Simulation of Electrical Field Induced Particle Transfer

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ABSTRACT

The controlled transfer of charged, densely distributed polymer particles across narrow air gaps is one of the basic mechanisms in modern printing technology. To understand the detachment and transport of charged particles by an electric field many-body simulation is employed. All relevant forces like Coulomb particle-particle, particle-field or adhesion forces are included. The results of the simulation are validated by experiments where charged polymer particles are transferred from one roller to a neighbouring one. Since polymer particles of the same polarity can form thick layers, short-ranging attractive forces (cohesion) were introduced in the simulation to prevent the particles from being scattered due to their surplus charge. Our computer simulations clearly show that an inter-particle charge transfer mechanism has to be included in the simulation model to get results that conform to the experiment.

Keywords: many-body particle simulation charged transport

1 INTRODUCTION

Many industrial printing processes use electrical fields to control the transport of charged particles across small air gaps. In this work we analyze in detail the detachment and transfer of charged, densely distributed polymer particles by the action of appropriately adjusted electric field forces in order to optimize the efficiency of the transfer mechanism. To this end we performed microscopic many-body simulations to investigate the motion of a large number of particles. The results of the simulations were compared to equivalent experiments with clearly defined boundary conditions. The experimental setup consists of two metallic rollers, where a constant voltage is applied in between. The rate and arrangement of the transferred particles can be monitored using optical and scanning electron microscopy. If the theoretical model describes all interaction forces correctly, computer simulations should be able to reproduce the experimental findings.

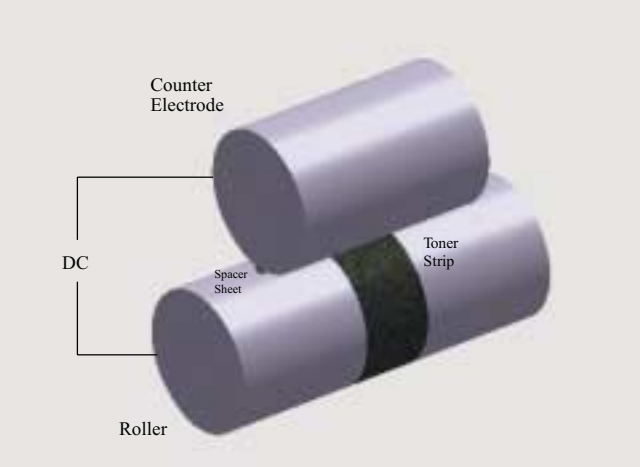

Figure 1: Transfer experiment with rollers

2 TRANSFER EXPERIMENT

An aluminum roller is covered by a thick layer of polymer particles which have been charged before. The thickness of the layer, as measured by laser triangulation, is about three times the average particle diameter. A second aluminum roller acting as counterelectrode is placed above the first roller (Fig. 1), resting on insulating spacer sheets and thus forming an air gap with accurately defined spacing. Both rollers are connected to a DC power supply unit.

After switching on the DC voltage for several seconds, which is a very long time compared to the approximate transfer time of the particles across the air gap, the resulting layer on the counterelectrode is measured: Visual inspection shows that the amount of transferred particles is very low. The layer on the counter electrode is very thin and the aluminum is still shimmering through, whereas in contrast the original layer was thick and black with no trace of aluminum visible.

Even after the experiment there is no perceptible change in the original layer; there are still enough particles left to cover the roller completely. The thickness of the transferred particle layer is measured to be below one third of the original thickness; this means that mainly single particles were transferred.

To investigate this in more detail the transferred particle layer was investigated using an optical microscope

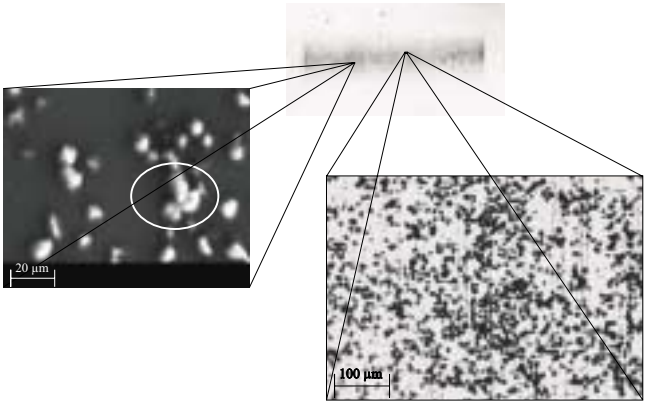

Figure 2: SEM micrographs showing the morphology of the transferred particle layer

and a scanning electron microscope (SEM, Fig. 2). The optical inspection confirms that a large part of the transferred particles consists of isolated particles and that indeed a large area of uncovered aluminum is visible. However, also several clusters are found. Since the optical microscope cannot resolte the spatial configuration of these clusters, SEM micrographs were made. These reveal that in some of the clusters a number of particles are placed above the ground layer on top of other particles without contact to the aluminium surface. It can be assumed that at least some of these clusters were detached and transported as a whole, and did not lump together during the deposition.

