Population and Orientation Transfer in Excited NaK Collisions
Sarah Carlus
Advisor: J. Huennekens
This work was funded by the National Science Foundation

The goal of this project is to study collisions between NaK molecules and He and K atomic perturbers. A polarization spectroscopy experiment by H. Salami et al. observed collisions with $|\Delta J| \leq 58$, which not only transferred population but also maintained substantial orientation. This prompted our study of the transfer of population and orientation in collisions to understand how orientation was preserved over such a large change in rotational quantum number. Two step OODR fluorescence and polarization spectroscopy are used to examine the collisions. We use a rate equation approach to relate the intensities of the fluorescence peaks to rate coefficients for the transfer of population and orientation to another level with a particular $\Delta J$ value. Collisions with He were found to show a strong propensity for $\Delta J$=even values, while collisions with K monotonically decrease with increasing $|\Delta J|$, but show a propensity for $\Delta J$=positive. Polarization spectroscopy signals are still being analyzed to find retention of orientation in collisions of NaK molecules with He atoms.
As a part of a series of inexpensive yet powerful experiments for students to engage in “real” material science and research, we have designed and built a simple apparatus for the accurate measurement of the thermal conductivities of glass and polymer samples. The apparatus is simple to construct, consisting of a heated aluminum block placed on the top side of the flat sample, and two tiered pedestal base on the cold side which provides an independent measurement of heat flow through the sample. Differential thermocouple pairs are used to sense both the temperature difference across the sample as well as the heat following through the base pedestal. Two low cost instrumentation amplifier ICs are used to convert the small signal from the thermocouples into a voltage range appropriate for measurement with a conventional meter. The cost of parts for the entire apparatus is less than $50. Our data is collected automatically using a student programmed low cost Basic Stamp microcontroller.

A good correlation was obtained for a collection of glass and plastic materials where literature values were available. We also measured thermal conductivities on a commercial thermal analysis instrument, TA’s Modulated DSC Q2000 for comparison. The Modulated DSC Method is listed as one of the ASTM standard methods for measuring the thermal conductivity of polymers and glasses in the range of 0.1 to 1.5 W/m°C. The results of this peer-reviewed method were compared with our apparatus. Our apparatus was found to be much simpler to use and gave more consistent sample to sample variation.
Hollow Shells Of Dipoles: A Group Theoretical Approach
Christopher Devulder. Advisor: Dr. Slava V. Rotkin
Lehigh University Department of Physics

Abstract: We use Group Theory to solve for the dipole interaction part of the Hamiltonian of various types of linear, circular and cylindrical lattices of dipoles. The fabrication of such structures has been recently achieved for various plasmonic devices, such as gold nanoparticles surrounding carbon nanotubes\(^1\). These systems present various levels of rotational and translational symmetry that can be put in correspondence with symmetry groups and their matrix representations. This mapping of our physical system onto mathematical groups enables us to use several powerful results and theorems from linear algebra to diagonalize the interaction potential tensor that appears in the Hamiltonian. This tensor is initially expressed in terms of a real vector space, whose basis set is rotated to a reciprocal space given by the irreducible representations of the symmetry groups under consideration. This enables us to re-express our Hamiltonian as a block diagonal matrix, which can be further diagonalized to display the eigenenergies of the system, while the columns of the change of coordinate matrix contain the eigenmodes. The response function of a cylindrical system with an arbitrary number of rings and dipoles can then be obtained for an incoming electric field with specified wave vector \(k\). By expressing the electric field in terms of cylindrical harmonics, it becomes possible to single out the eigenmodes that contribute to the various peaks in the response function.

Acknowledgment: This work has been supported by the Sherman Fairchild Center for Solid State Studies at Lehigh University.

