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## INTRODUCTION

Stony Brook University is proud to host the Research Experiences for Undergraduates (REU) Program in Physics & Astronomy. Sponsored by the National Science Foundation (NSF), this program gives undergraduate students an intensive hands-on research experience and involves them in all phases of the research process. This year, twelve summer researchers from colleges and universities throughout the country were selected from a select pool of over three hundred applicants. In carrying out their projects, REU participants worked alongside Stony Brook's faculty, post-docs, graduate students and other undergraduates. The summer activities culminated in a presentation of the students' work in a research symposium and in a written report.

As you read this collection of their abstracts, you will see evidence of their hard work, keen insight and enthusiasm, and be impressed at what they have accomplished in only eight weeks. I have no doubt that these individuals will continue on with successful academic and research careers.

—Erlend Graf, Director, REU Physics & Astronomy program, Stony Brook University

**Jacob Chamoun**  
Cornell University

## **Creating unconventionally polarized beams using stress birefringent wave plates**

Jacob Chamoun, Cornell University, MARTY COHEN and JOHN NOÉ, Laser Teaching Center,  
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This project investigated the use of a wave plate with spatially varying birefringence to produce cylindrical vector beams (CVBs), as suggested by the work of Spilman and Brown [1]. Birefringence is a property of materials in which incident polarized light is decomposed into two orthogonally polarized components - the ordinary and extraordinary ray - upon entry into the material. Because each ray travels at a different speed, a phase shift is incurred upon exiting the material. If the shift is 180 degrees, the material constitutes a half-wave plate and will rotate the polarization of linearly polarized light. In stress-induced birefringence, the fast and slow axes line up with the directions of principle stress, so a planar, inhomogeneous stress pattern can produce a wave plate whose fast axis orientation varies in space. These wave plates can be used to create unconventional polarization states, including cylindrical vector beams. CVBs are propagating solutions to the vector paraxial Helmholtz equation which contain a central polarization singularity. Such beams are of both theoretical and practical interest.

Spilman and Brown [1] mention a "discrete" wave plate composed of an angular arrangement of 8 half-wave plate wedges such that the fast axis rotates or "counterrotates" [1] at half the rate of the azimuthal angle. We made several such plates using birefringent transparency film and observed that the discrete wave plates rotated linearly polarized light in a way consistent with a discrete approximation to radially or azimuthally polarized light. Next, we built a stress-optical element (SOE) based on the previous work [1,2] to apply adjustable compressive stresses at 120° intervals around the perimeter of a 1/2 in. diameter, 3/8 in. thick plexiglass window. Spilman and Brown [1] calculated that such a stress pattern would produce a counterrotating fast axis — the continuous analog to the discrete plate — which could be used to produce a truly radial or azimuthally polarized beam. We chose plexiglass over glass [1,2] because its stress-optic coefficient is higher, so less compression is needed.

When we used an expanded green (532 nm) laser beam to illuminate our SOE between linear or circular polarizers, interesting polarization structures appeared. Between circular polarizers, the SOE exhibited a single dark ring of half-wave retardance. With the ring isolated by an annular mask, exposing the SOE to linearly polarized illumination and analyzing with a linear analyzer produced dark lobes that rotated with the analyzer, indicating the presence of a polarization vortex. A series of images of the SOE between various combinations of polarizer and analyzer were taken with a consumer camera and analyzed in MATLAB to extract the spatial pattern of Stokes parameters. This analysis confirmed that there is an annular region of counterrotating linear polarization at the half-wave radius. We are currently taking additional images with a more appropriate computer-based camera.

This work was supported by the National Science Foundation (Phy-0851594).

[1] A. K. Spilman, T. G. Brown, *Appl. Opt.* 46, 61-66 (2007)

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**Andriy Dotsenko**  
Stony Brook University

## **The Silicon Vertex Tracker upgrade project**

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The Relativistic Heavy Ion Collider (RHIC) is a powerful instrument for (spin, heavy ion/particle) physics. Since its first run in 2000 RHIC has observed the formation a dense nuclear matter called quark-gluon plasma (QGP) in energetic gold+gold nuclei collisions and has shown that gluons contribute very little to the spin of the proton. As new discoveries are made and as technology advances the RHIC detector systems undergo periodic upgrades. These upgrades allow us to gain an ever improving understanding of the QGP and the proton's spin constitution. The latest upgrade to be made to PHENIX, one of the two large detectors at RHIC, will be the addition of the Silicon Vertex Tracker (VTX). The VTX can resolve the decay vertices of heavy quark carrying particles. PHENIX can use the VTX to track heavy mesons traversing through the QGP which will render great insight into its properties. The purpose of this project was to work with a team of professionals in assembly and testing of the VTX.

