

**SYNTHESIS, CHARACTERIZATION AND  
MODELLING OF NICKEL NANOWIRES  
SYNTHESIZED VIA TEMPLATE-ASSISTED  
ELECTRODEPOSITION**

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We hereby declare that we have checked this thesis and in our opinion, this thesis is adequate in terms of scope and quality for the award of the degree of Master of Science in Mechanical Engineering

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I hereby declare that the work in this thesis is based on my original work except for quotations and citations which have been duly acknowledged. I also declare that it has not been previously or concurrently submitted for any other degree at Universiti Malaysia Pahang or any other institutions.

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## LIST OF SYMBOLS

$\lambda$	Wavelength of incident X-ray
$d$	Space between atomic planes in the crystalline phase
D	Diameter of crystallites
K	Crystallites shape factors
$\beta$	Full width at half maximum (radians)
$\sigma_y$	Yield strength
E	Young Modulus
$\sigma$	Stress
$\varepsilon$	Strain

## LIST OF ABBREVIATIONS

Ni	Nickel
NW	Nanowire
MNW	Metallic Nanowire
MD	Molecular Dynamic
LAMMPS	Large-scale Atomic or Molecular Massively Parallel Simulator
VMD	Visual Molecular Dynamic
1D	One Dimensional
AAO	Anodic Alumina Oxide
FESEM	Field Emission Scanning Electron Microscope
EDX	Energy Dispersive X-ray Detector
XRD	X-ray Diffraction
FWHM	Full width at half maximum
EAM	Embedded-atom-method
fcc	Face cubic centre

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## **ABSTRAK**

Struktur bahan dengan saiz nano telah menarik perhatian ramai kerana keunikan sifat mekanikal, elektronik, optik, elektrik dan sifat magnetnya yang telah membuka pelbagai idea untuk mengaplikasikan struktur bahan ini. Wayar nano logam adalah salah satu struktur nano yang mempunyai skala panjang dalam lingkungan 1-1000 nanometer, berbentuk pepejal dalam satu dimensi. Wayar nano logam seperti nikel dijangkakan memainkan peranan yang penting di masa akan datang. Pelbagai proses sintesis dan kaedah pencirian telah dijalankan untuk menghasilkan struktur ini, tetapi kerana sifat struktur ini yang memperkenan sifat-sifat yang berbeza pada keadaan sistesis yang berbeza, pengetahuan yang menyeluruh mengenai struktur ini masih pada peringkat awal. Selain itu, kerana saiz struktur ini yang sangat kecil, teknik pencirian mekanikal yang diaplikasikan kepada struktur bahan bersaiz makro tidak dapat digunakan untuk mengkaji sifat-sifat mekanikal struktur bahan bersaiz nano. Oleh itu, kaedah pemodelan dan simulasi akan menjadi kaedah alternatif untuk menganggarkan mekanisme dan sifat-sifat mekanikal struktur bahan bersaiz nano. Oleh itu, objektif kajian ini adalah untuk mensintesis wayar nano nikel melalui teknik pemendapan elektrokimia dengan bantuan templat dan untuk memahami pengaruh suhu pemendapan dan kepekatan asid borik kepada sifat-sifat fizikal wayar nano nikel. Dalam kajian ini, kepekatan asid boric diubah daripada 5 g / L, 37.5 g / L dan 60 g / L dengan suhu pemendapan 40 °C, 80 °C, dan 120 °C. Morfologi, analisis unsur dan sifat-sifat kristalografi dianalisis menggunakan FESEM, EDX, dan XRD. Huraian sifat-sifat fizikal wayar nano nikel diperoleh dengan mengambil kira kesan kepekatan borik asid dan suhu pemendapan kepada komposisi unsur, morfologi permukaan, panjang pertumbuhan, orientasi kristal dan saiz kristal wayar nano nikel yang disintesis dibincangkan. Sifat-sifat mekanik wayar nano nikel adalah dianggarkan melalui simulasi Molecular Dynamic (MD). Kajian ini telah mendapati wayar nano nikel dengan ketulenan yang tinggi (97.97% berdasarkan analisis EDX) berjaya dihasilkan melalui kaedah pemendapan elektrokimia dengan bantuan template. Analisis kualitatif daripada imej FESEM menunjukkan bahawa semua tekstur permukaan wayar nano nikel didapati kasar dan tidak stabil apabila peningkatan suhu pemendapan ditingkatkan. Analisis XRD menunjukkan bahawa semua wayar nano nikel yang dihasilkan adalah polikristal dan spektrum XRD yang diperolehi tidak menunjukkan apa-apa perubahan dalam orientasi kristal apabila keadaan sintesis yang berbeza telah diaplikasikan. Walau bagaimanapun, peningkatan dalam saiz kristal telah dikesan apabila suhu pemendapan meningkat, dan ia juga menunjukkan bahawa purata peningkatan saiz kristal dalam jumlah kecil apabila kepekatan asid boric dikurangkan. Dari simulasi MD, elastic modulus untuk wayar nano nikel yang dimodel dianggarkan antara 140.02-142.5 GPa, kekuatan tegangan adalah dalam anggaran 16.465-16.732 GPa dan kekuatan keterikan dihasilkan adalah antara 0.1181-0.1209. Penyelidikan ini mampu menyumbang kepada pemahaman yang lebih mendalam terhadap pengaruh parameter ketika sintesis dijalankan terhadap sifat-sifat fizikal nanowires logam, serta dapat memberi idea yang lebih baik untuk merekabentuk eksperimen untuk bahan-bahan nanostructure lain di masa akan datang.