An FTIR Study on the Effect of Tin in Ruby Glass

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Materials Science and Engineering Department, Lehigh University, Bethlehem, PA

Abstract

Ruby glass is produced when gold is introduced to a glass melt and allowed to form nanoparticles during annealing. The necessary annealing time is dramatically reduced by the addition of tin to the system. This study uses FTIR reflection analysis to examine the structural changes produced by the addition of gold or tin to the glass melt to better understand this process. Different compositions of sodium silicate glass, with up to one tenth of a molar percent gold or tin, were prepared by the melt-quench method, and subjected to FTIR analysis. The results of comparing the primary bridging and non-bridging oxygen peaks were inconclusive due to the slight sample variability, the minute size of the possible structural changes, and the shallow penetration depth of infrared radiation into the glass surfaces. Various sample preparation methods were used to achieve a reproducible surface but even in dry gas purged and desiccated environments, a change in the surface structure over time was observed.
Impact of Advances in Physics Basis of the Weiland Transport Model

Xiang Fan

Advisors: Prof. Arnold Kritz, Dr. Tariq Rafiq
Lehigh University REU 2012

August 3, 2012

Abstract

Recent advances in the Weiland drift wave model include new correlation length and new kink (peeling) terms as well as collisions on free electrons. The new model also includes electromagnetic effects on toroidal and poloidal momentum transport. These advances make the model suitable for simulating anomalous effects in transport barriers. In this study, particle, thermal, and momentum transport coefficients are computed in systematic scans over electron and ion temperature gradients, electron and ion temperature ratio, density gradient, magnetic $q$, trapped particle fraction, magnetic shear, plasma $\beta$ and elongation. Special consideration is given to the plasma parameter scans that correspond to the plasma edge region such as H-mode large temperature and density gradients, large magnetic shear and large magnetic $q$. The transport results yielded by the new Weiland drift wave model are contrasted with the results yielded by the earlier version of the model. Combined with high fidelity models for neoclassical effects such as NEO and XGC0 models, it is planned that the new Weiland model can be used to model H-mode pedestal buildup and recovery between ELM crashes.

Acknowledgement: This work is funded by National Science Foundation, Research Experiences for Undergraduates (REU) program grant 0849416.
This project explored rotationally inelastic collisions (at $T = 600K$) of He atoms with NaK molecules in the ($A^1\Sigma^+$) electronic state. The GAMESS code was used to determine the He-NaK potential surface at values of the NaK internuclear distance ranging from 6.0 to 11.0 $\text{a}_0$. Then theoretical calculations using the Arthurs and Dalgarno coupled channel formalism were performed to investigate the strong $\Delta j=\text{even}$ propensity found in rate constants determined experimentally at Lehigh for the $v$=16 vibrational level of the first excited ($A^1\Sigma^+$) state. Previous calculations in our group had assumed a fixed internuclear separation of NaK at the equilibrium distance (7.935 $\text{a}_0$); this assumption corresponds approximately to treating the $v$=0 state. This work did not reproduce the propensity measured experimentally. To better approximate the $v$=16 state, the oscillation of the molecule was taken into account in the calculations by averaging the potential over the NaK internuclear distance using the probability density of the vibrational wave function. Coupled channel scattering calculations then used the averaged potential to solve the Schrödinger equation for the nuclear motion of the atoms, giving cross sections used to estimate the theoretical rate constants. When compared to experiment, the new theoretical calculations show an excellent agreement. The difference in the results for $v$=0 and $v$=16 suggests that the propensity has a strong dependence on the vibrational state of the NaK molecule.

This research was made possible by the National Science Foundation, Research Experience for Undergraduates (REU) program and Lehigh University. My sincerest thanks are given to all those personally involved in the research and those who made it a possibility.
Abstract
Relaxor ferroelectrics exhibit phenomena such as strong dielectric dispersion, high electro-optic coefficients, and strong mode coupling in the lowest energy branches. KTN in particular exhibits electro-mechanical properties during phase transitions. The origins of these phenomena are considered to be due to the existence of polar nano regions (PNR) and polar nano domains (PND) which form after the crystal is cooled below certain critical temperatures. In this study, we are particularly interested in the transverse acoustic (TA) and transverse optic (TO) phonon properties. By using neutron scattering via a triple axis spectrometer, we seek to characterize crystal atomic structure at different wave vectors while subject to various temperatures. The primary types of inelastic neutron scattering scans used were constant energy (E) scans, and constant wave vector (q) scans. By fitting inelastic constant q scans with the mode coupling function, we have evidence that the transverse optic mode couples with the transverse acoustic mode. Furthermore, by analyzing the neutron scattering data, we are able to see significant evidence for interaction between the transverse optic mode phonon and PND.