3 MANY-BODY SIMULATION

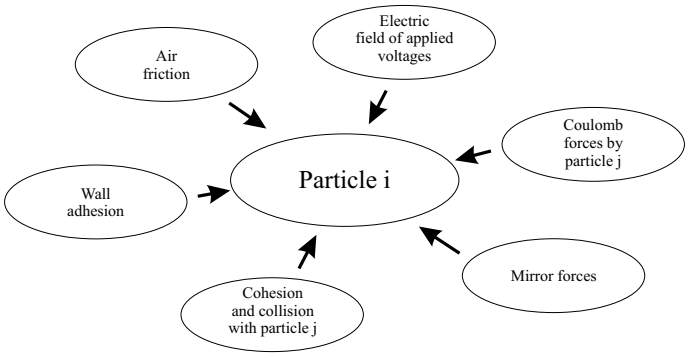

Figure 3: Forces on particle

The simulation of the behaviour of a many-body system is based on solving a coupled system of n second-order differential equations comprising the equations of motion for each particle:

$$m_i \ddot{\vec{x}}_i = \vec{F}_i(\vec{x}_i, \vec{x}_j, \dot{\vec{x}}_i)$$

The starting positions of the particles are chosen such that a compact layer with an average thickness according to the experimental value is formed. For the numerical integration of this system analytical expressions of the force terms are required. The total force comprises several contributions (Fig. 3)

$$\begin{aligned}\vec{F}_i(\vec{x}_i, \vec{x}_j, \dot{\vec{x}}_i) &= \underbrace{\sum_j \vec{f}_{el_{ij}}(\vec{x}_i, \vec{x}_j) + \sum_j \vec{f}_{coh_{ij}}(\vec{x}_i, \vec{x}_j)}_{particle-particle} \\ &+ \underbrace{\vec{f}_{mirror_i}(\vec{x}_i) + \vec{f}_{adh}(\vec{x}_i)}_{particle-roller} \\ &+ \underbrace{\vec{f}_{el,field}(\vec{x}_i)}_{particle-field} + \underbrace{\vec{f}_{vis}(\dot{\vec{x}}_i)}_{particle-air}\end{aligned}$$

3.1 Particle-particle forces

Since the particles were charged before the transfer experiment, Coulomb forces act between each pair of particles:

$$\vec{f}_{el_{ij}}(\vec{x}_i, \vec{x}_j) = \frac{q_i q_j}{4\pi\epsilon_0 \left|\vec{x}_i - \vec{x}_j\right|^3}(\vec{x}_j - \vec{x}_i)$$

The charging process employed here causes the majority of particles being charged with the same polarity. Therefore the Coulomb force will be mostly repulsive. Nevertheless a thick layer of particles can be deposited on the first roller without any indication that the particles would move away from each other. So obviously another, attractive force must be effective which compensates the Coulomb repulsion. This force has to be short-ranged compared to Coulomb repulsion because particles, once they are detached by the electric field, do not lump together but try to stay separate (see Fig. 2).

The physical origin of such a force, which shall be called cohesion force in the following could be the van-der-Waals mechanism, but also patch charges of opposite sign on the surface of the particle resulting in attractive dipole forces when two particles come into close proximity. A distance-dependence of $\frac{1}{r^4}$was chosen for this force. The amplitude of the cohesion force has still to be specified. This will be a major fitting parameter to calibrate the simulation model. A third force has to be introduced when two particles come into contact. Since the particles must not penetrate each other, a strong artificial repulsive force has to be added when the distance between the adjacent particle centers becomes smaller than the sum of their radii.

Fig. 4 shows the effective force between two particles approaching each other. It is important to use smooth transitions between the three parts of the curve to avoid numerical instabilities of the integration algorithm.

3.2 Particle-roller forces

Charged particles resting on a metallic surface experience a strong attractive force towards the surface.

