter $\Gamma$, screening constant $\kappa$, dust density $n_d$ and dust radius $r_d$. The simulations are performed with 900 particles for FCC crystal structure for following plasma parameters: $n_i = (1.5 \times 10^{14} - 4.0 \times 10^{14})/m^3$, $T_e = 2320K$, $T_i = 300K$, $T_d = 40K$ to 1000K. This lattice is used as initial condition. Each grain is assigned an initial velocity (random in magnitude and direction) such that the average kinetic energy corresponds to the chosen temperature $T_d$.

Newton's equation of motion is solved numerically using velocity Verlet algorithm for interaction potentials mentioned above. In MD scaling Newton's equation for the two cases take the following form:

Yukawa-Shadowing

$$\frac{d^2r_i'}{dt'^2} = \Gamma \kappa \left[ \left( 1 + \frac{1}{r_{ij}} \right) \frac{1}{r_{ij}} \exp(-r_{ij}') - \left( \frac{3}{8} \right) \left( \frac{r_d^2}{\lambda_{D,i}^2r_{ij}^2} \right) \right]$$ (5.2.3)

Yukawa-ODS

$$\frac{d^2r_i'}{dt'^2} = \Gamma \kappa \exp(-r_{ij}') \left[ \frac{1}{r_{ij}'} \left( 1 + \frac{1}{r_{ij}'} \right) - \frac{1}{2} \right]$$ (5.2.4)

where $r_{ij}' = r_{ij}/\lambda_D$, $r_d'/\lambda_D$ and $\lambda_{D,i}' = \lambda_{D,i}/\lambda_D$. From these results pair correlation function may be calculated that gives a picture of the structure of the particles. The pair-correlation function in 2D is defined as

$$g(r) = \frac{A \frac{N(r, \Delta)}{N}}{2\pi r \Delta}$$ (5.2.5)
where 'A' is the area of the simulated region, \( N \) the number of simulated particles, \( N(r, \Delta) \) the number of particles located in a circle of infinitesimal thickness \( \Delta \) from \( r - \Delta/2 \) and \( r + \Delta/2 \). One may study the solid, liquid, and gaseous phases of the system under different conditions from the above simulation.

5.3 Results and Discussions:

It is already mentioned that in this chapter a comparative study has been done between the Shadowing potential and ODS potential, keeping basic interaction as due to Yukawa potential. It is well known that dusty plasma described by Yukawa potential as described here transits from organized crystalline state to fluid state as the value of Coulomb parameter \( \Gamma \) decreases. Fig.5.1 shows variation of \( g(r) \) for different values of \( \Gamma \). It is seen that larger the value of \( \Gamma \), more pronounced are the peaks of RDF plot. The effect of both ODS and Shadowing force is to increase the height and sharpness of the peaks of RDF's. For almost all the values of \( \Gamma \), the contributions of Shadowing and ODS force almost overlap with each other. However, it is seen that Shadowing force is slightly more dominating than the ODS for relatively small values of \( \Gamma \). For large values of \( \Gamma \), the difference in the peak heights for the two cases is almost negligible.

Fig.5.2 shows the plot of RDF's both for Shadowing and ODS forces for different values of screening constant \( \kappa \). The simulations are performed keeping the value of \( \Gamma' \) fixed at \( 6.409 \times 10^3 \). For \( \kappa = 1.66 \), the two plots of RDF almost overlap with each other. The dust particles with this value of \( \kappa \) arrange themselves in crystalline state. With the increase in the value of \( \kappa \), a drastic change appears to the plots of RDF's. The contribution of Shadowing force no longer is same as that of ODS. It is seen that Shadowing force is not that affected with the increase in the value of \( \kappa \). The
Figure 5.1: Plot of $g(r)$ vs. $\tau/\lambda_D$ for Shadowing force and ODS for different values of $\Gamma$, taking $\kappa=1.6$
Figure 5.2: Plot of $g(r)$ vs. $r/\lambda_D$ for Shadowing force and ODS for different values of $\kappa$ with $\Gamma = 6.40924 \times 10^3$
shielding does not have much effect on Shadowing force. However, ODS potential has the tendency to take the system to gaseous state. For larger values of $\kappa$, the difference in both the peak height and shape, for the two cases, Shadowing and ODS is quite prominent. While the contribution of Shadowing force is still to maintain the crystalline state, that of ODS is completely opposite.

