Particle dynamics simulations of the effect of particle size distribution on triboelectric charging in granular insulator systems

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Abstract. Triboelectric charging occurs in granular materials composed of insulating particles even when all particles are composed of the identical material. Large scale particle dynamics simulations are used here to address triboelectric charging in such systems. The model used in the simulations is based on the presence of electrons trapped in high energy states, which can be released during collisions with another particle and transferred to the other particle. The simulations show that triboelectric charging in these systems can be attributed to a distribution of particle sizes, such that smaller particles tend to charge negatively and larger particles tend to charge positively. This polarity of charging has been observed in field studies and laboratory experiments involving granular systems.

1. Introduction
When granular systems flow, the collisions and rubbing between particles can lead the triboelectrical charging of the particles, even when all particles are composed of the same material. This triboelectric charging plays an important role in natural events such as sand storms [1], dust devils [2,3], and volcanic eruptions [4], in industrial processes such as fluidized beds [5] and pneumatic conveying [6], and in pharmaceutical dispersal devices such as dry powder inhalers [7].

Many studies suggest that in flowing granular materials, the smaller particles charge negatively while the larger particles charge positively [8-19]. Also, experiments have shown that the magnitude of triboelectric charging is larger when the system has a broad particle size distribution [20,21].

There are many aspects of this behavior that are not understood: For example, why net charge is transferred between particles when all particles are composed of the same material; why smaller particles tend to charge negatively; and why the particle size distribution affects the magnitude of triboelectric charging.

We suggest that these issues can be simply understood in terms of theoretical ideas introduced by Lowell and Truskott [22]. Electron states in insulators are spatially localized, and some electrons are trapped indefinitely in high-energy states. Contact with another surface can bring vacant low energy states on the other surface close to one of these high energy states, which allows trapped electrons to be released to vacant low energy states on the other surface. We showed previously how these ideas can be used to understand aspects of triboelectric charging in granular materials [23]. Here we extend our previous analysis with an improved simulation methodology. This approach is also described in more detail elsewhere [24].
2. Computational methods
Simulations are carried out to investigate the consequences of the hypothesis that electrons are trapped in high energy states, and are released in collisions and subsequently captured in low energy states of the other particle.

The simulations are carried out for ‘hard sphere’ particles that are impenetrable, which are confined in a cubic box with hard (impenetrable) walls. Each particle $\alpha$ is characterized by its diameter $\sigma_\alpha$, position $\vec{x}_\alpha$, and velocity $\vec{v}_\alpha$. All collisions of the particles with each other and with the walls are completely elastic. The simulations are carried out under the assumption that inertial effects on the trajectory dominate over electrostatic effects – i.e., the electrostatic interactions do not affect the particle trajectories.

2.1. Particle dynamics
The particle dynamics are simulated using an event-driven methodology, which consists of the following 3 steps [25]: (1) The times for all possible particle-particle and particle-wall collisions are determined; (2) the particles are moved at constant velocity until the first collision occurs; and (3) the collision alters the velocities of the colliding particles. These steps are repeated to generate the dynamic trajectory.

The time for the collision between particle $\alpha$ and particle $\beta$ is determined as

$$\Delta t_{\alpha\beta} = \frac{-\vec{x}_\beta \cdot \vec{v}_\beta - \left[ \left( \vec{x}_\beta \cdot \vec{v}_\beta \right)^2 - \vec{v}_\beta \cdot \left( \vec{x}_\beta \cdot \vec{x}_\beta - \sigma_{\alpha\beta}^2 \right) \right]^{1/2}}{\vec{v}_\beta \cdot \vec{v}_\beta}$$

where $\vec{x}_\alpha = \vec{x}_\beta - \vec{x}_\alpha$, $\vec{v}_\beta = \vec{v}_\beta - \vec{v}_\alpha$, and $\sigma_{\alpha\beta} = (\sigma_\alpha + \sigma_\beta)/2$. If the quantity within the square root is negative, or $\vec{x}_\beta \cdot \vec{v}_\beta > 0$, the particles do not collide; in these cases, $\Delta t_{\alpha\beta} = \infty$. For the collision between a particle and a wall, the time for the collision is obtained as

$$\Delta t_{\alpha i} = \frac{(L - x_{\alpha,i}) - \sigma_\alpha/2}{v_{\alpha,i}}, \quad v_{\alpha,i} > 0$$

$$\Delta t_{\alpha i} = \frac{x_{\alpha,i} - \sigma_\alpha/2}{v_{\alpha,i}}, \quad v_{\alpha,i} < 0$$

where $x_{\alpha,i}$ and $v_{\alpha,i}$ are the components of $\vec{x}_\alpha$ and $\vec{v}_\alpha$ along the $i$ direction, and $L$ is the length of the simulation box. The lowest of these collision times is designated $\Delta t_{\text{min}}$.

The particles are advanced at constant velocity until the first collision occurs. The position of each particle is updated as

$$\vec{x}_\alpha = \vec{x}_{\alpha,0} + \vec{v}_\alpha \Delta t_{\text{min}}$$

where $\vec{x}_{\alpha,0}$ is the position of particle $\alpha$ at the time of the previous collision (or, at the start of the simulation, $\vec{x}_{\alpha,0}$ is the initial position).

A collision alters the velocities of the colliding particles, as determined by the conservation of energy and momentum. After a particle-particle collision, the new velocities of the particles involved in the collision are determined by
and after a particle-wall collision, the new velocity of the particle is determined by

\[ \vec{v}_{a,i} = -\vec{v}_{a,i,0} \]

where the ‘0’ subscript represents properties at the instant preceding the collision.