The VTX consists of four concentric barrels of silicon detectors. The responsibility of my lab is to assemble and test the outer two barrels consisting of novel Strip Pixel sensors used for the first time for particle tracking. The barrels are made of chains of sensors assembled into ladders. After the sensors are precisely attached to the ladders, they are rigorously tested for quality. Routine tests tell us if dead channels are present as well as the noise signature of live channels. The ladders will undergo a final beta source test before being assembled into barrels. As we assemble and test the ladders, various precautions are taken to protect the sensors from static electricity discharges, dust, moisture, and human touch.

The project follows strict deadlines in order to finish the detector before Run 11 of RHIC in the winter of 2010-2011. Presently, all the ladders have been assembled and tested and await the final packaging as well as the beta source test.

This work was supported by the REU Physics program at Stony Brook University, and the National Science Foundation (PHY-0851594).

**Drummond Fielding**  
Johns Hopkins University

## **Sodium line strength as surface gravity indicator**

Drummond Fielding, *Johns Hopkins University*; MICHAL SIMON, *Department of Physics & Astronomy, Stony Brook University*

The motivation of this research was to develop a technique for estimating the age of stars a few tenths of the mass of the sun. This is useful to us because conventional youth indicators are not reliable for low mass ( $< 1$  Solar Mass), young ( $< 50$  million years old) stars. The stars we focused on are limited to a region of  $\sim 100$ pc around the sun because, although low mass stars are very numerous, they also have low luminosity. Young stars in the solar neighborhood are sometimes found in groups of stars of the same age moving together through the galaxy. We focused on the  $\beta$  Pictoris Moving Group (BPMG), which is spread throughout the sky so determining membership cannot rely on position and an observable age indicator is needed. We used surface gravity,  $g = G M/R^2$ , as a proxy for age since a young star decreases in radius as it collapses to its stable configuration as a main sequence star. We studied the use of the Na I doublets at 5890 and 5896 Å (Na D line) and at 8183 and 8195 Å ( $\sim 8200$  Å line) as surface gravity indicators for late K and M spectral type stars. I wrote several procedures in IDL to calculate the equivalent width (EW) of large number of observed spectra at different resolution and modeled theoretical spectra at very high resolution. By calculating the EWs of these doublets we show the demonstrated relation between EW of the spectral lines and the logarithm of the surface gravity,  $\log(g)$ . We found that for the Na D lines there is a clear distinction between known giant and main sequence dwarf stars; and that known and likely BPMG members lay in between but close to the main sequence stars. For the 8200 lines we found that the EWs are smaller but follow the same pattern. By choosing model spectra that corresponded to specific effective temperature and  $\log(g)$ , and comparing their EW with the EW of candidate BPMG stars and known stars of different sizes, masses, and ages, we demonstrated that EWs of the sodium doublets are a youth indicator.

This work was supported by a grant from the National Science Foundation (PHY-0851594).

**Simon Freedman**  
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## Verifying the efficacy of an ion source

Simon Freedman, *Illinois Institute of Technology*; Daniel Pinghero, *Clarkson University*; Victoria Yu, *Rutgers University*; THOMAS K. HEMMICK, Richard Lefferts, Andrzej Lipski, *Center for Accelerator Science and Education (CASE), Department of Physics & Astronomy, Stony Brook University*

Accelerator mass spectrometry (AMS) is a technique of measuring the mass content of an unknown sample to a high degree of accuracy using a particle accelerator. This involves creating a beam of negative ions whose velocity and direction can be manipulated by placing electric and magnetic fields of varying magnitude in their way. This work involved designing a relatively inexpensive negative ion beam source for the Van de Graaff tandem accelerator used in the Center for Accelerator Science and Education (CASE) that would be capable of producing a large amount of beam, while providing a mechanism for changing samples that does not require recalibrating the whole device. It was necessary to construct a test stand to evaluate the performance of the new ion source.