It is clear from these results that both Shadowing and ODS facilitate the formation of Coulomb crystal for $\kappa < 2$. The increase in $\kappa$ results in reduction in the values of shielding length $\lambda_D$. In ODS term, the exponential factor $exp(-r_{ij}/\lambda_D)$ dominates over the term $Q^2_d/2\lambda_D$ for small $\lambda_D$. The result is that ODS potential decreases very sharply with the decrease in the value of $\lambda_D$. Due to screening effect, Yukawa potential also decreases with the rise in $\kappa$. The effect of combined Yukawa and ODS potential is to cause phase transition of the crystalline state of dust particles to disordered gaseous state for large values of $\kappa$.

A reverse effect is observed for combined Yukawa and Shadowing force. Although with the rise in the value of $\kappa$, Yukawa potential decreases exponentially, the combined Yukawa and Shadowing forces still maintain the crystalline pattern. The absolute value of Shadowing force increases with the rise in $\kappa$ and the term due to this force plays the dominating role.

Thus it is seen that upto mean inter-particle distance $a = 1.608173 \times 10^{-4} m$ ($\lambda_D = 5.72927 \times 10^{-5} m, \kappa = 1.66$) the combined Yukawa-Shadowing and Yukawa-ODS overlap with each other and equally facilitate the process of crystallization. With the increase in inter-particle distance, the effect of ODS becomes gradually weak. However, even then shadow effect predominates and crystallization is possible with this term. It may be concluded that for large $\kappa$ ($\kappa > 2$), crystallization is possible only due to the effect of Shadowing force. The role of attractive force thus can not be neglected in dust crystal formation.

Fig.5.3 shows the comparison of RDF's for combined Yukawa-Shadowing and
Figure 5.3: Plot of $g(r)$ vs. $r/\lambda_D$ for Shadowing force and ODS for different values of dust number density.
Yukawa-ODS for four different values of dust density $n_d = 2.74 \times 10^{10}/m^3, 3.74 \times 10^{10}/m^3, 4.74 \times 10^{10}/m^3,$ and $5.74 \times 10^{10}/m^3$ respectively. It is known from earlier studies that higher the values of dust density, more is the probability of crystal formation. For large values of $n_d (> 4 \times 10^{10}/m^3)$, the effects due to Shadowing and ODS almost overlap with each other. Large values of dust density usually facilitate the process of crystallization. For relatively small values of dust density, the peak heights and positions for the two cases differ from each other. The Shadowing force shows sharper, prominent peaks with peak height higher than that of ODS. It is also seen that the peaks due to combined Yukawa-ODS shift towards smaller inter-particle distance. The dust particles attain gaseous state for Yukawa-ODS potential, whereas it is still showing crystalline pattern for Yukawa-Shadowing force. For small values of $n_d$, the contribution due to Shadowing force is very strong compared to ODS force.

When dust density is small, the particles are far apart from each other. Although Coulomb force is screened, Shadowing force can still be significant for distances larger than the Coulomb field screening length. The effect of combined Yukawa-Shadowing force is very strong to maintain the crystalline state of the particle. For ODS on the otherhand, closer the particles more effective is the overlapping and hence the attractive force. It is clear from the expression for ODS that small value of $n_d$ results in large inter-particle distance and hence small Yukawa-ODS potential. Simulation results also show that average inter-particle distance for the case $n_d = 5.74 \times 10^{10}/m^3$ is $1.6 \times 10^{-4} m$. It may be inferred that beyond $a = 1.6 \times 10^{-4} m$, Shadowing force dominates over ODS and becomes effective in Coulomb crystal formation. Both Shadowing and ODS potential are very sensitive to the change in dust density.

Results of our simulation have been compared with the plots of RDF obtained experimentally by Ramazanov et al.$^{197}$ They determined RDF from experiments carried out in a dc glow discharge set up. The experimental curves by Ramazanov et
al. have been compared with RDF's obtained for normal Yukawa potential, Yukawa-Shadowing and ODS potentials in our simulation and results are plotted in Fig. 5.4 - 5.7.

