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14. ABSTRACT

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RPPR Final Report
as of 28-Jan-2020

Agency Code:

Proposal Number: 67286PHREP **Agreement Number: W911NF-15-1-0535**

INVESTIGATOR(S):

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DUNS Number: 003135068 EIN: 540505990
Report Date: 20-Nov-2019 Date Received: 03-Nov-2019
Final Report for Period Beginning 21-Aug-2015 and Ending 20-Aug-2019
Title: Cubic Nonlinearity of Transition Metal Dichalcogenides in Atomic Layers for Defense Applications
Begin Performance Period: 21-Aug-2015 **End Performance Period:** 20-Aug-2019
Report Term: 0-Other

Submitted By: Felix Seo Email: jaetae.seo@hamptonu.edu
Phone: (757) 727-5152

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STEM Degrees: 5 **STEM Participants:** 9

Major Goals: The major goals of project were: 1) to characterize the cubic nonlinearity of 2-dimensional (2D) transition metal dichalcogenides (TMDCs, MX2; M=Mo or W; X=S and Se) atomic layers for DoD's nonlinear photonic applications; 2) to train the number of graduate and undergraduate students in emerging technologies related to the 2D atomic layers; and 3) to strengthen the pipeline of good students pursuing advanced degrees in science and technology through outreach activities involving local and regional schools.

Accomplishments: The following activities are accomplished under the goal during the reporting period:
? Material preparation of mechanically exfoliated atomic layers of two-dimensional transition metal dichalcogenides (TMDCs, MX2; M: Mo or W; X: S or Se) on Si-wafer, sapphire window, and liquid suspension for Z-scan and spatial self-phase modulation
? Study of cubic nonlinearity of TMDC atomic layer using the open and closed Z-scan and spatial self-phase modulation as functions of applied intensities and sample positions. The characterization includes: (1) nonlinear transmittance as functions of the sample positions in open z-scan for different excitation intensities; (2) nonlinear transmittance as functions of the sample positions in closed z-scan for different excitation intensities; (3) the magnitude and polarity of third-order nonlinearity; (4) nonlinear transmittance as a functions of the input intensity (I-scan) at the focal plane of open Z-scan, and the valley and peak positions of nonlinear transmittance in closed Z-scan for the potential applications of optical modulator and photonic devices; and (5) magnitudes and polarities of cubic nonlinearities of atomic layer liquid suspensions.
? Analyses of exciton polarization dephasing time of tungsten diselenide (WSe2) atomic layer. The analysis includes: (1) exciton dephasing time as functions of excitation intensity and exciton-exciton coupling strength; (2) exciton dephasing time as functions of temperature and exciton-phonon coupling strength; and (3) exciton dephasing time as functions of excitation intensity and temperature.
? Analyses of tunable bandgap and exciton formation entropy of TMDC atomic layers. The analyses include: (1) bandgap energy as a function of temperature; (2) bandgap energy as functions of temperature and coupling strength of electron-phonon; (3) bandgap energy as functions of temperature and acoustic phonon energy; (4) change in exciton formation entropy as functions of temperature and coupling strength of electron-phonon; (5) change in exciton formation entropy as functions of temperature and acoustic phonon energy; (6) bandgap energy as functions of the change in exciton formation entropy (variable electron-phonon coupling strengths for a constant phonon energy) and temperature; and (7) bandgap energy as functions of the change in exciton formation entropy (variable phonon energy for a constant electron-phonon coupling strengths) and temperature.
? Characterization of saturable and reverse saturable absorption transition between monolayer and bilayer/multilayer. The characterization include: (1) nonlinear transmittance as functions of the sample positions in open z-scan and excitation intensities; (2) nonlinear transmittance as functions of the sample positions in open z-

scan and the ratio of ground-state and excited-state absorption cross-sections; and (3) nonlinear transmittance as functions of the sample positions in I-scan and the ratio of ground-state and excited-state absorption cross-sections.

? The research results and finding were used to disseminate twelve (12) journal articles and sixty two (62) conference presentations. All disseminations were acknowledged by the ARO funding.

? The outreach activities include the Lab Demonstrations for high School students, Career Fair at Lake Taylor Middle School, High School Day Demonstration, Middle and High School Students' Research Activities, Middle School Student Training, Optics and Laser demonstrations to High School Students from Governor's STEM Academy at Harrisonburg, Annual Optics and Laser Science Summer-Workshop for High School Teachers, Optics and Laser Demonstrations at the Youth STEM Conference, and Physics Demonstrations Black Family Conference.

Training Opportunities: In the current research of cubic nonlinearity of transition metal dichalcogenides (TMDCs) in atomic layers for defense applications, four graduate students and five undergraduate students have been trained during the funding period. One graduate student completed his Ph.D. degree, and three undergraduate students completed their undergraduate degrees during the funding period.

Research training at the graduate level:
? Mr. Tikaram Neupane (Ph.D. candidate), Graduate student in Ph.D. Physics program was trained in the characterization of optical nonlinearity of TMDCs atomic layer with Z-scan, I-scan, and spatial self-phase modulation techniques. During the funding period, he authored and co-authored six (6) journal articles and fifty-two (52) conference presentation.
? Mr. Quinton Rice, graduate student in Ph.D. Physics program, was trained in time-resolved and temperature dependent properties of optical materials in order to develop efficient hybrid white LEDs. He was also trained on the quantum correlation of photon polarizations of exciton and bi-exciton transitions. His two manuscripts of tunable bandgap charaterizations and exciton formation entropy of transition metal dichalcogenides were accepted by the Journal of Nanoscience and Nanotechnology. In summer 2017, he successfully completed his dissertation research and, and earned his Ph.D. degree in Optical Condensed Matter Physics at Hampton University. He studied the exciton-plamon couplings for efficient lighting devices for six years under Dr. Seo's advisement since he was a junior. His research was involved in characterizing good candidates for white light generation based on II-VI and I-III-VI2 semiconductors to achieve highly efficient and bright white LEDs. He claimed that he is the top leading researcher in plasmon-coupled QDs for white LEDs. He authored and co-authored over 20 journal articles, and over 50 conference presentations. He received the Best Student Paper Award at the Virginia Academy of Science in 2014. His dissertation title was "Plasmon-coupled Excitons in Quantum Confined Semiconductors". From his Ph. D. dissertation, he would like to claim that he is the number one in the world in the area of plasmon-coupled quantum dot for white LEDs. He received three job offers including Optical Engineer at Thorlabs, Postdoctoral Research Associate at Hampton University, and Assistant Professor (Tenure-track) at University of North Carolina. Among those offers, he chose the Assistant Professor (Tenure-track) at University of North Carolina because he believed that he was trained enough in grant writing, research activities, teaching, and service.
? Mr. Dulitha Mahesh Jayakody Jayakodige, Graduate student in Ph.D. Physics program, was trained in nonlinear frequency conversion of optical emission. The nonlinear frequency conversion includes frequency down and up conversions. He also prepared a glove-box for preparing atomic layer materials, and was trained in the high-resolution multi-channel spectrometer. He authored and co-authored twenty-six (26) conference presentations.
? Mr. Taiwo Orogbangba, graduate student in MS Computer Science, involved in developing ZAVA programming to support the characterization of optical properties. He completed his MS degree in Computer Science with a comprehensive exam in summer 2017.

Research training at the undergraduate level:
? Mr. Taylor Jeremiah Osborne successfully completed his B.S. degree in Marine and Environmental Science in May 2019 and joined the Solar Energy Industry in both San Francisco, CA and Virginia Beach, VA. He participated in the laser spectroscopy of optical materials to characterize linear absorption, absorption cross-section, the concentration of quantum materials. He was also trained in the nonlinear spectroscopy for characterizing atomic layers. His experiment results and findings were disseminated through the School of Science Research Symposium.
? Miss Chanel Person also successfully completed her B.S. degree in Chemistry in May 2019 and joined the Applied Physics Laboratory at Johns Hopkins University in MD. She characterized the temperature-dependent (thermal effect) refractive index change of chemical molecules using a Mach Zehnder interferometer. The accuracy of refractive index was around 10-4. Her research results and findings were disseminated through the School of Science Research Symposium.
? Mr. Kyle Burney successfully completed his B.S. degree in Physics in May 2018, and joined the US Navy. During his undergraduate academic years at Hampton University, he was a Navy ROTC, and participated in the characterization on the temperature-dependence emission and time-resolved spectroscopy of quantum dots. He demonstrated his skillful data measurement and characterization which led to the successful preparation of his first co-authored manuscript entitled: "Broadband Light Source of Quantum Dots for Optical Sensing". He co-authored one manuscript and one conference presentation.
? Miss Ananda Ewing-Boyd, major in Psychology and minor in Physics, was trained in time-resolved spectroscopy (50-ps laser, spectrometer, streak camera (Hamamatsu)) and optical sensing. Her research findings and results were utilized for five conference presentations. She also prepared artificial atomic layers for potential electronic devices. Her research results and findings were disseminated through the School of Science Research Symposium.

? Miss Eden Duncan-Smith, major in Physics, was trained in lab safety, laser protection, laser alignment to study the temperature dependent-photoluminescence and Raman spectroscopy of nanomaterials. Her research results and findings were disseminated through the School of Science Research Symposium.

Results Dissemination: ? The research results and findings were utilized to disseminate twelve (12) journal articles in the Scientific Report, Optical Materials Express, Journal of Nanoscience and Nanotechnology, Optical Materials, Journal of Physics D: Applied Physics, Nanoscale, Applied Surface Science, and Physical Chemistry Chemical Physics. All disseminations through journal articles were acknowledged by the ARO funding.
? The research results and findings were utilized to present sixty two (62) conference presentations during the funding period. All disseminations through conference presentations were acknowledged by the ARO funding. The conferences include the 86th Annual Meeting of the APS Southeastern Section, the Annual Meeting of Viriginia Academy Science, the 16th International Conference on Nano Science and Nano Technology 2019, SPIE Defense and Commercial Sensing 2019, 6th International Conference & Exhibition on Advanced & Nano Materials, 49th Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics APS Meeting, 2017 Workshop on Innovative Nanoscale Devices and Systems (WINDS), 2017 Annual Meeting of the APS Mid-Atlantic Section, International Conference & Exhibition an Advanced & Nano Materials (ICANM), 22nd International Conference on Electronic Properties of Two Dimensional Systems (EP2DS22) and the 18th International Conference on Modulated Semiconductor structures (MSS18), 48th Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics, International Conference on NanoBio Sensing, Imaging, and Spectroscopy 2017, the 14th International Conference on NanoScience and NanoTechnology, the 83rd Annual Meeting of the APS Southeastern Section, and the 6th International Conference and Exhibition on Materials Science and Engineering.
? In addition to the direct analyses and characterization of 2D TMDC atomic layers, the students were trained in various spectroscopic techniques to prepare their skills for the atomic layer measurement.
? The research results and findings were also utilized for several outreach activities including School of Science Research Symposium; Lab Demonstrations for high School students; Career Fair at Lake Taylor Middle School; High School Day Demonstration; Middle and High School Students' Research Activities; Middle School Student Training; hands-on experience in materials, optics, laser science, spectroscopy, and microscopy to middle and high school students; Optics and Laser demonstrations to High School Students from Governor's STEM Academy at Harrisonburg; Annual Optics and Laser Science Summer-Workshop for High School Teachers; and Optics and Laser Demonstrations at the Youth STEM Conference.
? The research participants were actively involved in enhancing science teachers' education in the grades of 6-12, science demonstrations in local schools, and provide them with hands-on experience in optics and fun science.

Honors and Awards: It was honor that Dr. Felix Jaetae Seo serves as Director and PI of the NSF-funded Advanced Center for Laser Science and Spectroscopy, and Co-I of the NASA-funded Center for Atmospheric Research and Education at Hampton University. Also, Dr. Felix Jaetae Seo served as the Organizing and Scientific Committee for the International Conference and Exhibition on Advanced and Nano Materials 2017-2019. Dr. Felix Jaetae Seo also serves in the Editorial Board of International Journal of Optics Science; Editorial Board of International; Journal of Atomic, Molecular, and Optical Physics; Editorial Board of Photonics and Optoelectronics; Editorial Board of the Open Spectroscopy Journal; Editorial Board for Optics and Photonics Journal; Editorial Advisory Board of the Open Applied Physics Journal; and Editorial Board for International Journal of Advanced Physics Research. It is also a great advantage to the project that the PI, Dr. Felix Jaetae Seo, holds the certifications of Responsible Conduct of Research (RCR) by the Collaborative Institutional Training Initiative; and the Hazardous & Universal Waste Management (40 CFR parts 262, 273 & 279) & Hazardous Materials Transportation and Security (49 CFR Part 172 – Subject H).

Protocol Activity Status:

Technology Transfer: The characterization with Z-scan and spatial self-phase modulation revealed the reverse saturable absorption and saturable absorption, nonlinear refraction of atomics layers which can be utilized for optical modulators and photonic devices. Therefore, the results on the cubic nonlinearity of transition metal dichalcogenides (TMDCs) in atomic layers is important to make significant technological impacts on ultrafast laser mode-locking, passive Q-switching, optical power limiting, and quantum information processing. The technology transfer was not made during the funding period, but is anticipated near future.

PARTICIPANTS:

Participant Type: PD/PI

Participant: Felix Jaetae Seo
Person Months Worked: 8.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Faculty
Participant: Bagher Tabibi
Person Months Worked: 13.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)
Participant: Sheng Yu
Person Months Worked: 15.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)
Participant: Shopan Hafiz
Person Months Worked: 7.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

ARTICLES:

