

出國報告（出國類別：國際會議）

第 20 屆國際先進理論與計算化學研討會

服務機關：國防大學理工學院國科所

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摘 要

世界科學、工程及技術學會(World Academy of Science, Engineering and Technology, WASET)是個全球性的科研組織，統合多種專業領域的學者及研究人員，長年於各大洲舉辦國際性的學術研討會。2018 年規畫在新加坡辦理第 20 屆國際先進理論及計算化學研討會 (20th International Conference on Advanced Theoretical and Computational Chemistry)。此會議旨在匯聚權威科學家、研究人員及學者，交換及分享大家在先進理論與計算化學領域所有相關面向的經驗與成果，ICATCC 會議也提供一個重要的跨學科平台，給予研究者、從業者及教育家在此平台上發表及研討，就產業實務所面臨的挑戰，從計算化學領域近期創新、關注及未來趨勢發展，進行介接及交流，尋求有效的解決之道。

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一、本文

(1)目的

主要希望藉由參加國際研討會的機會，了解現今理論計算在化學及材料領域的應用及其未來的發展趨勢。採行理論模擬的方法，在自然與工程專業領域的實務問題研析中，經常可見搭配使用。然而，模擬運算的結果，雖多半未竟與實驗數據相吻合，仍能提供可靠的參考資訊，免卻資源的耗費。因此，透過參與會議聽取學術成果有關之技術分析報告及循由互動式的研討，可多元地汲取新知、學習新的理論計算法，以提升個人的研究能量，並能推展至更廣的研究面向。

(2)過程

此次研討會於 107 年 1 月 8-9 日，假新加坡雅亭假日飯店(Holiday Inn Singapore Atrium)舉行，為期兩天的會議，總計有包含美、英、德、日在內的 20 餘國，發表 110 篇研究論文(如附錄一會議論文輯索引)，並有數十位專家學者親臨與會，首日開場由大會議程主席 Wong 博士，以近年 WASET 論文的衝擊係數(Impact index)為題，分析說明歷來研討會收錄文章獲國際間學者、科研人員的重視及引用，對學術研究的推動，產生正面的助益。

接續在排訂的四個分組議程中，進行全文或電子海報的發表及意見交流，本人與博士研究生劉權文同學參與第 4 小組的研討，並由劉同學以電子海報方式發表 5 分鐘"電腦模擬檢視奈米鐵粒子的磁與吸波性質"之成果報告。過程中雖略顯緊張及生澀，終究順利地完成，相信是個不錯的活動體驗。議程研討間的茶敘時段提供與會學者持續地進行互動，大會規劃的階段活動，時間掌握得宜、流程順暢、獲得相當好的評價。

礙於會議只有兩天，大會無法安排新加坡當地的短程旅遊，而少了一覽知名景點的機會。所幸個人仍利用傍晚時間，造訪魚尾獅公園、中國城及體驗搭乘聖淘沙空中纜車欣賞海灣夜景，是此次赴外行程附帶的收穫。

(3)心得及建議

個人的研究專長為計算化學，主要係運用程式軟體(包含 Gaussian、Materials Studio . . 等)，致力於化學反應合成模擬及軍用材料特性分析等工作。近期指導博士生探討金屬(氧化金屬)/高分子複合材料的吸波特性的，已獲初步成果並在材料化學及物理(Materials Chemistry and Physics)發表期刊論文。此次研討會續將部分研究成果，定名為"電腦模擬檢視奈米鐵粒子的磁與吸波性質"進行發表，內容著重於採用材料工作軟件(MS)，輔以自編程式探討奈米層級金屬粒子構型對於複合材料吸波性質的影響，並與實驗研究結果相互比對。

在本次研討會的發表論文中，南韓朴教授提出多層結構的聚酯毯及混用毯聲波吸收材料的最佳化設計，他採行實驗法另輔以 Foam-X 軟體模擬，分別量測及計算多層聲波吸收材料的吸收係數，並進行比較與分析。研究成果可供軍、民用載具設備隔音材料開發及設計選用的參考。

