A Finite Element Study of Contact Resistance for a Flat Bilayered Au/MWCNT Surface

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***Abstract*—A gold-coated multi-walled carbon nanotube (Au/MWCNT) composite has been used as a contact material for low current MEMS application, and it has been shown that the application of the composite significantly improves the contact lifetime. To investigate the benefit of the composite on the mechanical behavior of electrical contact, a finite element (FE) contact model is developed, linked to the modified nano-indentation test, with a gold-coated 2 mm diameter stainless steel ball making contact with a Au/MWCNT or Au surface. The gold penetration into MWCNT is modeled as a bi-layered structure, with the top layer modeled as an elasto-plastic mixed material, and the under layer as pure MWCNT. The contact area is calculated from the modeling and the contact resistance is evaluated, and the results are compared to the experimental results. The use of Au/MWCNT results in a larger contact area and thus a smaller contact pressure than a gold-gold contact, which is assumed to improve the lifetime of electrical contacts.**

***Keywords*—electrical contacts; bi-layered structure; Au/MWCNT composite.**

I. Introduction

Gold-coated multi-walled carbon nanotubes (Au/MWCNT) composite has been used as a surface material of electrical contacts, for low current switching applications [1-4]. Compared to the counterpart gold-gold contact, the use of Au/MWCNT can provide a relatively low and stable contact resistance, and more importantly, it can prolong the lifetime of the electrical contacts significantly [3, 5].

The multi-walled carbon nanotubes are vertically aligned, like a forest. The nano-indentation show that the composite exhibits a high compliance to the gold metal conductive layer, and conform to the indenter probes, which reduces the impact of mechanical load [6]. By assuming the composite as a single material, the material properties can be calculated form the nano-indentation tests [6]. The evaluated elastic modulus is less than 1GPa, and the hardness is up to 1 MPa [6], which are much smaller than that of metallic material used in MEMS switches, like sputter Au and Au-alloys, whose hardness is about 1-2 GPa [8], or Ru and Rh, 10-25 GPa [9].

Due to the vertical gaps between carbon nanotubes, the gold film cannot form a uniform layer on the surface, but penetrates into the MWCNT forest [10]. A finite element contact model has been developed, and it is shown that the composite is best to model as a bi-layered structure, where the top layer is modelled as gold and MWCNT mixed material, and under layer as pure CNT [11, 12].

To investigate the electrical properties of the Au/MWCNT composite, a modified nano-indentation setup is developed, and the standard diamond tip is replaced by a stainless steel (SS) hemispherical ball. The modified tip allowed for integrating a four-wire measurement arrangement to measure the electrical contact resistance [7].

A finite element model is developed, linked to the modified nano-indentation tests. The contact area is evaluated from the modeling, and using the electrical resistivity measured with the 4-points probe method, we are able to calculate the contact resistance and compare to the measured values.

II. Sample Preparison and Expeeiments

A. *Sample Preparison*

Two contact pairs are investigated in the study, one is Au-Au contact, and the other is Au-Au/MWCNT contact. In both cases, the contact pair consists of a 2mm diameter stainless steel hemispherical probe and a substrate (see Fig. 1), which is with either Au/MWCNT composite, or gold-coated.

The stainless steel probe is sputtered with a 10 nm thick Cr layer, followed by a 500 nm thick Au. The counterpart gold sample is fabricated by sputtering 500 nm gold directly on to a silicon substrate with a 20 nm Cr adhesive layer.

The fabrication of the Au/MWCNT composite has been reported in [6]. Vertically aligned MWCNTs are growing using thermal chemical vapor deposition (CVD) method on a silicon wafer, and then a gold layer is sputtered onto the top of the nanotubes forest. The Au/MWCNTs composite in this study is gold coated on 50 μm high MWCNT forest, and three thicknesses of gold are studied: 300 nm, 500 nm and 800nm. A SEM image of a 500nm thick gold coated sample is presented in Fig. 2, showing the penetration of gold into MWCNT.

