International Journal of Nanoelectronics and Materials
Volume 15 (Special Issue) March 2022 [483-494]

Optimal Prediction on Stretchability Thickness of Graphene Conductive Ink by Numerical Approach

Ameeruz Kamal Ab Wahid[1,2], Mohd Azli Salim[2,3*], Nor Azmmi Masripan[2,3], Adzni bin Md. Saad[2,3], Mohd Zaid Akop[2] and Chonlatee Photong[4]

[1]Jabatan Kejuruteraan Mekanikal, Politeknik Sultan Azlan Shah,
Behrang Stesyen, 35950 Behrang, Perak, Malaysia
[2]Fakulti Kejuruteraan Mekanikal, Universiti Teknikal Malaysia Melaka,
Hang Tuah Jaya, Durian Tunggal, 76100 Melaka, Malaysia
[3]Advanced Manufacturing Centre, Universiti Teknikal Malaysia Melaka,
Hang Tuah Jaya, 76100 Durian Tunggal, Melaka, Malaysia
[4]Graduate School, Mahasarakham University, Khamriang Sub-District,
Kantarawichai District, MahaSarakham 44150, Thailand

ABSTRACT

This study determines the optimal graphene conductive ink thickness performance using maximum principal elastic strain and Von Mises stress analysis. It was performed by using finite element analysis (FEA) modeling approach. Previous studies of the comparative difference in strain and stress induced by stretching a screen-printed straight-line pattern (baseline) and a curved wave pattern using graphene conductive ink as material prompted the FEA modeling. Six straight-line patterns of conductive ink with the thickness from 0.05 mm to 2.0 mm were developed for FEA analysis. The mechanical properties from the previous study were used and FEA modeling was utilized to determine which thickness had higher elasticity by measuring the maximum principal elastic strain and equivalent stress (Von Mises stress). A modeling approach based on previous research of conductive inks patterns related to elasticity theories was proposed to be applied for the varying thickness effect of the 20% elongation stress. The fatigue in the pattern line's cross-section area was used to optimize the strain and stress difference during stretching. As the pattern thickness increased, the strain and stress value at sharp corners, as illustrated in the cross-section view, decreased. The 0.10 mm thickness gave a better thickness for graphene conductive ink because even it had a small thickness but good maximum principal elastic strain, which was 0.5451 and Von Mises stress of 8,060 MPa. After 20% elongation, the maximum principal elastic strain and Von Mises stress decreased for the thicknesses of 0.05 mm to 2.00 mm with the values of 0.5454 to 0.5449 and 8,078.9 MPa to 7,806.7 MPa, respectively. The mechanism clearly explains Hooke's law, which states that mechanical stress is directly proportional to strain.

Keywords: Graphene, conductive ink materials, maximum principal elastic strain, Von Mises stress

1. INTRODUCTION

Stretchable conductive ink is a unique technology for implementing electronics on clothing, accessories, and medical devices. The ink can be used to create a thin stretchable and flexible form-fitting circuit in wearable devices that provides both comfort and freedom. According to [1], wearable electronics applications have various obstacles, mainly due to the device's unobtrusiveness. Stretchable electronics serve as a major technique for reducing obtrusiveness. Stretchable electronics is a device that can be compressed, twisted, and adhered to a very complex shape. The mechanical and electrical compliances of stretchable electronics can pave the way for the advancement in health care, entertainment, and energy applications [2]. Because the

*azli@utem.edu.my

stretchable platform is always exposed to cyclic motion and deformation, it provides an advantage for widespread and unobtrusive sensor and display applications [3]. A circuit's flexibility allows it to be placed on an uneven surface or to change over time. Because of its flexibility, a circuit can be placed on an irregular or regularly changed surface.

Printed circuit boards (PCBs) are used in almost every industry nowadays, and they are still evolving into new ones and enhanced applications. In today's modern world, PCBs are the main functional centers of most electronics. In order to be aware of various trade-offs with different types of PCB materials and processes, PCB designers must consider many of these effects for higher frequencies, such as minimizing dielectric constant, copper roughness, and thickness variations, as they can all negatively impact the performance of the design [4]. When subjected to extreme pressure, the board is physically brittle or easily be broken. Low manufacturing costs, long-term durability, environmentally sustainable production processes, recyclability, lower energy consumption, improved efficiency, and electronic integration as part of other structures that are all essential new electronic properties [5].