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Journal: Optical Materials Express
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Volume: Issue: First Page #:
Date Submitted: 11/3/19 12:00AM Date Published:
Publication Location:
Article Title: Spatial Self-Phase Modulation in WS2 and MoS2 Atomic Layers
Authors: Tikaram Neupane, Bagher Tabibi, and Felix Jaetae Seo
Keywords: Spatial Self-Phase Modulation, Atomic Layers
Abstract: Laser field-induced spatial self-phase modulation (SSPM) in WS2 and MoS2 atomic layer liquid suspensions displayed the diffraction profile of concentric rings at the far-field due to the coherent superposition of transverse wave vectors with characteristic spatial nonlinear phases. The evolution of the number of rings indicated the spatial alignment of anisotropic atomic layers in the liquid base solution. The intensity-dependent number of symmetric rings revealed the nonlinear refraction coefficients of MoS2 and WS2 atomic layers which were estimated to be ~ - 1.96 x 10-16 m2/W and ~ -1.11 x 10-16 m2/W, respectively. The central interference profile and the diffraction pattern identified the negative polarity of nonlinear refraction. The vertically asymmetric diffraction ring indicates the phase distortion of optical field due to the heat convection.
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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Nanoscience and Nanotechnology
Publication Identifier Type: DOI Publication Identifier: 10.1166/jnn.2018.14956
Volume: 18 Issue: 2175 First Page #:
Date Submitted: 10/4/18 12:00AM Date Published: 3/1/18 5:00AM
Publication Location:
Article Title: Bandgap Tunability of Transition Metal Dichalcogenide Atomic Layers
Authors: Quinton Rice, Bagher Tabibi, and Felix Jaetae Seo
Keywords: Atomic layer, Bandgap, Transition Metal Dichalcogenides
Abstract: The temperature-dependent bandgap of transition metal dichalcogenides (TMDCs, MX2; M=Mo or W; X=S, Se, or Te) is analyzed using the O'Donnell and Chen relation with parameters including the average acoustic phonon energy ( ) and the electron-phonon coupling strength ( ). Wider (narrower) tunability of the bandgap results from the larger (smaller) electron-phonon coupling strength for a constant acoustic phonon energy. A 1.5 eV bandgap change was observed for weak electron-phonon coupling (=2) as well as with the strong electron-phonon coupling (=30). However, the weak electron-phonon coupling leads to a linear decrease in the bandgap energy as a function of temperature above ~85 K while the strong coupling exhibits similar behavior after ~60 K. Narrower (wider) tunability of the bandgap results from the larger (smaller) acoustic phonon energy for a constant electron-phonon coupling strength.
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Article Title: Exciton Dephasing in Tungsten Diselenide Atomic Layer
Authors: Tikaram Neupane, Quinton Rice, Sungsoo Jung, Bagher Tabibi, and Felix Jaetae Seo
Keywords: Exciton Dephasing, WSe2 Atomic Layer, Exciton–Exciton Coupling, Exciton–Phonon Coupling
Abstract: An intrinsic exciton dephasing is the coherence loss of exciton dipole oscillation, while the total exciton dephasing originates from coherence loss due to exciton–exciton interaction and excitonphonon coupling. In this article, the total exciton dephasing time of tungsten diselenide (WSe2) atomic layers was analyzed as functions of excitation intensity with exciton–exciton coupling strength and temperature with exciton–phonon coupling strength. It was hypothesized that the total exciton dephasing time is shortened as the exciton–exciton interaction and the exciton–phonon coupling are increased. The coherence loss analysis revealed that the exciton dephasing time of WSe2 atomic layers is due to mainly the temperature rather than the excitation intensity.
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Article Title: Third-Order Optical Nonlinearity in Tungsten Disulfide Nanoflakes with Resonant Excitation
Authors: Tikaram, Neupane; Bagher, Tabibi; and, Felix, Jaetae Seo
Keywords: Third-order optical nonlinearity, Atomic layer, WS2, Z-scan
Abstract: The third-order optical nonlinearity of tungsten disulfide atomic layer was characterized with open and closed Z-scan techniques with a resonant excitation near an exciton absorption peak using a pulsed laser which has a temporal pulse width of ~6 ns and a Gaussian spatial beam profile. The normalized transmittance traces with open and closed Z-scan for the WS2 atomic layers displayed positive nonlinear absorption and negative nonlinear refraction. The nonlinear absorption and nonlinear refraction coefficients of WS2 with the resonant excitation were estimated to be ~ 6.0 x10-8 m/W and ~-3.8 x 10-15 m2/W.
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Article Title: Piezoelectricity enhancement and bandstructure modification of atomic defect-mediated MoS
Authors: Sheng Yu, Quinton Rice, Tikaram Neupane, Bagher Tabibi, Qiliang Li, Felix Jaetae Seo
Keywords: MoS2 atomic layer; Bandstructure; Piezoelectricity
Abstract: Piezoelectricity appears in the inversion asymmetric crystal that converts mechanical deformational force to electricity. Two-dimensional transition metal dichalcolgenide (TMDC) monolayers exhibit the piezoelectric effect due to the inversion asymmetry. The intrinsic piezoelectric coefficient (e11) of MoS2 is ~298 pC/m. For the single atomic shift of Mo of 20% along the armchair direction, the piezoelectric coefficient (e11) of MoS2 with 5x5 unit cells was enhanced up to 18%, and significantly modified the band structure. The single atomic shift in the MoS2 monolayer also induced new energy levels inside the forbidden bandgap. The defect-induced energy levels for a Mo atom shift along the armchair direction are relatively deeper than the energy levels for a S atom shift along the same direction. It indicates that the piezoelectricity and band structure of MoS2 can be engineered by a single atomic shift in the monolayer with multi unit cells for mechano-electrical applications.
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Date Submitted: 10/4/18 12:00AM Date Published: 3/1/18 5:00AM
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Article Title: Exciton Formation Entropy Changes in Transition Metal Dichalcogenide Atomic Layers
Authors: Quinton Rice, Bagher Tabibi, Felix Jaetae Seo
Keywords: Transition Metal Dichalcogenides, Exciton Formation Entropy
Abstract: The atomic layers of transition metal dichalcogenides (TMDCs, MX2; M=Mo or W; X=S, Se, or Te) are of great interest in the areas of photonics and optoelectronics due to the correlation between valley orbital, spin, and optical helicity; the compositional tuning of exciton bandgaps in visible and near-infrared spectra; and the bandgap modification from indirect for bilayer or multilayer to direct for monolayer. The derivative of the O'Donnell and Chen relation is analyzed as a function of temperature and gives the relationship between the change in entropy of exciton formation and the bandgap energy. The analysis suggests the change in entropy of exciton formation with higher energy phonons (~100 meV) is constant until ~90 K while lower energy phonons (~10 meV) approaches a constant value of between ~250 K and ~300 K where is the strength of electron-phonon interaction and is the Boltzmann constant. Increased scattering and spontaneous decay probabilities explains the amplified elect
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Date Submitted: 10/4/18 12:00AM Date Published: 7/10/18 4:00AM
Publication Location:
Article Title: Emission Recovery and Stability Enhancement of Red Emission Inorganic Perovskite Quantum Dots
Authors: Wang, Hua; Sui, Ning; Zhang, Yu; Rice, Quinton; Seo, JaeTae; Colvin, Vicki; Yu, William
Keywords: Perovskite, Quantum dot
Abstract: Inorganic lead halide perovskite quantum dots (PQDs), especially red emission PQDs, are well-known to easily lose their luminescence emission with time, which shows from strong emission of fresh PQDs to no emission of aged PQDs. Here, we demonstrate that trioctylphosphine (TOP) can effectively and instantly recover the luminescence emission of aged red PQDs, making the “dead” PQDs “reborn”. Furthermore, TOP also works to improve the emission intensity of freshly synthesized PQDs. In this process, TOP does not make any detectable structural changes to PQDs. Besides, TOP can effectively enhance the stability of PQDs against long-term storage, temperature, UV irradiation, and polar solvents. This unusual emission recovery and stability enhancement by TOP shall promote the understanding of particle surface conditions and the development of PQD devices.
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Article Title: Piezoelectricity in WSe2/MoS2 Heterostructure Atomic Layers
Authors: Sheng, Yu; Quinton, Rice; Qiliang, Li; Bagher, Tabibi; and Felix, Jaetae Seo
Keywords: Piezo-electric
Abstract: A two-dimensional heterostructure of WSe2/MoS2 atomic layers has unique piezoelectric characteristics which depend on the number of atomic layers, stacking type and interlayer interaction size. The van der Waals heterostructure of p- and n-type TMDC atomic layers with different work functions forms a type-II staggered gap alignment. The large band offset of the conduction band minimum and the valence band maximum between p-type WSe2 and n-type MoS2 atomic layers leads to large electric polarization and piezoelectricity. The output voltages for a MoS2/WSe2 partial vertical heterostructure with a size of 3.0 nm × 1.5 nm were 0.137 V and 0.183 V under 4% and 8% tensile strains, respectively. The output voltage of an AB-stacking MoS2/WSe2 heterostructure was larger than that of an AA-stacking heterostructure under 4% tensile strain due to the contribution of intrinsic piezoelectricity and symmetric out-of-plane conditions.
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Article Title: Study of strain engineering at the ?-Al_2O_3/monolayer MoS_2 interface by first principle calculations
Authors: Sheng, Yu; Shunjie, Ran; Hao, Zhu; Kwesi, Eshun; Chen, Sh;, Kai, Jiang; Kunming, Gu; Felix, Jaetae S
Keywords: 2D semiconductors, Strain effect, Temperature effect
Abstract: With the advances in two-dimensional (2D) transition metal dichalcogenides (TMDCs) based metal–oxide–semiconductor field-effect transistor (MOSFET), the interface between the semiconductor channel and gate dielectrics has received considerable attention due to its significant impacts on the morphology and charge transport of the devices. In this study, first principle calculations were utilized to investigate the strain effect induced by the interface between crystalline ┐-Al_2O_3 (0001)/h-MoS_2 monolayer. The results indicate that the 1.3 nm Al_2O_3 can induce a 0.3% tensile strain on the MoS_2 monolayer.The strain monotonically increases with thicker dielectric layers, inducing more significant impact on the properties of MoS_2. In addition, the study on temperature effect indicates that the increasing temperature induces monotonic lattice expansion.
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Article Title: Piezoelectricity Enhancement and Bandstructure Modification of Atomic Defect-mediated MoS_2 Monolayer
Authors: Sheng, Yu; Quinton, Rice; Tikaram, Neupane; Bagher,Tabibi; Qiliang, Li; and Felix, Jaetae Seo
Keywords: Atomic layer, Defect
Abstract: Piezoelectricity appears in the inversion asymmetric crystal that converts mechanical deformation to electricity. Two-dimensional transition metal dichalcolgenide (TMDC) monolayers exhibit the piezoelectric effect due to inversion asymmetry. The intrinsic piezoelectric coefficient (e11) of MoS_2 is B298 pC m┐1. For the single atomic shift of Mo of 20% along the armchair direction, the piezoelectric coefficient (e11) of MoS_2 with 5 └ 5 unit cells was enhanced up to 18%, and significantly modified the band structure. The single atomic shift in the MoS_2 monolayer also induced new energy levels inside the forbidden bandgap. The defect-induced energy levels for a Mo atom shift along the armchair direction are relatively deepe than that for a S atom shift along the same direction. This indicates that the piezoelectricity and band structure of MoS_2 can be engineered by a single atomic shift in the monolayer with multi unit cells for piezo- and opto-electric applications.
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Authors: Sheng Yu, Tikaram Neupane, Bagher Tabibi, Qiliang Li, and Felix Jaetae Seo
Keywords: Spin-resolved Visible Optical Spectra, Electronic Characteristics of Defect-mediated Hexagonal Boron Nitride Monolayer
Abstract: The defect-mediated hexagonal boron nitride (hBN) supercell display the visible optical spectra and electronic characteristics. The defects in the hBN supercell include the atomic vacancy, antisite, antisite vacancy, and substitution of a foreign atom for boron or nitrogen. The hBN supercell with VB, CB, and NB-VN has the high electron density of states across the Fermi level which indicates the high conductive electronic characteristics. The hBN with defects including atomic vacancy, antisite vacancy, and substitution of a foreign atom for boron or nitride exhibit the distinct spin-resolved optical and electronics characteristics, while the defects of boron and nitrogen antisite do not display the spin-resolved optical characteristics. The hBN with positively charged defects has dominant optical and electronic characteristics at the longer spectral region.
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Authors: Felix Jaetae Seo, Quinton Rice, Bagher Tabibi, Sangram Raut, Ignacy Gryczynski, Rahul Chib, Zygmun
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Conference Location: Atlanta, Georgia
Paper Title: Role of Acoustic Phonon Energy and Electron-phonon Coupling on Exciton Formation Entropy Changes in Transition Metal Dichalcogenide Atomic Layers
Authors: Quinton Rice, Tikaram Neupane, Dulitha Jayakodige, Bagher Tabibi, and Felix Jaetae Seo
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Paper Title: Transition of Saturable and Reverse Saturable Absorptions between Monolayer and Bilayer/Multilayer
Authors: Tikaram Neupane, Quinton Rice, Dulitha Jayakodige, Bagher Tabibi, and Felix Jaetae Seo
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Authors: Quinton Rice, Sangram Raut, Kyle Burney, Zygmunt Gryczynski, Ignacy Gryczynski, Andrew Wang, Wil
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Authors: Ananda Ewing-Boyd, Albert Seo, Sheng Yu, Quinton Rice, Tikaram Neupane, Qiliang Li, Felix Seo, and
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Authors: Felix Jaetae Seo, Sheng Yu, Quinton Rice, Shopan Hafiz, Bagher Tabibi, and Qiliang Li,
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Paper Title: Quantum Nonlinear Interferometry for Occultation Satellite Remote Sensing
Authors: Felix Jaetae Seo, Jia Su, Quinton Rice, Dulitha Jayakodige, William Moore, Pat McCormick, and Baghe
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Authors: Quinton Rice, Tikaram Neupane, Dulitha Jayakodige, Bagher Tabibi, and Felix Jaetae Seo,
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Authors: Tikaram Neupane, Quinton Rice, Dulitha Jayakodige, Bagher Tabibi, and Felix Jaetae Seo,
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Authors: Tikaram, Neupane; Dulitha, Jayakodige; Bagher, Tabibi; Felix, Seo
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Authors: Tikaram, Neupane; Dulitha, Jayakodige; Bagher, Tabibi; Felix, Jaetae Seo
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Authors: Bagher, Tabibi; Sheng, Yu; Tikaram, Neupane; Felix, Jaetae Seo
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Authors: Tikaram, Neupane; Sheng, Yu; Bagher, Tabibi; and Felix, Jaetae Seo
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Research Results and Findings

The exemplary characterizations of cubic nonlinearity for transition-metal dichacogenide atomic layers are described below:

Third-Order Optical Nonlinearity of Tungsten Disulfide Atomic Layer with Resonant Excitation

The third-order optical nonlinearity of tungsten disulfide atomic layer was characterized with open and closed Z-scan techniques with a resonant excitation near an exciton absorption peak using a pulsed laser which has a temporal pulse width of ~6 ns and a Gaussian spatial beam profile. The normalized transmittance traces with open and closed Z-scan for the WS_2 atomic layers displayed positive nonlinear absorption and negative nonlinear refraction. The nonlinear absorption and nonlinear refraction coefficients of WS_2 with the resonant excitation were estimated to be ~ 6.0×10^{-8} m/W and ~-3.8×10^{-15} m^2/W.

1. Introduction

The tungsten disulfide (WS_2) atomic layer is an intriguing nonlinear optical material for optoelectronic applications of optical power limiting, optical modulation, Q-switching, and mode-locking [1-10]. The WS_2 atomic layer has inimitable optoelectronic and material properties including direct and indirect transitions for monolayer and multilayers [1], inversion asymmetry and symmetry for odd and even layers [2], polarization chirality [3], large exciton binding energy [4], and strong spin-orbital coupling [5]. The number of atomic layer dependent optical transitions and material properties of WS_2 affect the magnitude and polarity of third-order optical nonlinearity with the optical excitations at selected photon energies. The magnitude and polarity of nonlinear absorption and nonlinear refraction can be analyzed with the Z-scan technique [6].

The properties of resonant and non-resonant third-order optical nonlinearity of WS_2 depend on the excitation photon energy. The magnitude of resonant nonlinearity is relatively large, and the nonlinear optical process is relatively slow. The magnitude of non-resonant nonlinearity is relatively small, and the nonlinear optical process is relatively fast [7]. The polarity of nonlinear absorption includes a positive nonlinear absorption of reversed saturable absorption, and a negative nonlinear absorption of saturable absorption. The reversed saturable absorption or positive nonlinear absorption has relatively larger absorption cross-section of the excited state compared to that of the ground state [8]. The saturable absorption or negative nonlinear absorption has relatively smaller absorption cross-section of the excited state when compared to that of the ground state. The negative polarity of nonlinear refraction displays a peak-valley nonlinear transmittance as the optical sample passes through the focal point. The negative nonlinearity forms a focal plane after the lens focal plane along the wave propagation direction. The positive nonlinearity of nonlinear refraction exhibits a valley-peak nonlinear transmittance as the optical sample passes through the focal point. The positive nonlinearity forms a focal plane before the lens focal plane along the wave propagation direction [9]. The normalized transmittance as a function of applied peak intensity, I-scan, at the valley of open Z-scan or at the valley of closed Z-scan also verifies the intensity-dependent absorption and refraction beyond the chromatic absorption and refraction of WS_2 atomic layer [10].

This article reports the third-order optical nonlinearity of tungsten disulfide (WS_2) atomic layers in a base solution of 70% ethanol and 30% water. The electronic band structures for 1-4 layers were calculated by first principle calculations. The characteristics of layer number-dependent electronic band structures, absorption features, spectral shifts, and electronic transitions were analyzed. The properties of third-order optical nonlinearity for the tungsten disulfide (WS_2) atomic layers were characterized with Z-scan and I-Scan techniques with a resonant excitation.

2. Electronic band structure of WS_2 atomic layer

The resonant excitation includes both direct and indirect transitions from the valence to the conduction band depending on the number of atomic layers. The third-order nonlinear optical process through the phonon-assisted indirect transition is relatively slower than the optical process through the direct transition. The direct and indirect transitions and the electronic band structure depend on the number of atomic layers [1].

The electronic band structures of WS_2 atomic layers were calculated by first principle calculations using the Virtual Nanolab Atomistix ToolKit (ATK) package with the density functional theory (DFT). All atomic positions and lattice parameters were optimized by the generalized gradient approximations (GGA) with the maximum Hellmann-Feynman forces of 0.05 eV/Å, which was sufficient to obtain the relaxed structures. The lattice constant of WS_2 monolayer was optimized to be 3.19 Å. The calculation with spin-orbit interaction was based on the second-order generalized gradient approximation (SOGGA). A double zeta polarized (DZP) basis was used with a mesh cut-off energy of 150 Ry. The Pulay-Mixer Algorithm was employed for the iteration parameter with a tolerance value of 10^5. The self-consistent field iteration steps was 1000, and the electronic temperature 300 K. The periodic boundary condition was employed along all the three directions in the hexagonal lattice. The self-consistent field calculation ensured the complete convergence within the iteration steps.

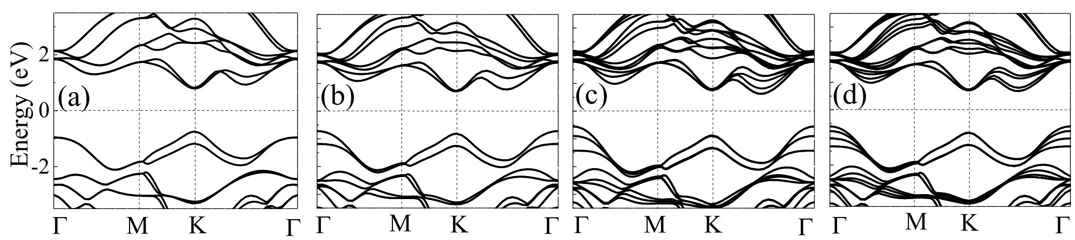

Fig. 1. Electronic band structure of WS_2 (a) monolayer, (b) bilayer, (c) tri-layer, and (d) quad-layer.