此外，印度坎達教授發表鋁鈦氧體摻雜鉛、釩金屬離子之陶瓷材料合成及特性分析。此種材料兼具高介電係數及低介電損耗等優點，可推廣至電容器應用;其鐵磁性質亦是匿蹤吸波功能設計時，可供選用的材料標的之一，相當值得以模擬與實驗並行的方式，投入後續研究。整體而言，此行參加 2018ICATCC 國際研討會後，廣開見聞、收穫豐碩。

本人於 107.1.9 完成參加研討會行程，過程順利圓滿。些許覺得遺憾的是陪同前往的博士生，過去 2 年在校研習期間，已發表(並獲刊登)頗具水準的國際期刊論文 6 篇，惟行前申請科技部補助研究生出席國際研討會時，未獲同意補助，殊為可惜!建議基於鼓勵優秀研究生多接觸國際以拓展視野的考量，能酌予經費補助，相信有助於激勵他們持續投入學術研究，推升國內的科研水準。

二、攜回資料及名稱

- (1) The 2018 World Academy of Science, Engineering and Technology : Conference Proceedinds. 研討會論文輯
- (2) The 2018 ICATCC Conference : Conference Program Manual. 研討會議程手冊
- (3) The 2018 ICATCC Conference : Compact Disc of Index of Paper Abstract. 論文摘要光碟

三、其他

感謝科技部給予經費補助，及國防大學理工學院院長、各級長官與行政同仁之協助，使個人有機會參加 2018 年國際先進理論與計算化學研討會，並發表論文。



四、發表論文

Computer Simulation to Investigate Magnetic and Wave-absorbing Properties of Iron Nanoparticles

Chuan-Wen Liu, Min-Hsien Liu, Chung-Chieh Tai, Bing-Cheng Kuo,
Cheng-Lung Chen, Huazhen Shen

Abstract—A recent surge in research on magnetic radar absorbing materials (RAMs) has presented researchers with new opportunities and challenges. This study was performed to gain a better understanding of the wave-absorbing phenomenon of magnetic RAMs. First, we hypothesized that the absorbing phenomenon is dependent on the particle shape. Using the Material Studio program and the micro-dot magnetic dipoles (MDMD) method, we obtained results from magnetic RAMs to support this hypothesis. The total MDMD energy of disk-like iron particles was greater than that of spherical iron particles. In addition, the particulate aggregation phenomenon decreases the wave-absorbance, according to both experiments and computational data. To conclude, this study may be of importance in terms of explaining the wave- absorbing characteristic of magnetic RAMs.

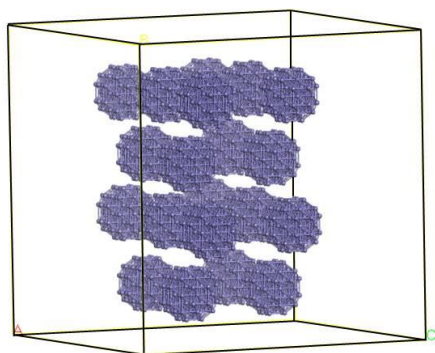
Combining molecular dynamics simulation results and the theory of magnetization of magnetic dots, we investigated the magnetic properties of iron materials with different particle shapes and degrees of aggregation under external magnetic fields. The MDMD of the materials under magnetic fields of various strengths were simulated. Our results suggested that disk-like iron particles had a better magnetization than spherical iron particles. This result could be correlated with the magnetic wave- absorbing property of iron material.

Keywords—wave-absorbing property; magnetic material; micro- dot magnetic dipole; particulate aggregation.

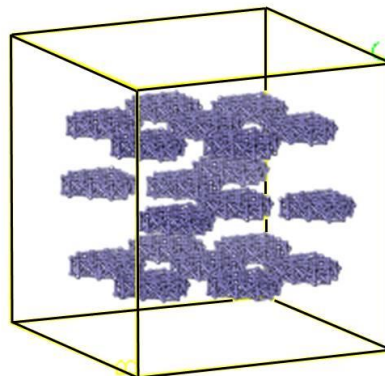
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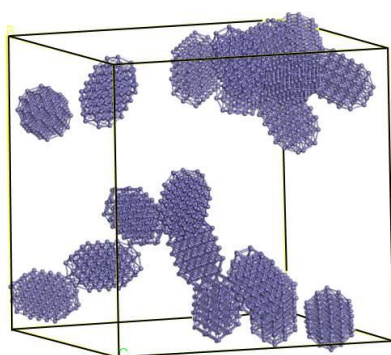
(a) System I-a