In order to generate an ion beam that accurately reflects the contents of the sample being analyzed, it is necessary to maintain high vacuum ( $10^{-8}$  to  $10^{-9}$  torr) within the test stand. The components of the test stand were thus sealed with Conflat, Dependex, and O-ring joints. The beam line was pumped down to the millitorr range using a roughing pump, and reached a minimum of  $2.0 \times 10^{-6}$  torr using a  $125 \frac{L}{s}$  turbo pump.

Although the initial acceleration of the beam is performed within the ion source itself, an Einzel lens with a variable voltage was attached to the test stand in order to keep the beam from becoming too wide (and hence missing the target) while traveling down the beam line of the test stand. Additionally, a magnetic dipole with a variable current was placed over a pipe in the test stand to prevent the beam from veering off course laterally.

Detection of the beam was accomplished by placing a quartz plate in the beam-line that would phosphoresce when hit by the beam. The intensity of the beam was measured by placing a Faraday cup in the test stand capable of measuring the beam's current. The test stand was implemented using an ion source of the same model as currently exists on the tandem accelerator. A bluish spot was seen whose radius would change depending on the voltage placed on the Einzel lens. Additionally, the current measured in the Faraday cup reached a maximum of  $1.5 \mu A$ , which is the same order of magnitude of how much beam is necessary to perform AMS. These preliminary results indicate that this test stand will be able to validate the performance of our new ion source.

This work was supported by a grant from the National Science Foundation (PHY-0851594), as well as funding for the Center for Accelerator Science and Education (CASE) at Stony Brook University.

**Vincent Gregoric**  
Mount Union College

## **A precise measurement of the speed of light in air from the frequency separation of longitudinal modes in an open-cavity HeNe laser**

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This project was motivated by an interest in the longitudinal modes of laser cavities, which are similar to standing wave harmonics on a string fixed on both ends in that the allowed modes are those in which an integer number of half-wavelengths exactly 'fit' within the laser cavity. From this condition, the frequencies of adjacent longitudinal modes are ideally separated by  $c/2nL$  where  $c$  is the speed of light,  $n$  is the refractive index of the medium in the cavity, and  $L$  is the cavity length. Thus by measuring the beat frequency between two adjacent longitudinal modes and the cavity length, one can in principle determine the speed of light.

D'Orazio et al. [1] have recently described an experiment which uses this general concept to determine the speed of light with enough precision to differentiate between its value in air and in vacuum. The key feature of their method is to use an open-cavity laser with a movable output coupler (OC) mirror. It is then sufficient to determine the intermode beat frequency as a function of the precise mirror position relative to some fixed reference point, rather than the absolute total cavity length. The light velocity obtained in the analysis depends on the index of refraction of the ambient air but not that of the laser gain medium and Brewster window within the laser cavity. Finally, as discussed in Ref. [1], the exact separation between two adjacent longitudinal modes can be effected by frequency "pulling" and "pushing." These effects can be minimized by using a scanning Fabry-Perot interferometer to monitor and then adjust both the absolute and relative intensities of the longitudinal modes.

Our experimental setup was similar to that described in Ref. [1]. The main modification was taking length measurements closely spaced over approximately 2 cm as opposed to the larger range of 16 cm used in Ref. [1]. We also determined distances from the micrometer driving the translation stage on which the OC mirror was mounted, rather than by using a separate caliper. The beam from our open cavity HeNe laser ( $\lambda = 632.8$  nm) was directed by a beam splitter into both a photodiode connected to an RF spectrum analyzer (HP model 8566A) and a scanning Fabry-Perot interferometer connected to an oscilloscope. The spectrum analyzer was used to measure the precise beat frequency between adjacent modes, while the Fabry-Perot was used to monitor the mode intensities. Two complete sets of data were taken, one with and one without using the Fabry-Perot to minimize frequency pulling/pushing effects. It was apparent from the results that frequency pulling and pushing does in fact have a significant effect on the observed beat frequency for a given cavity length. Our final result for the speed of light in air was  $2.9973 \times 10^8$  m/s. This result is comparable to that obtained in Ref. [1]. The accepted value of the speed of light is  $2.9979 \times 10^8$  m/s in vacuum and  $2.9971 \times 10^8$  m/s in air at standard temperature and pressure. We are currently seeking to determine the error in our final result by analyzing the uncertainties in the length and frequency measurements.

