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Computer aided simulation of mesoscale particles mixing for direct printable ink†

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Abstract

Conductivity is an important property of nano ink when considering printable electrical devices need low current loss and high frequency application. Some of the mechanical, chemical and physical characteristics that can affect the conductivity of nano ink are contact resistance, impurity, void volume, aspect ratio, particle shapes, and packing density. Increasing the packing density is one of the most important factors in increasing nano ink conductivity. A computer modeling code was developed to simulate 2 dimension packing factor (2D-PF: covered area by circle/total area of domain, %) using statistics and probability theory. The values calculated in the 2D-PF were similar to empirical 3 dimension PF (3D-PF; volume of occupied by particles/ total volume of system, %) values. The observed volume fraction of voids using spherical balls could be applied to printable ink. The highest 2D-PF calculated by 2D particles model simulation was 60% (binary) when the ratio of large to small particles size was 6. The fraction of void volume was observed empirically for binary packing systems using various ball sizes. The highest 3D-PF observed was 75.5% when the ratio of large particle to small particle was 10 and the volume fraction of small particles was 0.3. The 2D-PF results calculated using 2D computer simulation agreed with the results found in actual experiments. This work studies the relationship of how packing-density and surface-contact affects conductivity of patterns using printable nano inks.

Keywords: Conductivity; Printable ink; 2D Computer Simulation; 2-D 3D-PF

1. Introduction

The market for printable electronics such as displays [1-3] and circuit board [1-5] has greatly increased in 21st century. The conductivity of nano paste and inks using nano sized particles in media has been a crucial factor for electronics patterns for the advanced [1] and flexible electronic devices [3]. Electronic devices patterned with nano inks have conductivity in the range of ~30% [1-3] that of bulk state metal. The low conductivity of electronics patterned with nano particles is a prohibitive factor for using nano particle in high frequency electric devices [1-7]. Fig. 1 shows the direct writing head and particle packing patterns with printable inks. The most influencing factors on conductivity are particle size [1-5], concentration [4], contact resistance [4], shape [8], and void [1, 8]. It is believed that 3 dimensional particle packing factor (3D-PF) is a crucial factor in improving the conductivity of direct patterned devices [1]. In other words, conductivity can be improved by decreasing the amount of voids within the pattern [1-15].

In this study, systematic tests were carried out to determine the void quantities of particles packed body in a cylinder with spherical balls. For the accurate prediction of 2D-PF and volume of void in a system, series of simulation were carried out with various circle radii and mono-, and binary-dispersed particles mixture in a rectangular pattern. The computer simulation was designed to measure void site and particle covering. The results of 2D-PF and empty area were compared with 3D-

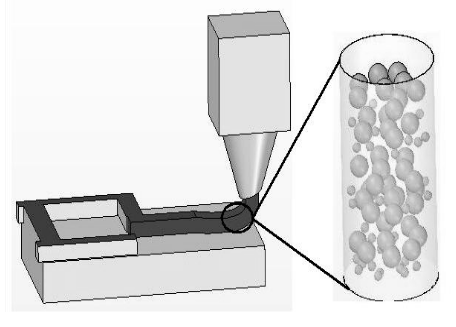

Fig. 1. Schematics of direct writing head and packing particle in pattern.

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PF data for each mixture of mono- and binary dispersed particle. This work deals with the correlation of how packing and particle contact points affect conductivity of nano inks for direct deposited patterns.

2. Procedure

A graphical packing (500X500 dimensionless rectangular pattern) simulation program developed for convenience and the ability to accurately predict the 2D-PF. Different size circles were used in the computer simulation program while rectangular patterned size was held constant. 2D-PF of each ratio circles, five different particle sizes which are 165, 100, 70, 55, and 45 were used. For the simulation the 50 sized circles was assumed to be in the domain then changed small sized circle ratio 1 to1/10 with 50 sized circles. The results of each simulation were calculated. The ratio of large to small particles was varied. The 2D-PF was then calculated. The binary circle covering simulation used four different circle combinations: A-B, A-C, A-D, and A-E (Table 1). The computer simulation program was used to calculate the packing of the different ratio combinations. The results were then determent the reliability of the computer simulation. The conditions were held constant for empirical experiments.