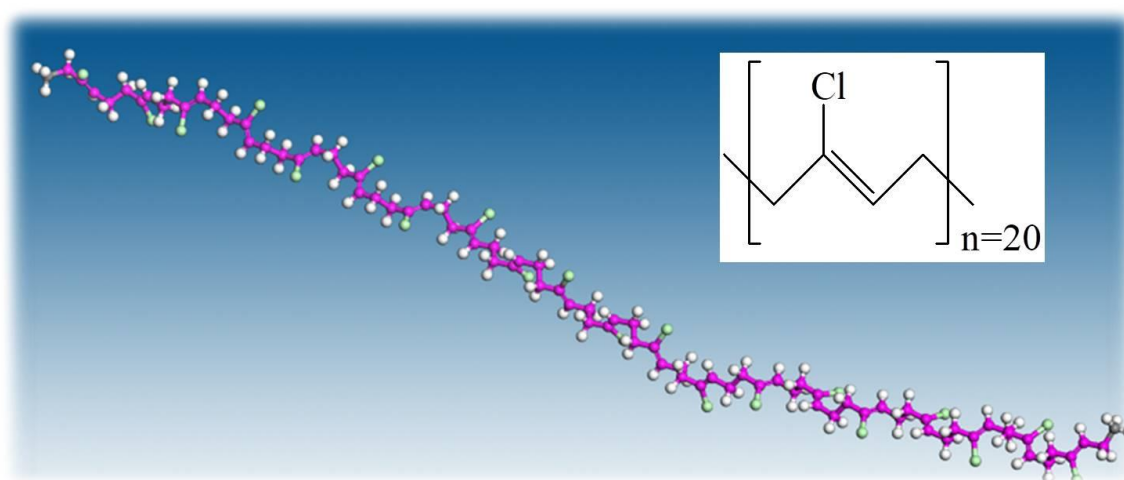
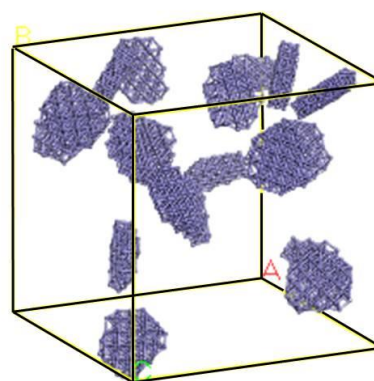
(b) System II-a

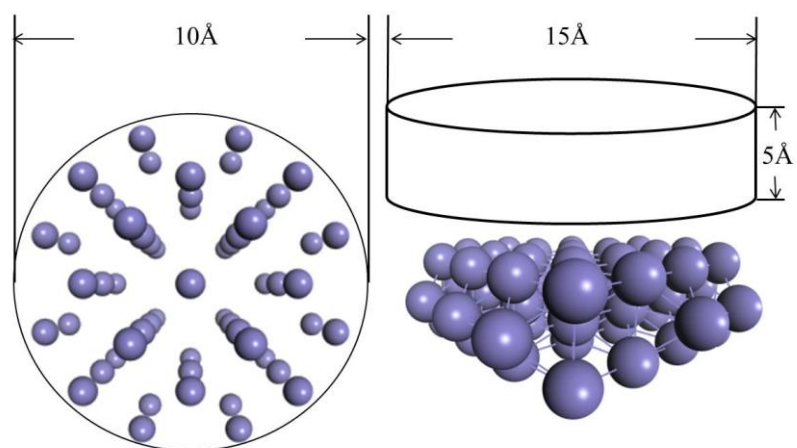


(c) System I-b



(d) System II-b

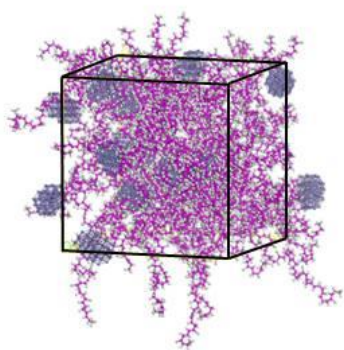




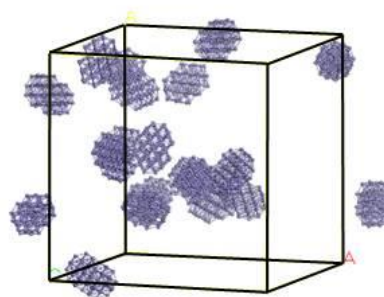
Iron ball-shaped
In diameter 10 Å
59 Fe atoms per ball-shaped

