出國報告（出國類別：參加國際研討會）

參加「2016 Fifth ICICE 國際研討會」

服務機關：國立高雄應用科技大學機械系

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派赴國家：大陸-陝西省西安市

出國期間：105.11.04-105.11.11

報告日期：105.11.25

摘要

2016 年 11 月本團隊參加大陸陝西省西安市 2016 Fifth ICICE 國際研討會。於 ICICE 的交流會議發表一篇標題為：Interface Friction of Double-walled Carbon Nanotubes Using Molecular Dynamics 相關奈米材料的研究論文，本研究為模擬方法主要探討雙壁奈米碳管在不同的溫度與結構方向下的摩擦特性研究。參加 2016 Fifth ICICE 國際學術會議可以促進本校的國際交流機會與建立學術友誼關係，並且激勵本校研究團隊在國際研討會上交流與分享更多工程發展與學術研究上的未來發展導向。

在大陸陝西省西安市雅致東方酒店，展開一系列的學術與工程交流。會議中，來自世界各國優秀的研究團隊發表關於研發成果，如技術與研究方法、學理分析、創新研究、科學發展與應用等導向值得我國教育與工程研究發展單位學習與仿效。由研究成果中充分表現了未來的新興工程與科學發展導向，而製程加工技術的跨領域結合與創新研究是未來工程科學發展之指標。

對於工程科學領域之創新研發、檢測技術以及材料應用發展等方面，我國學研單位應保持與全世界先進技術同步發展，並藉由培訓優秀的研究發展團隊、強化工程學識與拓展新興工程與專業科學領域。未來，可推薦優秀的產業開發團隊或學研技術開發專業人才能到國外學習與交流，以及成立良好的產學合作模式。未來，引進國外新穎的開發技術提升國內工程科學發展之需求，亦期許我國學術教育與工程材料等發展能早日與先進國家的優秀研發團隊並駕齊驅。

關鍵詞：大陸陝西省西安市、2016 Fifth ICICE E-RMS 國際研討會、研究論文。

目次

一、目的

1. 計畫目標

方得華教授團隊參加在大陸陝西省西安市 2016 Fifth ICICE 國際研討會。主要以新興的工程材料應用與科學發展趨勢方向進行國際學術討論與會議交流，並針對未來之學研發展範疇為目標，以創新材料應用與工程應用發展為指標進而培訓國內工程研發團隊與優秀的科學人才。

2. 主題

2016 Fifth ICICE 國際研討會於 2016 年 11 月 5 日至 10 日在大陸陝西省西安市舉行，將為科學研究人員提供一個會議交流平台，包括先進材料技術、創新設計、通訊科學與工程、工業設計、創意設計、應用數學、計算機科學、設計理論、管理科學、文化創意研究、機電工程、機械自動化工程，以及建築工程等相關領域。

3. 緣起

本研究團隊以分子動力學的模擬技術發展為根基，並以奈米材料應用與學術研究為發展導向。本研究團隊積極參與國際研討會與發表國際期刊，今年將其中一篇論文發表於 2016 Fifth ICICE 國際研討會，標題為: The field emission properties of multi-wall carbon nanotube grown on a flexible carbon cloth 相關的研究成果。

4. 預期效益與預達成事項

本研究團隊發表一篇標題為: The field emission properties of multi-wall carbon nanotube grown on a flexible carbon cloth，本研究為模擬方法主要探討雙壁奈米碳管在不同的溫度與結構方向下的摩擦特性研究。參加 2016 Fifth ICICE 國際學術會議可以促進本校的國際交流機會與建立學術友誼關係，並且激勵本校研究團隊在國際研討會上交流與分享更多工程發展與學術研究上的未來發展導向。所有被接受的優秀論文將被推薦發表至下列的 SCI 國際期刊。

