

The Structure of Toner Sediments Simulated with Random Ballistic Deposition

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Introduction

With high speed computers it has become possible to simulate the motion of toners and carriers in the electrophotographic process.[1-3] The motion of the particles can be analyzed to draw conclusions about the behavior of the particle system. However, there are many aspects of deposited toner films and granular systems that don't require a simulation including all the interparticle forces. We use the theory of random ballistic deposition to examine the relationships between particle size, the structure of a developed image, particle adhesion, and image quality. In random ballistic deposition, simulated particles are dropped one at a time from random locations above a surface, like snow falling on the ground. The structure of the deposited toner layer depends on the rules for deposition: the particles can restructure by rolling or they may just stick. The rules for deposition depend on the toner adhesion and geometry. Random ballistic deposition has been used to understand the compaction of the toner sediments in liquid development, the void fraction of fluidized beds, and the buildup of multiple layers. The theory can be used in a simple way to highlight the role particle size and size distribution has in these processes.

Theory

Random Sequential Adsorption

Random Sequential Adsorption (RSA) simulates the geometry of monolayer coverages of toner. The theory was originally developed to understand the adsorption of proteins on cell surfaces.[4] It is applicable to xerographic applications where only a monolayer of toner is developed. To simulate the structure of developed images using the RSA approximation to following algorithm is used. A random positions is picked on a surface and a particle is attempted to be placed at that location. However, if at this location it would overlap with a previously placed particle, the new particle is discarded. If this location is far enough away from other particles, the particle remains on the surface. The surface gradually fills up and the process is repeated until there is no more room for the particles to be deposited. The resulting structure arising from an RSA simulation is shown in figure 1.

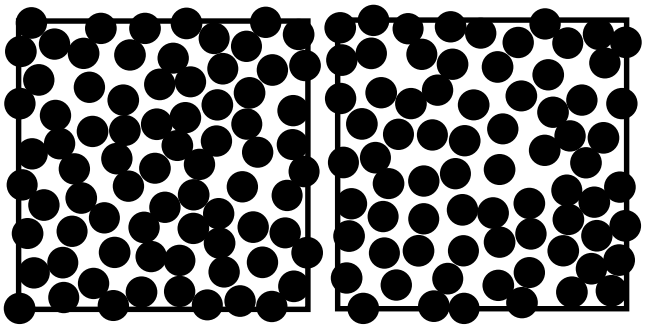

Figure 1. Toner monolayers simulated with RSA

Random Ballistic Deposition

RBD has been used over the past four decades to understand the geometry of agglomerates formed from sticky particles.[5] In the simplest model of RBD, the structure being built is assumed to be made from spherical particles (or circular particles in a 2D simulation). The particles are deposited on a flat substrate, shown in figure 2. The initial particle position is chosen from a random location far above the substrate. The charged particle feels an attraction towards the oppositely charged substrate and approaches it vertically. The particle will stop either when it hits the substrate, as illustrated in figure 2(a), or after enough particles start to build up on the surface, will stop where it hits another particle, as illustrated in figure 2(b) and 2(c). If there is a strong cohesion between particles, there will be no rolling or restructuring and the particles will stay as illustrated in the figure. Although the illustration is for two dimensions, we perform the simulation in three dimensions. The deposition process is repeated until films of sufficient thickness are simulated.

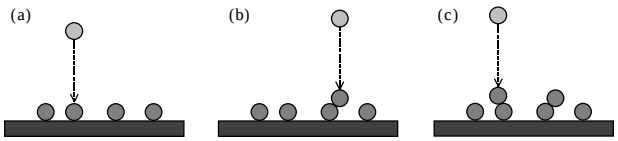

Figure 2. Technique for random ballistic deposition

Random Ballistic Deposition with Restructuring

In high electric fields increased attraction of the particle to the surface overcomes the interparticle cohesoin. The

particles can then roll over each other or restructure which causes an increase in packing fraction (figure 3a). Restructuring can be included in a model of random ballistic deposition. Complete restructuring has been investigated and the algorithm, described below, is the same as that developed by Meakin and Jullien.[5]

In RBD with restructuring, the particles are dropped sequentially. However, instead of sticking to the first particle they contact, they can continue to move to a position of lower potential energy. This movement is a sequence of rolling along previously deposited particles or falling from ledges until the substrate is hit or the particle is resting in a depression formed by three other previously deposited particles. The algorithm for forming a film with complete restructuring in three dimensions is illustrated in figure 3(b) and occurs as follows:

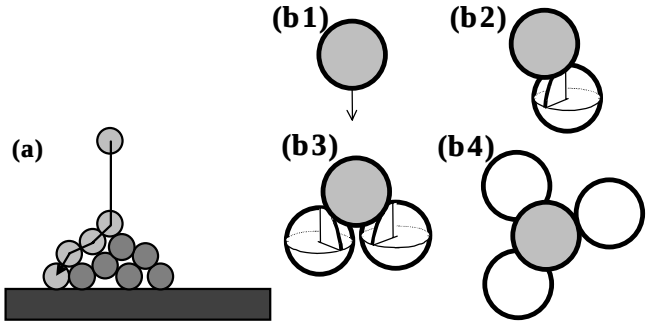

Figure 3. (a) Illustration of restructuring (b) Algorith for restructuring: 1 – Drop particle, 2 – Particle roll salong one other particle, 3 – Particle rolls along 2 other particles, 4 – Switch to another pair of particles.