Stretchable electronics technology has various advantages, which include reducing final product size and weight, greater circuit density, and elimination of cumbersome connections and wiring [6-8]. Stretchable electronics using screen printable conductive inks on stretchable substrates is a promising breakthrough. The human body is flexible, curvy, and stretchable. Electronic equipment must be compatible with the human body in order to function efficiently inside, on, and around it. Stretchable electronics technology varies from conventional integrated circuits, which are rigid, planar, or inflexible [9]. Nanoparticle inks can be manufactured in huge quantities, distributed at high concentrations, and produced electrical conductivities that are relatively good [10]. According to [11], advances in mechanics and materials provide routes to integrated circuits that have the electrical properties of traditional, rigid wafer-based technologies while also allowing them to be stretched, compressed, twisted, bent, and deformed into arbitrary shapes. The flexible electrical circuit must be insufficiently thin due to these structures and bending strains that decrease linearly with thickness. Due to microscopic changes in morphology or an increase in distance between the conductive fillers, the electrical resistance changes under mechanical strain [12–13].

Graphene has become a major source of research due to its numerous appealing features, including excellent electrical conductivity, mechanical efficiency, and elasticity [14]. Because of its exceptional electrical, mechanical, and thermal properties, graphene as a filler has the potential to increase the efficiency, reliability, and durability of numerous applications for the future generation of electronic devices, composite materials, and energy storage devices [15]. Graphene has the most potential as a high-performance absorption material because of its numerous appealing qualities, such as distinctive structural effects, high specific surface area, and high conductivity [16]. Strain sensors made of graphene can detect a wide range of strains induced by stretching, bending, and torsion, all of which are required for sensors to detect human body movements [17]. It is important to know the graphene content. Depending on the cross-section measurement, the graphene content can be calculated [18]. More percentages of graphene will result in more deformation and can show a significant impact on the results. An experimental investigation was conducted to explore the effect of the conductive ink thickness on the strain and stress in a circuit. The strain/deformation of an elastic object or substance is proportional to the stress applied, according to Hooke's law. Due to the fact that general stresses and strains may have numerous independent components, the "proportionality factor" may no longer be a single real value.

However, the assessment of stress induced by the attachments and the effect of conductive ink thickness and resiliency on stress dissipation is lacking. The maximum principal elastic strain and equivalent stress (Von Mises stress) can be estimated using experimental results as an input parameter for material properties in FEA modeling. The fatigue in the pattern line's cross-section area could also be used to optimize the strain and stress difference during stretching. Thus, the focus of the research was to show how stretching a screen-printed straight-line pattern with different thicknesses of graphene as conductive ink causes a significant variation in strain and stress. The maximum principal elastic strain and Von Mises stress produced by FEA modeling can be used to estimate them. The stress distribution in the conductive ink patterns was evaluated using Von Mises stresses because a larger Von Mises stress indicates a greater probability of failure [19]. Following the accomplishment of the above-mentioned objective, an attempt was made to find the best-printed conductor thickness with the optimum stretchability using maximum principal elastic strain and Von Mises stress acquired from FEA modeling.

1.1 Previous Studies on Pattern Analysis

[20] produced a graphene conductive ink formulation with various filler loading percentages to find and select the most functional conductive ink. The conductive ink was made with GNP as a filler, Araldite® as an epoxy resin, and Huntsman polytheramine as a hardener, all of which were used without modification. The electrical characterization analysis has obtained the sheet resistance values by using the In-Line Four-Point Probe. Then the sheet resistance data were analyzed to get the volume of resistivity for the FEA analysis application. For mechanical characterization analysis, a sample from the electrical characterization was used. Mechanical characterization study can be used to determine the material's strength that can be used in FEA mechanical properties.

