Surface State Models of Tribocharging of Insulators

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Abstract

Surface state models of tribocharging assume that charging results from the exchange of charge species among specific charging site on two contracting surfaces. The charging sites are generally assumed to be uniformly distributed in energy. In this paper, charging behavior is calculated for several different shapes of the energy distribution of charging sites. These calculations show that the success of surface state models in fitting observed tribocharging results is not strongly dependent on the particular distribution of energies of the charging sites. Very nearly linear plots of the mass-to-charge ratio of toner as a function of the mass ratio of toner to carrier present are generated when both surface contain charge-donating and charge-accepting surface states with board energy distributions. The dependence of the slope and intercept of these linear distributions on toner and carrier particle size agrees with experiment. Electric field effects appear to be unimportant for these surface state models.

Background

Surface state models of tribocharging assume that charging results from the exchange of charged species among specific charging sites on two contacting surfaces. The assumptions made for surface state models are:

1. Each surface can be characterized by charge donating and/or charge accepting sites that distributed in energy. The formalism of the model does not depend upon whether the charged entities exchanged are ions or electrons. All that is required is that there be sets of discrete sites.

2. Charging occurs by the exchange of charged species, which proceeds until thermodynamic equilibrium is established. That is, until the chemical potential, the charged species on the surfaces in contact becomes the same.

Lee was the first to propose such a model for tribocharging of two-component electrophotograghic developers. He assumed the surfaces of the toner and the carrier have partially filled sets of surface states uniformly distributed in energy.[1] In his model, when the developer is mixed, charged species are transferred from filled high-energy sites on one surface to unfilled sites of lower energy on the other surface. Charging continues until the energies of the highest occupied states on the two surfaces are equal.

Kondo[2] pointed out that the exchange of charge creates an electric field opposing further exchange. He developed a model of tribocharging of electrophotographic developers, which assumes that charging ceases when the electric potential caused by charge exchange is equal to the work function difference between the toner and the carrier. The magnitude of this potential is determined by the electrical capacitance of clusters consisting of a carrier particle and its associated toner particle. The higher the capacitance, the lower the potential difference developed by charged transfer. The electrical capacitance, in turn, is determined by the number of toner particles per carrier particle and the particle sizes of the toner and the carrier.

Recently, Schein[3] and Gutman and Hartmann[4] have combined Lee's and Kondo's models to consider the concentrations of charging sites on surfaces, the work function differences between the surfaces, and the effects of the electric fields created by charge exchange.

All of these surface state models agree with experiment. The predict that there should be a linear relationship between the mass-to-charge (M/Q) of the toner in a two-component developer and the mass ratio of toner to carrier (T/C). (Plots of M/Q vs. T/C are hereafter referred to as T/C series.) They further agree with experiment in that they predict the observed dependence of the slopes and intercept of T/C series plots on the particle sizes of the toner and the carrier. If toner size is held constant and carrier size increases, the slope of the T/C series plots increases while the intercept remains nearly constant. If carrier size is constant, and toner size increases, then the intercept of the T/C series plots increases while the slope remains constant.[1]

Schein[3] and Gutman and Hartmann[4] have shown that in the limit of very high density of surface states, the ratio of the slope to the intercept of T/C series plots,m/b, depends only on the toner and carrier particle sizes and their mass densities (Kondo's result). The model also predicts that in the limit of very low densities of states,m/b depends not only on the toner and carrier particle sizes, but also on the chemical properties of the surfaces (Lee's result). Anderson[5] has compared experimental results for a wide range of particle sizes with these predictions and found that m/b depends primarily on the particle sizes and densities. However, m/b is not completely independent of the chemical nature of the surfaces. He concluded that neither the high- nor the low-density limits of surface state models is sufficient to describe all of the experimental data.

The purpose of this study is to determine how the choice of a particular distribution of energies for surface charging sites influences the ability of surface state models to fit experimental data. In particular, is the choice of a constant, partially-filled density of states essential to the surface state model? To this end,a series of models has been explored for which M/Q can be calculated as a function of

T/C, particles size and the shape of the distribution of charging site energies.

Modeling Approach

The approach taken was to replace the constant density of states in the earlier models with a variety of functions: delta functions, Weibul distributions, Lorentzian distributions, or differential Fermi functions (DFD). The effects of the electric fields generated by charge exchange were included by incorporating Kondo's method for calculating the potential difference between a carrier particle and its associated toner particles. The equilibrium charge was found by adjusting chemical potential until the amount of charge transferred from the donating sites just equals the charge received by the acceptor sites. (The condition corresponds to overall charge neutrality of the mixture.)