This work was supported by funding from the National Science Foundation (NSF), Research for Undergraduates (REU) program.
Multi-Mode Model 7.1 Validation Study
Predictive Modeling of DIII-D Tokamak Discharges

Victor J. Genty*
Advisors: Professor Arnold Kritz, Dr. Tariq Rafiq
Lehigh University

Abstract

This research focuses on validating the Multi-Mode anomalous transport module MMM7.1, recently installed in the PTRANSP code. The MMM7.1 module is used to compute thermal, particle and toroidal angular momentum transport. MMM7.1 includes a model for ion temperature gradient, trapped electron drift modes and MHD modes as well as a model for electron thermal transport driven by electron temperature gradient modes and a model for drift resistive inertial ballooning modes. MMM7.1 is documented and organized as a standalone module, which complies with the National Transport Code Collaboration standards available at w3.pppl.gov/ntcc. Simulations of DIII-D tokamak discharges are carried out using the PTRANSP predictive integrated modeling code with time evolved boundary conditions. The discharges simulated in the validation study of MMM7.1 include DIII-D Ohmic, L-mode, H-mode plasmas and plasmas with co- and counter-rotations. The time evolution of temperature, toroidal angular frequency and current density profiles predicted using the MMM7.1 transport module are compared with corresponding data from DIII-D tokamak discharges for which analysis is available in the ITPA database. For each class of DIII-D discharges studied in this research, RMS deviations and offsets are reported. Differences in predictions of plasma profiles for different plasma parameter regimes are discussed.

*University of Texas at Austin REU student supported by the National Science Foundation, Research Experience for Undergraduates (REU) program grant 0849416.
Experiment on Non-equilibrium State: Jarzynski’s Fluctuation Theorem

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August 9, 2012

Systems which are far from thermal equilibrium can prove to be challenging to study. The vast range of possible non-equilibrium states prohibits formulation of a general theory from being developed. In 1997, Christopher Jarzynski presented a theorem which states that the change in the Helmholtz free energy \( F \) of a system undergoing a thermodynamic transformation along an arbitrary path between two equilibrium states is given by the ensemble average of the exponential of the work done during the transformation:\[1\]:

\[
\Delta F = -\frac{1}{\beta} \ln \langle e^{-\beta w} \rangle
\]

Here \( \beta^{-1} = k_B T \), where \( k_B \) and \( T \) denote the Boltzmann constant and temperature, respectively. This relationship is known as Jarzynski’s fluctuation theorem. It describes the response of the system as it is driven away from thermal equilibrium. With the ultimate goal of studying the theorem, we have initiated an experimental study of a two-dimensional system. It consists of a mixture of small ball bearings at two different sizes lying on a nearly horizontal cell bounded by a rectangular frame defining the cell’s edges. The thermal state of the system is excited by driving the base plate in two mutually orthogonal directions by two linear translation stages; the frame is held stationary, however. Each of the translation stages is independently driven by a stepping motor according to a chaotic algorithm. The thermal state of the system is mechanically changed by controlling the intensity of the motor drives and the angle of tilt of the base plate relative to the horizontal plane. The system relaxes initially into two Gaussian velocity distributions, one for each of the two groups of spheres with its own temperature; the two temperatures approach each other with significant fluctuations over a longer period of relaxation. The particle velocity is determined individually by imaging: high-resolution images are taken at 13.5 frames/s and they are analyzed to determine the positions of individual spheres, and their velocities, by means of the Hough transformation. From the sigma values of the respective Gaussians, the temperatures are determined for the x and y directions and for the two sets of spheres. The base plate is tilted at a small angle, and the evolution of temperatures is followed over time from an initial condition. The approach towards equilibrium is observed as the spheres mix together while the system runs. The system energy and work done on the system are tracked individually in this study.