Numerical workbench tools were used to perform the FEA of the patterns. Patterns were designed in CATIA modeling software, then converted as IGES files and imported into the workbench software. The model was then fine-meshed, and the computing process was expected to take a decent length of time. FEA of ink stresses on a wavy pattern and a straight-line screen-printed pattern were utilized to simulate the strain and stress behavior of the circuit under mechanical loads using ANSYS software. According to [20] FEA data, the straight-line pattern's stretchability after 20% strain exposure was 0.5451 and 8,060 MPa for maximum principal elastic strain and Von Mises stress, respectively.

[21] investigated the buckling properties of a fully profiled sandwich structure made of a polyethylene terephthalate (PET) substrate and thicker multi-wall carbon nanotubes (MWCNT) bonded together with distinct adhesives. Researchers used Rayleigh-Ritz and Comsol Multiphysics software was used to predict the critical buckling stress for various layer thicknesses of MWCNTs in their investigation. The finite element simulation exposed that a thinner MWCNTs/PET was more stable. The FEA results demonstrated the reduced thickness from 0.50 mm to 1.00 mm reduced Von Mises stress with corresponded values of 1.56078 GPa and 0.979473 GPa, respectively, proving Hooke's law theory of elasticity.

1.2 Mechanical Properties

The main objective of mechanical characteristics analysis is to determine the strength of a material. In nanocomposite materials, equal loadings have made a considerable and stable contribution to nanomechanical properties [22]. A nano-indentation machine was used to test the materials' hardness. Nanoindenter testing is based on the employment of a high-resolution actuator to push an indenter into the test surface, as well as a high-resolution to continually quantify the penetration that happens [23]. Because Young's modulus and maximum depth are feasible for this experiment, a maximum load of 150 mN was utilized based on previous experiments [20].

The following are the steps in a typical indentation experiment: (1) approaching the surface, (2) loading to 150 mN of peak load, (3) maintaining the peak load for 5 seconds, (4) unloading from 150 mN of maximum force, and (5) completing the unloading procedure. The holding phase was included to eliminate the effect of creep on the unloading characteristics because the unloading curve was utilized to obtain the elastic modulus of the material. One of the most interesting findings from this experiment was the shape of the hardness impression when the indenter was unloaded, and the material elastically recovered.

The maximum load was determined by the depth of penetration of the indenter into the surface [22]. To avoid the formulation from breaking and rupturing, and therefore losing its protective effect, the depth of the nano-indentation was carefully regulated. When measuring thin films, the indenter may penetrate too deeply if the load is too high. This becomes a major concern because the results would be influenced by the substrate's properties. The roughness of the specimen surface will influence the results if the load is too low. In addition, the elastic behavior of printed ink can also be determined using the nanoindenter test.

2. METHODOLOGY

2.1 Model Configuration

The research was carried out using data from earlier tests and FEA models. Graphene material characteristics from previous research, as well as simulated maximum elastic strain and Von Mises stress results, were utilized. The finite element program ANSYS Workbench was used to run the stress analysis simulations. The FEA model was created with patterns with an ink thickness of 0.1mm. A half model was used due to symmetrical geometry in the X-direction. [24] used a 20% of stretch to assess the lifetime of stretchable conductors under a specific strain. Figure 1 shows how 20% of elongation stress was applied uni-axially along the X-axis for this study.

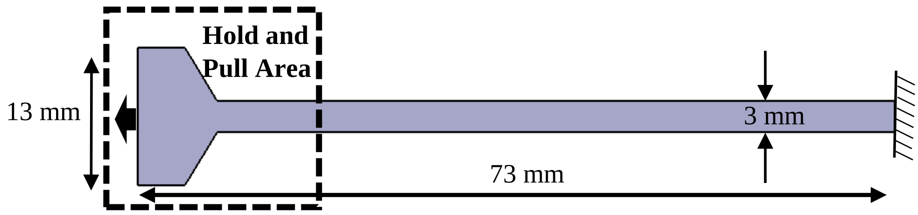

Figure 1. FEA straight-line model [20].