B. *Experimentals Setup*

The NanoTest Vantage system of Micro Materials® is used for the nano-indentation test. To integrate the 4-wire measurement arrangement in the nano-indentation system, the standard diamond contact tip is replaced by 2 mm diameter stainless steel hemispherical probe, which is also consistent with previous experimental studies [1, 4]. Fig. 1 shows the principle of the measurement system. The contact resistance is measured using a National Instrument Data Acquisition (DAQ) card, which applies the current source of 100 mA, and measures the voltage drop. Each sample was indented with 10 different loads from 0.2 mN to 2mN, and each indent was at a new surface location, separated by 500 µm distance [7]. The loading rate was kept constant and the maximum load was held constant for 30 seconds for each indent. The electrical data were only read during the static stage. Using this system, the contact force and the resistance can be measured simultaneously.

The sheet resistance of the composites are measured with a 4-point probe equipment Napson RT70V/RG-7.

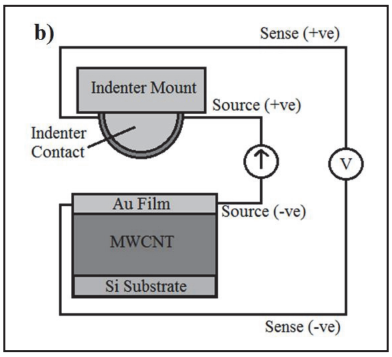

Fig. 1 Four-wire measurement system integrated into the nano-indentation, to measure the contact resistances. The current source and contact voltage drop are supplied and measured by a data acquisition module. (After [7])

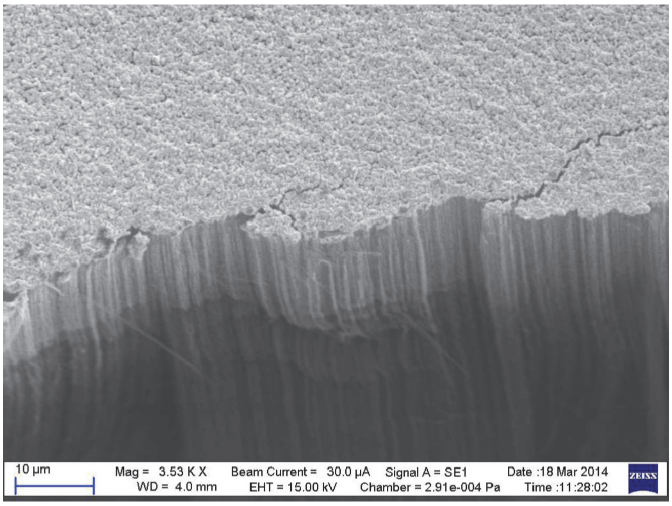

Fig. 2 SEM images of a 500nm Au/50 µm CNT composite, showing the penetration of gold into MWCNT.

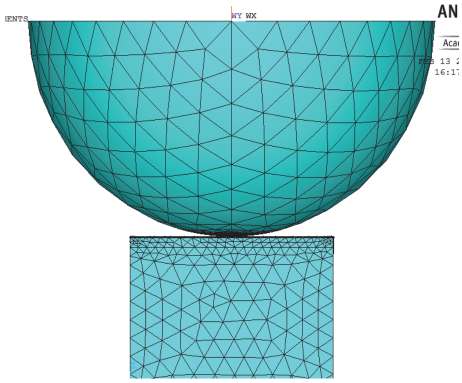

Fig. 3 Geometry of a finite element model of a 2 mm ball making contact with a Au/MWCNT substrate.

III. Finite ELement Modeling and Calculation

A. *Finite Element Smooth Contact Model*

A finite element smooth contact model is developed using ANSYS[14.5], linked to the modified nano-indentation test. The model consists of a 2 mm diameter ball making contact with a substrate, as shown in Fig. 3. Previous studies [11, 12] have used a 200µm ball. The adhesive Cr layer is not included in the modeling. The size of the substrate is modelled as 2 × 2 mm, and the thickness of the silicon is 675 µm. Two types of contact pairs are modelled, corresponding to the experiments: Au/MWCNT composite on silicon substrate for Au-Au/MWCNT contact, and gold coated silicon substrate for Au-Au contact.