(1) Materials(ISSN 1996-1944; IF: 2.651).
(2) Sensors(ISSN 1424-8220; IF: 2.245).
(3) Applied Sciences(ISSN 2076-3417; IF: 1.484)
(4) Micromachines(ISSN: 1432-1858; IF: 0.875)
(5) Eurasia Journal of Mathematics, Science and Technology Education(SSCI, ISSN: 1305-8223; IF: 1.016)
(6) Microsystem Technologies(ISSN: 1432-1858; IF: 0.875).
(7) Journal of Environmental Protection and Ecology(ISSN 1311-5065; IF: 0.838).
(8) Advances in Mechanical Engineering(ISSN: 1687-8140; IF: 0.575)
(9) Oxidation Communications (ISSN: 0209-4541; IF: 0.451)
(10) Integrated Ferroelectrics(ISSN: 1607-8489; IF: 0.357)

二、過程

11 月 04 日

由臺灣桃園國際機場直飛抵達大陸西安咸陽國際機場。

11 月 05 日

會議中心位於陝西省西安市雅致東方酒店完成註冊程序，報到後開始學術活動。

11 月 06 日

Title：Photocatalytic Study of Zinc Oxide with Different Bismuth Doping

Author：W.H. Lan, M.C. Shih, D.J.Y. Feng, Y.X. Ding, Y.J. Chiu, Y.J. Lin, W.J. Lin, S.Y. Lee, J.C. Lin, K.J. Chang, M.C. Wang, C.J. Huang

透過 450℃含有乙酸鋅和硝酸鉍前體的水溶液的噴霧熱解沉積製備具有不同鉍（Bi）摻雜的氧化鋅（ZnO）膜。 在紫外線光照射下，研究了這些 ZnO 膜的甲基橙的光降解。在單摻雜 ZnO 中，5％Bi 摻雜的 ZnO 顯示出相對高的光催化活性。實現了反應速率，並討論了可能的原因。發現通過增加表面摻雜可以提高反應速率。

11 月 07 日

Title：Deposition of inductively coupled plasma chemical vapor deposition siliconbased stacked layers for organic light-emitting diode encapsulation

Author：H.Y. Wu, Y.S. Lin, C.H. Hsu, S.Y. Lien, Y.L. Jiang, K.W. Weng, D.S. Wuu

通過電感耦合等離子體化學氣相沉積（ICP-CVD）系統沉積作為無機氧化矽（SiOx）和有機矽（SiCxHy）層的矽基薄膜。研究 SiOx 和 SiCxHy 堆疊層的厚度對水蒸氣透過率（WVTR）的影響以評估封裝能力。用於有機發光二極體（OLED）封裝的最佳 SiOx / SiCxHy 堆疊層可導致 OLED 器件的壽命從 7 小時增加到超過 2000 小時。

11 月 08 日

Title：Study on N2 Atom Thermodiffusion of FBG Sensor for High Temperature

Author：T.S. Hsieh, Y.C. Chen, C.C. Chiang

本文討論了熱光學模型和溫度敏感性的數值計算。分析光纖布拉格光柵（FBG）傳感器的氮（N2）氣體的熱致光行為。FBG 由適當選擇的具有熱光係數的光敏纖維材料組成。實驗和優化的熱光係數結果在溫度敏感性方面是一致的。在這些實驗中，發現 FBG 的溫度敏感性為 11.9 pm /℃ 。

11 月 09 日

Title：Novel electrospray deposited nanocrystalline CuOX hole transport layer for perovskite solar cell

Author：J.F. Li, I.Y.Y. Bu, S.J. Liu, S.B. Dai

鈣鈦礦太陽能電池通常通過使用有機電洞傳輸層（HTL）來製造，這可能導致性能不穩定性問題。在這裡，工業兼容的電噴霧沉積工法在鈣鈦礦太陽能電池中製備無機 HTL。使用電噴霧 CuOx 作為 HTL，已實現了 5.83％的太陽能電池功率轉換效率，其中短路電流密度（Jsc）為 17.22 mA /cm^2，開路電壓（Voc）為 0.7 V，填充因子 FF）為 0.48，優於使用常用的 PEDOT：PSS 膜（～4.01％）製造的鈣鈦礦太陽能電池（相同的器件結構）。

