Derek Chen
Research Plan
Category: Physics and Astronomy

Title: **Simulating Nanoscale Imaging of Plasmonic Excitations and Cancer Cells under Near-field Nanoscopy**

A. Rationale

Modern nanoimaging within the terahertz (THz) frequency range provide novel possibilities in imaging a variety of samples and phenomena [1], from cancer cells [2,3,4,5] to plasmonic modes and polaritonic excitations [1,6,7,8,9,10]. This is due to the low photon energy within the THz regime, which makes it applicable to biological samples which may be otherwise damaged by high-energy imaging methods [1,3]; moreover, THz imaging has been shown to be able to provide higher optical contrast and resolution in comparison to high-energy imaging methods [3]. In addition to this, THz imaging has been used with novel near-field imaging methods, such as scattering-type scanning near-field optical microscopy (s-SNOM), has been critical for the study of various materials, including strongly correlated quantum materials (SCQMs) [1, 11]. s-SNOM has been shown to be capable of spatial resolution down to 10 nm, and has been applied to the direct imaging of materials such as gold and hexagonal boron nitride [1,6,7,8,9,10]. Under s-SNOM, a probe is placed close to the surface of a sample, linking the optical properties of the sample to the probe; this thus allows for the propagation of a near-field signal, which cannot be measured through conventional optics [1]. s-SNOM, used in conjunction with THz imaging, shows promise for applications in fields ranging from the biomedical field to the field of condensed matter physics [1]. Developing accurate models for s-SNOM is thus critical for verifying experimental results; this is particularly true within the THz regime, in which high signal-to-noise ratios currently hinder experimental capabilities [1]. Accurate models are thus necessary for providing quantitative interpretation and validation of experimental results [1].

Modeling THz imaging with the usage of s-SNOM is of particular interest for cancer diagnosis, as cancer diagnosis relies on optical contrasts in imaging [3]. 25% of deaths within the United States can be attributed to cancer; to address this death rate, effective and efficient treatment necessary, which is in turn dependent on effective and efficient diagnosis, which in turn depends on precise imaging of cancer cells [3]. A possible THz probe for cancer diagnosis would address this issue due to its precision in imaging, while also being non-invasive [3]; in order to attain such a probe, accurate modeling of s-SNOM imaging in the THz range, especially with regards to cancer cells, is necessary.

B. Objectives

Research Question(s): How can s-SNOM be modeled analytically in the THz regime?

This study has several aims:

1) to create an accurate simulation method for s-SNOM microscopy and spectroscopy

2) to demonstrate the applicability of s-SNOM, especially in the THz regime, for a variety of applications, including in physics and in cancer cell imaging, through the usage of simulation. This would include the usage of this simulation method for plasmonic and polaritonic modes, as well as in the simulation of optical contrasts between normal and cancerous human cells.

The creation of an accurate and applicable simulation method would ultimately provide a method for providing more accurate verification of experimental and future results for s-SNOM and THz imaging, which could lead to novel methods for imaging materials, as well as novel methods for cancer diagnosis, such as possible probes relying on the principles of s-SNOM and THz imaging.

C. Procedures:

The semi-analytical discrete dipole approximation (DDA) [15,16,17] will be used to simulate various systems, including plasmonic modes in gold [9,10], polaritonic modes in hBN [7,8], and optical contrasts between normal and cancerous human cells [4,5]. Under the DDA, the tip-sample system of s-SNOM will be approximated using interacting dipoles [16,17,18], and has been previously applied to the study of evanescent waves with atomic force microscopy (AFM) [19] as well as near-field microscopy using total internal reflection [20]; however, the application of this simulation method to s-SNOM, particularly in the THz regime, has not yet been achieved.

The DDA will be adapted from existing Python source code [21] for s-SNOM and THz imaging. In order to do this, the source code will be adapted to create loops to sweep over spatial position; in addition to this, the source code will be adapted to create various sample and tip geometries, such as circular and triangular samples.

Risk and safety: No potential risks are applicable for this project.

Data analysis: Simulations produced will be compared against existing analytical, numerical, and experimental results for s-SNOM and THz. Spectroscopy simulations will be graphed against previous spectroscopy results [12,13], while microscopy simulations will be compared against previous analytical results [4,5,6,7,8,9,10].

References

[1] Chen, X., Hu, D., Mescall, R., You, G., Basov, D. N., Dai, Q., & Liu, M. (2019). Modern Scattering-Type Scanning Near-Field Optical Microscopy for Advanced Material Research [PDF]. *Advanced Materials*.

