UNIVERSITI TEKNIKAL MALAYSIA MELAKA

PREDICTIVE MODELLING OF STRETCHABLE CONDUCTIVE INK USING FINITE ELEMENT ANALYSIS

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DEDICATION

To my beloved mother and father.

ABSTRACT

Stretchable and flexible printed electronics, which utilize conductive materials made from graphene, have attracted considerable interest due to their cost-effectiveness, flexibility, and impressive ability to conform to various shapes. However, these materials often experience performance failures when subjected to strain, which poses challenges for diagnosing electrical conducting failures and predicting their behaviour. To address these issues, a numerical modelling and simulation method is needed to predict the performance of stretchable conductive ink (SCIs) based on graphene nanoplatelets (GNPs). Furthermore, when the SCI/substrate system is subjected to mechanical loadings like stretching, torsion, and bending, it can affect the functionality of the SCI, leading to electrical failures. To overcome these challenges, finite element analysis (FEA) can be employed to simulate and observe the electrical performance of the printed electronics. However, to the best of our knowledge, predictive modelling to forecast the electrical performance of the printed electronics based on the development of stress and strain energy is yet to be studied. This thesis focuses on predicting the performance of the SCI/substrate system using the FEA method. The main goal of this study was to optimize the geometrical parameters of SCI using design of experiment (DOE) software through incorporation with finite element (FE) method. In an independent study, different shapes of silver conductors (straight, zigzag, square, and sinusoidal) were compared in terms of their impact on stress, strain, and electrical performance. The straight pattern exhibited the highest average von Mises stress and maximum principal strain, while the zigzag pattern showed the lowest stress and strain. These results aligned with experimental findings, indicating that increasing stress and strain decrease the maximum strain before conductivity is lost. To validate the simulation model, input parameters were acquired by subjecting both the thermoplastic polyurethane (TPU) substrate and formulated SCI to uniaxial tensile tests. The simulated results were then compared with the experimental data, and the model exhibiting quasi-static loading with non-linear material behaviour demonstrated the closest fit with the lowest peak stress error. Lastly, the development of equivalent plastic strain was predicted using the DoE method, considering the thickness and width parameters of the conductor. Through the optimization of geometrical parameters, a printed circuit with a thickness of 0.04 mm and width of 2.66 mm was found to produce the lowest maximum equivalent plastic strain. These optimized geometrical parameters enhance the stretchability of the SCI system, allowing for greater strain tolerance and reducing the likelihood of electrical failure when subjected to mechanical deformation. In summary, this research provides insights into the performance prediction and optimization of stretchable and flexible printed electronics based on graphene conductive materials. The combination of numerical modelling, simulation, and experimental validation offers valuable tools for enhancing the reliability and functionality of these systems in various applications.