The empirical experiments were completed by filling a cylinder to a pre-designated depth with a single size of steel balls. The cylinder was than weighed. Next the cylinder was filled with water to the same depth and weighed. The weight difference was then determined and the volume of voids was calculated based on the weight of the water in the cylinder. The diameter of the cylinder used was $5.0X10^{-2}$m. Various trials were conducted to determine the optimum packing factor, which is to use five different sized that is 1.6 $X10^{-2}$m, 1.0 $X10^{-2}$m, 0.7 $X10^{-2}$m, 0.55 $X10^{-2}$m, and 0.45$X10^{-2}$m steel balls. The sizes used are shown in. Binary sized particle packing experiments were compared to single sized particle packing experiments. The binary experiments used four steel ball combinations of A-B, A-C, A-D, and A-E. (Table 2) In order to determine the relationship of particle packing with the affect of pressure on conductivity, conductivity was checked using a MITSUBISHI Loresta GP MCP-T610 4-pin probe.

Two methods were used the first packed one size steel balls in a cylinder and the other used two different sizes for packing. The cylinder size used was 8 mm, and the size of steel balls used was 0.8 mm and 0.04 mm. Fig. 2 shows the conductivity instrument layout.

Table 1. Radii of Circles used in binary computer simulation.

Circles	A	B	C	D	E
Radius (Unit-less)	50	35	25	15	5

Table 2. Sizes of steel balls used in binary packing experiments.

Ball bearing	A	B	C	D	E
Radius (m) $x10^{-3}$	5.0	3.5	2.5	1.5	0.5

3. Results

The optimum 2D-PF for single size particles is at R/r ratio of 10. After a ratio of ten the 2D-PF levels off. The computer simulation showed a maximum 2D-PF of 45%. The maximum Packing factor for Empirical 3D-PF is 62% and levels off at an R/r ratio of 10. Fig. 3 shows that the simulation and Empirical 3D-PF results. It is believed that trends of results are similar. Fig. 4 shows the results of computer binary sized particle covering. The R/r_1 ratio fixed at 10 and the ratio of large to small particles was varied. Fig. 4 the maximum 2D-PF is 62% when the particle size ratio is 1/10.

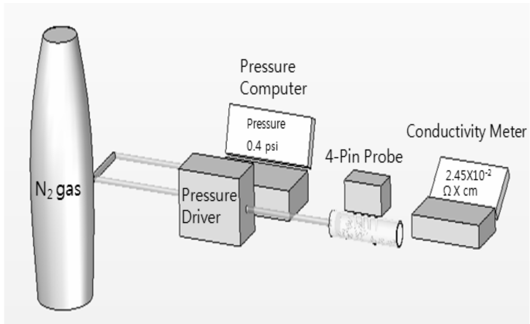

Fig. 2. Conductivity instrumentation layout.

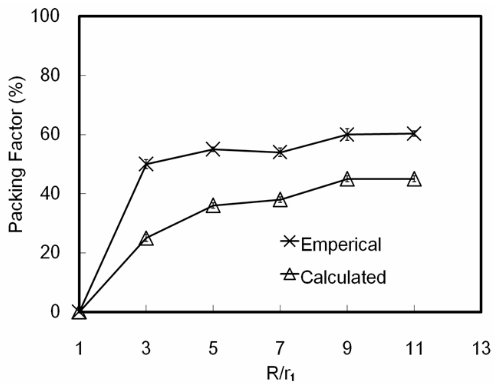

Fig. 3. Single sized particle packing factor in computer simulation and empirical packing (R is simulation program & cylinder size and r_1 is large sized circle or ball).

