Modelling of concrete composite material with phase-centered cell

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Modelling of concrete composite material with phase-centered cell

by

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in partial fulfillment of the requirements for the degree of

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(1.0) Motivation

The ability to self-sense in a concrete material yield to the smart concrete structure for buildings and pavement plays an important role in health monitoring purposes. Self-sensing is an attractive attribute that allows the structural materials to measure its own electrical properties output such as resistance and resistivity based on the stress applied, defects or other stimulus. It’s a more straight forward and easier modern way to perform the non-destructive evaluation (NDE) on the structure material for defect and damage detection compared to conventional NDE technique such as ultrasound and liquid penetrant testing.

In order to incorporate the self-sensing attribute to produce the smart concrete structure, the cement is filled conductive material such as currently trending carbon nanomaterial. The combination of the cementitious material and the conductive filler forms the composite material or smart concrete. Some of the famous carbon nanomaterials are carbon-black (CB), carbon nanotube (CNT), carbon fiber (CF) and carbon nanofiber (CNF).

Once the concentration of the conductive filler added into the composite material exceed the percolation threshold, the composite material would become conductive. Continuous infinite network of conductive particle and conducting path would be formed throughout the material beyond the percolation threshold. Some reference also referred those material with conductive filler that exceed the percolation threshold as percolation structure. We can reduce the percolation threshold therefore reduce the amount of conductive filler needed significantly by adding additional polymer to the composite material well [1].

Several studies have been made for different combination of cementitious material and conductive filler to verify various functionality and advantages of the composite material. Two of the most popular output measurements taken the papers are discussed in this report. First measurement is the resistivity measurement due to a stimulus such as strain, temperature or defects [2] [3] [4]. From the resistivity measurement, we can extract useful information such as the percolation threshold and the effect of polarization on composite material and by conducting these measurements on the composite materials we can evaluate and compare the performance of various composite material. Some composite material may have lower percolation threshold and lower tendency polarization but higher cost of producing the conductive filler and some may not.

Hence, we would want to make sure that the resistivity measurement is accurate. It is always preferred to test the specimen of smart concrete with a surface electrical contact, however it may not be easy or cheap to realize the surface contact depending on the concrete material and researcher’s equipment. Common mistake is to assume that the resistivity measurement is the same for both surface and non-surface electrical contacted specimen when $\rho = R \frac{A}{l}$ is used. The geometrical factor of $A/l$ is true for specimen with surface contact but not for non-surface contact.
specimen. Researcher may have made mistake such that the resistivity is overestimated or vice versa due to non-surface electrical contact specimen because the resistivity would mainly affect by its geometrical factor ($\text{GeoF}$) and not its resistance.

For 2D, it can illustrate as the following

$$R_{\text{square, surface contact}} = R \times GF_0 = R \frac{W}{l} \quad \text{where } \text{GeoF}_{2D} = \frac{W}{l}$$

$$R_{\text{square, non-surface contact}} = R \times GF_1 \neq R \frac{W}{l}$$

It’s rarely seen that a state-of-the-art would have problem with evaluating a conductive thin film with the general equation with geometrical factor of $W/L$. Most of the time the contact will be made across the perimeter of the thin film. Although it’s not a surface contact but because the thickness is very small and with four-probe measurement, the current and voltage contact is always far enough to ensure accurate measurement. Similarly, for 3D, the resistivity can illustrate as the following

$$\rho_{\text{surface/mesh contact}} = R \times GF_0 = R \frac{A}{l} \quad \text{where } \text{GeoF}_{3D} = \frac{A}{l}$$

$$\rho_{\text{non-surface/mesh contact}} = R \times GF_1 \neq R \frac{A}{l}$$

Specimen where the thickness is a key parameter is when some state of the art fails to predict the resistivity correctly and it’s often due to the inner voltage contact is not far enough from the from outer current contact. Due to the non-uniform current flow around the non-surface contact, the geometrical factor would not be linear thus the geometrical factor effect is more severe than we would expect.

Second popular measurement across the papers is the rate of resistance change, $\Delta R / R_{\text{NOM}}$ due to the strain, $\varepsilon$ [2] [3] [4]. From the measurement, we can obtain the gage factor to tell which composite material is more sensitive to the strain in term of the resistance. It also would tell us whether the composite material is suitable for the piezoresistive application by looking at the linearity of the rate of resistance change due to the strain. Gage factor can be defined as following:

$$\text{Gage factor} = \frac{\Delta R / R_{\text{NOM}}}{\Delta L / L_{\text{NOM}}} = \frac{\Delta R / R_{\text{NOM}}}{\varepsilon} = 1 + 2\nu + \frac{\Delta \rho / \rho}{\varepsilon}$$

where $\nu$ is the Poisson ratio and $\frac{\Delta \rho / \rho}{\varepsilon}$ is the ratio of rate of resistivity change to the strain. Some of the author fails to show or interpret the gage factor from the measurement by assuming that the gage factor is a constant when it’s not. Despite that, if the range of strain is still within the range of interest then the gage factor should still be correctly predicted. Gage factor is believed
to have some sort relationship with the geometrical factor and with a non-surface material, both geometrical factor and the gage factor would be non-linear. From the general equation, Poisson ratio is the ratio of the rate of lateral dimension change to the longitudinal dimension change of the specimen which is not related to the type of contact and $\frac{\Delta \rho/\rho}{\varepsilon}$ is often assumed to the 0 assuming that the volume of the specimen does not change or deform. The equation is not true for some of non-surface contact specimen.