PEMODELAN RAMALAN DAKWAT KONDUKTIF BOLEH REGANG MENGGUNAKAN ANALISIS UNSUR TERHINGGA

ABSTRAK

Elektronik bercetak boleh regang dan fleksibel menggunakan bahan konduktif graphene telah mendapat perhatian yang ketara kerana kosnya yang rendah, fleksibiliti dan kesesuaian yang tinggi. Walau bagaimanapun, bahan ini sering mengalami kegagalan prestasi apabila mengalami ketegangan, yang menimbulkan cabaran untuk mendiagnosis kegagalan pengalir elektrik dan meramalkan kelakuannya. Untuk menangani isu ini, kaedah pemodelan dan simulasi berangka diperlukan untuk meramalkan prestasi dakwat konduktif boleh regang (SCI) berdasarkan nanoplatelet graphene (GNP). Tambahan pula, apabila sistem SCI/substrat tertakluk kepada beban mekanikal seperti regangan, kilasan dan lenturan, ia boleh menjejaskan fungsi SCI, yang membawa kepada kegagalan elektrik. Untuk mengatasi cabaran ini, analisis unsur terhingga (FEA) boleh digunakan untuk mensimulasikan dan memerhati prestasi elektrik elektronik bercetak. Walau bagaimanapun, sepanjang pengetahuan kami, pemodelan ramalan untuk meramalkan prestasi elektrik bagi elektronik bercetak berdasarkan perkembangan tekanan dan tenaga terikan masih belum dikaji. Tesis ini memfokuskan kepada meramal prestasi sistem SCI/substrat menggunakan kaedah FEA. Matlamat utama kajian ini adalah untuk mengoptimumkan parameter geometri SCI menggunakan perisian reka bentuk eksperimen (DOE) melalui penggabungan dengan kaedah unsur terhingga (FE). Dalam kajian bebas, bentuk konduktor perak yang berbeza (lurus, zigzag, segi empat sama dan sinusoidal) telah dibandingkan dari segi kesannya terhadap tekanan, terikan dan prestasi elektrik. Corak lurus menunjukkan tekanan von Mises purata tertinggi dan regangan prinsipal maksimum, manakala corak zigzag menunjukkan tegasan dan regangan yang paling rendah. Keputusan ini sejajar dengan penemuan eksperimen, menunjukkan bahawa peningkatan tegasan dan terikan mengurangkan terikan maksimum sebelum kekonduksian hilang. Untuk mengesahkan model simulasi, parameter input diperoleh dengan menundukkan kedua-dua substrat poliuretana termoplastik (TPU) dan merumuskan SCI kepada ujian tegangan uniaxial. Hasil simulasi kemudiannya dibandingkan dengan data eksperimen, dan model yang mempamerkan pemuatan kuasi statik dengan gelagat bahan bukan linear menunjukkan kesesuaian paling hampir dengan ralat tegasan puncak terendah. Akhir sekali, perkembangan terikan plastik yang setara telah diramalkan menggunakan kaedah DoE, dengan mengambil kira ketebalan dan parameter lebar konduktor. Melalui pengoptimuman parameter geometri, litar bercetak dengan ketebalan 0.04 mm dan lebar 2.66 mm didapati menghasilkan regangan plastik setara maksimum yang paling rendah. Parameter geometri yang dioptimumkan ini meningkatkan keanjalan sistem SCI, membolehkan toleransi terikan yang lebih besar dan mengurangkan kemungkinan kegagalan elektrik apabila mengalami ubah bentuk mekanikal. Ringkasnya, penyelidikan ini memberikan pandangan tentang ramalan prestasi dan pengoptimuman elektronik bercetak boleh regang dan fleksibel berdasarkan bahan konduktif graphene. Gabungan pemodelan berangka, simulasi dan pengesahan eksperimen menawarkan alat berharga untuk meningkatkan kebolehpercayaan dan kefungsian sistem ini dalam pelbagai aplikasi.

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LIST OF ABBREVIATIONS

PCB	-	Printed circuit board
SMB	-	Small medium business
SCI	-	Stretchable conductive ink
CNT	-	Carbon nanotube
0-D	-	0-dimension
1-D	-	1-dimension
2-D	-	2-dimension
CP	-	Conducting polymers
AMOLED	-	Active-matrix organic light-emitting diode
OLED	-	Organic light-emitting diode
SEC	-	Stretchable electronic circuit
RFID	-	Radio-frequency identification device
EEG	-	Electroencephalogram
ECG	-	Electrocardiogram
PPy	-	Polypyrrole
PANI	-	Polyaniline
PT	-	Polythiophene
PPV	-	Poly(p-phenylenevinylene)
PEDOT	-	Poly(3,4-ethylenedioxythiophene)
PSS	-	Poly(styrene sulfonic acid)

LED	-	Light-emitting diode
COOH	-	Carboxylic acid
SWCNT	-	Single-walled carbon nanotube
MWCNT	-	Multi-walled carbon nanotube
PEG	-	Polyethylene glycol
LPE	-	Liquid-phase exfoliation
CVD	-	Chemical vapor deposition
GO	-	Graphene oxide
RGO	-	Reduced graphene oxide
GNP	-	Graphene nanoplatelet
UV	-	Ultraviolet
DMSO	-	Dimethyl sulfoxide
EG	-	Ethylene glycol
OH	-	Hydroxyl
PET	-	Polyethylene terephthalate
ITO	-	Indium-tin-oxide
RHCP	-	Right-hand circularly polarized
PDMS	-	Polydimethylsiloxane
FTCF	-	Flexible transparent conductive films
TPU	-	Thermoplastic polyurethane
TPE	-	Thermoplastic elastomers
FEA	-	Finite element analysis
NW	-	Nanowire
DOE	-	Design of experiment
DMA	-	Dynamic mechanical analysis

