Process Variation Characterization and Modeling of Nanoparticle Interconnects for Foldable Electronics

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Abstract—Designers require variational information for robust designs. Characterization of such information can be costly for the novel nanoparticle interconnect process, which utilize nanoparticle silver solutions. To reduce characterization cost and initiate circuit level considerations for foldable electronics, we provide nanoparticle interconnect models. We use SEM measurements to characterize nanoparticle size distribution. We conduct field solver simulations over the proposed model to obtain physics-based process variation impact on a nanoparticle interconnect resistance. Such methodology can be helpful to aid designers for circuits based on novel transistors, such as organic TFTs on low cost foldable substrates.

I. INTRODUCTION

Nanoparticle interconnects are becoming increasingly popular due to:

- Suitability for interesting application areas
- Being easy to integrate with different transistor types
- Being integratable on low cost substrates
- Low process stress
- Being an enabler for foldable electronics

Foldable electronics can provide applications such as books with plastic pages with integrated OTFTs (Organic Thin Film Transistors) [15], [12] or very large and cheap displays that can cover the walls in a house.

Nanoparticle interconnects can be manufactured on very low cost substrates, such as plastic [11], and even on a paper or on textiles [10] that are wearable.

Nanoparticle interconnects are a result of a process as summarized in Table I. The evaporation phase results in the silver particles flowing in the solution to start touching each other. At the end of this step, the particles conduct through each other yet the conductivity is low due to small surface area of connection between the particles.

The sintering process helps particles to join with each other. Adjustment of sintering time and temperature is an important process choice. Elevated temperatures would result in high stress gradients, which may bring reliability problems to the transistors on the polymer substrate. Increased time would increase the cost associated with the process.

It is desirable from an electrical performance to have:

1. Low resistivity
2. Low process variations
3. Low process time

TABLE I

PROCESS FLOW FOR NANOPARTICLE POLYMER INTERCONNECTS

<i>Consumable.</i> Nanoparticle silver inks obtained from a supplier
1. Print interconnects using the nanoparticle ink with an industrial ink-jet printer
2. Evaporate solvent in air
3. Sinter at an elevated temperature

4. Low stress

Given these targets, designers furthermore need process variation information. Such information can be obtained through characterization of hundreds of polymer chips. However, as polymer processing is new, most of the steps incorporate manual labor consisting of many man-hours. Furthermore, resources including supplies increase the cost significantly.

Given this overview and the need from designers, it is necessary to characterize process variations in nanoparticle interconnects. To achieve this, we model nanoparticle interconnects, use data from the literature and conduct Monte Carlo field solver simulations. We provide process variation information, given the process conditions and our models.

II. MOTIVATION

The final texture of a nanoparticle interconnect is correlated to the particle size distribution of a nanoparticle ink, which can be obtained through a supplier. Yet, nanoparticle sizes can vary significantly, as nanoparticle ink process is relatively new. Such process control inability can result in a nanoparticle size distribution with a large standard deviation.

It is known from conventional aluminum or copper interconnect technologies that resistance variations in interconnects can result in significant performance variability in circuits. Process variation models can enable fast characterization for nanoparticle interconnects, without wasting expensive consumables and lab time. Known variability needs to be modeled to the best extent.

III. PREVIOUS WORK

In [1], the authors have proposed simple analytic models which relate resistivity to linear shrinkage and densification given time, temperature and particle size. A resistivity vs. thermal cure model is proposed. Curtis et al. [2] have provided a maskless fabrication scheme for nanoparticle interconnects.

Park et al. [8] have analyzed the thermal behavior of printed silver nanoparticles.

In the area of organic electronics, Iyer et al. [13] and Forrest et al. [5] provide introductory tutorials for organic electronics. Lu et al. [14] have studied polymer composites as gate dielectrics for organic electronic applications. Marbell et al. [18] have provided high-level models for system implementation in electronic textiles. Nieuwoudt et al. [19] have provided a theoretical process variability analysis on carbon nanotubes.