The electronic band structures of WS_2 monolayer, bilayer, tri-layer, and quad-layer with the first-principle calculations are shown in figure 1. The electronic band structure of monolayer displayed the direct bandgap at the K-position in the momentum space in the first Brillouin zone [2]. The large band splitting in the valence band is attributable to the strong spin-orbital coupling. The magnitude of band splitting is ~435 meV at the K-position in the momentum space which is nearly independent on the number of atomic layers [2]. The electronic band structure with the first principle calculation also displayed the spin degeneracy at the Γ-position and the zero-splitting at M-position in the momentum space [11]. The confinement of potential energy at the Γ-position in momentum space was weakened as the number of layer was increased due to the interlayer interactions. As the number of atomic layers was increased, the highest level of valence band at the Γ-position in momentum space approached the Fermi level, and placed higher than the highest level of valence band at the K-position in the momentum space. The changes of potential-energy confinement and electronic band structure crossed over from the direct energy transition at K-position to the indirect energy transition which is assigned to the transition between the valence band maximum at the Γ-position to the conduction band minimum at the Λ-position (between K and Γ) [12]. The exciton energy transitions occurred at K-position with no gradient of electronic band structure and the large band-splitting due to strong spin-orbital coupling. Another exciton energy transitions transpired near K – Γ and Γ – M positions in the momentum space due to the band nesting with less gradient between the electronic band structures [22, 23]. The optical absorption due to the energy band structure gradient is related to the imaginary dielectric constant (ε_2) of [13]

$$\varepsilon_2(\omega) = \frac{4\pi^2 e^2}{\omega^2 m^2} \sum_{v,c} \frac{1}{(2\pi)^2} \int_{s(\omega)} \frac{1}{\left|\nabla_k (E_c - E_v)\right|} \left|\vec{\eta} \cdot M_{cv}(k)\right|^2 ds \quad (1)$$

where $\vec{\eta} \cdot M_{cv}(k)$ is the dipole transition matrix element, $\vec{\eta}$ is the radiation polarization, $M_{cv}(k)$ is the dipole matrix, and $\nabla_k (E_c - E_v)$ is the gradient between the lowest level of conduction band and the highest level of valence band at near Γ - K, and Γ - M positions in momentum space.

The WS_2 nanoflakes were prepared by a liquid exfoliation (Graphene Supermarket) [14]. The concentration of nanoflakes in a base solution of 70% ethanol and 30% water was ~26 mg/L. The nanoflakes include 1-4 number of layers with lateral size of ~ 50-150 nm. Figure 2 displayed the absorption spectrum of WS_2 nanoflakes using a UV-Vis absorption spectrometer. The distinct absorption peaks appeared at ~627, ~520, ~457, and ~345 nm. The absorption peaks at ~627 nm and ~520 were assigned to the optical transitions at K-position in momentum space with strong spin-orbit coupling [5][11][15][16] [17][18]. The peaks at ~457 nm and ~345 nm are attributed to the optical transitions due to the band nesting near at K - Γ, and Γ - M positions in momentum space [12] [13].

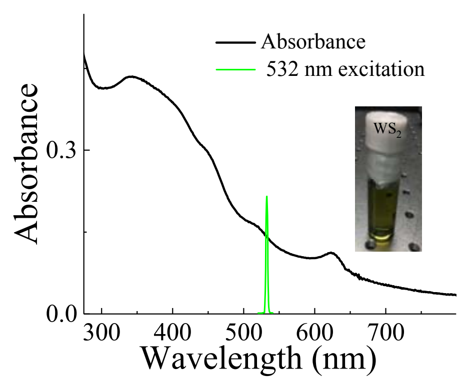

Fig. 2. Absorption spectrum of WS_2 nanoflakes in ethanol. The green spectrum indicates the laser excitation for the nonlinear optical characterizations.

3. Nonlinear spectroscopy

The third-order optical nonlinearity of WS_2 nanoflakes in the base solution was characterized using open and closed Z-scan with a boxcar averaged technique. The excitation source was a pulsed laser at 532 nm wavelength, 10-Hz repetition rate, and ~6-ns temporal pulse width. The effective focal length of the lens and radius of beam waist (w_o) at the focal plane were ~125 mm and ~15.1 µm respectively. The Rayleigh length ($z_0 = kw_0^2/2$) was ~2.02 mm which is larger than the sample thickness (~1 mm) [6]. A Gaussian beam was prepared using two irises for the Z-scan technique [19]. The first iris of diameter ~ 2 mm produced the Bassel beam through the circular aperture diffraction as shown in Fig 3 (b) [20]. The second iris of diameter ~ 5 mm at 35 cm apart from first iris generated the Gaussian beam as shown in Fig 3 (c) [19]. The beam profiles and images were captured by a CMOS Beam Profiling Camera (USB 3.0, Edmunds). The Fig. 3 (c) shows the intensity distribution of the Gaussian beam and their fitting. The diameter of Gaussian beam at the focusing lens was ~2.6 mm at FWHM for the Z-scan measurement.

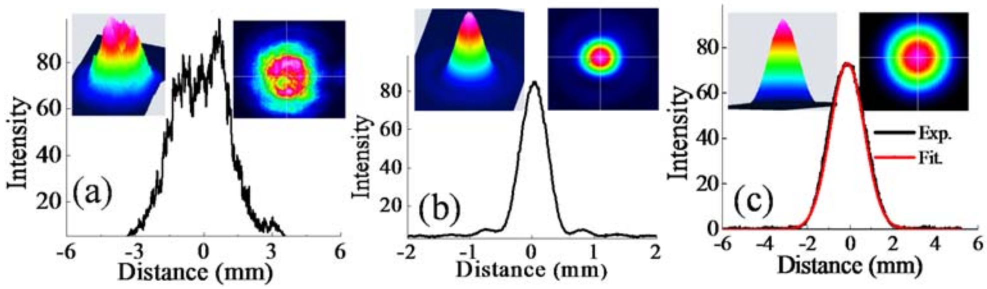

Fig. 3. Beam profiles of (a) initial laser beam; (b) Bessel beam profile after the first iris; (c) Gaussian beam profile. Each figure shows the image of top view (right) and side view (left) of beam profile.

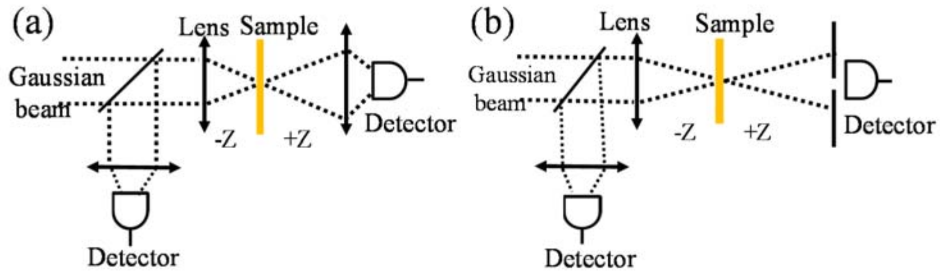

Fig. 4. Schematic diagrams of open (a), and closed (b) Z-scan setups for characterizing the magnitude and polarity of nonlinear absorption and nonlinear refraction.

The schematic diagrams of open and closed Z-scan setups are shown in Fig. 4 (a) and (b) respectively [16, 19]. The open Z-scan characterizes the polarity and magnitude of nonlinear absorption. The optical material has a reverse saturable (or saturable) absorption property of positive (or negative) nonlinearity if the nonlinear transmittance is decreased (or increased) as the sample approaches the focal plane in the open Z-scan [27, 28]. The nonlinear transmittance with open Z-scan for a Gaussian beam is given by [16, 17, 27],

$$T(z,S=1)=\sum_{m=0}^{\infty}\frac{\left(\dfrac{-q}{1+(z/z_o)^2}\right)^m}{(1+m)^{3/2}} \tag{2}$$

where z is the sample position, r_a is the radius of a finite aperture in front of an optical detector, $q(r,z,t) = \beta I_o L_{eff} < 1$ is the requirement for nonlinear absorption characterization with the negligible nonlinear phase distortion of $\Delta\Psi_o(t)=\beta I_o(t)L_{eff}/2$, $L_{eff}=(1-\exp(-\alpha_o L))/\alpha_o L$ is the effective sample length, L is the sample thickness, I_o is the peak intensity of excitation beam, α_o is the linear absorption coefficient, and β is the nonlinear absorption coefficient. Also, the closed Z-scan technique characterizes the magnitude and polarity of nonlinear refraction coefficient of optical materials. For the closed Z-scan, if the nonlinear transmittance displays a peak-valley (or valley-peak) trace as the optical medium moves to and from the focal plane, the optical material has a negative (or positive) refractive nonlinearity or a defocusing (or self-focusing) property [23]. The nonlinear transmittance of a closed Z-scan with a Gaussian beam is given by[19, 20],

$$T(S << 1) = 1 - \frac{4\Delta\phi_0 x + q(3 + x^2)}{(1 + x^2)(9 + x^2)} - \frac{4\Delta\phi_0^2(5 - 3x^2) - 8\Delta\phi_0 qx(9 + x^2) - q^2(40 + 17x^2 + x^4)}{(1 + x^2)(9 + x^2)(25 + x^2)} + .. \quad (3)$$

where w_a is the radius of beam waist at the focal plane, $q(r,z,t) = \beta I_o L_{eff} < 1$, $\Delta\phi_o = k\gamma I_o L_{eff} < 1$ is the phase distortion for the symmetric peak-valley nonlinear transmittance trace, γ is the nonlinear refraction coefficient, and $x = -(1/z_o)(z + (z_o^2 + z^2)/d - z) \sim z/z_o$ for the far-field condition of an aperture ($d >> z_o$) where $d \sim 2.0\ m$ is the distance between the focal plane and the aperture. The radius (r_a) of a finite aperture in front of the detector was ~0.75 mm which results in the linear transmittance of finite aperture of $S = 1 - \exp(-2r_a^2/w_o^2) \sim 0.01 < 1$. Since the nonlinear absorption and nonlinear refraction coefficients are associated with the imaginary and real parts of cubic nonlinear susceptibility respectively, the modulus of cubic nonlinear susceptibility is given by [10],

$$\left|\chi^{(3)}\right| = \sqrt{\left|\mathrm{Re}\,\chi^{(3)}\right|^2 + \left|\mathrm{Im}\,\chi^{(3)}\right|^2} \quad (4)$$

where $\mathrm{Re}\,\chi^{(3)} = (4/3)n_o^2\varepsilon_o c\gamma$ and $\mathrm{Im}\,\chi^{(3)} = (1/3\pi)n_o^2\varepsilon_o c\lambda\beta$ are real and imaginary components of cubic nonlinearity, n_o is the linear refractive index [24], ε_o is the dielectric constant of the vacuum, and c is the speed of light.

All optical nonlinearity measurement were conducted within the system linearity to avoid any additional nonlinear contributions from the electronic devices and the optics used in the experiments. Also, the third-order optical nonlinearity of both the base solution and the WS_2 atomic layer in the base solution were separately scanned to remove the nonlinearity from the base solution. As a reference, the nonlinear refraction of CS_2, an inset graph in Fig. 6, was estimated to be ~4.5×10^{-11} m^2/W with the closed Z-scan technique. The third-order optical nonlinearity of CS_2 was on the same order of the nonlinearity in the literature [25].

To characterize the nonlinear absorption of WS_2 nanoflakes in the base solution, the open Z-scan technique was used. Fig. 5 shows the nonlinear transmittance as a function of sample position (z) for the different peak excitation intensities of ~ 7.15 GW/cm^2, 3.7 GW/cm^2, 2.4 GW/cm^2, 1.22 GW/cm^2, 0.8 GW/cm^2 and 0.2 GW/cm^2 at the focus plane at Z=0 mm. The nonlinear transmittance at both negative and positive Z-positions was normalized to 1. The typical asymmetrical normalization fluctuations at the lower ~1.22 GW/cm^2 was also shown in the figure 5 [14, 20, 24, 25]. The nonlinear transmittance traces of WS_2 nanoflakes displayed a reverse saturable absorption (RSA) with a positive nonlinearity. It implies that the absorption cross-section at the excited state is larger than the absorption cross-section at the ground state [8]. The nonlinear absorption coefficient of WS_2 was extracted to be ~ 6.0×10^{-8} m/W after fitting with equation 2. The estimated value is comparable to the literature information. For example, the nonlinear absorption for 1-3 Layers was estimated to be ~ 1×10^{-7} m/W, 5.29×10^{-9} m/W, and 2.7×10^{-7} m/W with the fs laser excitations at 1064nm, 800 nm, and 515 nm respectively [28], ~ 3.07×10^{-8} m/W for the monolayer with the fs laser excitation at wavelength 1064 nm [27], and ~ 3.7×10^{-6} m/W for the monolayer with a fs laser excitation at 800 nm [29]. The nonlinear refraction (γ) of WS_2 nanoflakes in the base solution was also characterized using the closed Z-scan technique. The nonlinear transmittance as a function sample position for the different input intensities of ~5.1, ~2.3, and ~0.7 GW/cm^2 at the focal plane were shown in figure 6. The nonlinear transmittance of WS_2 nanoflakes displayed the peak-valley traces of negative nonlinearity or the defocusing characteristics. The nonlinear refraction coefficient of WS_2 was estimated to be ~ -3.8×10^{-15} m^2/W after fitting with equation 3. Then, the cubic nonlinear susceptibility of WS_2 nanoflake in the base solution was estimated to be $\left|\chi^{(3)}\right| \sim 9.55 \times 10^{-17}\ m^2/V^2$ which is comparable to the literature value [30].

The nonlinear transmittance of WS_2 in the base solution as a function of the input intensity, I-scan, was also characterized using the same z-scan experimental set up. The normalized transmittance depends on several parameters of excitation intensity and wavelength, nonlinear absorption, nonlinear refraction, and sample position, Rayleigh length, sample thickness, and linear transmittance of finite aperture [31]. The optical sample of WS_2 nanoflakes was placed at the valley (~2.5 mm) of closed Z-scan transmittance trace. The I-scan revealed that the normalized transmittance was decreased as the peak intensity was increased as shown in figure 7. It indicates that optical diffraction through nonlinear optical medium was enhanced as the input peak intensity was increased.

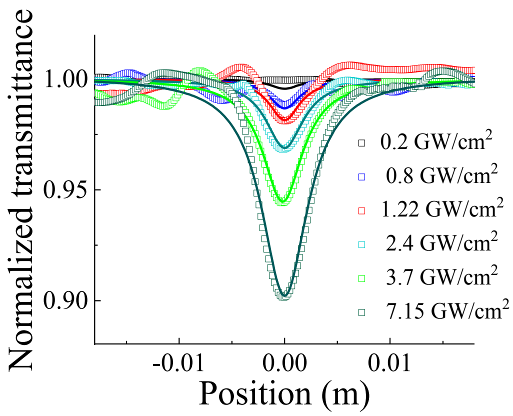

Fig. 5. Nonlinear transmittance as a function of the sample position along the open Z-scan for different input peak intensities

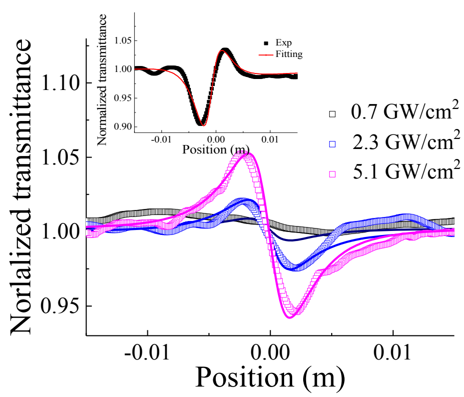

Fig. 6. Nonlinear transmittance as a function of sample position along the close Z-scan. The inset graph shows the nonlinear transmittance of CS_2 as a reference sample.

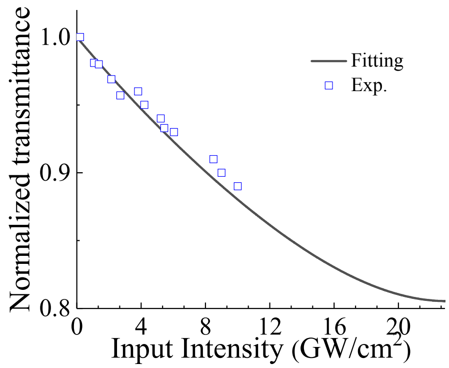

Fig. 7. Nonlinear transmittance as a function of peak intensity for the sample position at the valley of closed Z-scan trace.

4. Conclusion

The third-order optical nonlinearity of tungsten disulfide (WS_2) nanoflakes were characterized using the Z-scan technique with a Gaussian beam. The open Z-scan revealed reverse saturable absorption of positive nonlinearity, and the nonlinear absorption coefficient was estimated to be ~ 6.2 x10^{-8} m/W. The closed Z-scan exhibited the peak-valley nonlinear transmittance as a function of sample position through the focal plane. It indicates that the WS_2 nanoflakes have negative nonlinearity or defocusing properties. The nonlinear refraction coefficient was estimated to be ~ -3.8 x 10^{-15} m^2/W. Therefore, the third-order susceptibility of WS_2 nanoflakes was estimated to be $\left|\chi^{(3)}\right|$ ~ 9.55 x 10^{-17} m^2/V^2 with the resonant excitation. The I-scan revealed that the normalized transmittance at the valley Z-scan was decreased as the peak intensity was increased due to the negative nonlinearity or the defocusing property.