To simplify the modeling, the gold coated stainless steel ball is modelled as a gold solid ball. For the Au-Au/MWCNT contact, simulations results showed little difference between a SS ball and a gold ball, as the Au/MWCNT surface is very soft [6]. For the Au-Au contact, the differences between a SS ball and a gold ball is not negligible, and this will be addressed in the results.

The meshing elements are the same as in previous studies [12]. The top surface of the Au/MWCNT composite or gold film is modeled as a contact surface, and is meshed with the 3D surface-to-surface contact element CONTA174. The spherical surface of the probe ball is modeled as a target surface, and meshed with the target element TARGE170. The volumes of the substrate and the ball are modeled using 3D tetrahedral solid element SOLID187.

The augmented Lagrange method is used to seek the contact and large deformation is activated in the calculation. A uniform pressure is applied vertically on the top surface of the hemisphere, and a loading-unloading cycle is applied, with the contact force increasing gradually from 0.2 mN to 2 mN in 10 steps. It should be also noted that roughness is not included in the modeling, and will be investigated in further study.

B. *Material Properties*

It is shown in previous study [11, 12] that the Au/MWCNT is best modelled as a bi-layered structure. Considering the gold penetration into MWCNT (see Fig. 2), the top layer is modelled as a gold and MWCNT mixed material, whereas the under layer is modelled as pure CNT. The thickness of top layer is set as 6±1.5 μm, which is the thickness of the penetration of gold. The material properties in FE models are listed in Table I. The silicon substrate and the under layer of Au/MWCNT (i.e. pure CNT) are modelled as elastic material. Gold and the top layer of Au/MWCNT are modelled as elasto-plastic material, and the yield strength is defined as $H/2.8$, where H is the hardness of the materials. It should be noted that the material properties of the bi-layered structure are based on the extreme limits of the nano-indentation tests in [6], to try to capture the properties of the two layers in the modelling, and they are different from the values calculated automatically from the indentation tests in [6, 7], more details about the material properties of bi-layered structure see [11, 12].

TABLE I. MATERIAL PROPERTIES IN FE MODELING

Material		Material Properties		
		Elastic modulus (GPa)	*Hardness (GPa)*	*Poisson's ratio*
Au		80	1.008	0.42
Si		162.5	-	0.223
Au/ CNT	Top layer	1.242	4.05	0.21 [12]
	Under layer	50.82E-3	-	0[13], [14]

C. Contact resistance calculation

The contact resistance is calculated with Holm function $R_c = \rho/2a$, where a is the contact radius, and ρ is the equivalent resistivity of a contact pair, and equaling to the average resistivity of two parts for a bi-material contact pair, i.e. $\rho = (\rho_1+\rho_2)/2$.

IV. RESULTS AND DISCUSSIONS

A. Experimental results

Fig. 4 plots the results of contact resistance as a function of contact forces for Au-Au/MWCNT contact pair. As expected, the contact resistance decreases gradually as the force increases. The contact resistance also reduces with thicker gold layer on the top. The gold layer has double-edged effects on the contact resistance. On one hand, the electrical conductivity increases with thicker gold, as Fig. 5 shows, which reduces the resistance; On the other hand, the surface becomes harder and less compliant with thicker gold [6], which will reduce the contact area, resulting in higher resistance. Two effects work together, making the contact resistance decreases with thicker gold layer, as shown in Fig. 4.

Fig. 5 plots the measured sheet resistance (R_S) of Au/MWCNT composite from Napson 4-points probe measurement. For the Au/MWCNT composite, assuming the thickness of top layer of the bi-layered structure is the thickness of the conductive layer (t), the electrical resistivity can be calculated, as $\rho = R_S \times t$, and the results are listed in Table II, also the results for 500 nm gold only. The resistivity of 500 nm gold (last row of table II) is found to be significantly higher than that of bulk gold, and about twice of the measured values for sputter gold of same thickness from [15], i.e. 42.7 nΩ×m. This could due to the contamination, considering the sample has been stored in an atmosphere environment for a month.