11 月 10 日

Title：Omnidirectional Planar Loop Dipole Tag Antenna for UHF Band

Author：I.T. Tang, W.F. Chang, C.L. Hsu

提出並實驗研究了具有調諧短截線天線和雙環偶極天線的單環偶極天線與調諧短截線天線的設計。由於其高輻射電阻和高感抗，在該過程中選擇環形偶極天線。僅通過調整具有調諧短截線提出的環形偶極子天線的調諧短截線長度，可以獲得諧振頻率的阻抗匹配。提出了環形偶極天線設計和所構造的原型的實驗結果的細節。

11 月 11 日

由大陸西安咸陽國際機場直飛抵達臺灣桃園國際機場。

三、心得及建議事項

本屆會議以進材料技術、創新設計、通訊科學與工程、工業設計、創意設計、應用數學、計算機科學、設計理論、管理科學、文化創意研究、機電工程、機械自動化工程，以及建築工程等相關領域為議題，尤其是在創新理念與學理基礎方面關於各類科學與工程相關領域之議程進行交流與分享。世界各地的學術發展團隊與科學研究人才發表優異的研究成果，在成果發表方面值得我國學研單位與工程研發團隊學習與仿效。藉此國際學術會議與世界各地先進的研發成果進行交流可引導跨國學術研究研究與工程科學發展的潛力，並藉此國際會議的交流建立各國學術之間的友誼關係。

此次見識到世界各國研究團隊具有敏銳的工程開發潛力與科學革新之巧思，此方面是我國學研單位與研發團隊對於各類專業領域之科學研究與學術工程發展應保持努力與先進國家同步發展，強化專業學理根基與發展創新之潛能，對於優秀研究團隊與專業人才可建議校方與國家研究發展單位應該可以多多勉勵與積極培訓。未來，期待可協同各類工程領域的研究發展為前景和世界各地優秀學者攜手策畫拓展新興科學研究與開創具前瞻性的工程與學術價值。

除了建議：建立完備的國內外學術合作模式與結合多元的專業學識，除了學術教育與工程科學發展項目以外，亦包含國內外專業研究團隊的學者交流與跨領域合作。並期許未來可推薦優秀的產業開發團隊或學研技術研發專業人才能到國外學習與互訪，以及建立完整的產學合作模式。未來，引進國外新穎的開發技術提升國內工程科學發展之需求，亦期許我國學術教育與工程材料等發展能早日與先進國家的優秀研發團隊並駕齊驅。

最後，本次出國參加國際研討會能夠獲得 DBSD2 機械系結餘款&碩專班 D519 計畫結餘款之差旅費補助，在此特別致謝。

附錄

1. 會場相片

The Fifth

2016 The Fifth
International Conference on Innovation,

2016
TIKI
2016 The Fifth

2.接受函

2016 The Fifth International Conference on Innovation, Communication and Engineering

Taiwanese Institute of Knowledge Innovation

November 5 - 10, 2016, Xi'an, Shaanxi, P.R. China ||http://2016.icice.net/

Acceptance Letter

Paper No.: C160088
Paper Title: Interface Friction of Double-walled Carbon Nanotubes Using Molecular Dynamics
Authors: Cheng-Da Wu ,Chung Yuan Christian University; Te-Hua Fang ,National Kaohsiung University of Applied Sciences; Fu-Yung Tung ,National Kaohsiung University of Applied Sciences
Corresponding Author: Te-Hua Fang

Dear Prof. Te-Hua Fang,

I am pleased to inform you that the abstract you kindly submitted to the 2016 International Conference on Innovation, Communication and Engineering (ICICE 2016) has now been accepted and you are invited to attend the conference to present your paper. Please register by http://2016.icice.net before August 31, 2016.