This research was supported by a grant from the National Science Foundation (PHY-0851594).

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**Ewain Guatemala**  
Stony Brook University

## **Mode-locking a HeNe laser by extra-cavity acousto-optic modulation**

Ewain Guatemala, MARTY COHEN and JOHN NOÉ, *Laser Teaching Center, Department of Physics & Astronomy, Stony Brook University*

This project was motivated by an interest in the interaction between light and sound (acousto-optics) and in longitudinal laser modes. In this work we have demonstrated mode locking in a helium-neon laser through the use of an AO modulator placed outside the laser cavity, as suggested in Ref. [1]. Mode-locking of a laser occurs when the longitudinal cavity modes oscillate in phase. These modes generally oscillate with a random phase relationship but when in phase the laser will output pulses of higher peak intensity than the time-average intensity. A setup incorporating an AO modulator (AOM) can provide the frequency and phase shifts necessary to satisfy the mode-locking condition. In an AOM a propagating acoustic wave results in a traveling refractive index grating. The first order diffracted light is frequency shifted by the frequency of sound propagating in the crystal.

Our HeNe laser (Spectra Physics model 127) supports 8-11 longitudinal modes; it has a mode spacing of 160 MHz and a cavity length  $L = 93.7$  cm. The laser beam is incident at the Bragg angle on an Isomet AOM (model 1205C-2-804B) driven at half the mode spacing frequency. The first diffracted order is reflected back through the AOM to be further frequency shifted to 160 MHz and re-diffracted back into the laser cavity creating side band modes adjacent to the cavity modes. The optical path length (OPL) between the laser's output mirror and the reflecting mirror is controlled by placing the latter on a micrometer translation stage. This external cavity distance must be carefully matched to the OPL of the laser cavity. By setting this distance and the AOM frequency, the AO generated sidebands are coupled to the cavity modes, locking these in phase. The zero order beam is reflected to a beam splitter, which directs it to a Fabry-Perot analyzer and a fast Si photodetector (Thorlabs DET-210) connected to an oscilloscope (Tektronix 485) or spectrum analyzer (HP 8566A).

The spectrum analyzer was used to tune the sidebands to coincide with the cavity mode spacing; mirror adjustments resulted in shorter pulses with higher peak intensity. The pulses had the expected 160 MHz spacing and a peak pulse amplitude four times higher than the time-average intensity. Further refinements to the experiment will be aimed at finding the optimal external cavity length. This is complicated by mechanical instability of the mirror mount, which is very sensitive to vibrations. We hope to achieve stronger phase locking, resulting in pulse width values more consistent with theory, which predicts subnanosecond pulses.

We would like to thank Rich Migliaccio (East Coast Optical Technologies) for providing the Spectra Physics laser and Sam Goldwasser for providing the FP analyzer. This work was funded by URECA and by NSF-REU (grant no. PHY-0851594).

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**Heather Hill**  
Duke University

## Observing the Pancharatnam-Berry phase on the Poincaré sphere

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In 1984, Michael Berry discovered a geometric phase in quantum systems [1], which soon led to a whole new understanding of the importance of geometric phases in other fields. In particular, an optical phenomenon that had been discovered earlier by Pancharatnam [2] was realized to be a manifestation of a geometric phase. The Pancharatnam-Berry phase is the phase change that a monochromatic beam of light gains in a cyclic change in polarization. If one maps out the changes in polarization on the Poincaré sphere, this phase change is equal to half of the solid angle that the polarization trajectory traces out on the sphere.