2.2 Finite Element Analysis (FEA)

The findings were determined by numerically solving the governing equations at each node using the finite element method, which was generated from a mesh. The fine mesh option was applied with the sine wave model preference, and the computing process took a decent amount of time, as shown in Figure 2. The finite element was created using an element size of 1.9 x 10^{-4} mm that generated from 6,915 to 76,065 elements depending on the thickness of the patterns.

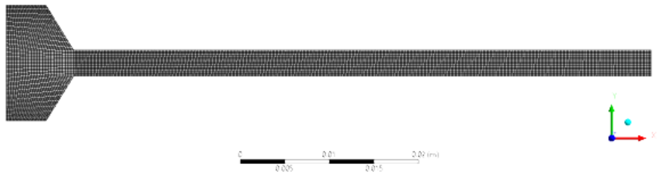

Figure 2. Mesh model of the straight-line sample [20].

The strain and stress behavior of the circuit under mechanical loading was simulated using FEA of ink stresses on a straight-line screen-printed pattern using ANSYS software. To imitate the screen-printing process, the ink was simulated as a layered structure. The goal of the study was to determine the thicknesses effect of straight-line printed shapes on the stresses of the printed pattern. Similar printing and curing procedures were used to print the forms on the same substrate. This research aimed to determine which thickness would have the least amount of strain and stress based on its maximum value respectively. The cross-sectional observations at maximum value strain and stress points were also discussed. The values for the material properties used in this paper were obtained from previous studies. The material properties used for this FEA research are presented in Table 1.

Table 1 Graphene properties used for FEA [20]

Materials	Properties				
	Young's Modulus (Pa)	Poisson's Ratio	Density (kg/m^3)	Thermal Conductivity (W/m °K)	Resistivity (Ω.m)
Graphene	15.49×10^9	0.149	2200	5300	0.249

3. RESULTS AND DISCUSSION

3.1 Percentage Change in Conductive Ink Thickness

Table 2 shows the percentage change in conductive ink thickness due to maximum principal elastic strain and Von Mises stress. The comparison of the percentage change of the graphene conductive ink thickness shows that the strain and stress of most of the samples decrease with the increase of the conductive ink thickness. The percentage change value of samples (a) and (b) is -0.06% for maximum principal elastic strain and -0.23% for Von Mises stress. It can also be stated that sample (b) decreases by 0.06% of the maximum principal elastic strain and decreases by 0.23% of Von Mises stress as compared to sample (a). Through the observation in Figures 3 and 4, the positions of the maximum value for the strain and stress are almost at the same spot, which is on the outside of the sharp corners of the samples. The pattern may be catastrophically broken at the corner area due to the severe stress created during this hogging condition [25]. The following equation was used to solve all percentage changes:

$$\%\ Change = \frac{(V2 - V1)}{[V1]} \quad (1)$$

where:
V1 = Initial maximum principal elastic strain or Von Mises stress value
V2 = Final maximum principal elastic strain or Von Mises stress value

According to Hooke's law theory of elasticity, mechanical stress is directly proportional to the strain, and the highest Von Mises stress results in the most stretchable and flexible conductive ink. Table 2 shows the results of maximum principal elastic strain and Von Mises stress from different thicknesses of graphene conductive ink, which are type (a) 0.05 mm, (b) 0.10 mm, (c) 0.20 mm, (d) 1.00 mm, (e) 1.50 mm, and (f) 2.00 mm. The numerical simulation shows that the maximum principal elastic strain of the conductive ink at 0.05 mm thickness of 0.5454 is slightly reduced by 0.06% at 0.10 mm thickness of 0.5451, but significantly increases by 1.23% at 0.20 mm thickness of 0.5518. When the thickness of graphene conductive ink is increased to 1.00 mm, 1.50 mm, and 2.00 mm, the maximum principal elastic strain values decrease sequentially to 0.5473, 0.5448, and 0.5449. Table 2 also shows that the strain value decreases when the thickness of graphene is multiplied by a huge margin.