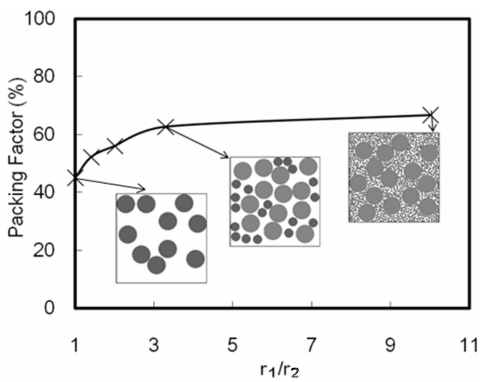

Fig. 4. Binary computer simulation 2D-PF (r_1 is large sized circle and r_2 is small sized circle).

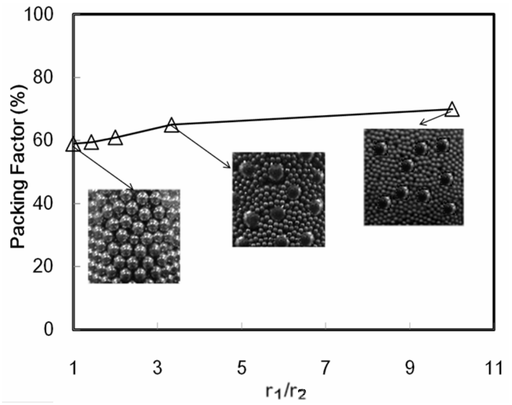

Fig. 5. Binary steel ball Empirical 3D-PF (r_1 is large sized ball and r_2 is small sized ball).

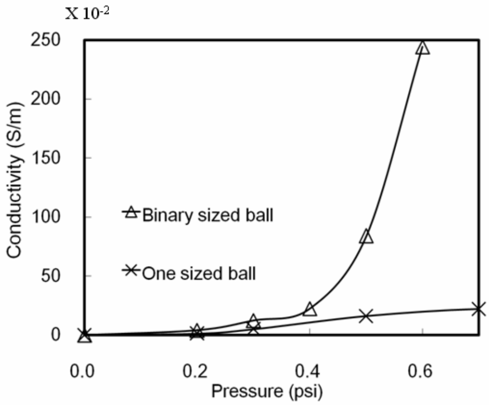

Fig. 6. Conductivity versus pressure for binary and single size particles.

The computer simulation and empirical results were similar in this application. Fig. 5 shows the results of the Empirical 3D-PF experiments. The Empirical 3D-PF is higher than in the computer simulation. The maximum Empirical experiment 3D-PF is 71%. Fig. 6 shows the relationship of the 3D-PF and the effect of pressure on conductivity for one sized particle packing. A 4-pin probe was used to measure the conductivity for single size particles. As the pressure increased the packed particle conductivity increased until pressure 0.5psi at which pressure the conductivity levels off. This is because as the pressure increased the particle packed void decreased in turn increasing the particle contact points and the conductivity. Fig. 6 shows one sized versus Binary sized particle packed conductivity. Binary sized packed particle conductivity is higher than single sized packed particle conductivity. It is believed that as the pressure increase the smaller steel balls deform increasing the packing factor and contact point. Conductivity rapidly increases when the pressure is over the 0.4 psi. These results show that binary sized particles have a higher packing factor than single sized particles with a corresponding increase in conductivity.

4. Conclusion

In 21st century, electronic manufacturers demand a printable ink that has a high conductivity. This research used a computer simulation program and empirical experiments in order to understand the compared relationship between packing factor and conductivity. Both methods were used to insure accuracy and to make a comparison of the results. The empirical experiment used a cylinder and steel ball with same sized ball and cylinder ratio as was used in the simulation program. This work shows the binary sized particle packing is higher than single mono dispersed sized particle packing. The conductivity was measured in each variation and showed that as the packing increased the conductivity also increased. This paper displays that particle packing and contact greatly influence the conductivity of the paste.

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