Jung et al. [9] have analyzed sintering process. They have identified that sintering 5 minutes at 250°C results in a rapid decrease in resistivity. The resistivity starts to increase slightly after 20 minutes and consequently reaches a constant. Murray et al. [3] also report resistivity values as a function of sintering temperature.

In terms of recent foldable electronics applications, Redinger et al. [7] and Molesa et al. [11] use ink-jet printed interconnects for RFID applications.

Polymer-metal composite interconnections can also be used in advanced packaging applications. Aggarwal et al. [16] provide a manufacturing processes using composites for packaging. Jiang et al. [17] presents highly conductive lead-free interconnects using polymers with silver nanoparticles.

Final particle sizes can still exhibit significant radius and alignment variations. Larger scale models are needed. Furthermore, designers require a simulation-based analysis for accurate process variation characterization to be able to design circuits without over-constrained limits, which restrict attainable circuit performance, and without under-constrained limits, which decrease yield.

IV. MODELING

In order to model the process variations for a nanoparticle interconnect, we first model the texture of a nanoparticle interconnect.

Characterization of Process Variations. We characterize the process variations of particles using the SEM measurement in Figure 1. Using the provided scale and on-screen measurements, we find the particle with the maximum radius and the minimum radius. We assume that these particle radii provide the plus- and minus-three sigma standard deviation around the mean, respectively. Assuming a Gaussian distribution, we then find the mean particle radius through an average of the maximum and minimum radii. From the SEM, we measure the minimum radius as 21nm and maximum radius as 55nm . We provide the parameters for a silver nanoparticle in Table II.¹

In Table II, ρ is the electrical resistivity, μ_R is the mean value of particle radius and $3\sigma_R$ is the three sigma of particle radius.

Modeling the Sintering Process. We model the sintering process such that there are no deformations to the rest of nano particles that are joining, other than the contact area. This model is shown in Figure 2. Initially, d , the distance between the centers of two particles, is $r_1 + r_2$, where, r_1 and r_2 are

¹Although we have used silver nanoparticles in our study, gold nanoparticles can also be used [6] for plastic-compatible foldable electronics.

Fig. 1. An SEM image, showing silver nanoparticles [4]. We extract particle size distribution from this image.

the radii of two particles. As the sintering process progresses in time, two particles in contact merge into each other and their centers approach each other along the arrows in Figure 2. The distance d becomes smaller over time.

Fig. 2. Model for initial stages of a sintering process [4].

Modeling Nanoparticle Interconnect Cross-section. To form an interconnect, multiple nanoparticles need to be present. The particles stack up with each other, forming the height of the interconnect, and also fill the width of the interconnect, which is printed using nanoparticle ink droplets. We model particles as spheres. A front cross-sectional view along the interconnect length is given in Figure 3. The model in Figure 3 corresponds to the end of the evaporation step 2 in Table I. Although the particles may be in touch with each other, the conduction area is negligibly small. We use a grid to align all the particles. The center of each particle falls into one of the grid points as shown in Figure 3. We furthermore extend the grid in 3D along the length of the interconnect. The resistance is measured between the planes at the two ends along the length, such that the planes include the grid points at either end. W and H in Figure 3 correspond to the printed width and height of an interconnect. We set the radius of each particle using random sampling from the particle probability density function.^{2,3}

At the initial time for sintering, let the distance between each grid point be d_0 . We model the sintering process such that as time progresses, d_0 decreases linearly by a constant rate ν , to yield the final d as:

²We use an uncorrelated sampling methodology, as the particles are initially floating in the nanoparticle solution, hence, there is no physical correlation as to what size two neighboring particles may be.

³We use a Gaussian density function assumption, although this function can be substituted by a more accurate one if additional characterization data is available from the solution supplier.