The Von-Mises stress value decreases slightly with the increase of thickness from 0.05 mm to 0.10 mm, which makes it 8,078.9 MPa to 8,060 MPa. The value of Von Mises stress is increased by 0.59% when the thickness is increased to 0.2 mm, making it 8,107.5 MPa. To assess a change in Von Mises stress, the thickness range is increased multiple times. Von Mises becomes 7,897 MPa at 1.0 mm, which is 2.6% lower than the previous value. As well as the results obtained at 1.5 mm and 2.0 mm thicknesses, showed a constant decrease in stress at 7,844.5 MPa and 7,806.7 MPa, respectively.

Table 2 FEA Results Summary of Graphene Conductive Ink with Different Thicknesses

Component	Type	Thickness (mm)	Maximum Principal Elastic Strain	% Change	Von Misses Stress (MPa)	% Change
Graphene Conductive Ink	a	0.05	0.5454	-	8078.9	-
	b	0.10	0.5451	-0.06	8060	-0.23
	c	0.20	0.5518	+1.23	8107.5	+0.59
	d	1.00	0.5473	-0.82	7897	-2.6
	e	1.50	0.5458	-0.27	7844.5	-0.66
	f	2.00	0.5449	-0.16	7806.7	-0.48

Figures 3 and 4 illustrate the condition of graphene conductive ink at various thicknesses as seen through a cross-section view. The maximum principal elastic strain in Figure 3 illustrates that when greater multiple values are given to the thickness of graphene conductive ink, the area of the maximum value shrinks. Maximum principal elastic strain can be seen at the same corner where the maximum stress is found as shown in Figure 3. The Von-Mises stress as shown in Figure 4 also can be seen at the same corner pattern where the maximum principal elastic strain is found in Figure 3. The maximum value is highlighted in red color and the minimum value is highlighted in blue. Type (c) in Figure 3, the maximum value of maximum principal elastic strain of 0.5518 with the red color code indicates the highest strain in the model that withstands more stress than the other samples.

The center of the straight-line pattern is fixed to restrict the motion of the node in the x-axis. The whole pattern deforms in all directions and shows a bending effect. Due to the larger size of the pull area than the fixed area in the pattern, the component shows deformation or expansion at a different rate that causes stresses. The corner pattern shows a maximum value of strain and stress. The corresponding red stresses are not visible almost to the whole side of the pattern, they are actually at the corner of the pattern. As the pattern thickness increases, the red region shrinks via the inside of the corner, as shown in Figures 3 and 4. This demonstrates that the thickness of the material has an effect on the strain and stress values, which can reduce failure and hence increase material flexibility. The equivalent stress value at the corner can be reduced as the thickness of the material increases [18].

The maximum principal elastic strain for each of the samples was determined using the FEA results, with the assumption that the samples with the lowest maximum principal elastic strain would have the best stretchability value [20]. As we can see in Figure 5, with the increase of the thickness of conductive ink thickness the maximum principal elastic strain goes on decreasing. The maximum principal elastic strain value for type (f) with a thickness of 2.0 mm is 0.5449, which is the lowest among the other types. Although type (f) has the largest thickness compared to the other types, the maximum principal elastic strain value of type (f) is only slightly different from type (b) which has a thickness of 0.1 mm, indicating that type (b) has a better thickness for graphene conductive ink because it has a small thickness but a good strain value. Since graphene can be generated cost-effectively on an industrial scale, and the graphene functional groups enable its hydrophilicity and processability of formulations, the majority of graphene and its application studies have concentrated on the reduction of graphene materials [26].