Specimen where the measuring contact is near the supplying current/voltage contact would have a non-linear resistance-length relationship. For example, with for four probe and perimetrically electrical contacted (band contact) specimen, if the inner measuring contact is too close to the outer supplying contact, the current measurement would be non-linear as we apply the strain. both Poisson ratio and the $\frac{\Delta \rho/\rho}{\varepsilon}$ does not take in account the non-linearity caused by the type of contact. The current densities across the specimen when compressed or elongated would be different as shown in the Figure 1.1. Thus, the Gage factor $= \frac{\Delta R/R_{NOM}}{\Delta L/L_{NOM}}$ would be non-linear as $\Delta R/R_{NOM}$ is non-linear as strain changes.

![Figure 1.1 Compressed specimen (left) Elongated specimen (right)](image)

The papers we would discussed in the later section clearly shows the plots of result where the rate of resistance change is not linear and the plot is a form of differential equation where part of it may be linear and part of it may be not.
(2.0) State of the Art

In this section, we would look at four state-of-the-art which the electrical contact has been made on the specimen such that the geometrical factor would affect the resistivity measurement. We are particularly looking at authors that uses $\rho = R \frac{A}{l}$ for non-surface electrical and discuss whether the accuracy of the measurement for the electrical contacts made. Also, we would look at how the authors evaluate the gage factor from a non-linear $\Delta R/R_{NOM}$ vs $\varepsilon$ plot.


The electrical contact of the specimen described in the paper is as the following:

“Specimens were rectangular bars of size 75 x 15 x 15mm. DC electrical resistance was made along the length of a specimen… Fours contact were made perimetrically… all perpendicular to the length of specimen with respect to the midpoint along length of specimen. The outer two contacts (50 mm apart) were passing current. The inner two contacts (40 mm apart) were measuring voltage.”

The distance between the current and voltage contacts on both ends are about 3 mm assuming the contacts are 2 mm wide. Below shows the rough cross-sectional sketch of the electrical flow for a band contact or perimetrically contacted rectangular bar. If the inner contact is too close to the outer contact, the current may not be flowing uniformly along the length direction yet. The current may well be flowing toward the midpoint along the height direction when the voltage measurement is taken. $\frac{A}{l}$ is used for the resistivity calculation when the geometrical factor is a differential equation due to the contact which causes the error in the resistivity shown in the paper.

Figure 2.1. Sketch of electrical flow in specimen fabricated in [6]

The sample is as described as the following:

“Samples consists of 70mm long prisms with a square base side of 50 mm. Four high temperature resistant Kanthal steel wire electrodes with diameter of 2.2mm were embedded symmetrically along central axis of samples with spacing electrodes set at 10, 20, and 10mm”

Figure 2.2. Sketch of electrical flow in specimen fabricated in [7]

By embedding the electrode rods as contacts, the current would leaks around the outer contact toward the other end. The leakage paths are shown in the sketch above where some current would leakage horizontally and vertically towards both side of the electrode. Let’s first talk about the first major measurement which is the resistivity. Imagine that 1mA is inserted into the outer contact and we would not get 1mA flow through the inner measuring voltage contact due to the current leakage caused by the contacts. In consequences, the resistance calculated would be lower than what it supposed to be as \( R = V*I \). The paper also commented the resistivity of the specimen so another possible mistake is the resistivity calculation by using the \( A/l \) as the geometrical factor for a non-surface contact.

The paper also shows the second major measurement which is the rate of resistance change due to strain. The resistance value is still lower than what it is supposed to be. The slope of the
\[ \Delta R / R_{NOM} \] vs \( \varepsilon \) is still linear for different samples, thus the constant gage factor shown in the paper for five different sample is valid and true. However, the gage factor ranges from 391 to 2392 for a titanium-doped specimen and the author can’t find correlation to the difference. One major factor which may causes the huge difference is the large variation of the current and resistance measurement for different sample. The dispersion and concentration of the titanium on the specimen can be different across the specimen. The electrical contacts are made such that the current paths are highly sensitive to the specimen content which therefore would causes the high variation. The higher gage factor specimen which means higher \( \Delta R / R_{NOM} \) may caused by the lower \( \Delta R / R_{NOM} \) of the leakage path around the contact; the dispersion of conductive filler on the leakage path is more to make the path more conductive.


The sample is as described as the following:

“The samples were cylindrical, 50.8 mm in diameter and 100 long. Four cooper electrodes were attached to the samples with silver paste to allow for four-probe resistance measurements.”

The inner contact distance is 60 mm and outer contact distance is 100 mm shown in [7]. From the figure and standard fabrication procedure, the copper paste is perimetrically applied to the cylindrical cement structure shown below;

Figure 2.3. Close-look picture of the contact on the specimen from [8]
Just like the first state-of-the-art we discussed, it is highly possible that the inner contact is too close to the outer contact considering that the distance between outer and inner contact is only about 10mm and the radius is 25.4 mm.