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Spatial Self-Phase Modulation in WS_2 and MoS_2 Atomic Layers

Laser field-induced spatial self-phase modulation (SSPM) in WS_2 and MoS_2 atomic layer liquid suspensions displayed the diffraction profile of concentric rings at the far-field due to the coherent superposition of transverse wave vectors with characteristic spatial nonlinear phases. The evolution of the number of rings indicated the spatial alignment of anisotropic atomic layers in the liquid base solution. The intensity-dependent number of symmetric rings revealed the nonlinear refraction coefficients of MoS_2 and WS_2 atomic layers which were estimated to be ~ - 1.96 x 10^{-16} m^2/W and ~ -1.11 x 10^{-16} m^2/W, respectively. The central interference profile and the diffraction pattern identified the negative polarity of nonlinear refraction. The vertically asymmetric diffraction ring indicates the phase distortion of optical field due to the heat convection.

1. Introduction

An optical field propagates through an optical material with its own characteristic spatial and temporal phase changes. The spatial phase of optical field includes linear and nonlinear phases. The linear phase of optical field in the medium changes with the linear refractive index, and the nonlinear phase of optical field is shifted by the characteristic nonlinear refractive index of optical material and the applied optical intensity. The nonlinear phase is mutated by the applied intensity, and the spatial nonlinear phase is modulated by the spatial distribution of intensity and the characteristic nonlinear refractive index of optical medium [1]. The coherent superposition of transverse wave vectors with characteristic spatial nonlinear phases display the diffraction profile of concentric rings at far-field [2]. The diffraction profile of spatial self-phase modulation (SSPM) reveals the nonlinear optical properties and the interaction characteristics of optical field and medium. The evolution of the number of rings implies the spatial alignment of anisotropic atomic layers in the liquid base solution. The intensity-dependent number of symmetric rings reveals the nonlinear refraction coefficients of atomic layers [3]. The central interference profile and the diffraction pattern identifies the polarity of nonlinear refraction. The asymmetric diffraction discloses the phase distortion of optical field due to the heat convection [4, 5]. The evolution of self-phase modulation with the spatial alignment of anisotropic atomic layers and the evolution of vertical asymmetric diffraction due to thermal convection are characteristic nonlinear optical processes in atomic layer liquid suspension, which can't be observed with a bare atomic-layer material.

The SSPM of carbon disulfide was observed by Callen et al in 1967 for the first time [6]. Recently, the nonlinear optical characterization of atomic layers with SSPM was reported [3, 5, 7] by multiple research groups. Wu and Zhao's group [7] proposed a "wind chime" model to describe the emergence of electron coherence from the nonlocal domains of nanoflakes which were driven by the SSPM. They reported the bandgap-dependent nonlinearity of nanoflakes using the SSPM with 200-fs lasers and CW lasers at visible and near-IR spectra, and all-optical switching by the two-color phase modulation. G. Wang and J. Wang's collaborators [3] characterized the nonlinear refractive index of atomic layers using the distortion of SSPM with a CW laser at 488 nm. Wu and Zhao's group [8] articulated the third-order nonlinearity of $MoSe_2$ flakes with SSPM and the threshold intensity as a function of photon energy, and the correlation between the third-order nonlinearity and absorption of $MoSe_2$ flakes. Jia and Xiang's collaborators [5] reported the broadband nonlinear optical nonlinearity at visible spectra, and all-optical switching two-color spatial cross-phase modulation (SXPM).

In this research, the spatial self-phase modulation in MoS_2 and WS_2 atomic layer liquid suspension was investigated by the SSPM using a pulsed laser which has a temporal pulse width of ~1.5 ps and a repetition rate of ~82 MHz. The nonlinear optical characteristics of atomic layers by the SSPM were revealed by the evolution of coherent superposition of transverse wave vectors, the intensity-dependent number of symmetric rings, the diffraction patterns and central interference profiles, the number of excitations and intensity-dependent asymmetric diffractions.

2. Theory

The refractive index changes the characteristic nonlinear refraction coefficient and the applied optical intensity. The intensity-dependent refractive index *n* is [5],

$$n = n_0 + \gamma I(r,z) = n_0 + \Delta n \tag{1}$$

where n_0 is the linear refractive index, γ is the nonlinear refraction coefficient, $I(r,z)$ is the spatially distributed input intensity, and Δn is the change in refractive index. The radial component of electric field in Gaussian profile is

$$E(z,r) = E(0,z)exp\left(\frac{-r^2}{w^2(z)}\right)exp\left(\frac{-\alpha L}{2}\right)exp(-i\phi(z,r)) \tag{2}$$

where $E(0,z)$ is the amplitude of electric field, $r=\sqrt{x^2+y^2}$ is the transverse coordination to the beam propagation direction, $w(z)$ is the beam radius, α is the absorption coefficient, *L* is the length of optical medium, and $\phi(z,r)=\phi_L(z,r)+\phi_{NL}(z,r)$ is the phase of electric field. The intensity-dependent nonlinear phase $\phi_{NL}(z,r)$ is [9],

$$\begin{aligned}\phi_{NL}(z,r) &= \frac{2\pi}{\lambda} n_{0,s}\gamma_m L_{eff} I(0) exp\left(\frac{-2r^2}{w^2(z)}\right)\\ &= k_s\gamma_m I(0)L_{eff}\, exp\left(-\frac{2r^2}{w^2(z)}\right) = \Delta\phi_{NL}(0)exp\left(-\frac{2r^2}{w^2(z)}\right)\end{aligned} \tag{3}$$

where $I(0)$ is the input intensity into the sample, L_{eff} is the effective length of optical sample path *L*, k_s is the wavenumber vector of base solution, and $\Delta\phi_{NL}(0)$ is the maximum nonlinear phase shift. If the maximum nonlinear phase shift $\Delta\phi_{NL}(0) = k\gamma I(0)L_{eff} \geq 2\pi$, the diffraction pattern at far-field will be displayed. The spatial change of nonlinear phase is the transverse propagation wave vector which is given by [2],

$$\delta k(r) = \frac{\partial\phi_{NL}(r)}{\partial r}\hat{r} = -4rk_s\gamma_m I(0)L\, exp\left(\frac{-2r^2}{w^2(z)}\right)\hat{r} \tag{4}$$

where $\hat{r}$ is the unit vector along the transverse direction. The nonlinear phase (equation 3) and the traverse propagation wave vector (equation 4) are shown in figure 1. If the transverse propagation wave vectors or the local changes of nonlinear phase are the same at different spatial positions at r_1 and r_2, the interference between the different phases of an optical wave occurs. If the nonlinear spatial phase shift $\Delta\phi_{NL} = \phi_{NL}(r_1) - \phi_{NL}(r_2)$ of an optical wave has an even or odd integer number of $m\pi$, the local phases of an optical wave will have the coherent superposition of in the form of constructive or destructive interference that provides the concentric diffraction rings at far-field.

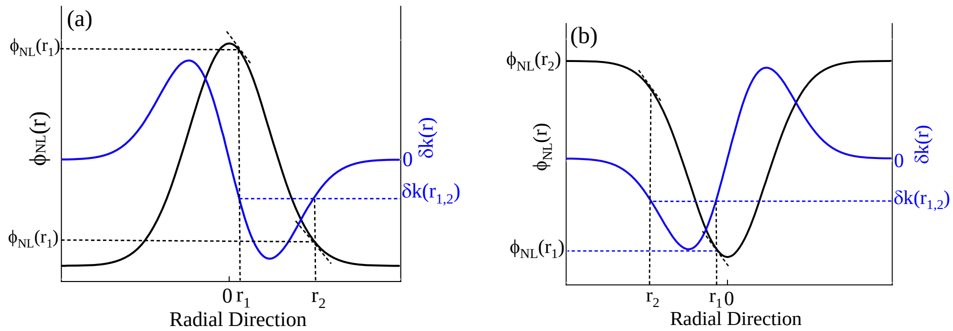


Fig. 1. Nonlinear phase (black curve, eq. (3)) and transverse propagation wave vector (blue curve, eq. (4)) as a function of radial position of *r* for (a) positive and (b) negative nonlinear refraction coefficients (γ).

The number of concentric rings depends on the maximum nonlinear phase shift $\Delta\phi_{NL}(0) = k\gamma I(0)L = 2\pi N$. The number of diffraction rings as a function of applied intensity has a slope of $k\gamma L/2\pi$ [1, 3],

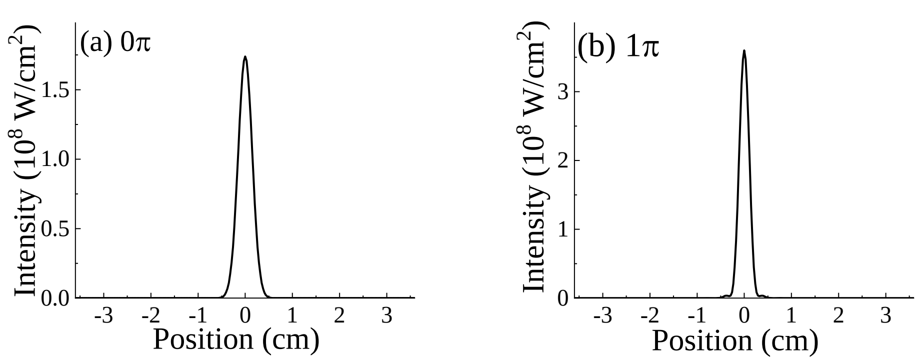
$$N = \frac{\Delta\phi_{NL}(0)}{2\pi} = \frac{k\gamma L_{eff}}{2\pi} I(0). \tag{5}$$

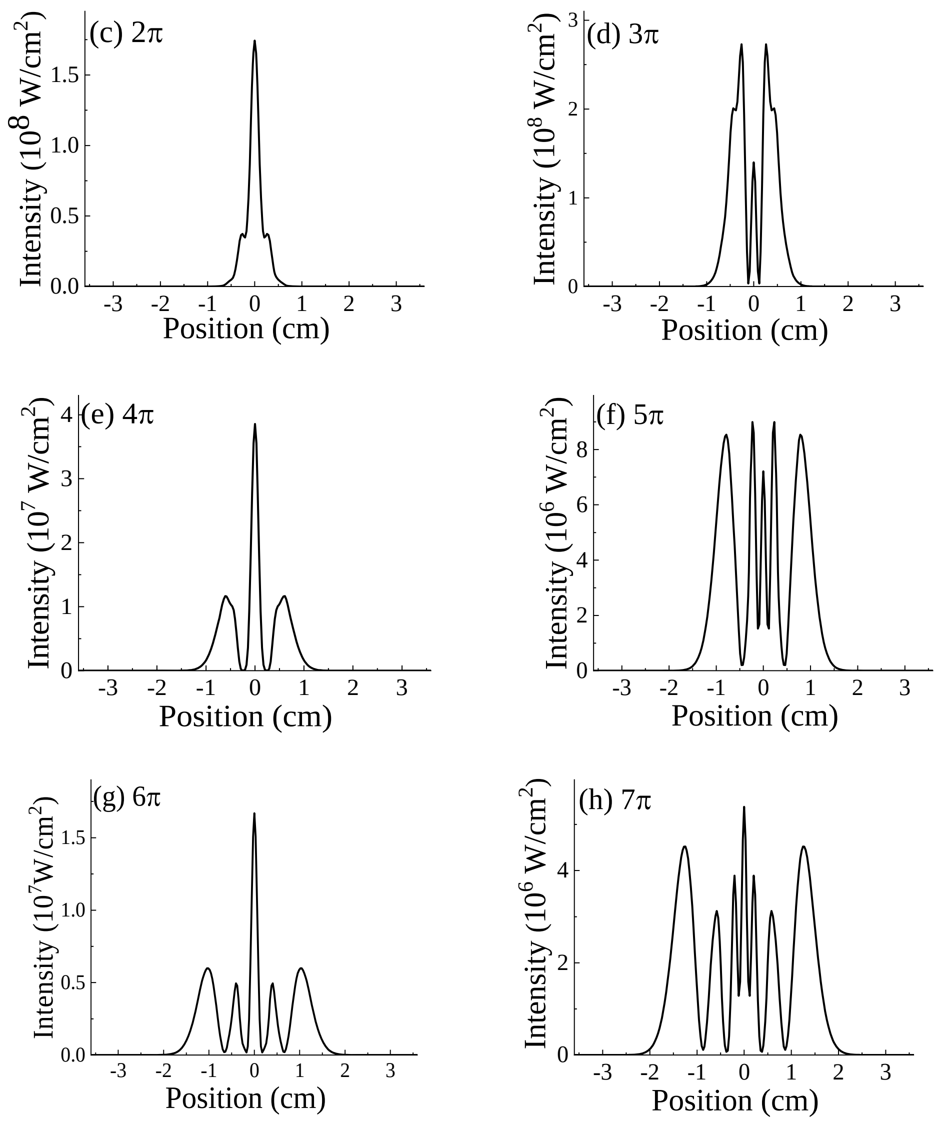
Then, the nonlinear refraction coefficients of atomic layers can be estimated from the slope of the number of diffraction rings as a function of applied intensity.

The far-field intensity with the Fraunhofer approximation of Fresnel–Kirchhoff diffraction is given by [10],

$$I = 4\pi^2 \left| \frac{E(0,z)exp(-\alpha L)}{i\lambda D} \right|^2 \left| \int_0^\infty J_o(k_0 r\theta) exp\left(\frac{-r^2}{w^2(z)}\right) exp(-i\phi(r)) r dr \right|^2 \tag{6}$$

where $J_o(k_0 r\theta)$ is the first kind of zero order Bessel function, and $\phi(r) = \phi_L(r) + \phi_{NL}(r)$ is the phase of optical field. Figure 2 and 3 displayed the diffraction patterns of SSPM for the positive radius of curvature (*R>0*) at the far-field and the different positive and negative maximum nonlinear phase shifts.





(c) 2π
Intensity (10^8 W/cm^2)
Position (cm)
(d) 3π
Intensity (10^8 W/cm^2)
Position (cm)
(e) 4π
Intensity (10^7 W/cm^2)
Position (cm)
(f) 5π
Intensity (10^6 W/cm^2)
Position (cm)
(g) 6π
Intensity (10^7W/cm^2)
Position (cm)
(h) 7π
Intensity (10^6 W/cm^2)
Position (cm)