We hope to observe and measure the Pancharatnam-Berry phase with an apparatus inspired by van Dijk et al. [3]. We will start with vertical linearly-polarized light (Point A on the equator of Poincaré sphere) and pass this through a quarter-wave plate to create circularly polarized light (Point B at the north or south pole). A linear polarizer at some angle  $\alpha$  to the vertical will then move this polarization state to another point C on the equator. Finally, a second linear polarizer will restore the light to its original state, point A. The experiment consists of comparing the relative phase of the initial and final polarization states in a Mach-Zehnder interferometer. We should observe that the fringe shift as a function of  $\alpha$  varies in proportion to the solid angle mapped out on the Poincaré sphere.

We found a number of unspecified quarter-wave plates in the lab and tested them to see which ones were effective at 632.8 nm wavelength. With careful adjustments, the best of these produces good quality circularly polarized light from the beam of our linearly polarized HeNe laser. The interferometer was set up and crisp fringes were obtained; the fringes are susceptible to air currents, mechanical vibrations, etc, but with care are sufficiently stable when the room is quiet.

Data taking will consist of recording the shift in fringe position while changing the first linear polarizer from  $\alpha = 0$  to other values  $\alpha < 180^\circ$ . The Pancharatnam-Berry phase is largest ( $\pi/2$ , or 1/4 of a fringe) for  $\alpha = 90^\circ$ , which corresponds to moving half-way around the equator of the Poincaré sphere. Unfortunately, as one approaches this angle the transmission of light in the active arm of the interferometer drops to zero. Our initial observations are a series of images of the fringe pattern with  $\alpha$  cycled between 0, 35 and 70 degrees. These images clearly show the expected geometric phase.

We thank T. van Dijk and Prof. T. D. Visser for their helpful responses to our emails. This research was supported by a grant from the National Science Foundation (Phy-0851594).

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**Maximilian Katz**  
Rensselaer Polytechnic University

## Testing and using a modern 1D stellar evolution code

Max Katz, *Rensselaer Polytechnic Institute*; MICHAEL ZINGALE, *Department of Physics & Astronomy, Stony Brook University*

The majority of what we know about stellar evolution has come from the use of one-dimensional computer codes which simulate such evolution. The standard codes, though, were written decades ago and can no longer efficiently utilize the multi-core processors which have become the standard today. The new project, Modules for Experiments in Stellar Astrophysics (MESA), is designed to combine efficient, modern code capable of true parallel processing, with the latest theoretical developments in stellar astrophysics. Although the most complex problems in the field can only be fully understood in multiple dimensions, many problems can at least be qualitatively understood through 1D simulations, and the relative savings in computational time usually justify this. In this regard, we found several areas in which MESA can be useful.

White dwarfs are the remnants of stars like the Sun; they are cool, compact stars which have roughly the mass of the Sun in an object the size of the Earth. When these have companion stars which eject matter in a stellar wind, the ejected mass can be accreted onto the surface of the white dwarf, and in many cases, this can lead to nuclear fusion, and possibly a thermonuclear runaway (nova), of the accreted material. MESA was used to simulate novae on a carbon/oxygen white dwarf. While complete understanding of these events requires multi-dimensional simulations, such simulations require good initial models. Since it is too expensive to run through the majority of the process in two or three dimensions, we used MESA to generate initial models sufficient for use in these more complex codes. It was found that these models are much more resolved than models generated in older codes. Additionally, it is important to know which nuclei are important in the nuclear reactions in the nova; keeping track of isotopes which do not play a significant part in the physics is simply too expensive. It was found that the proton-proton reaction chain, although important in the interior of stars like the Sun, is unimportant in typical novae; rather, the carbon-nitrogen-oxygen (CNO) process is responsible for the majority of hydrogen burning in these events. We also found particular isotopes in certain reaction channels that play relatively important parts in the dynamics, and were able to isolate only the ones which truly contribute to the nova.

Additionally, MESA was used to study the ratio of carbon to oxygen, by mass, in these white dwarfs. Stars with varying initial metallicity were simulated from the beginning of the main sequence to nearly the end of the asymptotic giant branch. It was found that in general there is a decline in the C/O ratio with initial metallicity, although there are exceptions in some cases.

This work was supported by a grant from the National Science Foundation (PHY-0851594).