We would like to thank the National Science Foundation's "Research Experiences for Undergraduates" program for funding our work along with Lehigh University's Physics Department
Surface plasmons (SPs) are electromagnetically excited coherent charge oscillations at a metal-dielectric interface. Nanoplasmonic biosensors utilize SPs to confine light at the nanoscale for sensitive detection of biomolecular binding events. These SP surface waves are extremely sensitive to the local surface conditions. Small changes, such as roughness, can cause them to scatter, which makes the sensor less sensitive. In order to lower surface roughness, a process called template stripping was used. By depositing a metal film on a very smooth silicon substrate, the interfacial surface can be made ultrasmooth. The metal film was then attached to an adhesive epoxy layer and peeled off from the silicon substrate, revealing the ultrasmooth metal surface. With this process, the RMS roughness of the metal film was lowered from 2.54nm (for the deposited metal) to 0.59nm. The refractive index of the substrate can also affect the performance of a particular biosensor called a Plasmonic Mach-Zehnder interferometer proposed by the Bartoli group. Due to the way in which SPs on opposite sides of the thin metal films interfere with each other, lowering the refractive index of the substrate increases the sensor sensitivity. To lower the refractive index of the substrate, two processes were used. A sol-gel solution to deposit silica was used for both. Dip coating created a very cracked surface, with RMS roughness of 5.09nm. Spin coating created a much smoother coating, with surface RMS roughness of 0.35nm. Although the refractive indexes of these coatings were not measured, it has been reported to be 1.46, which is lower than the 1.51 of the substrates this group previously used.
The Study of Cluster Formation in Janus Ellipsoids

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Colgate University

Advisor: Jim Gunton
Collaborators: Donovan Ruth, Wei Li
Lehigh University
August 3, 2012

Abstract:

Janus Particles are microscopic particles whose surface can be coated with two different chemical compositions for e.g., metal/polymer, hydrophobic/hydrophilic, etc. In our study, we make use of Janus oblate ellipsoids with aspect ratio of 0.6, in order to study their cluster formation through self-assembly. Our model assumes that the pair interaction between ellipsoids is given by the combination of hard-core repulsion and orientation dependent attractive square-well potential model. Using standard Monte Carlo simulations in NVT ensemble, we found that clustering is an effective means for Janus gases to become orientationally structured and thus retain their gaseous phase at higher densities. This study can prove to be effective in terms of giving us an estimate of the phase diagram of these Janus ellipsoids.

This research was made possible through the generous funding from the National Science Foundation.
Terahertz Technology, Spectroscopy, and Their Application to the
Examination of Glassy and Crystalline States

Samantha Jane Lampe, William Jewell College
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Lehigh University IMI-NFG REU 2012

Abstract

Implementation of a spectroscopic system designed to examine a portion of the terahertz region of the electromagnetic spectrum allowed us to further analyze a collection of materials: SiO$_2$ glass, SiO$_2$ crystalline quartz, LaBGeO$_5$ glass, and LaBGeO$_5$ polycrystal. This is an extension of an investigation conducted by Song, Ding, Gupta, and Jain$^{[1]}$ in 2010. Our THz absorption spectroscopic study using an FTIR spectrometer and a blackbody light source in the wavelength range of 20 μm to 200 μm (500 cm$^{-1}$ – 50 cm$^{-1}$) yielded several notable results. Three mysterious absorption peaks consistently occurred at approximately 21 μm, 23 μm, and 27 μm in all samples except LaBGeO$_5$ glass. We have confirmed that these were not due to sample holder adhesives or free molecular water absorbance – as data was gathered within a vacuum. It is possible that this phenomenon could have been generated by adsorption where OH or water molecules accumulate on the surface of the samples by means of weak van der Waals forces or chemisorption. Information regarding water absorbance – and adsorbance – is valuable in terahertz technology due to the many applications dependent upon water concentration. A more in-depth investigation of this phenomenon could be beneficial. A second notable observation was that, contrary to expected results, the LaBGeO$_5$ polycrystal was found to be more absorptive than the LaBGeO$_5$ glass at THz frequencies. This contradicts the expectation that glasses are typically more lossy. Further research – possibly reflection mode spectroscopy – is necessary to confirm our results for these materials. LaBGeO$_5$ is a material of particular interest to IMI because of its useful characteristics – specifically that it is a ferroelectric material that produces non-linear crystals. Thus, LaBGeO$_5$ has a strong potential for future applications within the field of photonics.

Acknowledgement: Funded by NSF supported International Materials Institute for New Functionality in Glass (IMI-NFG), Lehigh University (Grant DMR-0844014).

