Final Report for AOARD Grant FA2386-17-1-4020

Computational Electromagnetic at Fractional Dimensions

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Period of Performance: 4 April 2017 to 5 May 2019 (2 years of USD$100,000 in total)

Abstract:
The most important outcome of this grant is a comprehensive revision some traditional models based on Maxwell equations into fractional dimensions, namely fractional field emission models, fractional Mott-Gurney law, fractional Fresnel Coefficient, and fractional capacitors. The excellent agreement between the new models and experimental results have resulted the successful implementation of the computational fractional EM models developed in this proposal for applications in physics and engineering.

Introduction:
Fractional calculus is a branch of mathematics in taking n-power of a differential operator or integral, where the n is not necessary a positive integer number (n = 1, 2…). Its origin can be traced back to 30 September 1695, when derivative of n = ½ was described by Leibniz in his letter to L' Hospital. It has been studied by many great mathematicians such as Fourier, Euler, Laplace, Liouville, Riemann, Abel, and Weyl. For a long time, the research on fractional calculus is purely on scientific or mathematical interests without any specific applications. Not until the works of Mandelbrot on fractal geometry is early 1980s showing that most of the "practical" objects are in fractal dimensions. From Mandelbrot's work, it is clear that many objects are in fractional dimensions that the traditional calculus or differential equations are not sufficient. Thus, fractional models on differential equations (important to physicists) have emerged. Some earlier applications include fractional Brownian motion and anomalous diffusion. The field has greatly been expanded to other engineering fields in past 10 years, such as wave propagation in human cancellous bone and porous materials, speech signal modelling, modelling of Cardia tissue electrode interface, fractional order controllers of autonomous vehicles, theory of viscoelasticity, fractional image detection, and others. In this proposal, we aimed to create computational tools based on fractional differential equations, such as Maxwell equation, and/or Schrodinger equation to study various applications in Physics and Engineering.

Approaches:
For our theoretical models, we applied the "fractional differential operator" to reformulate the related coupled equations involving Maxwell and Schrodinger and Dirac equations. Using this new "fractional model", we will study various topics (see below) and compare with experimental results or full multi-scale simulation. On each new model, we will ensure the model will be able to recover to the traditional model at integer dimensions.

Results and Discussions [4 highlighted topics]

<u>Topic 1: Fractional field emission models</u>

Publication: M. Zubair, Y. S. Ang, and L. K. Ang, "Fractional Fowler-Nordheim Law for Field Emission from Rough Surface with Nonparabolic Energy Dispersion", IEEE Transaction on Electron Device 65, 2089 (June 2018). – 12 citations from google scholar

Abstract: The theories of field electron emission from perfectly planar and smooth canonical surfaces are well understood, but they are not suitable for describing emission from rough, irregular surfaces arising in modern nanoscale electron sources. Moreover, the existing models rely on Sommerfeld's free-electron theory for the description of electronic distribution, which is not a valid assumption for modern materials with nonparabolic energy dispersion. In this paper, we derive analytically a generalized Fowler–Nordheim (FN)-type equation that considers the reduced space-dimensionality seen by the quantum mechanically tunneling electron at a rough, irregular emission surface. The traditional FN equation is shown to be a limiting case of our model in the limit of a perfectly flat surface of a material with parabolic dispersion. The fractional dimension parameter used in this model can be experimentally calculated from appropriate current–voltage data plot. By applying this model to experimental data, the standard field-emission parameters can be deduced with better accuracy than by using the conventional FN equation.

Topic 2: Fractional Mott-Gurney law

Publication: M. Zubair, Y. S. Ang, and L. K. Ang, "Thickness dependence of space-charge-limited current in spatially disordered organic semiconductors", IEEE Transaction on Electron Device 65, 3421 (Aug 2018) – 9 citations from google scholar

Abstract: Charge transport properties in organic semiconductors are determined by two kinds of microscopic disorders, namely, energetic disorder related to the distribution of localized states and the spatial disorder related to the morphological features of the material. Froma semiclassical picture, the charge transport properties are crucially determined by both the carrier mobility and the electrostatic field distribution in the material. Although the effect of disorders on carrier mobility has been widely studied, how electrostatic field distribution is distorted by the presence of disorders and its effect on charge transport remain unanswered. In this paper, we present a modified space-charge-limited current (SCLC) model or Mott-Gurney (MG) aw for spatially disordered organic semiconductors based on the fractional-dimensional electrostatic framework. We show that the thickness dependence of the SCLC is related to the spatial disorder in organic semiconductors. This fractional MG model shows good agreement with several experiments on spatially disordered organic semiconductors. By applying this model to the experimental data, the standard charge transport parameters can be deduced with better accuracy than by using existing models.

Topic 3: Fractional Fresnel Coefficient

Publication: EDITOR PICK: M. Zubair, Y. S. Ang, K. J. A. Ooi and L. K. Ang, "Fractional Fresnel coefficients for optical absorption in femtosecond laser-induced rough metal surfaces", J Appl Phys 124, 163101 (10/2018) - 3 citations from google scholar

Abstract: The surface morphology of metal influences its optical absorptivity. Recent experiments have demonstrated that the femtosecond laser induced surface structures on metals could be dynamically controlled by the fluence of laser and the number of pulses. In this paper, we formulate an analytical model to calculate the optical absorption of a rough metallic surface by modeling the roughness as a fractal slab. For a given experimental image of the surface roughness, we characterize the roughness with a fractal parameter by using the box-counting method. With this parameter as an input, we calculate the absorption of an 800 nm laser pulse impinging on gold, copper, and platinum, and the calculated results show excellent agreements. In terms of physics, our model can be viewed as a fractional version of the Fresnel coefficients, and it will be useful for designing suitable surface structures to tune the light absorption on metals from purely reflective to highly absorptive based on different applications.