2.2. Trapped electron model

In the present model, electrons are trapped in high energy states, and can be released in collisions and subsequently captured in low energy states of the other particle. Each particle \( \alpha \) has \( n_{H,\alpha} \) electrons trapped in high energy states, and \( n_{L,\alpha} \) electrons captured from collisions into low energy states.

Initially, all particles have the same surface density of electrons trapped in high energy states; therefore, the initial number of trapped electrons on a particle, \( n_{H,\alpha,0} \), is proportional to the square of the radius of the particle. These trapped electron have defined positions on the particle surface, which are randomly distributed over the surface of the particle; an example of the distribution of these trapped electrons over the surface of the particle is shown in Figure 1.

When a collision between particles occurs, electrons may be transferred from trapped high-energy states on one particle to low-energy states on the other particle. All trapped electrons (on either particle) with positions within a cutoff distance \( d_{\text{cut}} \) of the point of collision are transferred to the other particle (note that since the particles are spheres, the collision occurs at a single point). For each electron that is transferred, the electron is removed from the list of electrons trapped in high-energy states of the original particle (and the value of \( n_{H,\alpha} \) of this particle decreases by 1), and the value of \( n_{C,\alpha} \) of the electron’s new particle increases by 1. The positions of these captured electrons do not need to be defined, since in this model they do not undergo any further transfers.

All particles initially have zero net charge. However, the particles can develop net charges due to the transfer of electrons during collisions. The net charge on a particle is determined as \( q_{\alpha} = n_{H,\alpha,0} - n_{H,\alpha} - n_{L,\alpha} \).

**Figure 1.** Example of the positions of electrons trapped in high energy states, which are randomly distributed over the surface of a particle.
2.3. Simulation details

Simulations are carried out for 864 particles. The distribution of particle sizes is characterized by radii randomly distributed between 0.1 \( \sigma \) and 0.9 \( \sigma \) (where \( \sigma \) defines the length scale). The particles have density \( 1 \text{ m}/\sigma^3 \) (where \( m \) defines the mass scale), and a surface density of trapped electrons of \( 100 \text{ e}/\sigma^2 \) – i.e., a particle with radius \( R \) has a mass of \( (4/3)\pi R^3 m \), and contains \( \text{int}(100*4\pi R^2) \) trapped electrons (where \( \text{int}(y) \) is a function that truncates \( y \) to an integer). The velocities are initially assigned random values, with each component uniformly distributed between -1 \( \sigma/\tau \) and 1 \( \sigma/\tau \) (where \( \tau \) defines the time scale). The simulation box is a cube with length \( L = 25.45 \sigma \). The simulations are carried out for a duration of 32 million collisions. Note that all results are given in terms of reduced units defined by \( \sigma \), \( m \) and \( \tau \).

3. Results

The simulation results for the time dependence of the electron populations are shown in Figure 2. Collisions act to transfer electrons trapped in high energy states to low energy states on other particles; thus, the number of electrons trapped in high energy states decreases with time, while the number of electrons captured in low energy states increases with time. During the course of the simulation, approximately 60% of the electrons trapped in high energy states have been released.

![Figure 2](image.png)

**Figure 2.** Average number of electrons trapped in high energy states per particle, and average number of electrons captured during collisions in low energy states per particle, as a function of time.

The transfer of electrons from high energy states on one particle to low energy states on another particle leads, on average, to a net transfer of electrons from the larger particles to the smaller particles. This result is evident in Figure 3. Figure 3a shows that the net charge \( q_0 \) on the particles is a monotonically increasing function of particle size, such that the charge is negative for small particles and positive for large particles. Figure 3b shows a snapshot of the system at the end of the simulation, in which positive and negative particles are shown with different colors –it is clear from this snapshot that the smaller particles are charged negatively and the larger particles are charged positively.

To understand why smaller particles charge negatively and larger particles charge positively, the electron populations of the high-energy and low-energy states are examined for each particle. As shown in Figure 4, all particles release approximately the same fraction of their electrons trapped in high energy states. However, since the large particles initially have a greater number of trapped
electrons, larger particles release more trapped electrons than smaller particles. Since the larger particles release more electrons, they develop a positive charge. Likewise, since the smaller particles release fewer electrons, they develop a negative charge. A further factor that leads to the smaller particles charging negatively is that they move faster due to their smaller mass, and thus undergo more collisions and capture more electrons in their low energy states; this effect is only significant for the smallest particles (it is a nonlinear effect since the mass scales as the cube of the radius).

**Figure 3.** (Left) Results for net charge on particles as a function of particle radius. (Right) Snapshot of system at end of the simulation. Lighter (red online) particles are charged negatively, and darker (blue online) particles are charged positively.

**Figure 4.** (Left) The number of trapped and captured electrons on each particle, at the end of the simulation. Also shown is the initial number of trapped electrons. (Right) Fraction of trapped electrons that are released during the simulation, for each particle.
4. Conclusions
We use particle dynamics simulations to show that the simple idea that collisions transfer electrons trapped in high energy states to low energy states on another particle can explain observed features of triboelectric charging in granular materials. In particular, this effect gives rise to a negative charging of smaller particles and positive charging of larger particles, which has been suggested in many experimental studies [8-19]. Additionally this effect leads to triboelectric charging that increases in magnitude with the breadth of the particle size distribution, which has also been observed in experimental studies [20,21].

We argue that the mechanism described here provides the driving force for triboelectric charging. However, many other factors will affect the magnitude of the charging. For example, it will be less likely that an electron will be transferred from a positively charged particle to a negatively charged particle, due to the electric field that opposes this transfer. This effect would oppose the driving force described here, and thus limit the magnitude of charging. Future studies will attempt to incorporate this effect, as well as others, into the model.

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