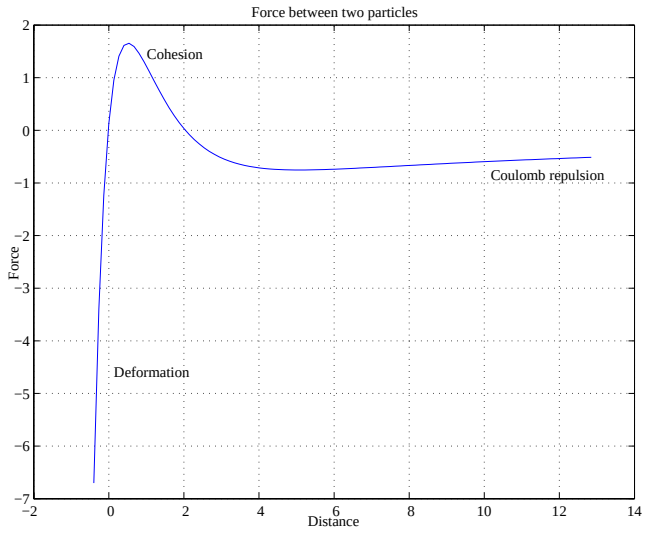

Figure 4: Effective force between neighbouring particles

This force results from induced mirror charges due to the surplus charge of the particle and from non-electrostatic effects which apply also to uncharged particles. Among those the dominant contributions are van-der-Waals forces and the surface tension of adsorbed water droplets.

The mirror force on an ideally conductive surface is

$$\vec{f}_{mirror_i}(\vec{x}_i) = \frac{1}{4\pi\epsilon_0}\frac{q_i^2}{(2r)^2}\vec{n}$$

where r is the distance between the particle center and the surface and $\vec{n}$ is a unit vector normal to the surface.

The influence of the non-electrostatic effects can be measured using a centrifuge experiment: Uncharged particles are spread on a small substrate which is exposed to centrifugal acceleration. Counting the rate of detached particles at subseqent acceleration steps allows to extract the underlying force distribution.

3.3 Particle-field and particle-air forces

The voltage applied between the rollers creates an electric field which causes and controls the particle transfer. The field distribution $\vec{E}(\vec{x}_i)$ can be calculated using finite element methods. The force exerted on a single particle is then

$$\vec{f}_{el,field}(\vec{x}_i) = q_i\vec{E}(\vec{x}_i)$$

After detachment the particles move across the air gap and experience a friction force due to the air viscosity. Assuming an approximately spherical shape of the particles the friction force according to Stoke's law is:

$$\vec{f}_{vis}(\dot{\vec{x}}_i) = -6\pi\eta_{air}r_i\dot{\vec{x}}_i$$

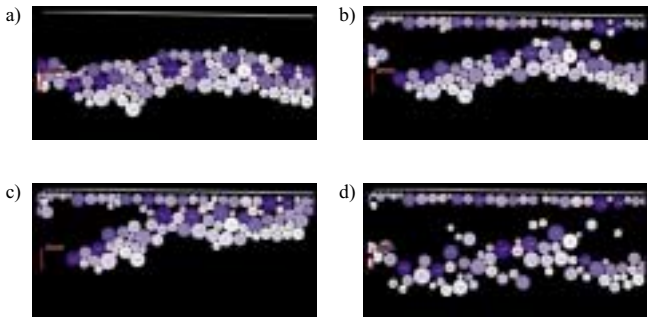

Figure 5: Particle detachment for various cohesion parameters

3.4 Simulation results

3.4.1 Cohesion variation

As mentioned above one important parameter to be determined is the maximum cohesion force occurring when two particles come into contact. Therefore several simulation runs were performed with varying cohesion forces. The results are displayed in Figure 5: Fig. 5(a) shows the effect of a very large cohesion force. The particle layer is completely detached as whole. In Fig. 5(b) the cohesion force is still large but smaller than the particle-roller adhesion. In this case all the particles are detached as one large cluster except for the ones directly connected to the roller. In Fig. 5(c) the cohesion force is of the same order of magnitude as the forces caused by the electric field. Clusters are detached where the charges are high enough, while at other locations they remain on the roller. Fig. 5(d) shows the case where the cohesion force is nearly zero. All the particles not in touch with the roller are detached and are almost instantaneously separated.

Unfortunately none of these four cases reproduces the behaviour observed in the experiment, where only a small fraction of the particles is detached. So additional effects not considered so far have to be taken into accound.

3.4.2 Charge transfer between particles

As an additional mechanism we envisaged the idea that electric charge might be transferred between indivual particles instead of being fixed on them. In this case the electric fields could cause a charge transfer from the particles near the roller towards the outer particles. This could explain the different behaviour of the outer particles compared to those in the interior. Measurements have shown that there is indeed a conductivity in polymer particle layers.