Both of the major measurements are evaluated in the paper. First, the resistivity computation is wrong because $A/l$ is used as the geometrical factor. Second, a non-linear $\Delta R$ due to strain plot is shown in the paper and the author does use hyperbolic equation for the rate of resistance change given a certain loading rate [kN/s]. However, when it comes to the $\Delta R$ due to strain is shown, the linear fitting curve is used while ignoring the high-strain part of the curve as shown in Figure 2.4. By having a second-order equation, the gage factor would be constant which is true for the range of interest and not true for a larger range of strain because the fractional change in resistivity, $\Delta \rho/\rho$ or the rate of resistance change $\Delta R/R_{NOM}$ is a differential equation.

![Fractional Change in Resistivity vs strain plot from [9]](image-url)

The fourth paper has a sample where it’s described as the following;

“the fresh mixture were cast into a cubic mold 50 x 50 x 50 mm³… To measure the resistance of the hardened specimens, the electrodes were designed in equivalent planes using silver paste to minimize the contact resistance between the composite matrix and the electrodes/ These had a width and height of 10 mm and 20 mm, respectively”

![Image](2.5. Specimen illustrated from [9])

The specimen has only partially surface electrical contact and yet the equation used to calculate the resistivity for different cementitious composites at # days of curing is no other than $R_s \frac{A}{l}$.

Some may debate that since the A is the cross sectional of the electrodes on the specimen and it is correct to some extent. Since it’s only a partially surface contact, the geometrical factor is not close to $A/l$. The resistance measured would have an error due to the current flow non-uniformly from one contact to the other which therefore changes the geometrical factor. Only resistivity is evaluated in this paper and it does not take in account the geometrical factor error induced due to the contact. Figure 2.6 shows the sketch of the electrical current flows from the top view.

![Image](2.6. Sketch of current flow for specimen [9])
(3.0) Research Work

A phase-centered cell is a model that contains resistors with certain resistance, $R$ and each side of the cell has a resistor connect from the side to the center.

![Figure 3.0.1. 2-D phase-centered cell](image1)

![Figure 3.0.2. 3-D phase-centered cell](image2)

The cell is often used to model a particular structure and its electrical properties such as resistance and resistivity is extracted out by applying a voltage on the material. In this section, we would use the 2-D phase-centered model then the 3-D cylindrical model and finally we would use the 3-D model and apply the model on one of the state-of the art mentioned in Section (2.0).

(3.1) 2-Dimensional Thin-Conductive film

Imagine a material that is modeled using a single phase-centered cell shown in Figure 3.1.1. The equivalent resistance of the material would be $2*R$ with the voltage source and ground connected as shown. It’s important to note that the tip resistance of the contact and contact resistance are neglected when we are modelling the test bench for the material. Since the W/L of the material is 1, the sheet resistance would simply be $R_{\square} = R_{eq} \frac{W}{L} = 2*R$.

![Figure 3.1.1. 2-D phase-centered cell simplified test bench](image3)
The cell is useful to get an insight of the current density in a material. Imagine a material that’s modelled with millions of the cells and therefore we could compute the current going through each resistor and draw out the current flow in the material with a bunch of current arrows and its density.

The individual are free to choose the number of phase-centered cell for a fixed size of a material. The higher the number of cells for a fixed size of material, the more insight we can get about the current flows. Figure 3.1.2 and 3.3.3 shows thin film with relatively small thickness compared to the width or length and modeled with the phase-centered cell on a 2-D plane.

By applying a voltage to the material we can easily obtain the resistance and resistivity. The equivalent resistance of the material can be obtained through the Ohm’s law since we know exactly what voltage we supplied and the current supplied from the voltage source. The general equation for calculating the resistivity of a thin material such as thin film is

\[ R\square = R \cdot GF = R \frac{W}{L} \]  
for 2-D structure where the thickness is neglected

where GF is the geometric factor, \( R\square \) is the sheet resistance and R is the resistance. Note that often times sheet resistance is used instead of the resistivity when we are characterizing a thin film. When we are increasing the number of per unit length, the resistivity would remain the same and that is 2*R. “Cell per unit” would be use often in this report to indicate the number of cell used per unit length so that we can imagine how wide or long is the material. For instance, Figure 3.1.2 and 3.1.3 has the same W/L but different cell per unit.
The resistivity equation and the geometric factor is accurate if the whole surface of the material (shaded region in Figure 3.1.4) is connected to the voltage source. In this report, it would often refered as the multiple contact material also and if the material is modeled using the phase-centered cell, it would like what is shown in Figure 3.1.5.