## ABSTRACT

Nanometer-sized structures have attracted lots of interest due to its unique mechanical, electronic, optical, electrical, chemical and magnetic properties; opening up a broad view of the application. Metallic nanowires classified as a nano-sized material with the characteristic length scale in the range of 1-1000 nanometers. As one of the most important one-dimensional (1D) nanostructures, metallic nanowire such as Nickel (Ni) expected to play a vital part in the future. Many synthesis and characterization method have been developed to produce this structures, but due to the nature of this structures which exhibits different behavior at different condition (environmental and synthesis), the comprehensive knowledge of these structures still in its early stages. Apart from that, due to the size of these structures, the well-established macro-scale mechanical characterization technique could not be used to determine the mechanical properties of these structures. As such, the modeling and simulation methods would be the alternate methods to provide further insights into various deformation mechanisms and mechanical properties. Therefore, the objectives of this research are to synthesize Ni nanowires via template-assisted electrochemical deposition technique; and to understand the influence of deposition bath temperature and stabilizer concentration on the physical properties. In this study, the stabilizer concentration was varied from 5 g/L, 37.5 g/L and 60 g/L with the deposition bath temperature of 40 °C, 80 °C, and 120 °C. The morphology, elemental analysis and crystallographic properties were analyzed using FESEM, EDX, and XRD. The elaboration of the physical properties of obtained Ni nanowires by taking into account the effect of stabilizer concentration and deposition bath temperature on the elemental composition, surface morphology, growth length, crystal orientation and crystal size of the synthesized Ni nanowires discussed. The mechanical properties of Ni nanowires are estimated through molecular dynamic (MD) simulation. Key research insight from the present investigation concludes that the template-assisted electrochemical deposition approach successfully synthesized high purity Ni nanowires (97.97% based on EDX analysis). Qualitative analysis from FESEM images showed that all the surface texture of Ni nanowires found to be rough and flaky with rough surface texture when the deposition temperature increase. XRD analysis suggests that all the grown Ni nanowire is polycrystalline in nature and the obtained XRD spectrum does not show any change in the crystal orientation when different synthesis condition was applied. However, increase in crystal size was noticed when deposition temperature increased, and it is also noted that the average of crystal size increase in small amount when the stabilizer concentration reduced. From MD simulation, the estimated elastic modulus for Ni nanowires is between 140.02 to 142.5 GPa, the yielding stress between 16.465 to 16.732 GPa and the yielding strain between 0.1181 to 0.1209. The present research contributes to the understanding the influence of processing parameter towards the physical properties of metallic nanowires, as well as designing experimental procedure for future extension to other nanomaterials.

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