Effect of Boron Addition on In-Vitro Degradation of Sol-Gel-Derived Calcium Silicate Bioactive Glass

Christine LaPorte, Ukrit Thamma, Himanshu Jain

Abstract:

Bioactive glass scaffolds with compositions 30%CaO-70%SiO2 and 5%B2O3-30%CaO-65%SiO2 were prepared using a polymer templated, sol-gel preparation and particle sintering technique. A mesoporous structure was confirmed by nitrogen absorption, with two pore size distributions at 5 and 10 nm due to a solvent exchange during aging of the sol-gel. In-vitro bioactivity analysis of scaffolds in simulated body fluid was performed to study the degradation behavior of the glass. The in-vitro bioactivity was studied under static and quasi-dynamic fluid conditions, and analyzing the concentration of boron, phosphorus, silicon and calcium in solution via inductively coupled plasma-optical emission spectroscopy. Nitrogen absorption and scanning electron microscopy (SEM) were performed to evaluate the scaffold structure. Although SEM imaging shows phase separation of some borate out the B2O3-CaO-SiO2 network, a calcium borosilicate structure had been confirmed through in-vitro bioactivity analysis, and changes in the pore sizes. The addition of borate seems to have resulted in more calcium phosphate deposition in the in-vitro bioactivity/scaffold degradation analysis, and yield increased surface area of scaffolds. Due to the increased bioactivity, this method of preparing calcium borosilicate sol-gel-derived glasses shows significant progress toward preparing scaffolds with 3-dimensional architecture.

Acknowledgements:

This work was supported by International Materials Institute for New Functionality in Glass through the NSF Grant (DMR-0844014). The author would like to thank Lehigh summer research program, Dr. Himanshu Jain and Mr. Ukrit Thamma for their support in research.
This summer we determined the third-order hyperpolarizabilities of a series of small organic molecules with conjugation lengths ranging from zero to five triple bonds. These molecules are similar to the DDMEBT molecule that has been previously studied, with minor variations that might cause differences in their nonlinearities. The two major nonlinear optical techniques we used are the degenerate four wave mixing (DFWM) and the third-harmonic generation (THG). The samples used in the DFWM measurement are solutions of the molecules with various weight percent concentrations, whereas the samples used in the THG measurement are thin films which we fabricated by a vapor deposition process. In addition, we performed ab initio calculations of the molecules using computational chemistry software to determine their hyperpolarizabilities in comparison to our experimental results. Due to time limit we have not finished all of our measurements, but future work will show a trend of nonlinearity in these molecules. We also developed a corona poling set up in addition to the measurements described above, which will allow us to explore any possible orientations in the molecules under high voltage at elevated temperature.

This research has been sponsored by the National Science Foundation (NSF) and the Karas Undergraduate Research Internship.
A Model for Actin Filament Bundling and Cable Formation in Fission Yeast Cells

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Summer 2012

Abstract

In growing fission yeast cells, formin proteins associated with cortical sites at the cell tip polymerize actin monomers into filaments. These filaments bundle to form actin cables that span the cell and guide the movement of vesicles toward cell tips. There has been little theoretical investigation into what processes and factors are required for the assembly of actin filaments into cables. We used computer simulations to determine whether actin polymerization, filament turnover and filament cross-linking were sufficient to reproduce the observed actin cable morphology. Our computer simulations modeled actin filaments in two dimensions as semi-flexible polymers and cross-linking as an elastic attractive interaction among filaments, modifying the code developed in [1]. Confinement by the cell membrane was implemented as a short-range repulsive boundary. Filaments polymerized away from cortical sites located at the boundaries that represent the cell tips. We determined a range of cross-linking parameters with which the cable assembly behavior was reproduced, and showed how that range changed with the persistence length and the number of filaments. We showed that the cross-linking and filament turnover processes were sufficient to reproduce cable formation behavior in computer simulations.

Probing the Physics of LS I +61° 303

Sean Napier & M. Virginia McSwain (Lehigh University)

Be stars are a subclass of B-type stars with rapid rotation and large circumstellar disks which display several distinct emission lines in their spectra, especially the H-Balmer lines. LS I +61° 303 is a high mass X-ray binary system comprised of a Be star and a compact companion, which is most likely a neutron star, that emit in the radio, optical, X-ray and γ-ray regimes. The system has periodic emission over the 26.496 day orbit as well as a 1667 day super-orbital period. Here we present recent optical spectra collected at the KPNO Coudé Feed Telescope during December 2011-January 2012. We present new equivalent width measurements of Hα and report a burst of emission near orbital phase 0.4. We also present new radial velocity measurements for the Be star which are consistent with previous results. Finally, we also investigate the super-orbital modulation to better understand the interactions between the Be star and the compact companion.