In [7], the electrical resistivity is also calculated with Holm equation from the measured resistance, assuming the plastic deformation,

$$\rho = 2R_C\left(\frac{F}{\eta\pi H}\right)^{1/2} \qquad (1)$$

Where ρ is the electrical resistivity, R_C is the contact resistance, F is the contact force, η is the reduction coefficient of electrical resistivity due to the contamination or insulating films, and H is the hardness of softer material in a contact pair. It should be noticed that the calculation in [7] is assuming the Au/MWCNT composite as a single-layer material, whereas the composite is modelled as a bi-layered structure in the finite element modeling, and the deformation mechanism is different form the purely plastic deformation (see discussion in IV. B). To calculate the contact resistance based on the simulated contact radius, the measured sheet resistance is used instead of the values from [7].

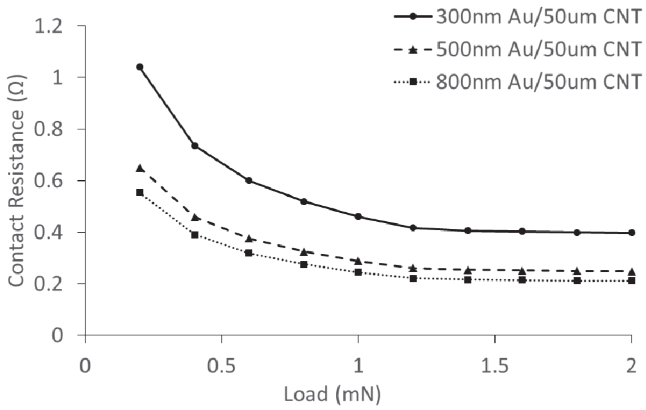

Fig. 4 Contact resistance results from nano-indentation tests as a function of contact forces, for the composites with different layer configurations.

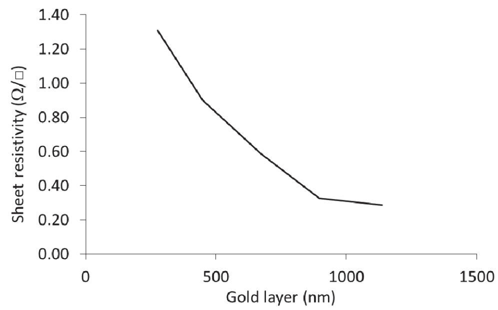

Fig. 5 Sheet resistance as a function of the thickness of nominal sputtering gold layer, the gold is coated on 50 μm CNTs.

TABLE II. ELECTRICAL RESISTIVITY OF SAMPLES WITH DIFFERENT LAYER CONFIGURATION

Au/CNT (nm/μm)	Electrical properties		
	Sheet resistance (Ω/□)	*thickness of film (μm)*	*Resistivity (nΩ×m)*
300/50	1.196	4	4721.7

Au/CNT (nm/µm)	Electrical properties		
	Sheet resistance *(Ω/□)*	*thickness of film* *(µm)*	*Resistivity* *(nΩ×m)*
500/50	0.696	6	4378.5
800/50	0.096	8	2435.3
500 (Au only)	0.175	0.500	87.5

B. Simulation Results

1) Au-Au contact pair

For a Au-Au contact pair, the deformation behaves elastically for the whole loading process, and the deformation is 6 nm at 2 mN load with a gold target ball, resulting in a contact radius of 2.3 µm, as shown in Fig. 6. The calculated contact resistance of Au-Au contact is plotted in Fig. 7, with the stainless steel (SS) ball and the gold ball. The maximum difference between two materials are about 10%. The experimental results are 0.4-0.04 Ω for the load ranging of 0.2 mN to 2 mN [7], and about 5-10 times higher than the calculated ones with gold ball, i.e. 0.037-0.020 Ω (see Fig. 7). The difference is assumed to come from the hydrocarbon, as discussed in [17], and also the effect of thin film resistance [15,19].