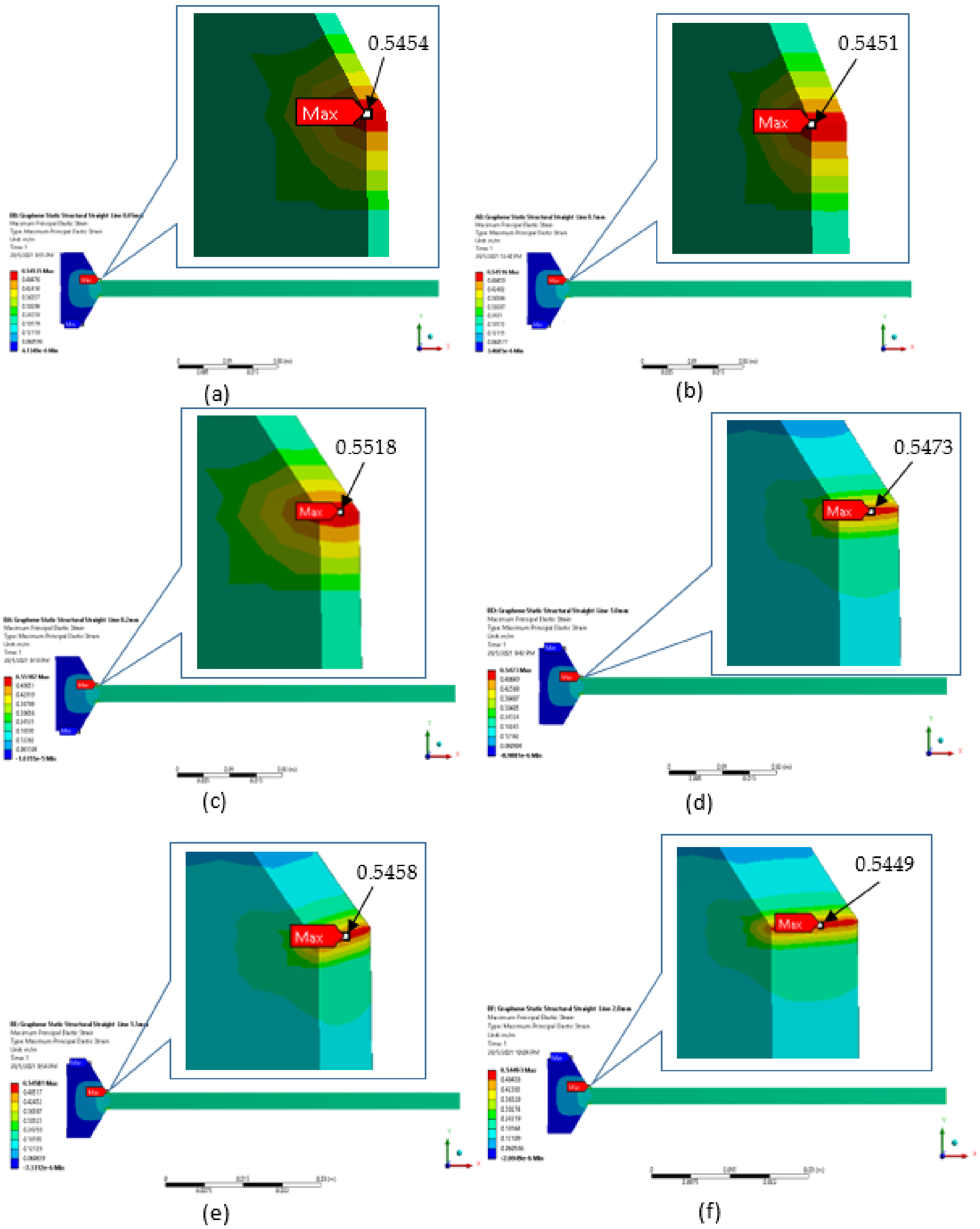

Figure 3. Maximum principal elastic strain of graphene conductive material cross-section view with different thickness. (a) 0.05 mm; (b) 0.10 mm; (c) 0.20 mm; (d) 1.00 mm; (e) 1.50 mm, (f) 2.00 mm.