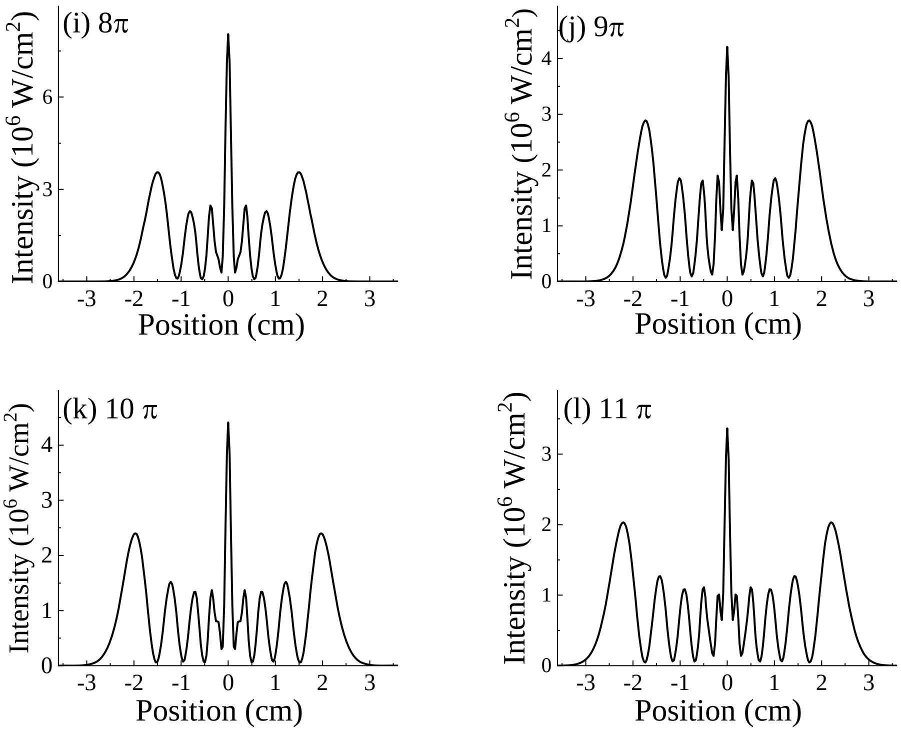
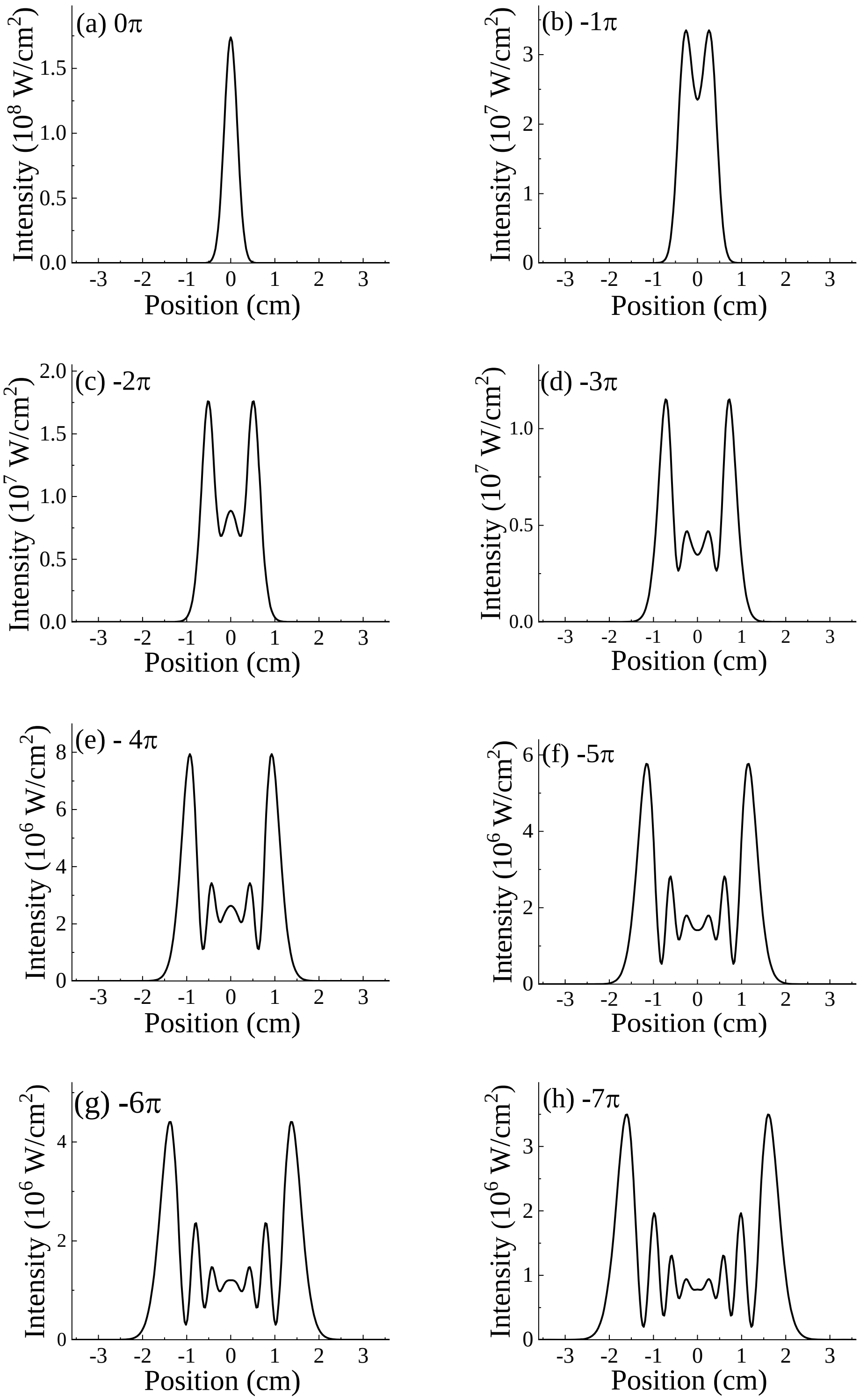


Fig. 2. Diffraction patterns at far-field due to the SSPM in optical medium with different nonlinear phase shifts $\Delta\phi_{NL}(0)$ of (a) 0π, (b) 1π, (c) 2π, (d) 3π, (e) 4π, (f) 5π, (g) 6π, (h) 7π, (i) 8π, (j) 9π, (k) 10π, and (l) 11π.

Figure 2 shows the diffraction patterns at far-field due to SSPM in optical medium with different positive nonlinear phase shifts. The central peak of diffraction pattern is due to the positive nonlinearity or self-focusing property of an optical medium. The number of diffraction rings is increased as the maximum nonlinear phase shift is increased. The intervals between the outer rings are larger than those between the inner rings. No diffraction pattern for zero nonlinear phase shift is shown in figures 2 (a) and 3 (a). The diffraction pattern for $\Delta\phi_{NL}(0) = 2\pi$ exhibited the side wings. The diffraction pattern for $\Delta\phi_{NL}(0) \geq 3\pi$ displayed the number of interference patterns. The positive nonlinear phase with positive nonlinear refraction coefficient displayed a distinct central peak which was disappeared with the negative maximum nonlinear phase with negative nonlinear refraction coefficient. The width and strength of the outermost diffraction ring are larger due to the larger deformed wavefront for lesser nonlinear phase change at the margin of propagation wave [11]. The interference fringe is proportional to the derivative magnitude of the angular deformation of wavefront to the nonlinear phase change [11]. Figure 3 shows the diffraction pattern due to SSPM in optical medium with different negative nonlinear phase shifts. The suppression or disappearance of central peak indicates the negative nonlinearity or self-defocusing property of an optical medium.


(a) 0π
(b) -1π
(c) -2π
(d) -3π
(e) - 4π
(f) -5π
(g) -6π
(h) -7π
Intensity (10^8 W/cm^2)
Intensity (10^7 W/cm^2)
Intensity (10^6 W/cm^2)
Position (cm)

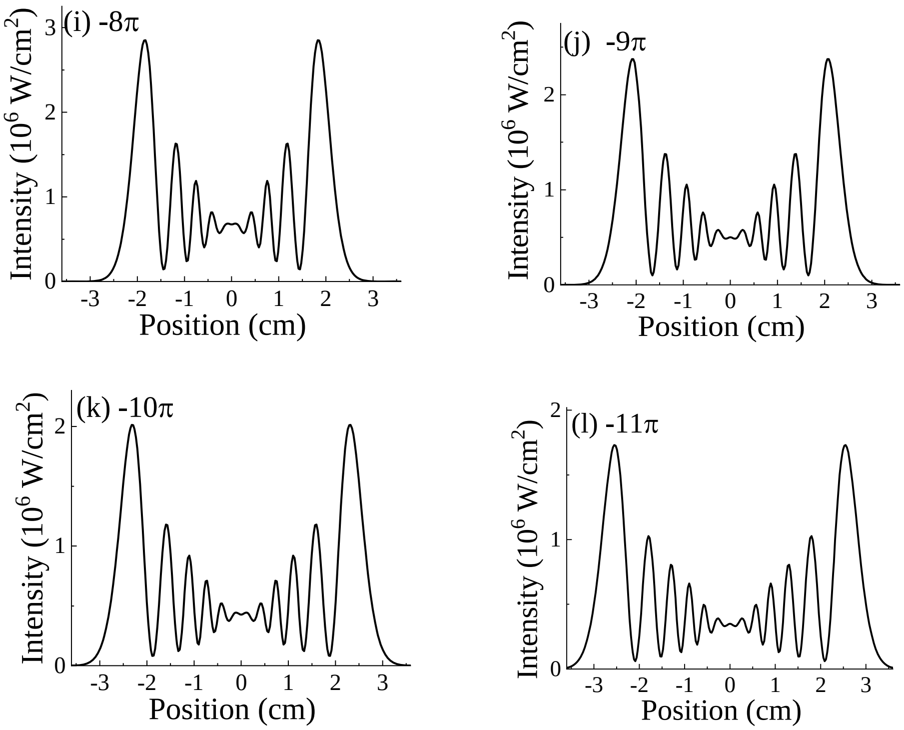


Fig. 3. Diffraction patterns at far-field due to the SSPM in optical medium with different nonlinear phase shifts $\Delta\phi_{NL}(0)$ of (a) 0π, (b) -1π, (c) -2π, (d) -3π, (e) -4π, (f) -5π, (g) -6π, (h) -7π, (i) -8π, (j) -9π, (k) -10π, and (l) -11π.

In addition to the intensity-dependent nonlinear phase changes, the asymmetric diffraction rings due to the heat convection of optical medium characterizes the thermal-induced nonlinear refraction coefficient which is estimated by the ratio of distortion angle θ_D to the half-cone angle θ_H [5],

$$\Delta\gamma = \frac{\theta_D}{\theta_H}|\gamma|. \tag{7}$$

The equation (7) indicates that the larger thermal distortion of diffraction pattern has the larger nonlinear refraction change within the diffraction angle.

3. Materials and Methods

The WS_2 and MoS_2 atomic layer liquid suspensions were purchased from the Graphene Laboratory [12]. The concentration of WS_2 atomic layer was ~26 mg/L. The number of layers were ~1-4 atomic layers with the lateral sizes of ~50 - 150 nm. The concentration of MoS_2 atomic layers was ~18 mg/L. The number of layers were ~1-8 atomic layers with the lateral sizes of ~100 - 400 nm.

The excitation source for the SSPM of atomic layers was a pulsed laser with temporal pulse width of ~1.5 ps and a repetition rate of ~82 MHz. The spectral peak was ~800 nm (~1.55 eV) at the optical band edge of atomic layers. The beam waist at the focal point was ~40 μm and the Rayleigh length was ~9.0 mm. The diffraction profile at the far-field from sample was collected by a CCD USB 2.0 camera (DCU223C, Thorlabs, Inc.).

The nonlinear refraction coefficients of MoS_2 and WS_2 atomic layers were characterized by the number of diffraction rings as a function of applied intensity at the fixed time duration of excitation. The polarity of nonlinear refraction was identified by the central interference and diffraction profiles at the far-field. The evolution of number of rings revealed the spatial alignment of anisotropic atomic layers in the liquid base solution. The asymmetric diffraction analyzed the thermal phase distortion of optical field.

4. Experiment Results and Analysis

Figure 4 shows the optical absorption spectra of WS_2 and MoS_2 atomic layer liquid suspension in 70% ethanol and 30% water. The weak characteristic absorption peaks of WS_2 and MoS_2 atomic layers at the visible region are assigned to the distinct exciton transitions of A and B exciton peaks which are related to the spin-orbital coupling at the K/K′ position in momentum space in the first Brillouin zone. The broad bands of absorption at the higher energies, which are called as C and D exciton peaks, are most likely linked to the band nesting near the Γ-Λ and Γ-M positions [13, 14].

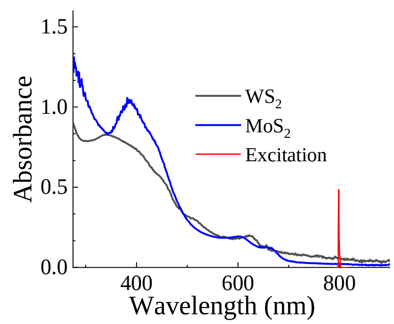


Fig. 4. Absorption spectra of MoS_2 (blue) and WS_2 (black) atomic layers, and optical spectrum of excitation laser (red).

Figure 5 (a) and (b) display the laser-induced diffraction rings of MoS_2 and WS_2 atomic laser liquid suspension for the different time durations of laser excitations which has a temporal pulse width of ~1.5 ps and repetition rate of ~82 MHz. The applied input intensity was ~0.7 GW/cm^2. The temporal evolution of diffraction rings within 0.48 seconds attributed to the spatial alignment of anisotropic atomic layers. The horizontal radius of diffraction ring was stabilized after 0.48 seconds as shown in figure 5 (c), but the upper vertical radius of diffraction ring was squeezed due to the heat convection of atomic layers as shown in figure 5 (d) [5, 8]. No diffraction rings of SSPM for base solution was observed for the same experiment conditions. It indicates that the SSPM and thermal distortion are originated from the atomic layers instead of the base solution.

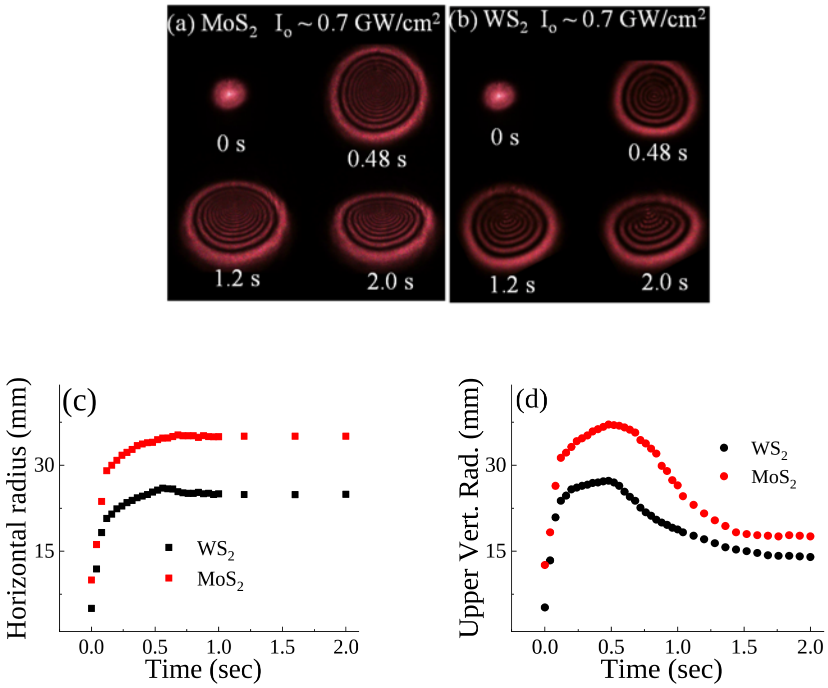


Fig. 5. Diffraction patterns at far-field due to the SSPM in (a) MoS_2 atomic layer liquid suspension and (b) WS_2 atomic layer liquid suspension for different time durations of laser excitation at the applied intensity of ~0.7 GW/cm^2. (c) Horizontal radius and (d) upper vertical radius of diffraction ring as a function of time duration of laser excitations at the applied intensity of ~0.7 GW/cm^2.

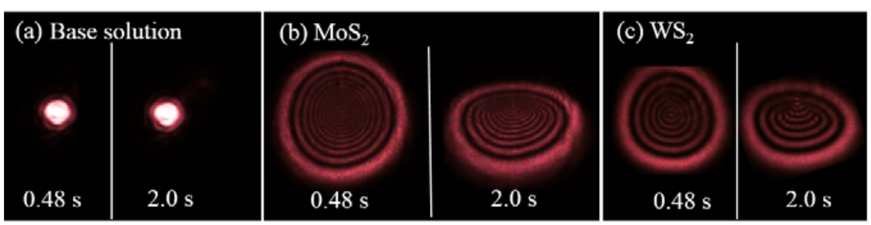


Fig. 6. Diffraction patterns at far-field due to the SSPM in (a) the base solution (70% ethanol and 30% water), (b) the MoS_2 atomic layer liquid suspension, and (c) the WS_2 atomic layer liquid suspension at the applied intensity of ~0.7 GW/cm^2.

The number of diffraction rings as a function of applied peak intensity for (a) MoS_2 and (b) WS_2 atomic layer liquid suspensions at the time duration of 0.48 seconds are shown in figure 7. The number of rings were linearly increased as the input intensity was increased. The nonlinear refraction coefficients of MoS_2 and WS_2 atomic layer liquid suspensions were characterized using the slope $(k\gamma L_{eff}/2\pi)$ for the number of diffraction rings as a function of applied peak intensity. The nonlinear refraction coefficients of MoS_2 and WS_2 atomic layer liquid suspensions were estimated to be ~-1.96×10^{-16} m^2/W and ~-1.11×10^{-16} m^2/W, respectively.

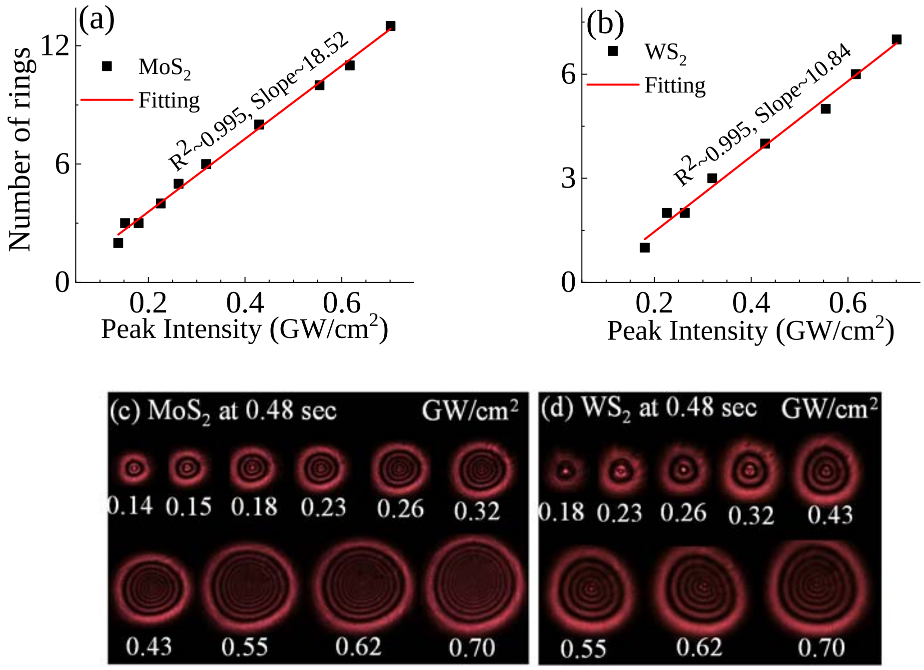


Fig. 7. Number of diffraction rings at the far-field due to the SSPM in atomic layers as a function of applied peak intensity for (a) MoS_2 and (b) WS_2 atomic layer liquid suspension at the time duration of ~0.48 seconds. Diffraction rings at the far-field due to the SSPM in (c) MoS_2 and (d) WS_2 atomic layer liquid suspensions for different applied intensities.