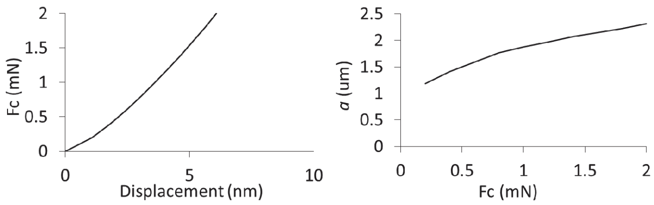

Fig. 6 Simulation results of Fc-D and *a*-Fc results for the Au-Au contact, the simulation is with gold solid ball, and *a* is the contact radius.

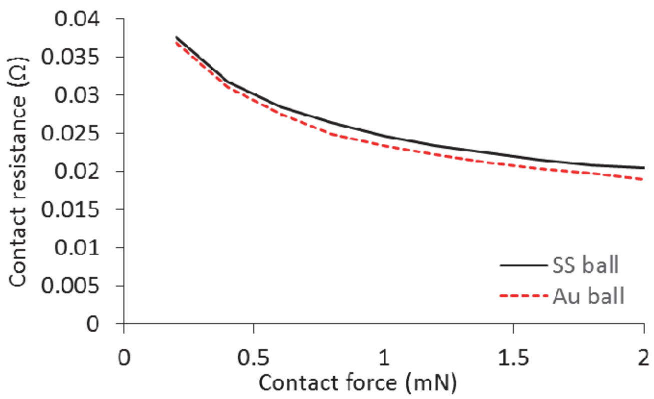

Fig. 7 Comparison of the contact resistance from the simulation and the experiments.

2) Au-Au/MWCNT contact pair

Fig. 8 plots the simulated force-displacement results of Au-Au/MWCNT contact pairs. As expected, because the top layer is harder than the CNT, the deformation is smaller with thicker gold coated on CNT. Also, the contact pair behaves less elastically with thicker gold, and more residual deformation is found after unloading. The critical displacement ω_c, at which the deformation changes from elastic to elastic-plastic regime, can be calculated by [16]:

$$\omega_c = \left(\frac{\pi K H}{2E}\right)^2 R \qquad (2)$$

Where H is the hardness of material, K is the hardness coefficient, can be calculated by K=0.454+0.41ν, ν is the Poisson's ratio. E is the Hertz elastic modulus and be defined by (3), and R is the radius of indenter probe.

$$\frac{1}{E} = \frac{1-\nu_1^2}{E_1} + \frac{1-\nu_1^2}{E_2} \qquad (3)$$

For the Au-Au/MWCNT contact, the critical deformation calculated with (2-3) is 7.65 nm, and the corresponding contact force is 0.0036 mN, which is lower than the smallest load in the modeling, suggesting that the top layer has started plastic deformation at the very beginning of loading process. However, due to the soft CNT under layer, the plastic deformation is restrained to a small value, as shown as the residual deformation in Fig. 8.

The contact radius is calculated from the simulation, and the results of force-contact radius for different samples are plotted in Fig. 9. Once again, because the Top layer is harder than CNT under layer (see Table I), the contact radius decreases with thicker gold.

Compared to the Au-Au contact pair, the Au-Au/MWCNT contact results in a much larger contact area (Fig. 9), and thus a smaller contact pressure, which is assumed to improve the lifetime of electrical contacts.

The contact resistance can be calculated using Holm function with the simulated contact radius and the measured electrical resistivity (see Table II). Fig. 10 plots the calculated contact resistance as a function of contact forces for different samples, and the values are found smaller than the measured resistances (see Fig. 4).

It should be noticed that the FEA model used is based on a smooth contact with no roughness. With surface roughness the effective contact area will be reduced further thus leading to an increase in the constriction and thus contact resistance. Also, the thin film effect is not included in the electrical resistance calculation, which will also result in a higher contact resistance [15, 19].