**Daniel Pinghero**  
Clarkson University

## Optical design considerations for a negative ion source

Daniel Pinghero, Clarkson University; Simon Freedman, Illinois Institute of Technology; Victoria Yu, Rutgers University; Rich Lefferts and THOMAS HEMMICK, Department of Physics & Astronomy, Stony Brook University

A new negative ion source is to be designed to bring full Accelerator Mass Spectrometry (AMS) capabilities to Stony Brook University. The new ion source, to be designed in conjunction with a sophisticated sample switching apparatus, is based on the Purdue University PRIME source. The design features a spherical ionizer made of molybdenum. As is common to all cesium sputter ion sources, cesium vapor will be allowed to strike the heated ionizer surface, causing Cs<sup>+</sup> ions to form and accelerate toward the sample opposite the ionizer due to the differences in electrical potential. The desired target area of these ions is very small; a circle of one millimeter diameter was the goal for this design. As in traditional optics, a spherical lens does not focus parallel beams (or cesium ions) optimally — a range of foci are created based on the distance of the ion from the central axis of the lens. It is desirable that all the cesium focus at the same point — on the sample — and so an additional optical element is required to correct for the spherical aberration. This element, the “shroud,” will be a custom built piece of stainless steel, thermally isolated from the ionizer but at the same electrical potential; the shroud will provide electric field correction but will not contribute significantly to the cesium ion production due to its low temperature. To further reduce the diffuse focusing of the lone ionizer, the body of the ionizer will be machined to a less spherical shape.

In addition to its optical benefits, the shroud will allow for more optimal placement of the cesium expulsion vents. Not all cesium atoms will ionize upon initial contact with the ionizer; introducing the cesium in a manner inducing several contacts, (similar to the bounces of a billiard ball) is desired. The shape of the shroud will allow the vents to send the neutral cesium vapor on trajectories that are likely to intersect the ionizer body up to four times (thus allowing four independent chances for ionization) before it enters the vacuum at random.

A second correctional optical element is also required for the new ion source. The produced negative ion beam must fit through the ionizer’s central hole (about 2.5 mm in radius). Without any correction, the initial one millimeter beam will diverge too greatly — further focusing of the beam will be required. To accomplish this, a thin circular plate of stainless steel, with a radius of just less than 4 mm will be placed just in front of the sample holder, and raised to a slightly less negative potential. This “immersion lens” has a negligible effect on the positive cesium ions, as their energy is quite high by the time they reach this element, but it provides sufficient focusing of the negative ion beam.

These elements were modeled on a computer using SIMION 8.0, an ion trajectory calculation program. A cross section of the cylindrically symmetric design is displayed in figure one. The combination of shroud design and ionizer alterations allow for slightly greater than 80% of cesium ions to hit the above described 1 mm target on the sample, and all of the resulting negative ions to emerge through the ionizer in a well focused beam.

This work was supported by a grant from the National Science Foundation (PHY - 0851594).

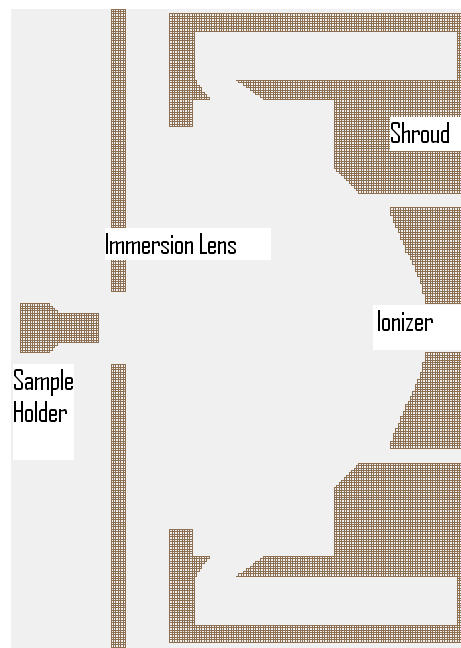


Figure 1 – Cross Sectional View of Interior of Ion Source

**Katya Sergan**

University of California, Davis

### **Creating a switchable diffraction grating in a liquid crystal cell**

Ekaterina Sergan, University of California, Davis, JOHN NOÉ, Laser Teaching Center, Department of Physics & Astronomy, Stony Brook University

This project focused on the study of polymer stabilized liquid crystals (LCs).