Topic 4: Fractional Capacitance for planar capacitor
Publication: PIERS2017, Singapore, 19 – 22 November (2017) – 2 papers below

Y. W. Low, S. Athalye, Y. S. Ang, M. Zubair, and L. K. Ang, Numerical and Experimental Study on Electrostatic Properties of 3D Printed Fractal Capacitors

Abstract: The dielectric properties of heterogeneous media are of increasing interest as many applications exploit the usage of dielectric property detection in bio-imaging, scanning, microwave tomography and other electromagnetic applications. It can be complex to model such media due to non-smooth and irregular interfaces. However, where there is fractality involved in the geometry of the material, it is possible to model the electrostatic properties of the media accurately using the application of non-integer dimensions onto Laplace's equations. Using this approach, we provide a numerically and experimentally validated analytical model to describe the capacitance of materials that accommodates the fractal nature of dielectrics. We achieve this by deriving the proposed fractal-dimensional electromagnetic models for static potentials using Laplace's equations but with dimensions D generalised to non-integers. We perform both practical experiments on 3D printed structures with LCR meters and computer simulations on COMSOL for dielectrics exhibiting different fractal geometries (Cantor Sets,Cantor Bars, Sierpinski Carpets, and Menger Sponges). The chosen geometries are cubical in nature so that they are easy to implement with a parallel plate setup. The experiment / simulation is carried out to determine the capacitance across the ends of the dielectric with fractality along at least one of the coordinate axis. We demonstrate that the experimental measurement can be well described by our theoretical models. The analytical non-integer dimensional model developed here may provide a powerful tool to simply the formidable electromagnetic simulation of nonhomogeneous media.

S. Athalye, Y. W. Low, Y. S. Ang, M. Zubair, and L. K. Ang, Electrostatic Properties of Heterogeneous Medium with Inclusion of Fractal Geometry

Abstract: The aim of this research is to study the electrostatic properties of heterogenous media that have fractal geometries. The existing models treat composite dielectrics as those that have regular geometric structures (integer-valued dimensions) and an isotopic, homogenous dielectric permittivity; but, in reality, the dielectric permittivity is affected by the irregular interface between different materials. These complicated irregularities can often be approximated using fractal geometry. In this work, a numerically and experimentally validated analytical model for describing the electrostatic properties of dielectric materials with fractal irregularities is developed based on recently proposed fractional-dimensional electromagnetic models. We investigated the effects of the fractal irregularities on the capacitance of parallel-plate geometry in the following ways: (i) by making the distance between the two electrode plates fractal but keeping the plate area non-fractal; (ii) by making the plate area fractal but keeping the distance between the plates non-fractal; and (iii) by making both the plate area and the distance between the plates fractal. Full-wave simulations using COMSOL, and experiments are employed to verify our model in various fractal geometries including 3D cube/cuboid and 2D square/rectangle. The fractal geometries are constructed by dividing the region between the electrode plates into alternating parallel layers of dielectric and air, with the thickness of each dielectric layers set to the length of the components of a Cantor set of certain removal factors (3, 4, 5, 6, and 7) at the 4th iteration. Each removal factor results in different fractal dimension as determined by Hausdorff's formula. The capacitance obtained from analytical model and full-wave 2D COMSOL simulations are validated in experiments using 3D printed fractal blocks. The proposed model provides a simple method of characterizing the effective dielectric properties of heterogeneous fractal media from thickness and area scaling of its capacitance. Our results reveal a new viable direction towards the modelling of electromagnetic properties of complex media using non-integer dimension approach.

List any interactions with industry or with Air Force Research Laboratory (AFRL) scientists AOARD window of science award to attend AFOSR program review, and presentations in universities

L. K. Ang, Computational Electromagnetics at Fractional Dimensions, USA AFRL (Wright Patterson) Sensor Directorate Seminar, Dayton, Ohio, USA 30 July (2018).

L. K. Ang, Electron emission from 2D materials and Fractional modeling, USA AFOSR Programme Review, Arlington, VA, USA 24 – 26 July (2018).

L. K. Ang, Applying Fractional Calculus in Modelling for Electromagnetism and Electronics, Seminar, Department of Computational Mathematics, Science and Engineering, Michgan State University, 13 April (2018).

L. K. Ang, Electron Emission from Two-Dimensional Novel Materials and Applications, Michigan Institute of Plasma Science and Engineering (MIPSE) Colloquium, University of Michigan, 11 April (2018)

L. K. Ang, Fractional modeling in computational physics and engineering, Zhejiang University, Seminar, China 25 April (2019)

L. K. Ang was elected as IEEE NPSS distinguished lecturer (DL)
https://ieee-npss.org/distinguished-lecturers/dr-lay-kee-ricky-ang/
One of his 4 talks under NPSS DLS is to present the results from this grant:

Title: Some applications of fractional modeling in physics and engineering

In modelling or simulation, it is common to solve coupled differential equations in one-, two- or three-dimensions (1D, 2D, or 3D) with corresponding boundary conditions. For complicated objects, the dimension may not be strictly 1D, 2D or 3D, where the normal computational approach may be expensive as it will involve multiple scale computation. By using fractional models developed mathematicians, a complicated object is projected into a "fractional" dimension in order to solve the relevant equations in this non-integer dimension with the assumption that the effects at smaller scales can be ignored. In this talk, we will present some recent results of using such "fractional" models on problems such as fractional high current from rough cathode, fractional high current transport in organic diode, fractional tunneling law, fractional Fresnel coefficients for laser absorption, fractional capacitor, and others. These new fractional models will provide useful fractional parameters that can be characterized by experimental measurements. The calculated results will be compared with available experimental results or normal numerical results.