We are grateful for support provided by NSF awards PHY-0849416, AST-1109247 and for the support of Lehigh University.
Probing Laser Induced Space Charge with Optical Spectroscopy
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Abstract

LiNbO₃ is an important optical material due to its favorable properties. Defects in the material can give rise to an internal space charge field when illuminated by a laser that can cause undesirable modifications of the material properties through the electro-optic effect. The emissions of an erbium dopant in the sample can be used to study this internal electric field buildup. As the energy levels of erbium are affected by the presence of an electric field, a shift in the center of gravity of the erbium emission peaks indicates a change in the electric field. When exciting a crystal of Er:LiNbO₃ with a 488 nm laser at 4.1 K, a space charge buildup of 26 kV/mm was created. When exciting crystal of Fe:Er:LiNbO₃ under these conditions, a space charge again built up, but the effect was mostly obscured by a broadening of the spectral peaks, most likely due to interactions between the iron and erbium defects in the crystal.

This work was supported by the National Science Foundation, Research Experience for Undergraduates Program, grant No. DMR-1008075.
Optophoresis and electrophoresis: motion of an optically trapped polystyrene particle in an electric field

Kathryn Reddy

Dr. H. Daniel Ou-Yang

August 3, 2012

Abstract:

It is well known that electrophoretic motion, the movement of a particle due to an external electric field, can be used to quantify particle charge. However, previous techniques assume the viscosity of a sample to be known. Using an optical tweezer-based setup we can both measure the viscosity of a sample directly and obtain reliable charge measurements. Here we studied the electrophoretic motion of a 1.5 µm polystyrene particle using an optical tweezers setup. A lock-in amplifier provided amplitude and phase measurements, and a function generator provided an AC electric field to our sample chamber. Optophoresis, in the form of optical tweezers, was used as a tool to quantify the electrophoretic effects. The setup used standard illumination and quadrant photodiode detection. This allows for extremely accurate calibration of the optical tweezers and precise measurements of particle motion. Manipulation of the relevant equation of motion allowed us to calculate particle charge and electrophoretic mobility. We found the charge of our particles to be $1.26 \times 10^{-16}$ C and the electrophoretic mobility to be $8.563 \times 10^{-9}$ m$^2$/V·s. We are able to validate the consistency and accuracy of such a setup through error analysis and comparison with previously published data.

This research was made possible through funding from the National Science Foundation’s Research Experience for Undergraduates program and support of NSF-DMR-0923299.
Antimony SulfoIodide (SbSI) glasses display high pyro-optic and pyroelectric coefficients, which make them suitable in uncooled pyro-optic IR detectors. The surface or bulk crystallization mechanisms that characterize these glasses determines their applications, including their piezoelectric properties and potential use for laser and E-beam induced fabrication of SbSI single crystal architecture in glasses. Previous EDS research indicates that the chemical composition of the glass is approximately 35.5% Sb, 40.1% S, and 24.4% I, or 82SbSI-18Sb$_2$S$_3$. We are interested in understanding the crystallization mechanisms that the glass undergoes when subject to thermal analysis. Through Differential Scanning Calorimetry (DSC), Thermal Gravimetric Analysis (TGA), Powder X-Ray Diffraction (PXRD), and different-sized samples, we have been able to identify the basic crystallization mechanisms in SbSI glasses.

This project has been funded by the National Science Foundation through IMI Grant DMR 0844014.
Gamma-Ray Emission from LS I +61°303
Leigh C. Schaefer (Lehigh University, Bryn Mawr College)
Advisor: M. Virginia McSwain (Lehigh University)

ABSTRACT
LS I +61°303 is a high-mass gamma-ray binary with known orbital and super-orbital variability in the radio, optical, X-ray, and gamma-ray wavelengths. The compact companion is probably a neutron star but remains unconfirmed. Here, we use data from the Fermi Gamma-ray Space Telescope to examine LS I +61°303’s gamma-ray emission over both its orbital and its super-orbital period. We find that the emission peaks at orbital phases of 0.3 and 0.5, and that the energy spectrum follows a log parabola model. We also find that there is gamma-ray variability in the 1667-day super-orbit, but further investigation will be required to determine the exact parameters of this variability. We interpret these results as possible evidence for a mass stream flowing from the optical star’s circumstellar disk and colliding with a pulsar’s wind, emitting across the electromagnetic spectrum.