The calculated Fc-Rc curves show the same trend as the measured values (Fig. 4), a factor of 8.5 is then used to multiply the calculated resistances of 500nm Au/50 µm CNT composite (labelled as '505' in figures), and the multiplied values are plotted in Fig. 11. Similarly, factors of 12 and 13 are used for the composite withe 300 nm Au and 800 nm Au coated on 50 µm CNT, respectively. These are arbitrary values which show that the trends are matching, and account for the surface roughness and thin film effect which is not included in the current model.

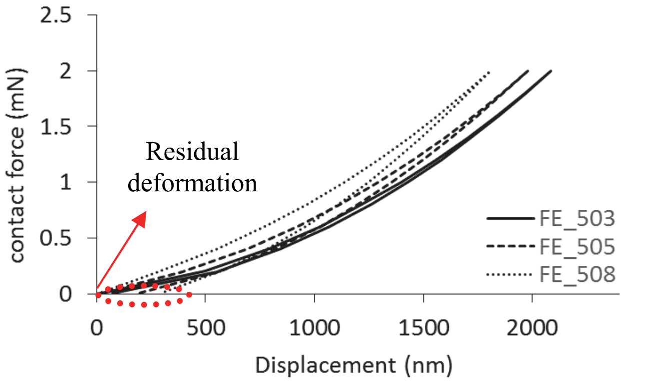

Fig. 8 Simulated force-displacement results for the samples with different layer configuration. 503, 505, 508 in the legends means 300 nm, 500 nm and 800 nm gold coated on 50 µm CNT.

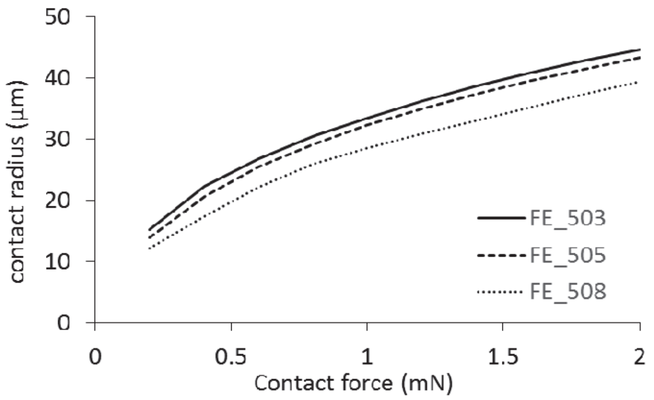

Fig. 9 Simulated force-contact radius results for the samples with different layer configuration.

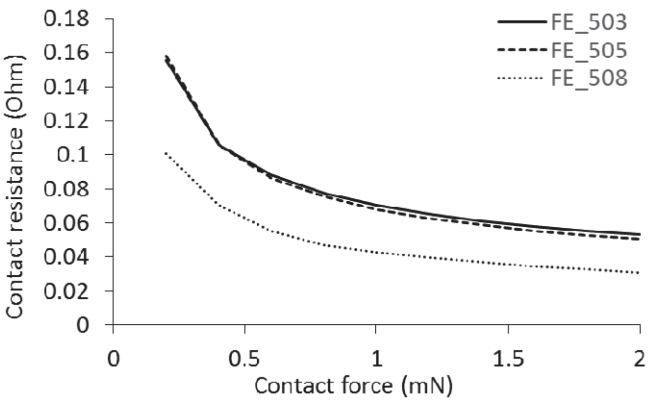

Fig. 10 Calculated contact resistance based on the FE modeling and the measured sheet resistance, for the composites with different layer configurations.