Iron disk-shaped
In diameter 15 Å
60 Fe atoms per disk-shaped

(a)

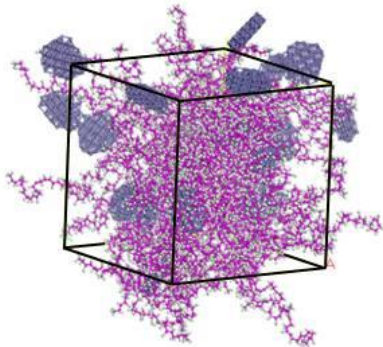


System I

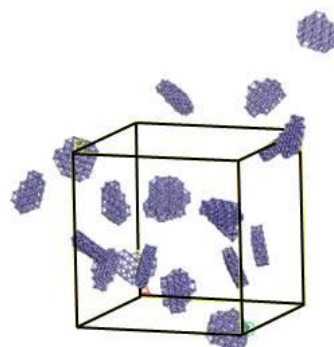


System I (only iron ball)

(b)

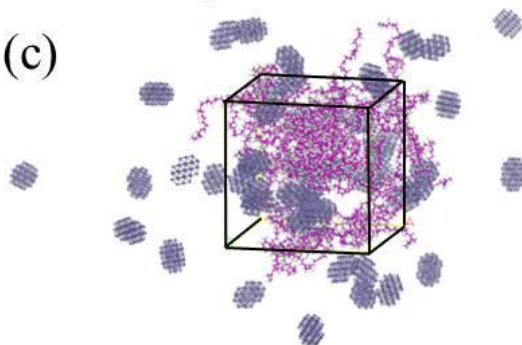


System II

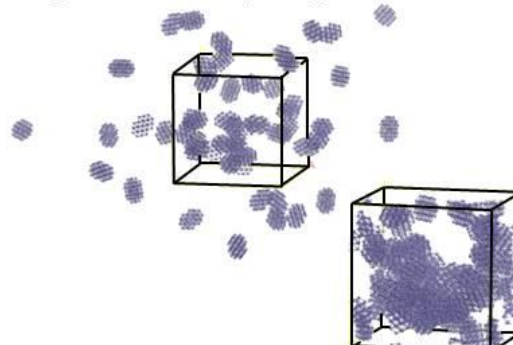


System II (only iron disk)