In some situations, the deposited toner films may be intermediate between the unrestructured and restructured films. We can simulated films of particle restructuring by defining a critical angle θ_c. If in steps b2-b4 of figure 3 the angle the gray particle makes with previously deposited particles is less than θ_c, then the particle is frozen in this position.

The justification of defining a critical angle for restructuring is justified by looking at the forces between the particles. Suppose the test particle is contacting the lower particle at a polar angle θ as illustrated in figure 4. If the upper particle has a charge *q*, then there is a downward force of *qE* on the particle, where *E* is the applied electric field. At the contact point there will be a component of this force normal to the contact and a component tangential to the contact. There is also a nonelectrostatic adhesion F_a between the two particles. In addition, there is a frictional force proportional to the normal force opposing the tangential force. Referring to the figure, we see that the toner will fall when the tangential force downwards exceeds the opposing tangential force. The critical angle for restructuring occurs when these two forces are balanced. Solving for θ_c gives

$$\theta_c = \sin^{-1}\left(\frac{\mu F_a}{qE\sqrt{1+\mu^2}}\right) + \tan^{-1}\mu$$

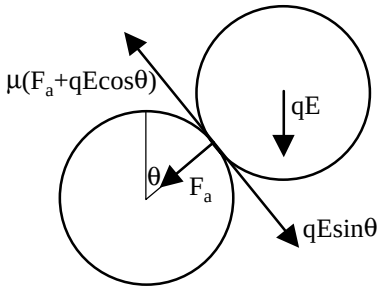

Figure 4. Forces between two particles

Applications

RSA Jamming Limit

There are situations where it is important to be able to estimate the area coverage or mass of a monolayer of toner. A metering blade may reduce the toner coverage on a donor roll to a monolayer for example. One can assume hexagonal closed packing or square packing and arrive at a fraction coverage of 0.907 and 0.785 respectively, but these ordered structures usually do not arise. The random structures in figure 1 are more representative of toner layers. The maximum amount of toner that can be deposited on a surface before there is no open spaces to allow more toner is called the jamming limit. RSA simulations show that the jamming limit occurs when the fractional area coverage is 0.517, independent of particle size. This coverage is much smaller than the ordered structures. For a 10 μm diameter toner with a density of 1 g/cm^3, a monolayer would occur at 0.345 mg/cm2.

Low density packing fraction

In liquid ink development the toner is dispersed in a fluid. When it is developed, the fluid remains in the spaces between the toner and must be removed so a robust image can be created. Measurements of the percent toner and percent fluid for a particular set of materials found that they were typicall <20% and >80% respectively. The small fraction of toner seemed surprising. However, it could be explained using the RBD theory.

Liquid toner particles are typically about 1μm in diameter, so multiple layers are built up in an image. The materials used in the experiments are cohesive in the fluid, so RBD theory applies. In figure 5 we show a two dimensional RBD simulation for the buildup of a multiple layer. Dendritic structures form as particles adhere to the top of the film and prevent other particles from moving past them to fill in the voids. Although figure 5 illustrates the two dimensional situation, we perform a 3 dimensional calculation. We simulated the deposition of over 10^6 particles and found a packing fraction of 14.69+/-0.04%

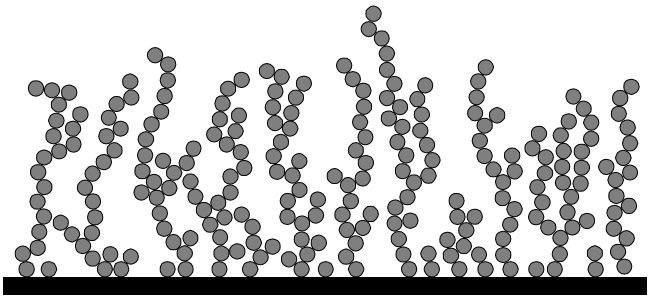

Figure 5. 2D RBD simulation

Toner is not monodisperse. RBD can be performed where the particle diameter for each deposited particle is picked from a polydisperse distribution. One might expect that the presence of the smaller toner particles might fill in the voids and result in a higher packing fraction. However, simulations show that this is not the effect and in fact the packing fraction is *independent* of the particle size distribution. The smaller particles are not able to fill in the voids because they contact another particle and stick before they reach them.

Fluidized Bed

RBD also can be used to understand some cohesive properties of dry toners. Toner cohesion can be explored with a fluidized bed.[5] Toner is put in a jar with a porous material on the bottom, with pores big enough for air to flow through but small enough so toner doesn't get through. Air is pushed through the porous bottom of the container and up through the granular toner material. As the velocity of the air increases, it breaks the contacts between the toners. As each bond is broken, the toners are pushed apart, and the toner bed begins to rise. When all the bonds are broken, the powder behaves as a fluid. If one can determine the number of toner-toner contacts in the powder at its initial condition, one can determine the average toner cohesion from the pressure drop across the bed when it becomes completely fluidized. However, the number of toner-toner contacts is not experimentally accessible. They depends on the structure of the toner powder.