However, when the material only has a single-point contact (shown in Figure 3.1.6) instead of surface or multiple contact, the resistivity equation $R_{\square} = R*GF = R*\frac{W}{L}$ would fail to predict the sheet resistance depending on the size of the material. A hypothesis can be drawn where if the long material (its $W/L$ is very small) then the general resistivity equation would correctly predict the sheet resistance. The geometric factor of a single-contact material is no longer equal to $\frac{W}{L}$.
Thus, in this section we would show the resistivity of a thin film that is modelled as a 2-D structure with the phase-centered cell with both surface contact and single-point contact. For surface contact model, the general equation of resistivity would accurately predict the geometrical factor and resistivity of the structure and they are:

$$ R_{\square, \text{surface contact}} = R \cdot G_F = R \cdot \frac{W}{L} $$

where $G_F = \frac{W}{L}$

For the single-contact structure, we would observe that as we increase the $W/L$, the error of the sheet resistance would increase when we are still using the general resistivity equation $R \cdot \frac{W}{L}$.

$$ R_{\square, \text{single contact}} = R \cdot G'_F \neq R \cdot \frac{W}{L} $$

A SPICE netlist of schematic with a bunch of resistors depending on the two different type of contact would be generated from the Microsoft Visual Studio.

The wire resistance, contact and contact’s tip resistance would be neglected as we discussed. Tip resistance is the most tricky factor that can caused error between the resistance calculated using the simulation model and the real-life material.
Tool Verification:

Through the discussion in the earlier section W/L, cell per unit and resistance of each resistor in the phase-centered cell would be our degree of freedom where the users can choose how many cell they desired in a structure. In this section, we would verify that the code written in Visual Studio would generate the SPICE netlist based on the circuit we desired. Surface-contact or multiple-contact structure is not shown and only the single-contact structure is shown in this tool verification section.

The equivalent resistance and resistivity multiple-contact structure can be easily calculated given the W/L and cell per unit. We would see later in the result section that it’s impossible to compute the resistance and resistivity of the a single-contact structure even when the material is modeled with the phase-centered model and simplified to a circuit that contains only resistors assuming the there’re hundreds or thousands of cell are used to model the structure. If the cell per unit is small and W/L is close to 1, it’s pretty easy to compute equivalent resistance of the material by realizing it’s just few resistors in parallel as shown in Figure 3.1.8.

Figure 9 shows a material with W/L = 1 and cell per unit = 2. Note that the resistors that has floating node in either end of it has been removed from the circuit schematic. It should be obvious that I₁ will be more than I₂ due to its lower resistance path. The equivalent resistance is simply \( R_{eq} = R + (2R \parallel 6R) + R \).

Now, we would discuss on how the code is written and how the generated SPICE netlist is verified. The code is written such that it would computes the matrix of the cell based on the W/L and cell per unit of the user input using the .exe extension file. For instance, if the W/L = 1 and cell per unit = 3, then it’s a 3X3 cell matrix; if the W/L = 2 and cell per unit = 3 then it’s a 3X6 cell matrix. The code would generate lines of resistor in SPICE format.
Since we are not specifying what type of material we are expecting, resistance of resistor in the phase-centered cell become a degree of freedom; therefore, R is defined as 10k Ohms by default in the code. At the beginning, the code will generate the resistors column by column for the first row in the order of top, right, bottom and left order as shown in Figure 3.1.9. Once first row is filled, it goes to second row and generate the resistors column by column with the same order, then third row and so on.

All the resistors that has floating node in either side such as the top resistor in top row cells for single-contact structure and the right resistor in the rightest column cells is would be ignored and not written in the netlist.

Because of how the code is written, the code is verified at cell per unit > 2. We wish the cell per unit to be large so it makes sense to have it at least 2. Nevertheless, there’s also a tracker to save the voltage middle node shown in Figure 3.1.9 of each cell so that we are able to compute the current flowing through each resistor.

The code would generate a text file and by changing the extension from .txt to .cir. We can simulate the SPICE netlist in Pspice software.
The current supplied by the voltage source simulated (Figure 3.1.10) using the SPICE netlist match with what we would expect from a circuit schematic as shown in Figure 3.1.11.

Note that Multisim has the capability of generating the circuit schematic given a SPICE netlist as shown in Figure 3.1.12. The attempt of importing the W/L = 1 and cell per unit of 3 netlist is shown below. However, if the cell per unit is extremely large, it would take enormous amount of time for the importing process and it is hard to identify if the netlist has been imported correctly given the enormous amounts of resistor and connection.
Another example with W/L = 3 and cell per unit of 4

Figure 3.1.13. Circuit schematic W/L =3 and cell per unit = 4 with current supplied of 19.2uA

Figure 3.1.14. Netlist generated for W/L =3 and cell per unit = 4 with correct current supplied of 19.2uA
Results and Discussion

For the multiple contact simulation where the top surface and bottom of the material under test are connected to the voltage source and ground respectively, the equation for sheet resistance $R_{\square} = \frac{\rho}{W}$ predict the sheet resistance perfectly. However, that is not the case for a single contacted material. From the data, as we increase $W/L$, the current would allocate more to the side near the voltage source and more and more space that has no current which cause the conventional resistivity question to fail to predict the real resistivity, shown in Figure 3.1.16.

![Figure 3.1.15. 2-D Multiple- and Single-contacted SPICE Simulation result](image)

![Figure 3.1.16. Simplified current flows in 2-D single contacted structure](image)
Figure 3.1.17. W/L versus resistivity error

Figure 3.1.18. Downward flowing current MATLAB xyz plot
A MATLAB script is written to clarify the reasoning where the current doesn’t flow through whole space of the material which therefore overestimated the sheet resistance as the structure is single contacted and W/L getting larger.