The two-dimensional diffraction profiles of WS_2 and MoS_2 atomic layer liquid suspension has no distinct central peak of interference as shown in figure 8 which indicates the negative nonlinear refraction of atomic layers [10]. The theoretical simulations of diffraction profile (red color) at the far-field due to the SSPM in (a) MoS_2 and (b) WS_2 atomic layers with $\phi_{NL} < 0$ and $R > 0$ are shown in figure 8. The theoretical fitting parameters were (a) $\Delta\phi_{NL}(0)$ =-16π phase shift for MoS_2 atomic layers and (b) $\Delta\phi_{NL}(0)$=-10π phase shift for WS_2 atomic layer at the input intensity of ~0.70 GW/cm^2. The negative nonlinear phase shift $\Delta\phi_{NL}(0) = k\gamma I(0)L_{eff}$ indicates the negative nonlinear refraction coefficients of MoS_2 and WS_2 atomic layers [13]. Figure 9 shows the diffraction patterns at the far-field due the SSPM in (a) MoS_2 atomic layers with $\Delta\phi_{NL}(0)$ of -16π and 16π; and (b) WS_2 atomic layers with $\Delta\phi_{NL}(0)$ of -10π and 10π for WS_2 atomic layers. The central interference patterns and diffraction profiles due to the SSPMs in atomic layers identify the nonlinear refraction coefficients.

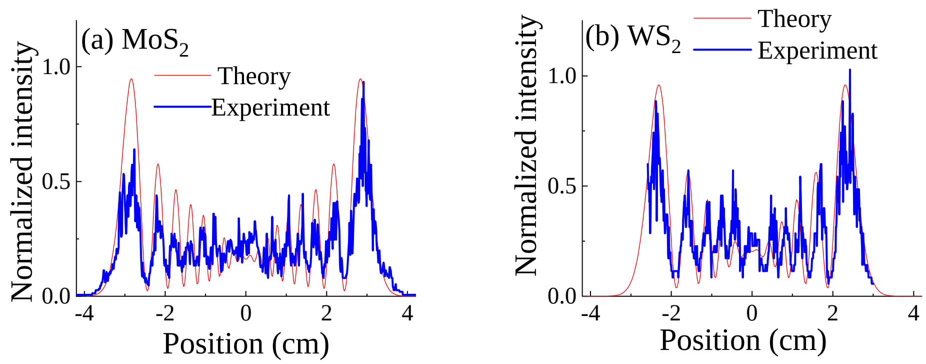


Fig. 8. Two-dimensional diffraction pattern (blue color) at the far-field due to the SSPM in (a) MoS_2 and (b) WS_2 atomic layer liquid suspensions. Theoretical fittings (red color) of (a) maximum nonlinear phase shift $\Delta\phi_{NL}(0)$=-16π for MoS_2 atomic layers and (b) maximum nonlinear phase shift $\Delta\phi_{NL}(0)$=-10π for WS_2 atomic layers. The fitting parameters include k_o = 7.85×10^6 m^{-1}, $w(z)$ = 4.01×10^{-4} m, I_o = 0.70 GW/cm^2, and D = 2.3 m.

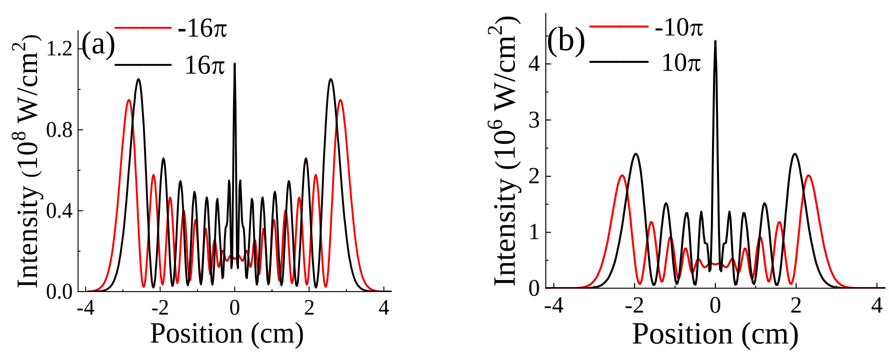


Fig. 9. Diffraction simulations at the far-field due to the SSPM in (a) MoS_2 atomic layers with the maximum nonlinear phase shifts $\Delta\phi_{NL}(0)$ of -16π and 16π; and WS_2 atomic layers with maximum nonlinear phase shifts -10π and 10π. The fitting parameters include k_o = 7.85×10^6 m^{-1}, $w(z)$ = 4.01×10^{-4} m, I_o = 0.70 GW/cm^2, and D = 2.3 m.

Figure 10 (a) shows the schematic sketch of the half-cone and distortion angles of diffraction profiles at the far-field where the half-cone angle was measured at the excitation time duration at 0.48 seconds and the distortion angle of diffraction profile was measured at the excitation time duration at 2.0 seconds. Figure 10 (b) and (c) include the distortion and half-cone angle ratio of θ_D/θ_H as a function of applied peak intensity for (b) MoS_2 and (c) WS_2 atomic layers, respectively. Figure 10 (d-k) and (l-m) show the images of diffraction profiles of for different applied peak intensities for MoS_2 and WS_2 atomic layers, respectively. The distortion radius for the upper half of diffraction profile is due to the laser-induced heat convection atomic layers in liquid base solution [3, 4, 15, 16]. The laser-induced temperature fields was proven by the simulation [17], and the laser-induced heat convection of atomic layers in base solution has an analogy with the heat convection due to a heating wire in liquid [18].The change in nonlinear refraction coefficient due to thermal effect was estimated by equation (7) as shown in figure 10 (b) and (c) [1, 3-5]. The changes in nonlinear refraction coefficients for MoS_2 and WS_2 atomic layers were ~0.7×10^{-16} m^2/W and ~0.4×10^{-16} m^2/W at the applied intensity of ~0.7 GW/cm^2, respectively, using the equation (7), while the nonlinear refraction coefficients of MoS_2 and WS_2 atomic layers were estimated to be ~-1.96×10^{-16} m^2/W and ~-1.11×10^{-16} m^2/W, respectively, using the equation (5).

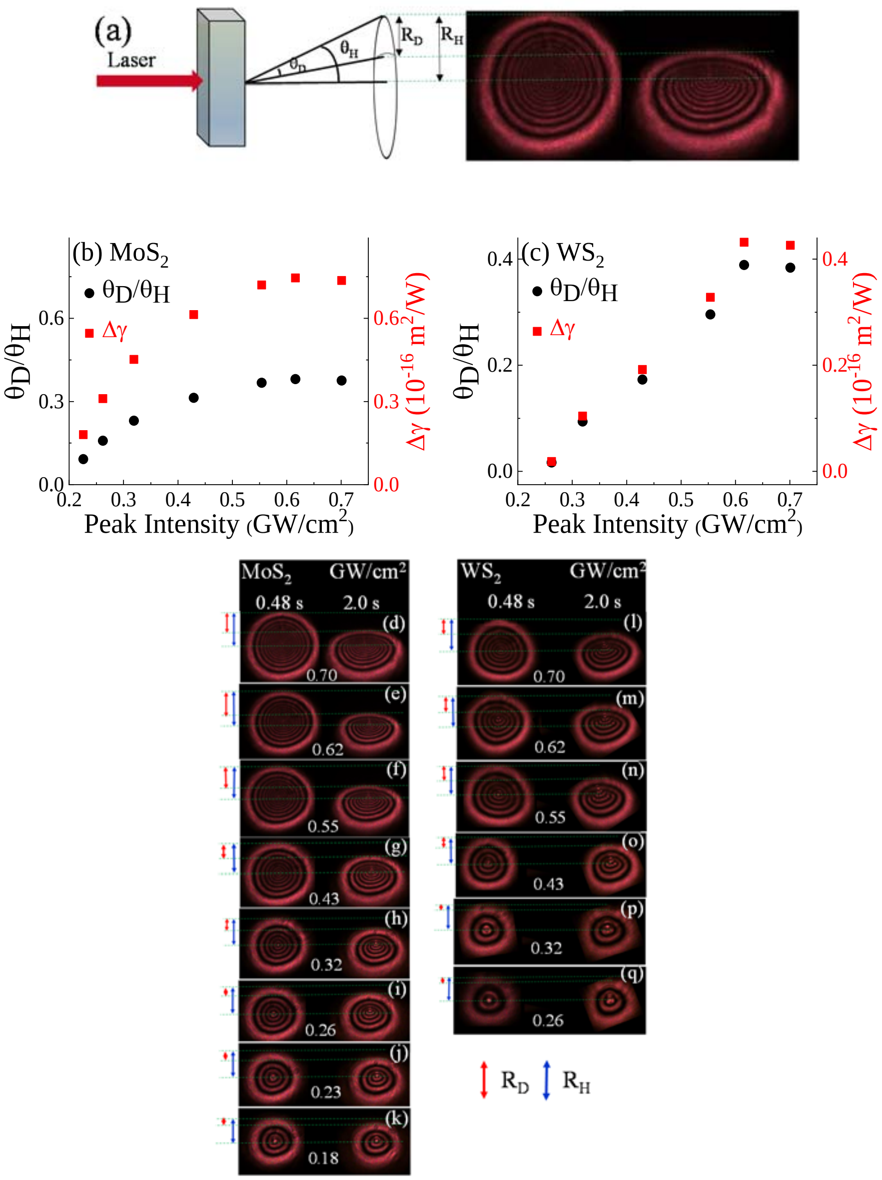


Fig. 10. (a) Schematic sketch of the half-cone and distortion angles of SSPM, (b) half-cone and distortion angles as a function of applied peak intensity; the ratio of θ_D/θ_H (left y-axis) and change in nonlinear refraction coefficient (right y-axis) as a function of applied peak intensity for (b) MoS_2 and (c) WS_2 atomic layer liquid suspension, respectively; (d-k) and (l-m) represent the half-cone and distortion radii of MoS_2 and WS_2 atomic layer liquid suspension for different applied peak intensities, respectively.

5. Conclusion

The laser intensity-induced SSPM in MoS_2 and WS_2 atomic layer liquid suspension displayed the concentric diffraction rings at the far-field. The formation of concentric diffraction rings is due to the coherent superposition of transverse wave vectors. The liquid suspension of atomic layers provided a unique material system to characterize the cubic nonlinearity with the SSPM in atomic layers for photonic applications which can't be achieved with bare atomic layers. The temporal evolution of diffraction ring morphology indicated the spatial alignment of atomic layers, maximum diffraction rings at the intermediate time, and thermal distortion of the upper vertical ring of SSPM at the longer time duration of laser excitation. The vertically asymmetric diffraction ring indicates the phase distortion of the optical field due to heat convection. The number of rings as a function of applied peak intensity revealed the magnitude of nonlinear refraction coefficients. The slope of the number of rings as a function of applied peak intensity revealed the nonlinear refraction coefficients of $\sim$-1.96×10^{-16} m^2/W and $\sim$-1.11×10^{-16} m^2/W for MoS_2 and WS_2 atomic layers, respectively. The simulation of two-dimensional diffraction pattern of SSPM as a function of the radial position identified the polarity of nonlinear refraction. The ratio of distortion and half-cone angle of SSPM as a function of applied input intensity revealed the change of the nonlinear refraction coefficient due to the thermal effect.

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Outreach Activities during the Fiscal Year 2015-16

1. Annual Optics and Laser Science Summer Workshop for 6-12 Science Teachers in 2016

An Annual Optics and Laser Science Summer Workshop was offered to the selected middle and high school science teachers at Hampton University from June 20 to 24, 2016 to promote science educations in the local area. Among the applicants from forty-nine public and private high-schools in the Hampton Roads area (Chesapeake, Hampton, Jamestown, Newport News, Norfolk, Portsmouth, Suffolk, Virginia Beach, Williamsburg and Yorktown in the state of

Virginia), thirteen science teachers were selected for the workshop. The teachers performed several optics and laser experiments which can be utilized in their classrooms. In the first set of experiments, the participants were trained in the diffraction, reflection, and refraction of light. In the second set of experiments, the science teachers involved in the spectroscopy of emission spectra from atomic lamps. In the third set of experiments, the teachers learned the constructive and destructive interferences with a Michelson interferometer. In addition, the workshop organizer, mentors, and participants developed optics and laser science educational modules to promote science education in middle and high schools.

2. Outreach Activities at Lake Taylor Middle School

The research team at HU participated in the Virginia STEM Innovation Network at Lake Taylor Middle School at Lake Taylor Middle School on July 14, 2015. The research team provided the interactive and hands-on experience in optics and laser to the middle school students. The mission of Virginia STEM Innovation Network is to actively engage in improving the students' learning performance in science, technology, engineering and mathematics. The Virginia STEM Innovation Network provides the instructional activities that can build STEM-related talent and proficiency for each and every child in Norfolk, Virginia.

3. Science Technology Engineering and Mathematics (STEAM) Expo and Fantastic Voyage at Hampton University

Dr. Felix JaetaeSeo, Dr. BagherTabibi, Mr. Quinton Rice, Mr. Tikaram Neupane and Mr. Dulitha Mahesh Jayakody Jayakodige provided the demonstrations of 'Fun Physics' to the K-12 students during the Black Family Conference at Hampton University, March 14-18, 2016. The Fun Physics include: (1) dispersion of light by a prism; (2) disappearance by refractive index matching; (3) total internal reflection of light; (4) 3D hologram with a cell phone; (5) optical microscope with a cell phone; (6) hydrophobic surface of elephant leaf; (7) magnetic force microscope; and (8) Van de Graaff Generator

4. Canadian Family Tour

A Canadian family visited our lab at the Graduate Physics Research Center on March 23, 2016. Mr. Quinton Rice, Graduate Student in Ph.D. program, provided them a research laboratory tour. They were excited to know about laser Physics and its applications. According to them, they made a very good decision to visit our lab among many labs in Hampton University.

5. Career Fair at Lake Taylor Middle School

Mr. Tikaram Neupane and Mr. Dulitha Mahesh Jayakody Jayakodige (Adviser Dr. Felix Jaetae Seo) participated in the Career Fair at Lake Taylor middle school, Norfolk, VA on April 21, 2016 in order to discuss the prospective career opportunities with a physics degree. The display of exemplary career opportunities includes: (1) business career like Mr. Elon Reeve Musk who is the CEO of SpaceX, Pay-Pal, Tesla motor, SolarCity, and OpenAl; (2) scientist at national labs, academia, and industry; (3) political leader like Angela Dorothea Merkel, Chancellor of Germany. In addition to the career opportunities, the graduate students demonstrated the disappearance of beaker, total internal reflection, and optical microscope with a cell phone to the middle school students.

6. Youth STEM Conference at Lake Taylor Middle School

The youth STEM (Science Technology Engineering Math) conference was held at Lake Taylor middle school on July 12, 2016. The purpose of the conference was to work with community partners to reach out and spark student interest in different STEM fields. Mr. Tikaram Neupane and Mr. Dulitha Mahesh Jayakody Jayakodige offered several physics demonstrations at the conference. The demonstrations included: (1) the observation of various light spectra by using spectrometer; (2) refractive index matching to indicate the speed of light varies in different materials; (3) demonstration of total internal reflection of light; (4) three dimensional hologram in the cell phone; (5) use of a cell phone optical microscope to identify very tiny particles; (6) the working principle of magnetic force microscopes; and (7) the attraction and repulsion of charges as well as magnetic poles.

Outreach Activities and Education Activities during the Fiscal Year 2016-17

1. **Lab Demonstrations for High School Students from Governor's STEM Academy at Harrisonburg High School**

On June 21, 2017, Mr. Andrew Jackson (Co-Director, Engineering Instructor), Mr. Seth Shantz (Engineering Instructor), and twelve (12) selected students from Governor's STEM Academcy at Harrisonburg High School visited the Graduate Physics Research Center to see the advanced research activities at Hampton University. Harrisonburg High School Governor's STEM Academy educates a diverse group of students, with a variety of interests, strengths, and backgrounds, to be academic and technical leaders in STEM related fields by creating a culture of collaboration and dynamic participation through integration of multiple disciplines and technologies utilizing distinct pathways involving advanced coursework in mathematics, science, engineering, and computer science.