The toner bed is initialized by fluidizing the toner with a powerful airflow, and then allowed to slowly settle. The volume of the toner bed is determined as a function of the airflow and pressure across the bed. One can assume locally that the rules of RBD with restructuring apply, with the electrostatic force replaced by a gravitational force. Using the RBD theory, one can relate the packing fraction, which is measurable, to the average number of toner-toner contacts.

We simulated the deposition of 10,000 particles in a square of sides 20 times the particle's diameter. We calculate the packing fraction and count the number of contacts between particles. To go from disperse to compact structures, we varied the critical angle for restructuring. The result of this simulation is plotted in figure 6. From this plot and a packing fraction measurement, the number of contacts per particle can be found and used to relate the pressure drop across the bed for fluidization to the toner-toner cohesion.

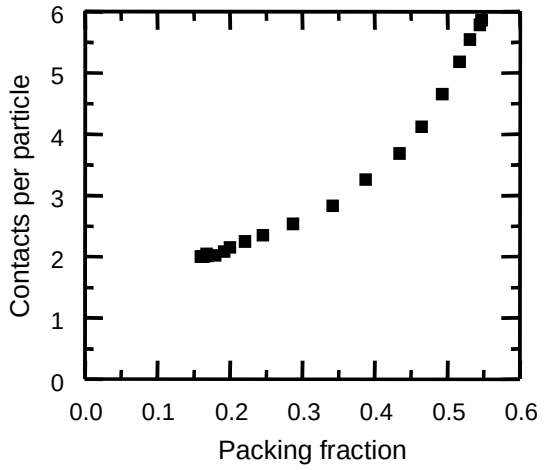

Figure 6. Particle contacts in a fluidized bed

Toner Surface vs. Toner-Toner Contacts

To transfer a toner layer from one surface to another, the toner-substrate adhesion must be overcome. For a submonolayer, uniformly dispersed toner layer, each toner is touching just the substrate and not touching other toners. However, as the toner coverage increases, some will touch not only the substrate, but also other toner particles. For these particles, toner-toner cohesion must be overcome for the toners to transfer. The removal force may be different than the toner-substrate adhesion and may cause transfer to occur at different fields.

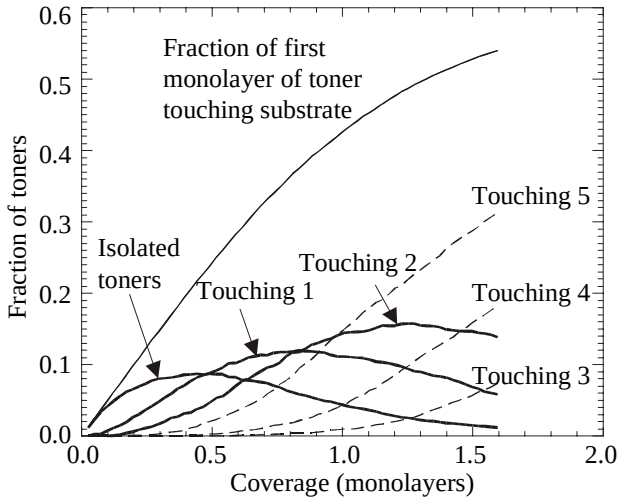

Figure 7

The relative number of toners touching the substrate and touching other toners can be simulated for spherical particles using RBD with complete restructuring. In an RBD simulation for a thin layer, each toner is categorized as to

whether it is touching the substrate and how many other toners it is touching. The surface coverage is given in units of the projected area of all the deposited toners over the area of the substrate on which they are deposited. More specifically this is $N\pi r^2/A$, where N is the number of particles deposited, r is a toner radius, and A is the area of the substrate where toner is deposited. This quantity can be thought of as the fraction of a monolayer.

The different categories are plotted as a function of coverage in figure 7. At the lowest coverages the only type of toners are those touching the substrate, but at higher coverages, there begins to be toners touching other toners. At the quite low coverage of 0.3 monolayers, only half the toners on the substrate are isolated.

Conclusion

The are a number of physical processes in xerographic printing where knowledge of the interparticle structure is needed to better understand the process. For example, how much toner does it take to put a randomly dispersed monolayer on the surface? What is the structure of loosely packing liquid toner deposits? How can toner-toner cohesion be measured using a fluidized bed? How does the fraction of toner-toner and toner-surface contacts change with coverage? Random sequential adsorption and random ballistic deposition allow the toner geometry to be estimated. The predictions these theories give for the microscopic toner structure give further insight into the physics of the xerographic process.

References

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Biography

Howard Mizes received his B.S. degree in Physics from the University of California at Los Angeles in 1983 and a Ph.D. in Applied Physics from Stanford University in 1988. Since 1988 he has worked in the Wilson Center for Research and Technology at Xerox Corporation in Webster, NY. His work has primarily focused on the development process, including toner adhesion, toner transport and image quality issues. He is a member of the IS&T and the American Physical Society.