Any number of software packages and algorithms can be used for this purpose. In this work Newton's method was used in a spreadsheet program (QuattroPro SE). An initial value for the chemical potential was assumed. It was varied by a small amount and the change in net charge was noted. The slope of the net charge as a function of chemical potential was calculated by dividing the change in net charge by the change in the chemical potential. The slope was used to estimate a new value for the chemical potential. This procedure was repeated approximately 20 times until the calculated net charge dropped to the order of 10^{-20} Coulombs. Calculations of this type were carried out for assumed T/C's ranging from 1% to 50%. The results were used to plot T/C series.

Results

The first case considered was charge exchange among narrow distributions of the density of states (delta functions) on the toner and the carrier. The concentration of surface state on each component of the mixture was maintained below 10^{14} cm^{-2}, which is equivalent to approximately one state per surface atom. It was found to be necessary for the donor and acceptor states to be separated by less 0.5 eV in order for the charge transferred to be of the magnitude normally observed for electrophotgraphic developers. The calculated TC series plots show some curvature. The magnitude of the curvature is small. Given experimental errors in measuring M/Q (±5-10%) and the relatively narrow range of T/C (a factor of 3-4) over which M/Q is normally measured, the curvature might not be detectable.

Calculated T/C series plots for charge exchange among narrow density of states distributions can be made linear if the electric field effects are increased by a factor of 10^4 to 10^6 . However, when this is done, the calculated charges are smaller than normally observed for electrophotographic developers.

The second case considered was charge exchange between a broad distribution of charge-donating surface states on the toner and a broad distribution of charge-accepting surface states on the carrier. The concentration of surface states on each component of the mixture was maintained below one per surface atom, 10^{14} cm^{-2}. As for exchange among narrow density of states, charges calculated for exchange among broad densities of states are found to be in the range expected for electrophotographic developers, and the calculated T/C series plots are curved. In this case also, the curvature is such that it might not be noticed in T/C series measured over a small range of T/C.

The curvature can be reduced by assuming electric field effects larger by a factor of 10^4 to 10^6 than those calculated using Kondo's model. But, as with narrow distributions, the resulting calculated charges are lower than normally observed. The curvature is also greatly reduced if the toner and the carrier are assumed to have both charge-donating and charge-accepting sites with broad distributions. In this case, the T/C series plots are quite linear, and the calculated charges are reasonable.

In all of the cases considered above where the T/C series plots are very nearly linear, the calculated effects of varying particle sizes are similar to those that are observed experimentally. This is illustrated in Table I, which presents the results for exchange among broad bands of different shapes. The energy separation between the peaks of the charge-donating and charge-accepting states in all cases was about 3 eV. The distributions had half widths at half height of approximately 0.5 eV. Total charging states in each band was of the order of 10^{12}–10^{14}. The calculated charge-to-masses were 10-100 μC/g.

Table I. Effect of toner and carrier particle size on the slope and intercept of T/C series calculated for three forms of broad distributions of energy.

Toner Size (μ)	Carrier Size (μ)	Slope			Intercept		
		Weibul	Lorentz	DFD	Weibul	Lorentz	DFD
0.5	15	0.0166	—	0.092	0.0036	—	0.0021
1.0	″	0.0167	0.065	0.093	0.0071	0.006	0.0076
5.0	″	0.0170	0.061	0.096	0.0355	0.031	0.0180
10.0	″	0.0170	0.060	0.100	0.0710	0.062	0.0346
5.0	15	0.0170	0.061	0.096	0.0355	0.031	0.0180
″	25	0.0282	0.106	0.157	0.0355	0.030	0.0186
″	50	0.0561	0.218	0.310	0.0356	0.030	0.0195
″	75	0.0837	0.320	0.463	0.0356	0.030	0.0199
″	100	0.111	0.438	0.616	0.0356	0.029	0.0202
″	150	0.166	0.660	0.927	0.0357	0.029	0.0206
″	200	0.221	0.884	1.23	0.0357	0.029	0.0207

Conclusions

These calculations show that the success of surface state models in fitting observed tribocharging results is not strongly dependent on the particular distribution of energies of the charging sites. Nearly linear behavior over narrow ranges of T/C is predicted for almost any configuration of densities of states distributions. Truly linear behavior over a wide range of T/C is not predicted for any configuration of narrow energy distributions, except the special case where all of the distributions have the same energy.[6] When charge is exchanged between a broad distribution of charge-donating surface states and a broad distribution of charge-accepting surface states, the T/C series plots are also curved. As with narrow distributions, this curvature might not be noticed if M/Q is measured over a narrow range of T/C. Very nearly linear T/C series plots are generated when both surfaces contain charge-donating and charge-accepting surface states with broad energy distributions. The dependence of the slope and intercept of these linear distributions on toner and carrier particle size agrees with experiment. Electrical capacitance and electric field effects appear to be unimportant for these surface state models.

References

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