We are grateful for support provided through NSF grants AST-1109247 and PHY-0849416.
Abstract

Er$^{3+}$ is a trivalent rare earth ion which can be doped within GaN to form Erbium doped Gallium Nitride (Er:GaN). The interaction of each ion with its surrounding electric field (also called the crystal field) breaks the degeneracy of its multiplets in a phenomenon called the Stark effect. This results in the splitting of each multiplet into a number of distinct sublevels/splitting which depends on the J value of the multiplet. Its interaction with magnetic fields can produce an analogous result through a phenomenon called the Zeeman effect. Both of these effects can be used to probe the crystal’s electric and magnetic properties, the latter which could be potentially utilized in new magnetic systems. Therefore studying the Stark splittings will help build a foundation toward better understanding the Zeeman splittings and developing these Er:GaN integrated devices. By stimulating its emissions with an 800 nm range laser, we were not only able to use Combined Excitation and Emission Spectroscopy (CEES) to obtain data found to be consistent with transitions between the $I_{11/2}$, $I_{13/2}$, and $I_{15/2}$ multiplet sublevels (mapped in earlier research), but also expanded upon this by quantifying the splittings in the $I_{9/2}$ multiplet.
Characterization of SWNT using spectroscopy for Dielectrophoresis

Ashish Shah, Drew University
Lehigh University, 2012 Physics Summer REU
Advisor: Dr. Slava V. Rotkin

Carbon Nanotubes (CNTs) have a tremendous amount of potential as the building blocks for nanoelectronics. Extraordinary mechanical and electronic properties of the Single-Wall Carbon Nanotubes (SWNT) allow them to be perfect candidates for biosensors, electronic transistors and photosensors. Dielectrophoresis (DEP) is the movement of the particle in non-uniform electric field. It describes the translational motion of particles due to the application of non-uniform electrical fields. DEP uses predominantly AC fields to align CNTs in solution on electrodes. DEP trapping of CNT networks represents a more reproducible method for forming CNT-FETs. It is quick and inexpensive with recent reports demonstrating parallel FET array fabrication. Presence of both metallic and semiconductive carbon nanotubes in solution is the main reason why forming single nanotube conductance channels is unreliable. The dielectrophoretic forces on CNTs are influenced by the electronic properties of the CNTs and cause a separation of metallic and semiconductive nanotubes. Spectroscopy techniques such as Absorption spectroscopy and Photoluminescence (PL) spectroscopy can allow optimization of DEP.

SWNTs can either be semiconductive, semimetallic or metallic depending on the symmetry of the tube defined by unique indices $n$ and $m$. Spectroscopy techniques such as absorption spectroscopy and photoluminescence (PL) spectroscopy are very efficient ways to characterize the different types of tubes in a solution. PL spectroscopy is a very efficient method in deducing ($n$, $m$) indices since different nanotubes absorb and emit at different wavelengths. The peaks in the PL/PLE (PL excitation) map define ($S_{22}$, $S_{11}$) pairs, which correspond to excitonic transitions in 1$^{st}$ and 2$^{nd}$ subbands for the unique ($n$, $m$) index of a tube.