S-S	-	Stress-strain
ASTM	-	American society for testing and materials
FE	-	Finite element
UTM	-	Universal tensile machine
FTIR	-	Fourier-transform infra-red
VMS	-	Von mises stress
BC	-	Boundary condition
BC1	-	Boundary condition at fixed end x = 0 mm for longitudinal loading and y = 0 mm at lateral loading
BC2	-	Constraint from rotational displacement in all directions and translational displacement normal to the model
BC3	-	Reference point at the center of the cross-sectional area opposite to BC1
CAE	-	Complete Abaqus environment
DMA	-	Dynamic mechanical analysis
RF	-	Reference point
C3D8R	-	8-node linear brick element featuring reduced integration and hourglass system
IGES	-	Initial graphics exchange specifications
STEP	-	Standard for the exchange of product data
SCP	-	Suspended colloidal particles
PUF	-	Phenol-urea-formaldehyde
TPU_1	-	First sample of bulk TPU
TPU_2	-	Second sample of bulk TPU
TPU_3	-	Third sample of bulk TPU

MPS	-	Maximum principal strain
ANOVA	-	Analysis of variance

LIST OF SYMBOLS

Cu	-	Copper
Ag	-	Silver
Au	-	Gold
F	-	Volume of conductive fillers
f^*	-	Threshold volume fraction of fillers
σ_f	-	Conductivity of fiber
σ_c	-	Conductivity of composite
T	-	Conductivity exponent
R	-	Resistance
Tn	-	Tin
Zn	-	Zinc
R_s	-	Sheet resistance
R_o	-	Initial resistance
V	-	Volume fraction or weight percentage of filler
C	-	Composite
P	-	Particulate phase
M	-	Matrix
V_m	-	Volume fraction of PEDOT: PSS solution
E	-	Elastic modulus or Young's modulus
F	-	Minimum force

V_L	-	Loading speed
T	-	Holding time
D	-	Indentation depth
G	-	Correction factor
V	-	Voltage
I	-	Current
σ_1	-	Principal stress in x-axis
σ_2	-	Principal stress in y-axis
σ_3	-	Principal stress in z-axis
Σe	-	Equilibrium stress
μ	-	Poisson's ratio
ϵ_1	-	Principal strain in x-axis
ϵ_2	-	Principal strain in y-axis
ϵ_3	-	Principal strain in z-axis
ϵ_{yt}	-	Yield point strain
σ_{yt}	-	Yield point stress
∂_z	-	Expansion of the simulation model
θ_z	-	Contraction of the simulation model
ΔL_x	-	Total displacement for longitudinal stretch of biaxial load (3.0 mm)
ΔL_y	-	Total displacement for lateral stretch of biaxial load (9.5 mm)
ΔL_{x1}	-	Positive longitudinal stretch = 9.5 mm (uniaxial loading) and 1.5 mm (biaxial loading)
ΔL_{y1}	-	Positive lateral stretch = 3.0 mm (uniaxial loading) and 4.75 mm (biaxial loading)

ΔL_{x2}	-	Negative longitudinal stretch = 1.5 mm (biaxial loading)
ΔL_{y2}	-	Negative lateral loading = 4.75 mm (biaxial loading)
ΔL_{total}	-	Total displacement of biaxial tensile loading
$\sigma_{TPU,max}$	-	Highest peak stress among three TPUs
$\bar{\sigma}_{TPU}$	-	Average peak stress of three TPUs
$\sigma_{TPU,min}$	-	Lowest peak stress among three TPUs
Ω/sq	-	Ohm/square
Ω.m	-	Ohm meter
Σ	-	Population standard deviation
x_i	-	Individual value from population
M	-	Mean of the population
N	-	Sample size of the population
$\sigma_{max,1}$	-	Peak normalized stress for the first specimen of bulk GNP/PEDOT: PSS ink
$\sigma_{max,2}$	-	Peak normalized stress for the second specimen of bulk GNP/PEDOT: PSS ink
σ_{avg}	-	Average Von Mise stress for elastic model
σ_{max}	-	Maximum Von Mises stress for elastic model
σ_{min}	-	Minimum Von Mises stress for elastic model
E_i	-	Input strain

LIST OF PUBLICATIONS

Azli, D.A.M., Zakaria, M.S., Ramli, M., Omar, G., Nordin, M.N.A., Syaifuddin, S., Ramle, Z., Dziaudin, A.F. and Abdullah, A.H.L., 2023. Equivalent Plastic-Strain Analysis of Copper Stretchable Electronic Circuit Using Finite Element Analysis. *Journal of Advanced Research in Applied Sciences and Engineering Technology*, 30, 31-43.

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