For the visiting high school students, Mr. Tikaram Neupane, Mr. Dulitha Jayakodige, Ms. Ananda Ewing-Boyd, and Dr. Sheng Yu (Dr. Felix Jaetae Seo's research group) demonstrated and discussed their research activities including liquid-helium low-temperature spectroscopy, nonlinear spectroscopy with lasers, ultrafast time- and spectrum-resolved spectroscopy with a streak camera, nanoscale materials and atomic layer preparation, and computer simulation of atomic layers. The high school students were eagle to discuss not only the physics principles of our research activities, but also the laser safety. In addition, the graduate students provided them the fun physics demonstrations of (a) refractive index matching of materials; (b) demonstration of the total internal reflection of light; (c) three-dimensional hologram in the cell phone; and (d) optical microscope to see very tiny particles using a cell phone. Dr. Felix Jaetae Seo and Dr. Bagher Tabibi explained the importance of study, research, and career opportunities in STEM area.

2. Career Fair at Lake Taylor Middle School on April 06, 2017



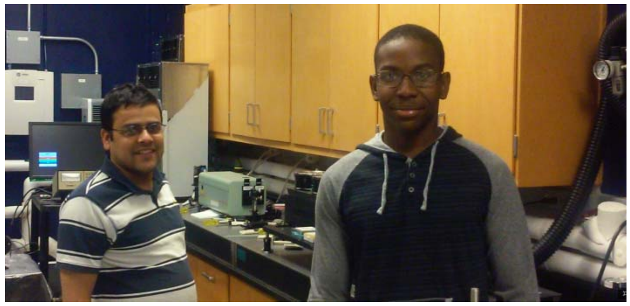
Mr. Quinton Rice and Dr. Shopan Hafiz (Dr. Felix Jaetae Seo's group) participated in the Career Fair at Lake Taylor Middle School, Norfolk, VA on April 6, 2017 to inform the students about future career opportunities with a physics degree. The possible career ventures include: (1) Business path: Mr. Elon Reeve Musk, the CEO of SpaceX, Pay-Pal, Tesla motor, SolarCity, and OpenAl; (2) Science/Research path: National lab scientist, professor, and/or an industrial career; (3) Political path: Angela Dorothea Merkel, Chancellor of Germany with Ph. D in Physical Chemistry. In addition to prospective career, they demonstrated several fun physics of the disappearance of a beaker, total internal reflection, cell phone optical microscope, and 3D hologram projections at the career fair.

3. High School Day on April 07, 2017

Dr. Felix Jaetae Seo (Physics), Dr. Senobia Crawford (Physical Therapy, Chair), Dr. Cecile Andraos-Selim (Biological Science), and Dr. Michelle Kimberly Waddell (Chemistry) setup a recruitment and information table for high school graduates in the Student Center on Friday April 07, 2017. The objective of this event was to inform students about opportunities and facilities in STEM available in Hampton University.

Mr. Quinton Rice, Mr. Tikaram Neupane, and Dr. Felix Jaetae Seo prepared the physics information table to recruit the under-represented minority students in the Science and Technology building. They displayed research posters, informed them the physics program, the research and education opportunities, and the prospective future careers. Among those visitors, around 30% of visiting high school students participated in laboratory tours of the Graduate Physics Research Center (GPRC). The lab tour included a slide show of research highlights, and several experiment demonstrations for the visitors. Mr. Maurice Roots, Mr. Dulitha Jayakodige, Mr. Tikaram Neupane, Mr. Quinton Rice, Dr. Sheng Yu, Dr. Shopan Hafiz, and Dr. Felix Jaetae Seo encouraged the minority high school students to join STEM-related fields for their future careers.

4. Lab Tour for High School Student



Mr. Aaron Jones, a junior studying at Hampton Christian Academy, was looking for a good physics program for next year. He visited GPRC on April 19. 2017, Mr. Tikaram Neupane (Graduate Student, Advisor: Dr. Felix Jaetae Seo) provided him a lab tour. Mr. Neupane discussed about color, wavelength, and lasers; laser safety using a suitable goggle; various research activities using lasers; and applications in daily life. During the visit, Aaron Jones showed his strong interest in the applications of research such as eye protection via optical power limiting. It was one of successful recruitment for under-represented minority students in STEM area. Mr. Aaron Jones joined the physics at Hampton University in fall 2018. He is a sophomore student in physics in fall 2019.

4. Meeting with Hampton City Mayor

Dr. Felix Jaetae Seo, Mr. Bill Thomas (Director of Governmental Relations), and Mr. Donnie Tuck (Hampton City Mayor) had a casual meeting in the Turner Hall on June 29, 2017. At the meeting, Mr. Thomas mentioned that Dr. Seo is an outstanding faculty and scientist at Hampton University.

5. Quinton Rice who changed his title from Mr. to Dr. with his Ph.D. in Optical Condensed Matter Physics in summer 2017

Mr. Quinton Rice (Advisor: Dr. Felix Jaetae Seo) earned his Ph.D. in Optical Condensed Matter Physics at Hampton University in summer 2017. He studied the nanophotonics of semiconductor quantum dots for efficient lighting devices for six years under Dr. Seo's advisement since he was a junior. His research was involved in characterizing good candidates for white light generation based on II-VI and I-III-VI_2 semiconductors to achieve highly efficient and bright white LEDs. He claimed that he is the top leading researcher in plasmon-coupled QDs for white LEDs. He authored and co-authored over 20 journal articles, and over 50 conference presentations with an anticipated graduation date in the summer of 2017. He received the Best Student Paper Award at the Virginia Academy of Science in 2014. His dissertation title was “Plasmon-coupled Excitons in Quantum Confined Semiconductors”. From his Ph.D. dissertation, he would like to claim that he is the number one in the world in the area of plasmon-coupled quantum dot for white LEDs. Before his graduation, he received three job offers including Optical Engineer at Thorlabs, Postdoctoral Research Associate at Hampton University, and Assistant Professor (Tenure-track) at University of North Carolina. Among those offers, he chose Sthe Assistant Professor (Tenure-track) at University of North Carolina because he believed that he was trained enough in grant writing, research activities, teaching, and service.


101 JOBS
Infrared Radiation
METAMATERIALS
Sir Isaac
1642-1727
Augustin-Jean
1788-1827


SPIE

5. Group Alumni of Laser Spectroscopy and Materials Modeling Group

Ms. Dominique Covington, Dr. Quinton Rice, Dr. Shopan Hafiz, and Mr. Taiwo Orogbangba have left the Laser Spectroscopy and Materials Modeling group to further develop their professional careers. Ms. Dominique Covington (MS) joined Merck Co. as a Process

Improvement Engineer, Dr. Quinton Rice joined the University of North Carolina as an Assistant Professor (Tenure-Track), Dr. Shopan Hafiz joined the Intel as a Processing Engineer. Mr. Taiwo Orogbangba (MS) would like to develop his career in machine learning human computer interaction in the Intel Corp.

6. Degree Completions

Ms. Dominique Covington completed her MS degree in Chemistry in summer 2016. Her thesis title was "Synthesis and Spectroscopic Studies of Vinylene-Bridged Heterocyclic Organic Semiconductors".

Mr. Taiwo Orogbangba completed his MS degree in Computer Science with a comprehensive exam in summer 2017.

Dr. Quinton Rice completed his Ph.D. degree in Optical Condensed Matter Physics in summer 2017. His dissertation title was "Plasmon-coupled Excitons in Quantum Confined Semiconductors". From his Ph.D. dissertation, he would like to claim that he is the number one in the world in the area of plasmon-coupled quantum dot for white LEDs.

Outreach Activities and Student Degree Completion during the Fiscal Year 2017-18

Lab Demonstrations for high School students on October 18th, 2017

Ten selected high school students in Virginia visited the Graduate Physics Research Center (GPRC) to discuss their prospective research projects at Hampton University. Mr. Tiaram Neupane, Mr. Dulitha Jayakodige, Ms. Ananda Ewing-Boyd, and Ms. Eden Duncan-Smith (Advisor: Dr. Felix Jaetae Seo) demonstrated and explained the prospective research opportunities in the GPRC. The research opportunities include the ultrafast time-resolved spectroscopy, low-temperature spectroscopy, nonlinear optical characterization, and quantum optics. Dr. Felix Jaetae Seo and Dr. Bagher Tabibi informed them the importance of scientific research and broader impacts.

Career Fair at Lake Taylor Middle School, Norfolk, Virginia on March 29, 2018

Mr. Dulitha Jayakodige and Dr. Felix Jaetae Seo participated in the Career Fair at Lake Taylor Middle School, Norfolk, Virginia on March 29, 2018. Mr. Jayakodige and Dr. Seo informed the career opportunities with a physics degree to 10 middle school teachers and over 100 middle school students at the Lake Taylor Middle School. The information of exemplary career opportunities included: (1) 101 jobs in optics and photonics; (2) examples of successful careers with physics degree including Sally Kristen Ride (first American women in space), Elon Reeve Musk (CEO of SpaceX), Turi Milner (successful entrepreneur), Angela Merkel (Chancellor in German), Brian May (legendary rock guitarist), Wu-Tang Clan(hip-hop musician), David X. Cohen (television cartoon writer), Mike Judge(writer and producer), and historical physicists Albert Einstein, Isaac Newton, and Thomas Alva Edison. The middle school students also learned the advantages of learning physics including “the top 10 reasons why you should take physics” and “the 7 myths about high school physics” and received the information of training programs and learning opportunities at Hampton University. In addition, an electrostatic flying object was demonstrated to motivate them to study physics and the applications.

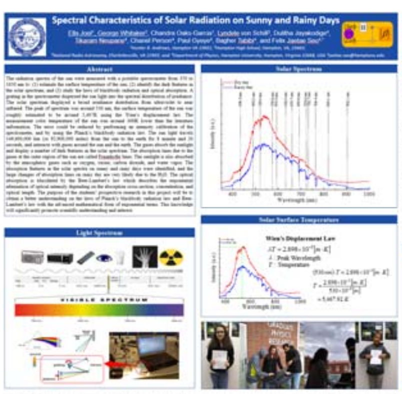
High School Day on April 6, 2018

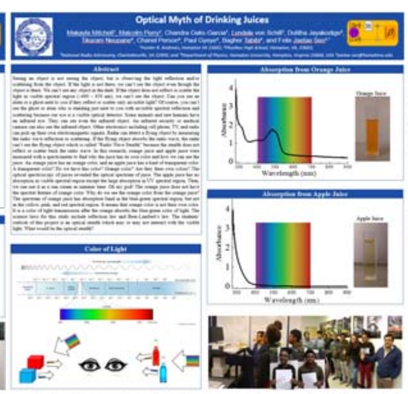
Hampton University hosted an Annual High School Day on April 6, 2018. The recruitment event took place in the Science and Technology building with the participation of over 100 high school students from all around the country. Mr. Dulitha Jayakodige and Mr. Tikaram Neupane (Advisor: Dr. Felix Jaetae Seo) prepared a recruitment table, and informed the physics program at HU including research and education opportunities in optical and material physics, nuclear physics, and medical physics to high school students and their parents. The high school students were very excited to hear the future career opportunities with physics degree.

Middle and High School Students' Research Activities at Graduate Physics Research Center

Dr. Felix Jaetae Seo's research group trained six middle and high school students in optical science at the Graduate Physics Research Center (GPRC) in spring 2018. Mr. Dulitha Jayakodige (graduate student) mentored Mr. Greorge Whitaker (Hampton high school) and Miss Ella Joel (Hunter B. Andrews School) for measuring solar spectrum to calculate the solar temperature in a cloudy and a sunny day. Miss Chanel Person (undergraduate student) mentored Miss Jerrel Griffin (Hampton high school) and Mr. Terrel Barnes Jr. (Hunter B. Andrews School) for measuring the optical spectra of room light and standard spectral lamps. Mr. Tikaram Neupane (graduate student) mentored Miss. Makayla Mitchell (Hunter B. Andrew School) and Mr. Malcolm Perry (Phoebus High School) for measuring the optical absorptions of various fruit juices. The students' research findings were presented at the 23rd Annual School of Science Research Symposium on March 23, 2018.

Student Presentations at SoS Research Symposium, HU on April 11-12, 2018





Six middle and high school students at the 23rd School of Science Annual Research Symposium on April 11th and 12th, 2018. The middle and high school students were Ella Joel, George Whitaker, Makayla Mitchell1, Malcolm Perry, Terrell Banes Jr, and Jerrell Griffin from Hunter B. Andrews Middle School, Phoebus High School and Hampton High School. Mr. Dulitha Jayakodige, Mr. Tikaram Neupane, Dr. Bagher Tabibi, and Dr. Felix Jaetae Seo trained and mentored the six middle and high school students.

Middle and High School Students:

Name	School
George Whitaker	Hampton High School, Hampton, VA 23669
Jerrell Griffin	Hampton High School, Hampton, VA 23669
Malcolm Perry	Phoebus High School, Hampton, VA 23663
Miss. Ella Joel	Hunter B. Andrews Middle School, Hampton, VA 23661
Terrell Banes Jr	Hunter B. Andrews Middle School, Hampton, VA 23661
Makayla Mitchell	Hunter B. Andrews Middle School, Hampton, VA 23661

Middle School Student Training at Graduate Physics Research Center

Mr. Dulitha Jayakpodige, Mr. Tikaram Neupane, and Ms. Chanel Person (Advisor: Dr. Felix Jaetae Seo) also trained another six students from Hunter B. Andrews Middle School at the Graduate Physics Research Center. The students' projects in the H_2O program include: 1) hologram projector; and 2) beaker disappearance by refractive index matching.

Middle School Students:

Name	School	Grade
Astro Isaiah Bren	Hunter B. Andrews Middle School, Hampton, VA 23661	7th grade
Na'Imah Patterson	Hunter B. Andrews Middle School, Hampton, VA 23661	6th grade
Jaidan Pauls	Hunter B. Andrews Middle School, Hampton, VA 23661	7th grade
John A. Barnett II	Hunter B. Andrews Middle School, Hampton, VA 23661	8th grade
Isyss London	Hunter B. Andrews Middle School, Hampton, VA 23661	7th grade
Gavyn Mayorquin	Hunter B. Andrews Middle School, Hampton, VA 23661	8th grade

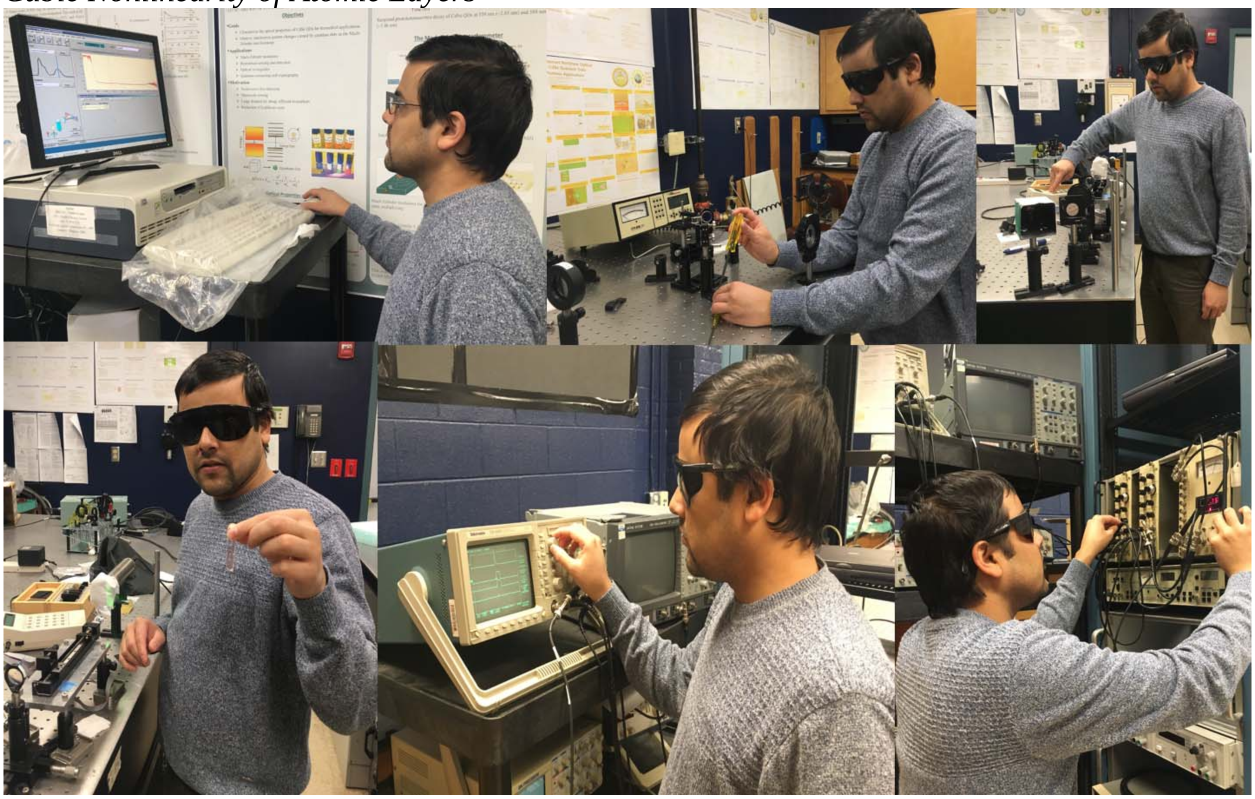
Degree Completion

Mr. Kyle Burney successfully completed his B.S. degree in Physics in May 2018, and joined the US Navy. During his undergraduate academic years at Hampton University, he was a Navy ROTC, and participated in the characterization on the temperature-dependence emission and time-resolved spectroscopy of quantum dots. He demonstrated his skillful data measurement and characterization which led to the successful preparation of his first co-authored manuscript entitled: "Broadband Light Source of Quantum Dots for Optical Sensing".