Figure 3.1.18 shows the downward current of a 2-D of single contact of W/L = 10 with cell per unit of 20. To show the downward flowing current, the additional SPICE line is added into the netlist to save the node voltages operating point of the phase-centered cell. The voltages are then imported into MATLAB to calculate the current through the Ohms law.

Leftward and rightward flowing current is not shown because downward flowing current is sufficient to observe how far the current is flowing away from the edge of the voltage source. In Figure 3.1.17, the peak current is flowing out from the voltage source to the ground along the length axis. The currents should divide throughout the resistive network modelled and as predicted that due to the single-contacted structure, current doesn’t flow all the way from one end to the another end along the length axis. Another way to think about that is the effective resistance path from the point A to point B shown in plot is high that almost no current is flowing from A to B.

From simulation results of single-contacted structure, we would obtain the overall current and therefore equivalent resistance of a structure. Since the sheet resistance or resistivity remain unchanged as we change the size, we can easily know the sheet resistance which is 2*R as discussed in page (fill here). By having the resistance and sheet resistance on hand, we can compute the actual geometrical factor (GF₁) that would yield the correct sheet resistance when a structure is single-contacted.

\[ R_{\square, \text{single contact}} = R \times GF₁ \neq R \times \frac{W}{L} \]
Figure 3.1.19. Single-point and multiple-contact geometrical factor comparison

From Figure 3.1.19, we can see that the geometrical factor for single-point contact (SC) and multiple contact (MC) start to diverge around W/L = 0.05. Once W/L goes beyond 1, the geometrical factor of SC remains constant. Instead of a linear relationship of MC geometrical factor with the L/W, the SC geometrical factor is not equal to L/W and has a power or negative sloping exponential relationship between the geometrical factor and W/L.

Now that we have a data for the actual geometrical factor of a SC structure, we can derive a generic equation to compute the correct geometrical factor for any W/L.
Using MATLAB Curve Fitting Toolbox, 3 different power functions are formed as shown in the MATLAB plot below:

Blue function : \( f_1(W/L) = 1.029(x)^{-0.9955} + 4.2 \)
Red function : \( f_2(W/L) = 1.01(x)^{-0.9995} + 4.66 \)
Green function : \( f_3(W/L) = 0.9994(x)^{-1} + 3.774 \)

Note that the green function doesn’t plot any W/L beyond W/L = 1. Blue and Red function can be used for any W/L, however, an maximum error of \(~10\%\) for blue function and \(~17.5\%\) error for red function would be introduced in the sheet resistance calculated from the simulation resistance (R) and geometrical factor calculated from the functions (GF₁).

\[ R_{\square, \text{single contact}} = R \cdot GF_{SC} \]
Another approach of deriving the function is realizing that the geometrical factor remains unchanged for any W/L larger than 1. Then, we can just derive the function for any W/L lesser than 1 and come up with the following condition:

\[
GF_{SC} = 0.9994^* (x)^{3.774} + 3.774 \quad \text{for } x = W/L \geq 1 \\
GF_{SC} = 4.66 \quad \text{for } x = W/L > 1
\]

With the conditional function above, we can estimate the sheet resistance of a 2-D thin film for any W/L. This approach of deriving the geometrical factor for a particular specimen with certain type of electrical contact can be applied to any structure as long as we have the true geometrical factor data simulated using the phase centered cell model.

Now, the question would be that the conditional function is good enough under what condition. Imagine that we have a W/L = 100 and cell per unit of 10, then we would have a total number of resistor of 100*10*5 = 5000. The testing condition setup in the simulation or netlist connects only one of the 5000 resistors to the voltage source and another resistor at the other end along the length axis to the ground. The reason we need to pay attention to the probe size relative to the size of the resistive network is to make sure the probe effect is considered in the real life measurements.

When L >> W such that the diameter of the tip of the probe is very small, the probe resistance \( R_{\text{TIP}} \) would go to \( R = R_\square \frac{L}{W} \) infinity. Since the \( R_{\text{TIP}} \) is in series with the overall resistance from the voltage source to ground, when \( R_{\text{TIP}} = \text{infinity} \), the current would approach 0. The longest 2D structure simulated is 10000 X 20 phase-centered cell or W/L of 500 with 20 phase-centered cell per unit, so the tip is still not molecularly small compared to the length but we can expected a noticeable probe resistance due to the 1/10000 probe size in reality. However, there are a few papers published to eliminate the probe resistance factor in the measurement such as four probe measurement that uses current sourcing and voltage sensing. We are also assuming the probe and material surface are homogenous; the molecular or atomic non-uniform interface between the probe and material under test that may cause a more complicated contact resistance is neglected.

The second factor that would affect the accuracy of the conditional function derived is the position of the contact on the 2-D thin film. All the simulation results shown has the contact at the corner of the 2-D thin film, however contacts are usually made on the center for a film. In the next section, we would see a more realistic scenario for the contact location on a 3-D cylindrical structure.

Further research is needed to measure the current and equivalent resistance of a phase-centered cell modeled structure by improving the electrical contact connection in the netlist generation to have a more realistic contact. By having the conditional function which has been derived in the previous page would be useful to predict the sheet resistance of a thin film and therefore able to use the correct dimension size for other purposes such as conductive films used in personal electronic devices, and solar panels.
(3.2) 3-D Cylindrical Model

Just like 2-D structure, different contact on a 3-D structure regardless of whether it’s a block-shaped or cylindrical shape would yield different geometric factor. Below shows the test bench of four different common contact on a test structure of a carbon-filled cement material.