[2] Yang, X., Zhao, X., Yang, K., Liu, Y., Liu, Y., Fu, W., & Luo, Y. (2016). Biomedical Applications of Terahertz Spectroscopy and Imaging [PDF]. *Trends in Biotechnology*. https://doi.org/10.1016/j.tibtech.2016.04.008

[3] Yu, C., Fan, S., Sun, Y., & Pickwell-MacPherson, E. (2012). The potential of terahertz imaging for cancer diagnosis: A review of investigations to date [PDF]. *Quantitative Imaging in Medicine and Surgery*. https://doi.org/10.3978/j.issn.2223-4292.2012.01.04

[4] Truong, B. C. Q., Tuan, H. D., Fitzgerald, A. J., Wallace, V. P., & Nguyen, H. T. (2015). A Dielectric Model of Human Breast Tissue in Terahertz Regime [PDF]. *IEEE Transactions on Biomedical Engineering*. https://doi.org/10.1109/TBME.2014.2364025

[5] Truong, B. C. Q., Tuan, H. D., Fitzgerald, A. J., Wallace, V. P., Nguyen, T. N., & Nguyen, H. T. (2015). Breast Cancer Classification Using Extracted Parameters from a Terahertz Dielectric Model of Human Breast Tissue [PDF]. *Conference Proceedings - IEEE Engineering in Medicine and Biology Society*. https://doi.org/10.1109/EMBC.2015.7318974

[6] Basov, D. N., Fogler, M. M., & Garcia de Abajo, F. J. (2016). Polaritons in van der Waals materials. Science. https://doi.org/10.1126/science.aag1992

[7] Dai, S., Fei, Z., Ma, Q., Rodin, A. S., Wagner, M., McLeod, A. S., . . . Basov, D. N. (2019). Tunable Phonon Polaritons in Atomically Thin van der Waals Crystals of Boron Nitride. *Science*. https://doi.org/10.1126/science.1246833

[8] Dai, S., Tymchenko, M., Yang, Y., Ma, Q., Pita-Vidal, M., Watanabe, K., . . . Basov, D. N. (2018). Manipulation and Steering of Hyperbolic Surface Polaritons in Hexagonal Boron Nitride. *Advanced Materials*.

[9] Garcia-Etxarri, A., Romero, I., Garcia de Abajo, F. J., Hillenbrand, R., & Aizpurua, J. (2009). Influence of the tip in near-field imaging fo nanoparticle plasmonic modes: Weak and strong coupling regimes. *Physical Review B*, *79*. https://doi.org/10.1103/PhysRevB.79.125439

[10] Hillenbrand, R., & Keilmann, F. (2001). Optical oscillation modes of plasmon particles observed in direct space by phase-contrast near-field microscopy. *Applied Physics B*. https://doi.org/10.1007/s003400100656

[11] Liu, M., Sternbach, S. J., & Basov, D. N. (2017). Nanoscale electrodynamics of strongly correlated quantum materials. *Reports on Progress in Physics*. http://dx.doi.org/10.1088/0034-4885/80/1/014501

[12] Chen, X., Fan Bowen Lo, C., Zheng, W., Hu, H., Dai, Q., & Liu, M. (2017). Rigorous numerical modeling of scattering-type scanning near-field optical microscopy and spectroscopy [PDF]. *Applied Physics Letters*. https://doi.org/10.1063/1.5008663

[13] Cvitkovic, A., Ocelic, N., & Hillenbrand, R. (2007). Analytical model for quantitative prediction of material contrasts in scattering-type near-field optical microscopy. *Optics Express*. https://doi.org/10.1364/OE.15.008550

[14] Knoll, B., & Keilmann, F. (2000). Enhanced dielectric contrast in scattering-type scanning near-field optical microscopy. *Optics Communications*.

[15] Purcell, E. M., & Pennypacker, C. R. (1973). Scattering and Absorption of Light by Nonspherical Dielectric Grains. *The Astrophysical Journal*.

[16] Draine, B. T. (1988). The Discrete-Dipole Approximation and its Application to Interstellar Graphite Grains. *The Astrophysical Journal*.

[17] Draine, B. T., & Flatau, P. J. (1994). Discrete-dipole approximation for scattering calculations. *Journal of the Optical Society of America A*.

[18] Yurkin, M. A., & Hoekstra, A. G. (2007). The discrete dipole approximation: An overview and recent developments. *Journal of Quantitative Spectroscopy & Radiative Transfer*. https://doi.org/10.1016/j.jqsrt.2007.01.034

[19] Loke, V. L. Y., & Mengüç, M. P. (2010). Surface waves and atomic force microscope probe-particle near-field coupling: discrete dipole approximation with surface interaction. *Journal of the Optical Society of America A*. https://doi.org/10.1364/JOSAA.27.002293

[20] Ruan, Y., Li, K., Lin, Q., & Zhang, T. (2018). Tip-Nanoparticle Near-Field Coupling in Scanning Near-Field Microscopy by Coupled Dipole Method. *Chinese Physics Letters*. Retrieved from https://iopscience.iop.org/article/10.1088/0256-307X/35/4/044203/meta

[21] Juluri, B. K. (2016). Coupled Dipole Approximation in Python. Retrieved from http://juluribk.com/2016/07/20/coupled-dipole-approximation-in-python/

1. Human participants research: Not applicable
2. Vertebrate animal research: Not applicable
3. Potentially hazardous biological agents research: Not applicable
4. Hazardous chemicals, activities & devices: Not applicable

NO ADDENDUMS EXIST