An additional simulation step was introduced: Whenever two particles come into contact, a certain percentage of the charge on the inner particle is transferred to the outer particle, with the percentage chosen propor-

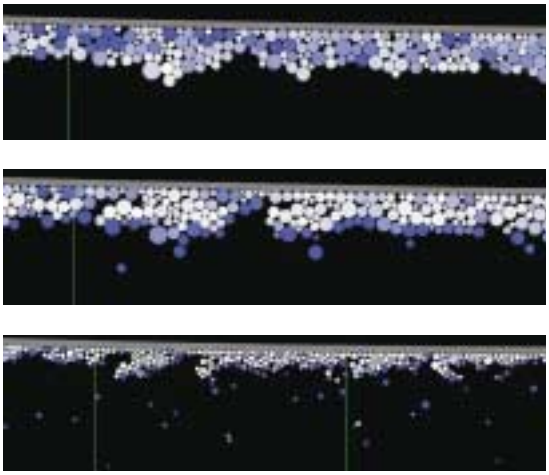

Figure 6: Charge transfer and detachment

tional to the electric field.

Fig. 6 shows the results. The upper two pictures illustrate the transfer of charge, while in the third picture isolated particles are detached.

3.4.3 Cohesion force distribution

The experiments have shown that the particles are transferred in form of isolated particles as well as in clusters, but with charge transfer alone only the detachment of single isolated particles can be reproduced. Hence still another mechanism has to be involved to explain the experimental finding. So far the cohesion force was assumed to be constant for the whole particle ensemble. But as all the particles are of different size and charge, this assumption seems rather unrealistic. So we improved the model by including variable cohesion forces, which have a distribution similar to the one known from the particle-roller adhesion force. In this way we assign each particle its individual cohesion force f_{coh_i}. The force used for the interaction of two particles i and j is calculated from the geometric mean of the two cohesion forces $f_{coh_{ij}} = \sqrt{f_{coh_i} \cdot f_{coh_j}}$. The simulation based on this enhanced model shows a transferred particle layer (Fig. 7) which is very simular to the experimental observations.

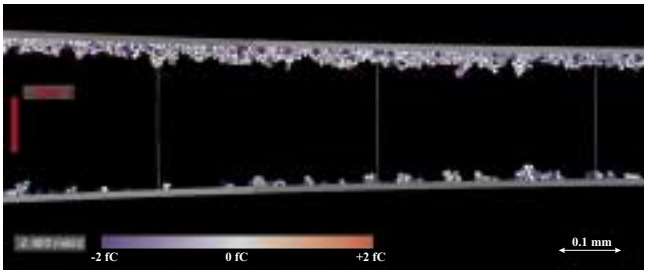

Figure 7: Realistic simulation of particle transfer

In this simulation about 27 percent of the original particle layer was transferred as single particles and clusters, which is about the same number as determined by the experiment.

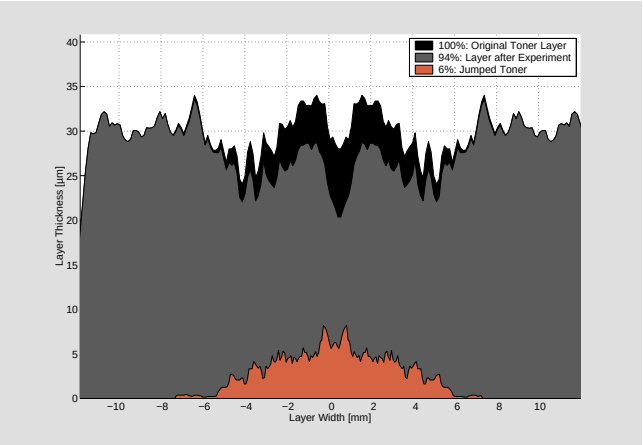

Figure 8: Layer thickness of original and transferred particles

4 CONCLUSION

It has been shown that many-body simulation can be used to reproduce the effects observed in electrical transfer experiments. Microscopic influences like short-ranged attractive particle-particle forces must be accurately modeled to simulate the macroscopic behaviour correctly. Also charge transfer between particles must be included in the simulation to explain the different behaviour of particles lying on top of the original layer and the others.

Further improvement of the predictiveness of our model may be optained by including also the simulation of the deposition process of the original layer, so that the initial conditions of the simulation would be closer to reality.

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