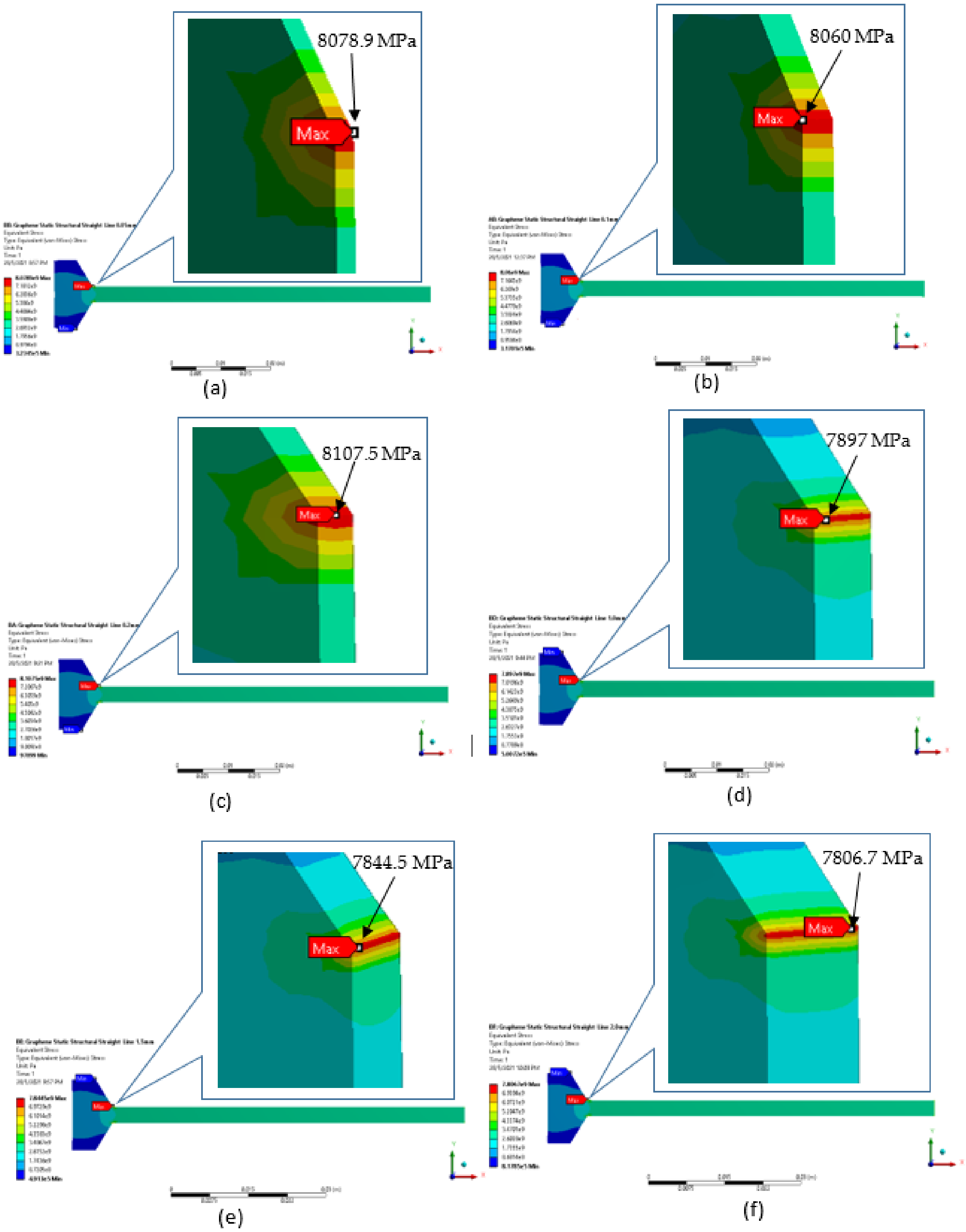

Figure 4. Von-Mises stress of graphene conductive material with different thickness. (a) 0.05 mm; (b) 0.10 mm; (c) 0.20 mm; (d) 1.00 mm; (e) 1.50 mm, (f) 2.00 mm.