Experimental data, based on which simulations are performed have been listed in Table.5.1. From all the figures of 5.4 - 5.7, it is clearly seen that RDF due to Yukawa-Shadowing potential is closer to the experimental curve than the curves due to ODS potential or Yukawa potential. The curve due to Yukawa-Shadowing potential is almost within the experimental errors (10-15 percent) mentioned in Ramazanov's plots.
Figure 5.5: Experimental and Simulational $g(r)$ vs. $r/\lambda_D$ for $\Gamma=239$, $\kappa=2.67$, $n_d=3940\text{cm}^{-3}$, $n_e=2.1 \times 10^{10}\text{cm}^{-3}$, $Z_d=2.1 \times 10^4$
Figure 5.6: Experimental and Simulational $g(r)$ vs. $r/\lambda_D$ for $\Gamma = 68.50$, $\kappa = 1.68$, $n_d = 10712\text{cm}^{-3}$, $n_e = 2.4 \times 10^{10}\text{cm}^{-3}$, $Z_d = 2.1 \times 10^4$
Figure 5.7: Experimental and Simulational $g(r)$ vs. $r/\lambda_D$ for $\Gamma=40.68$, $\kappa=1.48$, $n_d = 20995\, cm^{-3}$, $n_e = 2.4 \times 10^{10}\, cm^{-3}$, $Z_d = 2.1 \times 10^4$
Table 5.1: Summary of simulative data.

<table>
<thead>
<tr>
<th>$Z_d$</th>
<th>Dust number density</th>
<th>Electron number density</th>
<th>Ion temperature $T_i$</th>
<th>Coulomb coupling parameter $\Gamma$</th>
<th>Screening constant $\kappa$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^4$</td>
<td>$n_d = 2.1 \times 10^{16} \text{m}^{-3}$</td>
<td>$n_e = 2.96 \times 10^{16} \text{m}^{-3}$</td>
<td>$T_i = 203K$</td>
<td>121</td>
<td>1.79</td>
</tr>
<tr>
<td>$10^4$</td>
<td>$n_d = 3.940 \times 10^{16} \text{m}^{-3}$</td>
<td>$n_e = 2.1 \times 10^{16} \text{m}^{-3}$</td>
<td>$T_i = 167K$</td>
<td>239</td>
<td>2.67</td>
</tr>
<tr>
<td>$10^4$</td>
<td>$n_d = 1.0712 \times 10^{16} \text{m}^{-3}$</td>
<td>$n_e = 2.4 \times 10^{16} \text{m}^{-3}$</td>
<td>$T_i = 221K$</td>
<td>68.50</td>
<td>1.69</td>
</tr>
<tr>
<td>$10^4$</td>
<td>$n_d = 2.0995 \times 10^{16} \text{m}^{-3}$</td>
<td>$n_e = 2.4 \times 10^{16} \text{m}^{-3}$</td>
<td>$T_i = 240K$</td>
<td>40.67</td>
<td>1.49</td>
</tr>
</tbody>
</table>

It is also seen that for relatively small values of $\Gamma$ and $\kappa$, the curves corresponding to experiment, Shadowing potential and ODS potential almost overlap with each other. The deviation from the experimental curve is maximum for pure Yukawa potential. For $\gamma = 239$, $\kappa = 2.67$, the deviation from experimental curve is found to be maximum (Fig. 5.5). However, in almost all the cases, the results due to Yukawa-Shadowing potential agree with the experimental results. From this analysis it is clear that attractive potentials like Shadowing potential and ODS potential play a major role in determining crystal structure. Consideration of Yukawa-Shadowing potential or ODS potential leads to better agreement with the experimental results rather than mere Yukawa potential.

5.4 Conclusion:

In this Chapter, the effect of attractive ODS and Shadowing potential on structure
of 2D strongly coupled dusty plasma has been compared. The results have clearly showed that both ODS and Shadowing potentials equally dominate for small values of screening parameter $\kappa$ and large values of dust density. On the otherhand, Shadowing potential plays a dominating role over ODS potential for large values of screening parameter $\kappa$ and small values of dust density. For relatively large values of $\kappa$, Shadowing potential can dominate Yukawa repulsive potential and ODS attractive potential. For a dusty system considered here, it is seen that crystal structure is no longer maintained beyond an inter-particle distance $r_{ij} = 1.6029 \times 10^{-6} m$ with Yukawa-ODS as the interaction potential. On the otherhand, Yukawa-Shadowing potential maintains the crystal structure even beyond this distance. For longer inter-particle distance, Shadowing attractive potential becomes more effective and cannot be ignored. The comparison of this simualtional results with the experimental observation clearly reveal that Yukawa-Shadowing force is close to the real situation.