![Figure 3.2.1 Surface contact](image1)
![Figure 3.2.2 Mesh contact](image2)

![Figure 3.2.3 Band/Ring contact](image3)
![Figure 3.2.4 Point/Single Contact](image4)

The general equation for calculating resistivity is

\[
\rho = R \times GF = \frac{R \times A}{l}
\]

for 3-D structure where thickness isn’t neglected

where \( A \) = cross sectional area of the structure and \( l \) = length/height of the structure. The general equation above would perfectly predict the resistivity of a surface contacted structure shown in
Figure 3.2.1. If a good mesh contact where the contact cover most of the surface and the current void that doesn’t flow through small part of the structure near the contact is neglected, then it’s safe to predict that the geometrical factor of a mesh contact structure is close to the geometrical factor of the surface-contact structure. However, the general resistivity equation would not correctly predict the true resistivity of the specimen in Figure 3.2.3 and Figure 3.2.4 because the geometrical factor would be different and greatly affect the resistivity measurement.

We would model the structural material with the phase-centered cell again. The difference between the 2-D cell used in the previous section compared to the 3-D cell is that there would be resistor that connects the top and bottom cell as shown in Figure 3.2.5 (instead of just 4 sides, there would be 6 surfaces with cell adjacent to each other). The goal of the task is to show that the geometrical factor would be different for a phase-centered cell modelled 3-D cylindrical structure with surface, band and point contact.

Since we are looking at a cylindrical structure, we can view the 3-D cylindrical structure as pieces of 2-D circles with 2R resistor connected vertically between the middle node of the 2-D circles pieces that is adjacent to each other vertically as shown in Figure 3.2.6. Since we do not have a circular shape of phase-centered cell, we would model the 2-D circle piece with the square shape of phase-centered cell. Imagine that we have a circle sit on an infinite number of phase-centered cell, then we can eliminate the cell that is not engulfed by the circle. Thus, during the modelling or netlist generation through the program, we would eliminate the cell where the middle node of the 2-D phase-centered cell is not present. Notice that every middle node of the cell is located inside the circle. The method to determine the number of 2-D phase-centered cell need for each 2-D circle piece would be explained in detail later in the Tool Verification section.
Figure 3.2.6 Cylindrical Structure modelled with 3-D phase centered cell.

Notice that if we assumed the cylindrical structure is surface-contacted specimen, then the top resistor (pointing up vertically) which is not shown in Figure 3.2.6 would be present and connected to the voltages source. If we assume we have mesh contact, then most of the top resistor (pointing up vertically) would be present, though few resistor would be absent because the other end would be left floating. If we assume we have band contact then all the outer resistor would be connected to the voltage source. If we assume we have point contact, then only one outer resistor would be connected to the voltage source. Next, we would see how the Visual Studio code would generate the netlist of the 3-D cylindrical structure modelled with the phase-centered cell as shown in Figure 2.6.
Tool Verification

Similar to 2-D netlist generation, Visual Studio is used to generate the netlist and pSPICE is used to run the netlist. As mentioned earlier, we would place the circle in the infinite plane of the 2-D phase-centered cell and removed any cell where the middle point or node is not inside the circle. Assuming the circle is sitting on top of a \( a \times a \) matrix of phase-centered cell where \( a \) should be an even number and as big as possible for better precision and accuracy in modelling the circle with squares. \( a/2 \) would be the radius of the circle. In the example, we assume that we have the circle sitting on 8 X 8 matrix of cells so quarter of the circle sits on a 4 X 4 cell matrix as shown in Figure 3.2.7.

![Quarter of the circle on the 4 X 4 phase-centered cell](image)

**Figure 3.2.7 Quarter of the circle on the 4 X 4 phase-centered cell**

Red-colored dots represent the middle node of the 2-D phase-centered cell. Black-colored cross represents the points coordinate of the circumference of the circle and the y-coordinate of the crosses is the half of the cells. For instance, the y-coordinate of the crosses would be 0.5, 1.5, 2.5 and 3.5. Since we know the radius and y-coordinate of the crosses, we can obtain the x-coordinate of the crosses using Eq (2) after computing its angle using Eq (1);

\[
\begin{align*}
y &= \text{radius} \times \sin(\Theta) \quad \text{---- Eq (1)} \\
x &= \text{radius} \times \cos(\Theta) \quad \text{---- Eq (2)}
\end{align*}
\]
After that, we would make comparison of x-coordinates between the crosses and the red dots row-by-row such that whenever x-coordinates of cross is more than x-coordinate of red dot, then the count of box would increment by one. We would have the count of box needed each row for quarter of a circle. We would obtain count of box needed for a half of a circle by multiplying the count of box by two. Then, we would have the schematic where we need to create a netlist for. The resistors are written in the netlist in the similar manner as the 2-D model generation with additional coding.