TABLE II
PARTICLE VARIATIONS EXTRACTED FROM SEM AND RESISTIVITY

ρ	$1.59e^{-8}\Omega m$
μ_R	19 nm
$3\sigma_R$	8.5 nm

Fig. 3. Cross-section view of a modeling grid for a nanoparticle interconnect.

$$d = d_0 - \nu * dt \quad (1)$$

This decrease results in particles merging with each other over time. In Equation (1), dt corresponds to the time difference between a given time and the initial time when the sintering process starts. We set d_0 equal to twice the mean of the particle radius density function. We also define $1 \leq \alpha \leq 2$ as $2d/d_0$. We decrease α and monitor the change in resistance. A decrease in α indicates that two particles have increasingly joined with each other.⁴

To introduce another degree of variability to particle locations, we shift the layers row by row as a group in Figure 4. We set the shift amount per row by random sampling from a Gaussian density function with standard deviation equal to that of the particle density function. Positive or negative values define a shift to the right or left, respectively.

The state of the model after a given amount of sintering and using random sizes for the particles is illustrated in Figure 5.

⁴The parameter α can be found by comparing the mean resistivity with published data for given process conditions.

Fig. 4. Modeling of layer shifts in the grid.

Fig. 5. Modeling of particle size variations and sintering amount.

Fig. 6. Snapshot from one Monte Carlo Raphael simulation using proposed models with $\alpha=1.75$.

V. EXPERIMENTAL RESULTS

We use Raphael as the field solver in our simulations to implement our models. We conduct 10,000 Monte Carlo simulations using shell scripts and PERL. Each simulation utilizes 250,000 nodes and takes approximately 30 seconds to run on a 2GHz computer. We use reflective boundary conditions in our simulations. We compute the resistance using the simulator and record the resistance value. The input to our simulator is:

- i. 3D finite element model for nanoparticle interconnects
- ii. Particle size mean and standard deviation from Table II.
- iii. Particle resistivity value at given temperature
- iv. Sintering time from process

To reduce the simulation time, we only simulate a portion of the model. We provide a snapshot of our simulation structure in Figures 6 and 7 for α equal to 1.75 and 1.5, respectively. A 4 by 2 array of nanoparticles with 2 particles long is simulated for each Monte Carlo run. To find the resistance for a printed width, height and length, we scale the simulated resistance using:

$$R = R_{sim} * \frac{W * H * L}{(p_x - 1) * (p_y - 1) * (p_z - 1) * (\mu_R \alpha)^3} \quad (2)$$

In Equation (2), R is the resistance for the printed width (W), height (H) and length (L) of an interconnect; R_{sim} is the resistance for the simulated structure; p_x , p_y and p_z are the number of particles simulated in each direction and μ_R is the mean particle radius.

Density histograms for α equal to 1.75 and 1.5 are given in Figures 8 and 9, respectively. The mean resistance decreases as the sintering process continues, i.e., from 0.3496Ω to 0.2207Ω . Furthermore, the standard deviation of variation in resistance also decreases, i.e., from 0.0368Ω to 0.0135Ω , hence resulting in a $3\sigma/\mu$ reduction from 31.5% to 18.3%. Such analyses can provide process engineers with optimal time/resistance/variability point and designers with resistance variation bounds, enabling low cost process and design optimization and characterization.

Fig. 7. Snapshot from one Monte Carlo Raphael simulation using proposed models with $\alpha=1.5$.

Fig. 8. Density histogram for the resistivity with $\alpha = 1.75$.

VI. CONCLUSIONS

We provide models for nanoparticle interconnects and conduct 3D field solver simulations using the proposed models. We use SEM images to characterize particle size distributions. Models for nanoparticle interconnects can provide process variability information without the need to conduct analyses that may involve many hours of manual labor and consumption of consumables. With the models for nanoparticle interconnect process variability, designers will have the necessary nanoparticle interconnect resistance bounds to design circuits in foldable electronics technologies.

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Fig. 9. Density histogram for the resistivity with $\alpha = 1.5$.