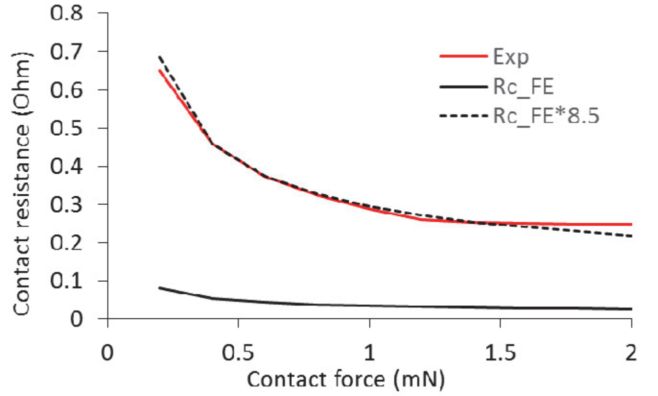

Fig. 11 Comparison of the contact resistance from the simulation and the experiments for the composite 500 nm Au/50 µm CNT, also the simulated one with an applied factor to account for surface roughness and thin film effect.

C. Discussions

For the differences of the contact resistance between the simulation and the experiments of Au-Au/MWCNT contact pair, there can be other reasons.

One is the contact radius from the finite element modeling. Fig. 12 shows the SEM images of the failed site at different force load for the composite 500 nm Au/50 µm CNT [5]. A circle is used to fitting the failed site, and the circle can be considered as the approximate failed contact area, thus the radii of failed area can be calculated, and the results are plotted in Fig. 13, alongside with the simulated contact radii. The simulated contact radii are found to be smaller than the failed radii. However, it should be kept in mind that the switching tests are done with the current of 100 mA, which will result in larger failed area than the cold switching [18], and there is no thermal effect included in FEM; also the failed area is found to be larger than the contact area at the very beginning of switching tests [18]. By dividing the failed radii by 2, the results match the simulated contact area better. This suggest that the simulated contact area is comparable to the real contact area.

On the experiments side, the contamination on the surface is not avoidable. It is difficult for gold to generate oxide film on the surface, but it is very likely to form a hydrocarbon layer [17].

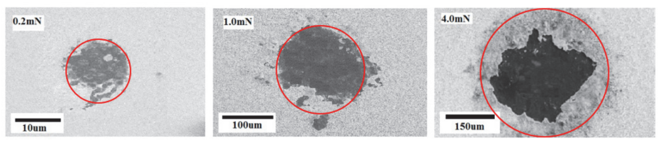

Fig. 12 SEM images of the failed sites on the 500 nm Au/50 µm MWCNT composite for loads 0.2 mN, 1 mN and 4 mN (after [5]).

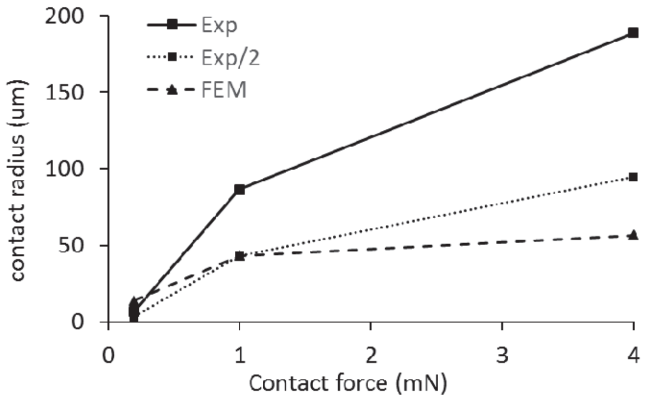

Fig. 13 The simulated contact radius for the loads 0.2 mN, 1mN and 4 mN, compared to the values from the fitting circles of the failed area in Fig. 12.

V. CONCLUSIONS

A finite element contact model of a smooth surface is developed, linked to a modified nano-indentation set up for the Au-Au/MWCNT contact and Au-Au contact. The Au/MWCNT is modelled as a bi-layered structure as previous research proved. Contact area is obtained from the modeling, and the contact resistances are calculated based on the simulated contact area and the measured sheet resistance. The calculated force-resistance results show the same trend as the experimental results, but are about 10 times smaller than the experimental ones, for the Au-Au/MWCNT contact, as well as Au-Au contact. The reasons of the differences are discussed. On the simulation side, a model including surface roughness and thin film effect will result in higher contact resistances, whereas the carbon contamination is considered to be the main reason for the high contact resistance in the experiments.

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