![Figure 3.2.8 Full circle modelled with phase-centered cell](image)

Those resistors which happen to have floating node on one side would be ignored and not included into the netlist. Thus, depending on the type of contact, some resistor may not be needed in the schematic. For instance, as mentioned when the structure is band-contacted then the resistors that are connected to the outer surface (highlighted blue in Figure 3.2.8) would be connected to the voltage source while for point-contacted then only one resistor out of all the resistors that are connected to the outer surface (highlighted blue in Figure 3.2.8) would be connected to the voltage source. The middle node of each phase-centered cell would be saved so that when the next 2-D piece of circle is written on the netlist, a 2*R resistor can be added easily.
The code is written such that user are able to decide the height of the cylindrical structure. The parameter, \( h \) is the number of 2-D circle piece in between the top and bottom 2-D circle piece. For instance, with the \( h = 1 \), there would be only one extra piece of 2-D circle in between the top and bottom pieces. Since the diameter and height of the cylindrical structure is dimensionless, to estimate the size of the structure in real world, we can use the ratio of the height to the diameter. For each unit, we would observe that the resistance is 2R in between. Thus, by taking Figure 3.2.9 as an example again, the height would be 2 and the diameter would be 8 which is four times the height. The ratio of height to diameter would be 0.25 which means depicts a pretty short cylindrical structure. The netlist generated does get verified although not shown.

![Figure 3.2.9 Example of quarter of circle 3-D structure](image)
Result and Discussion

The following result should not be taken and relate to third state-of-the-art discussed in Section 2 because the simulation done is meant for specimen with two-probe measurement.

Cell per unit \((u)\) and height given to the UI have to be odd number and more than one respectively. Parameter “\(u\)” indicate the width and length of the square where the circle lies on. Half of \(u\) would be the radius of the circle and \(u\) is basically the diameter. Below shows the result for band contact cylindrical structure by fixing \(W/L = 1\) and changing the radius by adjusting \(u\). The purpose of the simulation is to see at what ratio of height to radius does the error of resistivity start to become very small when using the standard resistivity equation \(\rho = R \frac{A}{l}\). The geometrical factor would pretty much be \(A/l\) with a non-contact specimen despite the non-surface contact.

<table>
<thead>
<tr>
<th>Voltage</th>
<th>W/L=1, (u)</th>
<th>(h)</th>
<th>Resistance (Ohms)</th>
<th>Current (A)</th>
<th>Resistivity ((\rho A/l))</th>
<th>Measured G factor</th>
<th>G factor using theoretical resistivity</th>
<th>Error in Resistivity</th>
<th>Error in G factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>20</td>
<td>20</td>
<td>2.05E+03</td>
<td>4.86E-03</td>
<td>32320.91207</td>
<td>6.36E-02</td>
<td>1.02E-01</td>
<td>61.60%</td>
<td>38.12%</td>
</tr>
<tr>
<td>10</td>
<td>20</td>
<td>50</td>
<td>3.95E+03</td>
<td>2.53E-03</td>
<td>24854.7253</td>
<td>1.59E-01</td>
<td>1.97E-01</td>
<td>24.17%</td>
<td>19.47%</td>
</tr>
<tr>
<td>10</td>
<td>20</td>
<td>100</td>
<td>7.12E+03</td>
<td>1.46E-03</td>
<td>22344.18673</td>
<td>3.18E-01</td>
<td>3.58E-01</td>
<td>11.72%</td>
<td>10.49%</td>
</tr>
<tr>
<td>10</td>
<td>20</td>
<td>150</td>
<td>1.02E+04</td>
<td>5.93E-04</td>
<td>21505.23773</td>
<td>4.77E-01</td>
<td>5.14E-01</td>
<td>7.53%</td>
<td>7.00%</td>
</tr>
<tr>
<td>10</td>
<td>20</td>
<td>200</td>
<td>1.34E+04</td>
<td>7.44E-04</td>
<td>21090.17625</td>
<td>6.36E-01</td>
<td>6.71E-01</td>
<td>5.45%</td>
<td>5.17%</td>
</tr>
<tr>
<td>10</td>
<td>20</td>
<td>300</td>
<td>1.97E+04</td>
<td>5.07E-04</td>
<td>20671.0926</td>
<td>9.54E-01</td>
<td>9.87E-01</td>
<td>3.36%</td>
<td>3.25%</td>
</tr>
<tr>
<td>10</td>
<td>20</td>
<td>400</td>
<td>2.60E+04</td>
<td>3.84E-04</td>
<td>20463.7357</td>
<td>1.27E+00</td>
<td>1.30E+00</td>
<td>2.32%</td>
<td>2.27%</td>
</tr>
<tr>
<td>1</td>
<td>30</td>
<td>19</td>
<td>1.18E+03</td>
<td>8.48E-04</td>
<td>43881.89537</td>
<td>2.68E-02</td>
<td>5.89E-02</td>
<td>119.41%</td>
<td>54.42%</td>
</tr>
<tr>
<td>1</td>
<td>30</td>
<td>49</td>
<td>2.02E+03</td>
<td>4.95E-04</td>
<td>29142.78899</td>
<td>6.93E-02</td>
<td>1.01E-01</td>
<td>45.71%</td>
<td>31.37%</td>
</tr>
</tbody>
</table>

From the simulation data, we can achieve less than 5% of resistivity error when the ratio of height to radius is 300/10 = 30. The ratio is large as one would not think of fabricating a 300 mm long specimen when the radius is only 10 mm. If the radius is 25 mm like the specimen in the [9], the specimen would need to be 750 mm long to have a resistivity error that is less than 5%. Note that it’s assumed that the two-probe measurement is used which is often not the case in most of the paper because four-point measurement is inexpensive and provides many benefits.
The simulation result for specimen with single-contact is shown below:

The purpose of showing the simulation data for single-contact specimen is to show that the error introduced is severe because the current flow is highly not-uniformly across the length or height of the specimen. Note that the highest ratio of height to radius simulated is only 60/15 = 4. It would be easy to modify the SPICE netlist script such that it has 4-probe contact which is true for most of the paper published.