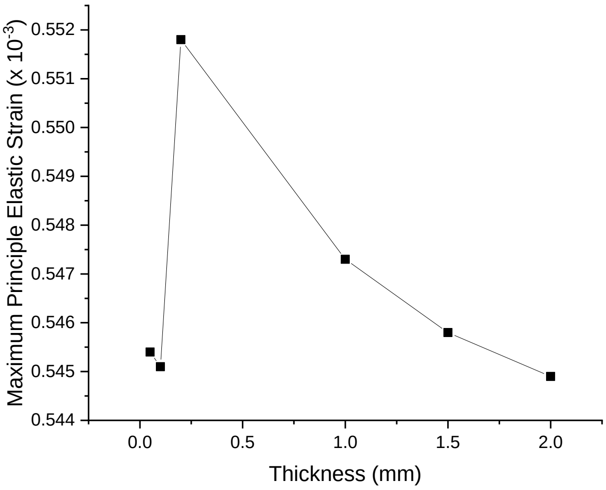

Figure 5. Maximum principal elastic strain of graphene conductive ink with different thicknesses.

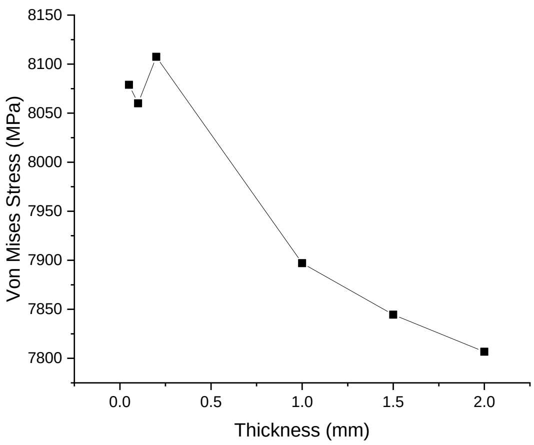

Figure 6. Von Mises stress of graphene conductive ink with different thicknesses.

The thickness of 2.00 mm or type (f) in Figures 6 attains the smallest amount of Von Mises stress among all the six types because according to Hooke's law, larger thickness is less flexible and cannot bend easily. The thickness of the pattern gives an effect to the stress and strain value. After 20% strain penetration, the FEA shows a decrease in Von Mises stress from 8078.9 MPa to 7806.7 MPa for the thickness of 0.05 mm to 2.00 mm, respectively. The mechanism clearly explains the theory of elasticity defined by Hooke's law. The maximum value of Von Mises stress on the corner decreases with respect to the width to thickness ratio, as predicted by mathematical models. However, the critical load is inversely proportional to the carbon-based conductive ink thickness when using the finite element model [21]. This FEA value is based on a perfect scenario with no ink-to-substrate delamination, no tension cycling, and no manufacturing process changes. Figures 5 and 6 show that type (c) thickness has the highest maximum principal elastic strain and Von Mises values of all the conductive inks. As compared to other conductive inks, this means that it has a very high level of hardness. The high-stress value is due to the influence of type (c) thin thickness. The thinner materials are more bendable and flexible [27-28].

4. CONCLUSION

The study was carried out successfully in demonstrating the optimal stretchability performance of differences thickness by using maximum principal elastic strain and Von Mises stress analysis. For the varied thickness effect of the 20% elongation stress, a modeling procedure based on previous research on conductive inks patterns related to elasticity theories was proposed to be used. In terms of maximum principal elastic strain and Von Mises stress, the 0.1 mm thickness provided a better thickness for graphene conductive ink because it had a small thickness but a good strain value. The small thickness provides an advantage in terms of low material consumption which in turn can be generated cost-effectively on an industrial scale. The red region was reduced via inside the corner pattern in the cross-section view, demonstrating that the thickness had an effect on strain and stress values, reducing failure and increasing material flexibility. The FEA showed that a decrease in maximum principal elastic strain and Von Mises stress from 0.05 mm to 2.00 mm of thickness corresponded to 0.5454 to 0.5449 and 8,078.9 MPa to 7,806.7 MPa, respectively, after 20% elongation. The mechanism clearly explains Hooke's law, which states that mechanical stress is directly proportional to the strain.

ACKNOWLEDGEMENT

Special thanks to the Advanced Manufacturing Centre (AMC) and Fakulti Kejuruteraan Mekanikal (FKM), Universiti Teknikal Malaysia Melaka (UTeM) for providing the laboratory facilities.

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