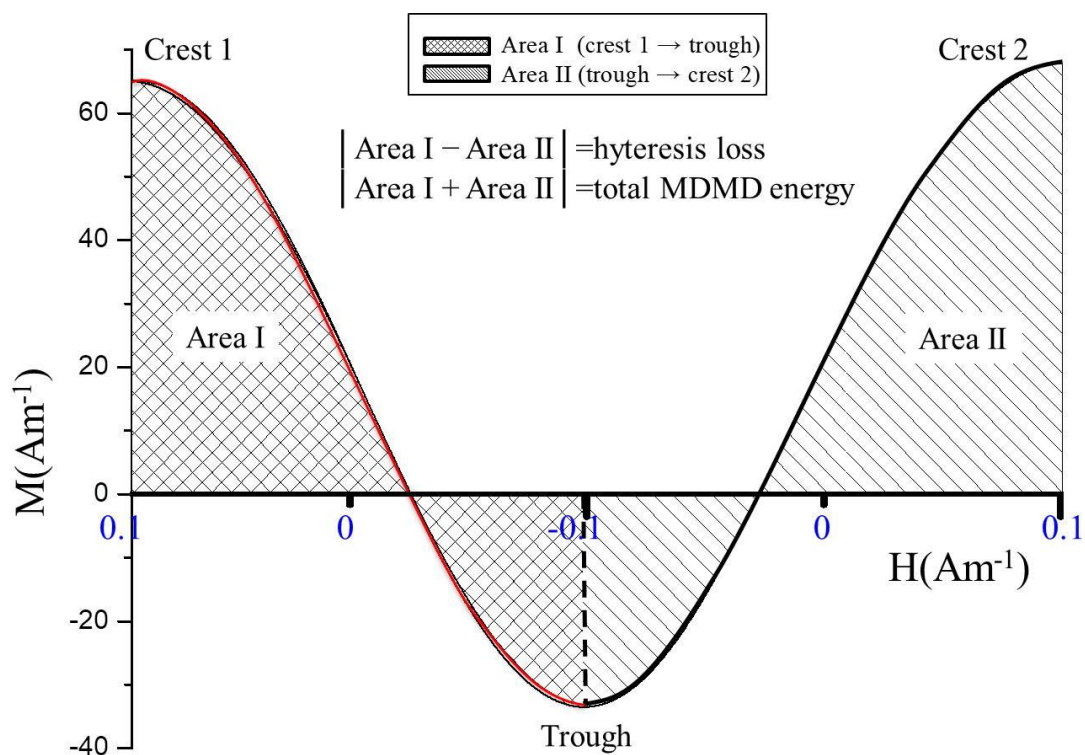
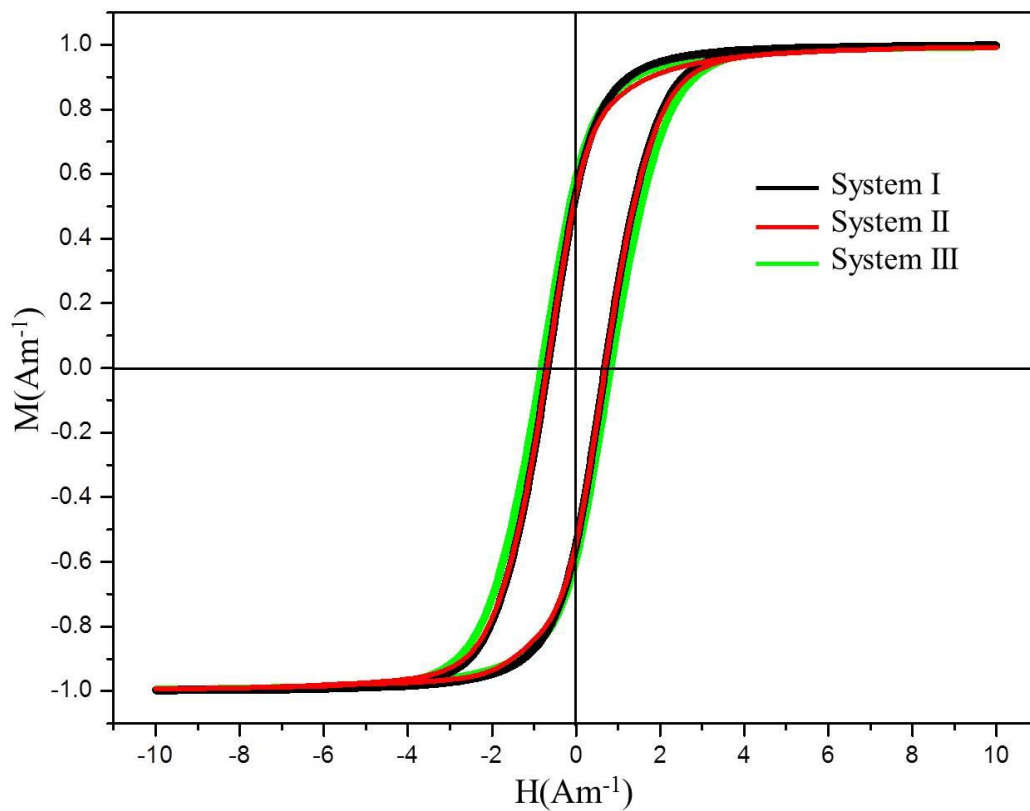
(c)



System III



6
System III (only iron ball)



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