A MATLAB script was also written to compute the center voltage (shown Figure 3.2.10) of the cylindrical specimen to observe the current flow. The initial thought was to compute the voltage to calculate the current density across the specimen. The current density is the highest near the contact and slowly decrease as it moves away. Any sort of defect or crack would cause variation in resistance near the crack and it can be manifested as resistance change in the specimen that is modelled as phase-centered model. By knowing the current density, we may be able to predict or calculate the resistivity change due to the resistance variation that is caused by the crack. Further research is needed to compute the resistivity due to change in height and the defect.

Figure 3.2.10 MATLAB center voltage of a cylindrical specimen cross-section
So far, we have been discussing about the resistivity measurement; we can also relate the simulation data with the gage factor. Gage factor is the rate of resistance change due to strain. Since we can simulate the model with any height, once we know or even estimate the height of the specimen due to the strain we are going to apply, we would know the $\Delta R$. That is also one of the advantage of the phase-centered model which is able to simulate up and predict the gage factor ahead.

### (3.3) State-of-the-Art Model

In this section, we would model the specimen in [5] with phase-centered model to clarify that the type of contact used would cause error in the resistivity measurement.

Figure 3.3.1 shows that the specimen dimensions assuming the contact is 2 mm wide. If the contact is wider than 2 mm we can expect the error to increase because the distance between the outer current contact and the inner voltage contact would decrease.

Assuming that $1 \times 1 \times 1 \text{mm}^3$ is equal to a 3-D phase center cell and we are looking at one end of the outer current contact, we would have the resistive network as shown in Figure 3.3.2. The script and model is verified by hand with a $2 \times 2 \times 50$ structure by setting $W$ and $L$ equal to 2.

Figure 3.3.2 Specimen [5] modelled with phase-centered cell
We can also increase the number of the model cell to four for a 1 x 1 x 1 mm$^3$ to better understand how the current density is distributed in the specimen but we will leave that for future research. The objective here is to compute the error introduced when you use the general resistivity equation on a non-surface contact specimen. It shows that the geometrical factor is not $A/l$ and the true geometrical factor which is about 0.1773 is 5.28% lesser than $A/l$.

In order to prove the phase-center model accuracy, we would need two similar specimens from state-of-the-art [5]; one with band contact as fabricated and one with modified surface or mesh contact for the current and voltage contact. Since we are very sure that the geometrical factor of the surface contact specimen is $A/l$, the prediction is that we would be able to see that the specimen with band contact would have 5.02% lesser resistivity.

<table>
<thead>
<tr>
<th>Current (mA)</th>
<th>W/L</th>
<th>Resistance (Ohms)</th>
<th>Voltage (V)</th>
<th>Resistivity</th>
<th>Measured G factor (using standard equation)</th>
<th>G factor using theoretical resistivity</th>
<th>Error in Resistivity</th>
<th>Error in G factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>3546</td>
<td>3.546</td>
<td>18996.42857</td>
<td>0.186666667</td>
<td>0.1773</td>
<td>5.02%</td>
<td>5.28%</td>
</tr>
</tbody>
</table>

True resistivity = 20 kOhms

\[ \text{R} \times 15 \times 15 / 42 \]
(4.0) Conclusion

Many different kinds of contacts on the smart concrete can be done and some can be valid depending on the application. For example, if we want to characterize the rate of resistance change due to strain using any kind of contact in the laboratory; that’s fine as long as same contact is used in the application for correlation purposes. Some applications that are built based on the resistivity of the material would prefer to have an accurate resistivity or conductivity measurement; therefore surface-contact is recommended in the lab.

In this report, we have looked first, at how a non-surface contact specimen would cause the resistivity error due to the misunderstanding that the geometrical factor is $A/l$ regardless of the contact made on the specimen. Secondly, we looked at how the gage factor can be incorrectly interpreting as a constant if someone assume that the rate of resistance change is linear which is often times not the case due to the natural phenomena such as deformation. Despite that, if the range of strain is still within the range of interest then the gage factor should still be correctly predicted just like what is discussed in [9].

This research work mainly focuses on the first measurement of resistivity aspect. The objective is to show that with a non-surface contact, the geometrical factor would not be $W/L$ (thin film) and not $A/l$ (cylindrical concrete) and show how much error would be introduced if the general geometrical factor is used. The research work data is not considered as the data for the second measurement of gage factor because strain or $\Delta L/L$ is not analyzed in the simulation process.
(5.0) References