Your interest in ICICE 2016 is very much appreciated. I look forward to meeting you at the conference.

INTL. CONF. INNOV. COMM. ENG. ICICE 2016

Prof. Artde Donald Kin-Tak Lam, Ph.D
Program Chairman of ICICE 2016
August 05, 2016

3.海報全文

Interface Friction of Double-walled Carbon Nanotubes Using Molecular Dynamics

Cheng-Da Wu [a], Te-Hua Fang [b*], Fu-Yung Tung [b]

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[b] Department of Mechanical Engineering, National Kaohsiung University of Applied Sciences, Kaohsiung 807, Taiwan

The interface friction characteristics of double-walled carbon nanotubes (DWCNTs) are studied using molecular dynamics simulations based on the Tersoff potential. The effects of DWCNT type, outer shell diameter, and temperature are evaluated. The simulation results show that when an inner shell is being pulled out from a DWCNT, the friction force and normal force between shells increase with increasing outer shell diameter and temperature. The zigzag-zigzag and armchair-armchair DWCNTs exhibit larger friction forces and smaller normal forces compared to the chiral-chiral DWCNTs.

Keywords: double-walled carbon nanotube; interface friction; friction coefficient; molecular dynamics

1. Intorduction

Carbon nanotubes (CNTs) are an important class of carbon-based materials due to their excellent physical properties, such as high mechanical strength, thermal conductivity, and electric conductivity, low density, and large specific area [1]. Due to these remarkable properties, CNTs have many potential applications in micro-electromechanical systems (MEMs) [2], nano-electromechanical systems (NEMs) [3], strain sensor [4], and adsorbent of flue gases [5]. In addition, the low interaction between adjacent shells of multiwalled CNTs has inspired studies for CNT oscillators and resonators.

The understanding of the interfacial tribology between shells of double-walled carbon nanotubes (DWCNTSs) is important for above applications. Molecular dynamics (MD) simulation is a powerful sciential tool for studying material interactions. Atomic simulation avoids experimental noise and turbulence problems, and can reduce cost. In this work, MD simulations are performed to analyze the interfacial friction between shells of a DWCNT by pulling an inner shell out from it. The effects of DWCNT type, outer shell diameter, and temperature are studied in terms of atomic trajectories, friction force, and normal force.

2. Methodology

Figure 1 shows a MD physical model of a DWCNT. The model consists of an inner shell and an outer shell, and both lengths are 30 nm, respectively. The diameters of outer and inner shells are 2.73 and 2.4 nm, respectively. The space between the shells was set at 0.34 nm. Two layers of atoms on the left-hand side end of outer shell were set as fixed layers to support the whole system. Another two layers of atoms next to the fixed layers were set as isothermal atoms. The rest of the material was set as Newtonian layers of atoms. In contrast, the fixed, isothermal, and Newtonian layers of atoms for the inner shell were set from its right-hand side end. In order to analyze the interfacial friction between both shells of DWCNTs during a relative motion process, the inner shell was moved by its fixed layers with a constant velocity of 40 m/s toward the Y-direction. A total movement of 27.5 nm was applied. No periodic boundary conditions were used in the model. The Tersoff-Brenner many-body potential function [6] was used to model the carbon-carbon atom interactions. This potential takes account of the coordination and angular dependence of the atoms and is well-suited to describing both the intrashell covalent bonds. The long range interactions of carbon were characterized using the Lennard-Jones 12-6 potential [7]. The parameters of cut-off radius, time-step and temperature in the simulation were set at 1.0 nm, 1 fs, and 300 K, respectively.

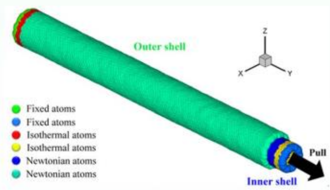

Figure 1. MD model of DWCNT. The model consists of an inner shell and an outer shell, and both lengths are 30 nm. Diameters of outer and inner shells are 2.73 and 2.4 nm.