Outreach Activities and Student Research Activities during the Fiscal Year 2018-2019

Graduate Student Research Activities

Cubic Nonlinearity of Atomic Layers



Mr. Tikaram Neupane is a Ph.D. candidate in the Department of Physics at Hampton University. He characterized the cubic optical nonlinearity of semiconductor atomic layers with Z-scan, I-scan, and spatial self-phase modulation for the passive Q-switch, all optical switching, and optical power limiting. He also participated in characterizing the exciton dephasing time of atomic layers.

His spatial self-phase modulation (SSPM) characterization revealed the magnitudes and polarities of nonlinear refraction coefficients for the molybdenum disulfide (MoS_2) and tungsten disulfide (WS_2) atomic layers. The laser intensity-induced SSPM in MoS_2 and WS_2 atomic layer suspensions in liquid solution displayed the concentric diffraction rings at far-field. The formation of concentric diffraction rings is due to the coherent superposition of transverse wave vectors. The liquid suspension of nanoflakes provided a unique material system to characterize the cubic nonlinearity with the SSPM in atomic layers for photonic applications which can't be achieved with bare atomic layers. The temporal evolution of diffraction ring morphology indicated the spatial alignment of nanoflakes, maximum diffraction rings at the intermediate time, and thermal distortion of the upper vertical ring of SSPM with long time duration of laser excitation. The vertically asymmetric diffraction ring indicates the phase distortion of the optical field due to heat convection. The number of rings as a function of applied peak intensity revealed the magnitude of nonlinear refraction coefficients. The slope of number of rings as a function of applied peak intensity revealed the nonlinear refraction coefficients of MoS_2 and WS_2 in base solution which were estimated be ~ - 1.96 x 10^{-16} m^2/W and ~ -1.11 x 10^{-16} m^2/W, respectively. The simulation of two-dimensional diffraction pattern of SSPM as a function of radial position identified the polarity of nonlinear refraction. The ratio of distortion and half-cone angle of SSPM as a function of applied input intensity revealed the change of the nonlinear refraction coefficient due to the thermal effect.

An intrinsic exciton dephasing is the coherence loss of exciton dipole oscillation, while the total exciton dephasing originates from coherence loss due to exciton-exciton interaction and exciton-phonon coupling. The total dephasing time of WSe_2 monolayer was analyzed as functions of excitation intensity and temperature. The exciton-phonon coupling is dominant at a higher temperature, whereas the exciton-exciton interaction has a major contribution at higher excitation intensity. At higher temperatures, the temperature-mediated exciton-phonon coupling effect on the total dephasing time is more dominant than the excitation intensity mediated exciton-exciton interaction. But at higher excitation intensity, the exciton-exciton interaction effect on the total dephasing time is much stronger than the exciton-phonon coupling contribution. However, the contributions of exciton-exciton interaction and exciton-phonon coupling to the total dephasing time are negligible at a weaker excitation intensity and at lower temperature, respectively. Larger phonon densities at higher temperature and larger exciton densities at higher excitation intensity increase the likelihood of scattering and the elastic collisions. Consequently, the coherency of exciton dipole oscillations is disturbed. It indicates that the modulation of exciton-exciton interaction and exciton-phonon coupling is crucial for ultrafast optoelectronics using the WSe_2 atomic layer.

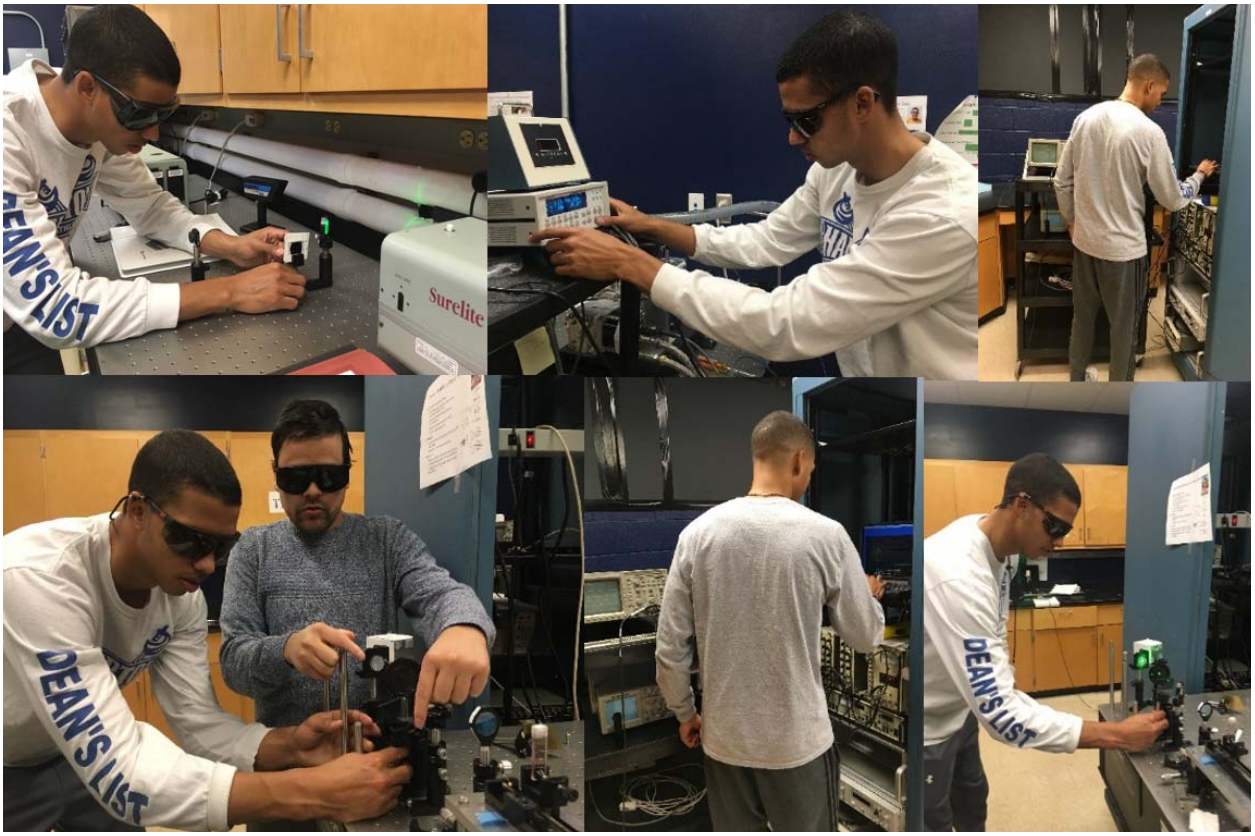
The research results and findings were disseminated through the scientific journals. An article was published in the Optical Materials, two articles were accepted by the Journal of Nanoscience and Nanotechnology, and one is submitted to the Optical Materials Express. Also, the research results and findings were presented at numerous meetings and conferences.

Nonlinear Interferometry for Quantum Ghost Imaging and Gas Sensing

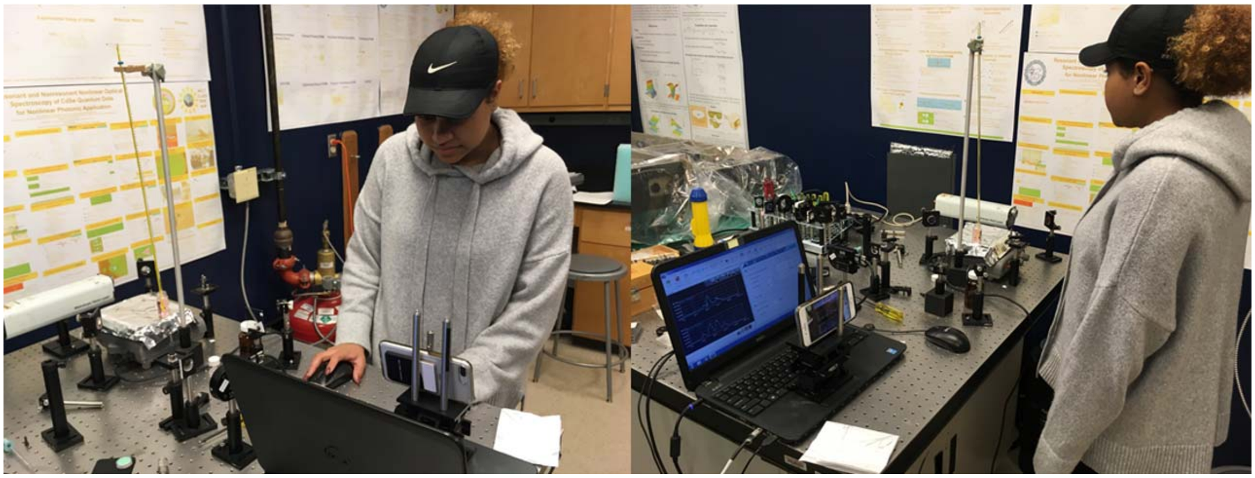
Mr. Dulitha Mahesh Jayakody Jayakodige is a Ph.D. candidate in the Department of Physics at Hampton University. He is working on the theoretical models and computational codes for nonlinear interferometry of quantum ghost imaging and sensing with intensity and phase objects for the carbon dioxide gas measurement. A nonlinear interferometry with spatial nonlocal correlation of two photons has excellent scientific and technical merits for the mission of DoD. The nonlinear interferometry has two nonlinear processes of spontaneous parametric down conversions which preserve the momentum and energy conservations between an input photon and two output photons of signal and idler in each conversion. If the signal and idler in each nonlinear conversion has a spatial nonlocal correlation, and the idlers between two nonlinear conversions keep the coherency without amplification, the idler's information interacting intensity or phase object is the signal's information. The idler in an invisible frequency interacts with an object or atmospheric gases, and experiences various optical processes including absorption, scattering, reflection, and phase change, while the signal in the visible frequency does not interact with the object or atmospheric gases. The coherency without amplification and indistinguishability with no-which-source information of idlers and the spatial nonlocal correlations of idler and signal preserve the interference of signals. Therefore, the information of idler's optical interaction with the object is the measurement of signal's ghost object because of the spatial entanglement of signal and idler beams.

The research results and findings were presented multiple meetings and is being articulated to publish in the scientific journals.

Undergraduate Research Activities



Mr. Taylor Jeremiah Osborne (Marine and Environmental Science, Senior) worked on the laser spectroscopy of optical materials to characterize linear absorption, absorption cross-section, the concentration of quantum materials. He was also trained in the nonlinear spectroscopy for characterizing atomic layers. His experiment results and findings were disseminated through the School of Science Research Symposium.



Ms. Chanel Person (Chemistry, Senior) characterized the temperature-dependent (thermal effect) refractive index change of chemical molecules using a Mach Zehnder interferometer. The accuracy of refractive index was around 10^{-4}. Her research results and findings were disseminated through the School of Science Research Symposium.

High School Student Research Activities

Mr. Alex Kwong (Senior, Governor's School for Science and Technology) characterized the optical power limiting properties of tungsten disulfide atomic layers in the academic year 2018-19 in the Quantum Optics and Nano Photonics group at Hampton University. He presented his research results and findings at the School of Science Research Symposium in Spring 2019. He graduated from the Big Bethel High School in Hampton, VA in June 2019, and joined the Engineering Program in The University of Virginia with a merit-based scholarship in Fall 2019.

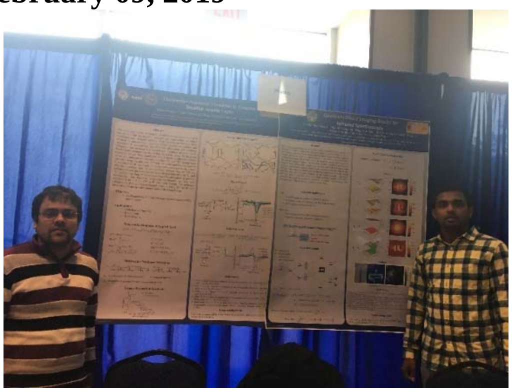
Student Training in the Lidar Laboratory

Miss. Ananda Ewing-Boyd (Psychology, Junior), Miss. Chanel Person (Chemistry, Senior), and Mr. Alex Kwong (High School Student, Senior) were trained with Hampton University's lidar system. The train included the operation and measurement techniques and analysis methodology.

School of Science Annual Research Symposium on April 17, 2019

The Hampton University's School of Science Annual Research Symposium was held on the 17th of April 2019. Mr. Tikaram Neupane, Mr. Dulitha Jayakodige, Miss. Chanel Person, Mr. Taylor Osborne, Miss. Lanijah Flagg, Miss. Angel Christopher, Mr. Alex Kwong (Advisor: Dr. Felix Jaetae Seo) presented their research activities. The students had the opportunity to network with fellow students in the scientific community while gaining feedback and appreciation for their works.

Outreach Activities
Graduate college Day on February 09, 2019



Hampton University graduate college hosted the graduate college day on 9th Feb 2019. Mr. Tikaram Neupane and Mr. Dulitha Jayakodige (Advisor: Dr. Felix Jaetae Seo) in the Physics Ph.D. program participated in the Graduate College Day event. The event introduced the information of all graduate degree programs at HU, admission requirements and procedures, financial aid, and research opportunities. The visitors also had opportunities to meet faculty and graduate students to discuss their interests.

Virginia Space Grant Consortium Visitors on April 04, 2019

The scholars and fellows of Virginia Space Grant Consortium visited the Graduate Physics Research Center (GPRC) on April 04, 2019. The visitors includes undergraduate students from The University of Virginia, Virginia Tech, Old Dominion University, and The College of William and Mary. Dr. Felix Jaetae Seo, Mr. Tikaram Neupane, and Mr. Dulitha Jayakodige informed them the research activities at GPRC.

High School Day on April 5, 2019

Hampton University hosted 41st Annual High School Day on April 5, 2019. The recruitment event for the Physics Department took place in the Science and Technology Building with the participation of over 200 high school students. Dr. Felix Jaetae Seo, Mr. Tikaram Neupane, Miss. Angel Christopher, and Mr. Dulitha Jayakodige prepared a recruitment table and explained them the physics program including classes, research and scholarship opportunities, social environment in the physics department, and career opportunities with a physics degree.

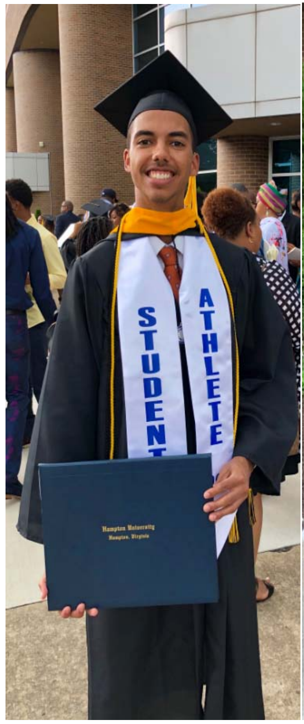
Career Fair at Lake Taylor Middle School on April 11, 2019

Dr. Felix Jaetae Seo, Mr. Tikaram Neupane, and Mr. Dulitha Jayakodige participated in the Career Fair at Lake Taylor Middle School, Norfolk, Virginia on April 11, 2019. They informed to the middle school students about career opportunities with physics. The information of career opportunities included exemplary successful careers with a physics degree such as Sally Kristen Ride (first American women in space), Elon Reeve Musk (CEO of SpaceX), Turi Milner (successful entrepreneur), Angela Merkel (German chancellor), Brian May (legendary rock guitarist), Wu-Tang Clan (hip-hop musician), David X. Cohen (television cartoon writer), Mike Judge (writer and producer), and historical physicists Albert Einstein, Isaac Newton, and Thomas Alva Edison. “The top 10 reasons why you should take physics” and “7 myths about high school physics” were also posted to encourage them to have interest in physics. An electrostatic flying object was demonstrated an example of physics concept and application.

Student Accomplishment

Mr. Tikaram Neupane (Ph.D. Candidate in Physics) completed his dissertation research entitled “Nonlinear Spectroscopy of Transition Metal Dichalcogenide Atomic Layers,” and is writing his dissertation for his Ph.D. degree. During the last fiscal year, he published three journal articles, submitted two manuscripts, and presented his research findings at the conferences and other institutions. His Ph.D. defense is scheduled in spring 2020.

Degree Completions



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