Optical absorption is routinely used to quantify quality of the carbon nanotube powders. The spectrum is analyzed in terms of intensities of nanotube-related peaks, background and pi-carbon peak. Absorption in nanotubes originates from electronic transitions from the v2 to c2 (energy E22) or v1 to c1 (energy E11) levels, etc. The peaks corresponding to the transitions are relatively sharp and they can be used to identify nanotube types in a solution. Absorption spectra can also provide the relative concentration of the tubes present in the solution. Absorption and PL spectroscopy are very efficient techniques to characterize SWNTs for applications such as optimization of DEP.
IR Spectroscopy of Hydrogen Impurities and Free Carriers in In$_2$O$_3$
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Hydrogen impurities recently have been predicted to contribute significantly to $n$-type conductivity in In$_2$O$_3$, a transparent conducting oxide widely used in the modern electronics industry.$^1$ In this work, we studied the effects of annealing temperature on O-H centers in In$_2$O$_3$ and on the free carrier absorption seen in the same samples using Fourier transform infrared (FTIR) spectroscopy, similar to a previous study with SnO$_2$.$^2$ Although multiple O-H lines exist in as-grown In$_2$O$_3$, annealing in an H$_2$ ambient at 500 °C significantly increases the O-H line intensities along with the free carrier absorption detected at lower frequencies.$^3$ In order to investigate the possible correlation between hydrogen defects and the free carriers in In$_2$O$_3$, both have been examined as a function of annealing temperature. In addition to six O-H lines with frequencies ranging between 3306 and 3418 cm$^{-1}$, an anomalous peak was found at 1889 cm$^{-1}$. With the exception of this anomalous line, the annealing behavior of the O-H vibrational absorption was found to be correlated with the free carrier absorption. The absorption due to free carriers significantly decreased in intensity beginning at an annealing temperature of 600 °C, at which point the hydrogen centers were also found to become unstable.


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Characterization and Efficiency Enhancements of mono-Si Solar Cells

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Abstract

Increasing the efficiency of photovoltaic cells is of interest to industry and consumers alike. In order to quantify the properties of a solar cell that give rise to its efficiency, various methods of characterization must be utilized. These methods include external quantum efficiency testing and current-voltage (I-V) curve analysis. We tested the external quantum efficiency of commercial solar cells using a QE/IPCE measurement kit to establish baseline data. The I-V measurements of the solar cells were also taken and analyzed for parameters such as open circuit voltage, short circuit current, max power, series resistance, shunt resistance, and energy conversion efficiency. Microlens technology similar to that used in III-Nitride LED efficiency improvement research was proposed as a way to enhance the efficiency of solar cells. The deposition of SiO2 microlenses was performed on the surface of the GaN semiconductor LEDs, and the same method will be applied to the surface of the solar cells by using the rapid convective deposition and melting of polystyrene microspheres. In continuing research, the solar cells will be characterized after lens application in order to determine the improvement in collection efficiency of the cells. In the future, research will include applications to advanced multi-junction solar cells.

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Abstract: Understanding the properties of rare earth metals in various glass and crystal compositions is essential to industries involved in their production and utilization for applications such as, optical fibers, and lasers. One important rare earth metal frequently utilized and studied is erbium (Er$^{3+}$). Nevertheless, little literature exists regarding erbium when doped in lanthanum borogermanate (LaBGeO$_5$) glass and crystals. LaBGeO$_5$ is an interesting material due to its useful electric and non linear optical properties as well as the fact that its composition is the same for both the glass and crystal phase. In order to learn more about Er:LaBGeO$_5$ glasses and crystals, we utilized various luminescence techniques including Raman and fluorescence spectroscopy. These methods allowed us to analyze the spatial distribution of erbium throughout a laser-crystallized line embedded within a bulk Er$_{0.002}$La$_{0.998}$BGeO$_5$ glass, and the effects of stoichiometric variations on the erbium fluorescence within LaBGeO$_5$ glass and crystals. We prepared LaBGeO$_5$ glasses with 0.2%, 1%, and 4% concentrations of erbium. After crystallizing these corresponding concentrations, via furnace we uncovered interesting behaviors among the polycrystals in relation to the laser-induced single crystal. After analyzing the laser-induced single crystal via Raman and fluorescence spectroscopy, we observed that an apparent erbium fluorescence enhancement previously observed is inhomogenous over the cross-section of the crystal structure, which, along with the general lack of spatial coordination implies a physical ion accumulation in addition to enhancement due to crystal field. Lastly, comparing the stoichiometric variations we found that the emission energies of erbium appear to be functions of erbium concentration and crystallization mechanism, while intensity ratios seem to depend solely on the crystallization mechanism. As the quest to uncover the mysterious characteristics of Er:LaBGeO$_5$ glasses and crystals progresses, further research will include polarized Raman scans of glass and crystals, the comparison of laser-induced single crystals of various stoichiometric variations, and lastly, the classification of Er$^{3+}$ energy levels in LaBGeO$_5$.

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