3. Results and discussion

A. Effect of DWCNT type

To study the effect of DWCNT type, four different DWCNTs, zigzag-zigzag (31,0)@(22,0), zigzag-armchair (31,0)@(12,12), armchair-armchair (18,18)@(12,12), and chiral-chiral (20,15)@(14,10), were used, respectively. Figure 2 shows the variation of friction force between the shells with time for the four DWCNTs. The friction force curve decreasingly oscillates with increasing time due to a decrease in number of interaction atoms. For zigzag-zigzag and armchair-armchair DWCNTs, their inner and outer shells meet the lattice matching requirement, i.e., commensurate contact between two grapheme sheets; therefore they exhibit larger friction forces and smaller normal forces. The chiral-chiral DWCNTs thus have larger normal forces due to the incommensurate contact.

B. Effect of outer shell diameter

To study the effect of size of outer shell diameter (*D*), three *D* values, 2.73, 2.93, and 3.26 nm, were used, respectively. A chiral-chiral (20,15)@(14,10) DWCNT was used in the simulation. Figures 3 and 4 show the variations of friction force and normal force between the shells with time for three D values. The average friction forces are 2.29, 2.49, 2.84 nN for *D* values of 2.73, 2.93, and 3.26 nm, respectively. The friction force and normal force increase with increasing *D* value due to an increase in number of interaction atoms. The normal force reaches its maximum at the beginning and decreases with increasing time.

C. Effect of temperature

A zigzag-zigzag (31,0)@(22,0) DWCNT with diameters of inner and outer shells of 1.75 and 2.47 nm, respectively, was used in the simulation. With increasing temperature (150~500 K), the shell surfaces get more corrugated due to an increase in kinetic energy of atoms. The corrugation height is in a range of 0.24 – 0.27 nm for the outer shell surface when temperature is increased from 150 to 500 K, and that is in a range of 0.1 – 0.16 nm for the inner shell surface, respectively. Figures 5 shows the variation of friction force with time for three temperatures. The friction force curve increasingly oscillates with increasing temperature. For these tested temperatures, they have an approximate average friction force of about -1.42 nN. However, the average normal force increases with increasing temperature.

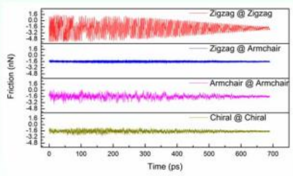

Figure 2. Variation of friction force between shells with time for four DWCNT types.

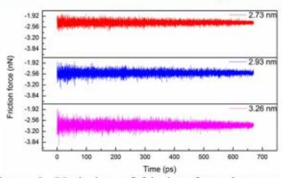

Figure 3. Variation of friction force between shells with time for three outer shell diameters.

4. Conclusion

MD simulations were used to investigate the effects of DWCNT type, outer shell diameter, and temperature on interfacial friction of DWCNTs. The following conclusions were obtained:

(1) The friction force and normal force between shells increase with increasing outer shell diameter and temperature.

(2)The zigzag-zigzag and armchair-armchair DWCNTs exhibit larger friction forces and smaller normal forces than those of the chiral-chiral DWCNTs.

Acknowledgments

This work was supported by the National Science Council of Taiwan under grants MOST 104–2221–E-033-062-MY2 and MOST 104–2622–E–033-006-CC3.

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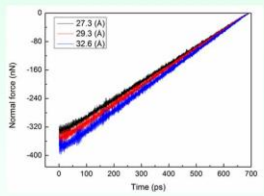

Figure 4. Variation of normal force between shells with time for three outer shell diameters.

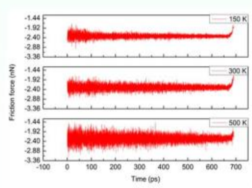

Figure 5. Variation of friction force between shells with time for three temperatures of 150, 300, and 500 K.