Nematic LCs are birefringent rod-shaped molecules that respond to an electric field. In our case, the applied field polarizes the molecules along their long molecular axis and re-orient them along the field direction. Creating a polymer network at the boundaries of an LC cell disables the ability of the LC molecules to respond in this way. If the polymer network is periodic, then a voltage-controlled *grating* can be created. The polymer network is formed by irradiating the cell with a wavelength of light that activates the photoinitiator. At the same time a relatively high voltage is applied across the cell to not only re-orient the LC molecules but also drive the polymer precursor (monomer) to the two substrates of the cell. After the voltage is removed, the areas that were not exposed to the light relax back to their original planar orientation and a variable phase shift between the ordinary and extraordinary waves of polarized light incident normally to the cell results in a spatially varying head-on retardation. Applying a switching voltage switches the planar areas between high and low retardation.

We used LC cells (gap ~20 microns) that were filled with a mixture of an LC material, about 1% of a photo-curable monomer, and about 0.01% of a UV (~300 nm) sensitive photoinitiator. The high voltage used was 120 VAC (rms) and the light source was a conventional RadioShack blacklight. The cell was irradiated for about 30 minutes through a mask with an approximately 50-50 pattern and a period of slightly greater than 1.0 line/mm.

The ability of the pattern to diffract light was studied by illuminating it with red light (633 nm) from an unpolarized HeNe laser. We observed a diffraction pattern that consisted of several fringes and a bright central spot. The fringe pattern changed as an AC control voltage was applied to the cell. The largest pattern (about 20 visible fringes) was observed at a peak to peak voltage of 3.00 V. The spacing in the pattern was consistent with the spacing in the mask to better than 10%. We are currently analyzing this spacing more carefully, in part to see if it is affected by the applied switching voltage. The diffraction pattern could be turned off by applying > 40 V peak-to-peak. From this we conclude that we did indeed create an electrically controlled diffraction grating. Some very interesting polarization effects were also observed. In one orientation of a linear polarizer only fringes could be seen, while in the perpendicular orientation only the undiffracted beam spot was visible. The polarizer had the same effect whether it was placed before or after the grating.

We thank the Optics Lab at California State University Sacramento for providing the prepared LC cells. We would also like to thank T. Sergan, V. Sergan and H. Metcalf for their invaluable contributions. This work was supported by the National Science Foundation (PHY-0851594).

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**Spencer Thomas**  
Stony Brook University

## **Potential energy comparisons between *ab initio* water simulations and classical analogs**

Spencer Thomas and MARIVI FERNANDEZ-SERRA, *Department of Physics & Astronomy, Stony Brook University*

Despite the prodigious growth of computational power available to physicists, *ab initio* Molecular Dynamics Simulations (AIMDS) remain prohibitively expensive. Even for the "simple" water molecule (our main focus), practical simulations are generally limited to 32 to 128 molecules. *Ab initio* calculations are expensive by nature and scale non-linearly with system size. Building on previous work, which determined spatial distribution functions for *ab initio* water simulations, we run tests on an analogous classical system.. We generate a classical potential energy landscape for a system of two water molecules and compare with analogous data from *ab initio* simulations.

Our algorithm takes one molecule at a "standard" position on the xy plane at the origin and places another molecule at all locations (within a precision parameter) on concentric spheres around the origin. For each spatial location (measured at the oxygen atom), the minimum potential energy configuration is determined. A field of all relaxed energy values is created and optimal (minimal-energy) locations are recorded for study. This method is repeated for the SPC/E, Tip4p, and Tip5p water charge models as well as a dipole case. A Gaussian smoothing function is applied to the discretized energy information for functional fits. Another program takes time-averaged coordinate data from *ab initio* simulations and calculates Gibbs free energy for the same coordinate data. With this, we have a direct comparison between the energy predicted in *ab initio* simulations and our classical analog. We can also observe differences between the various electronic charge models and build a base with which to test more. Additional work by W. Cancek et al (Phys. Chem. Chem. Phys., 2008, 10, 4716-4731) performs a direct energy analysis of *ab initio* models. This provides another layer of data with which to compare our relatively inexpensive classical model.

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## **Design of a sample changing ion source**

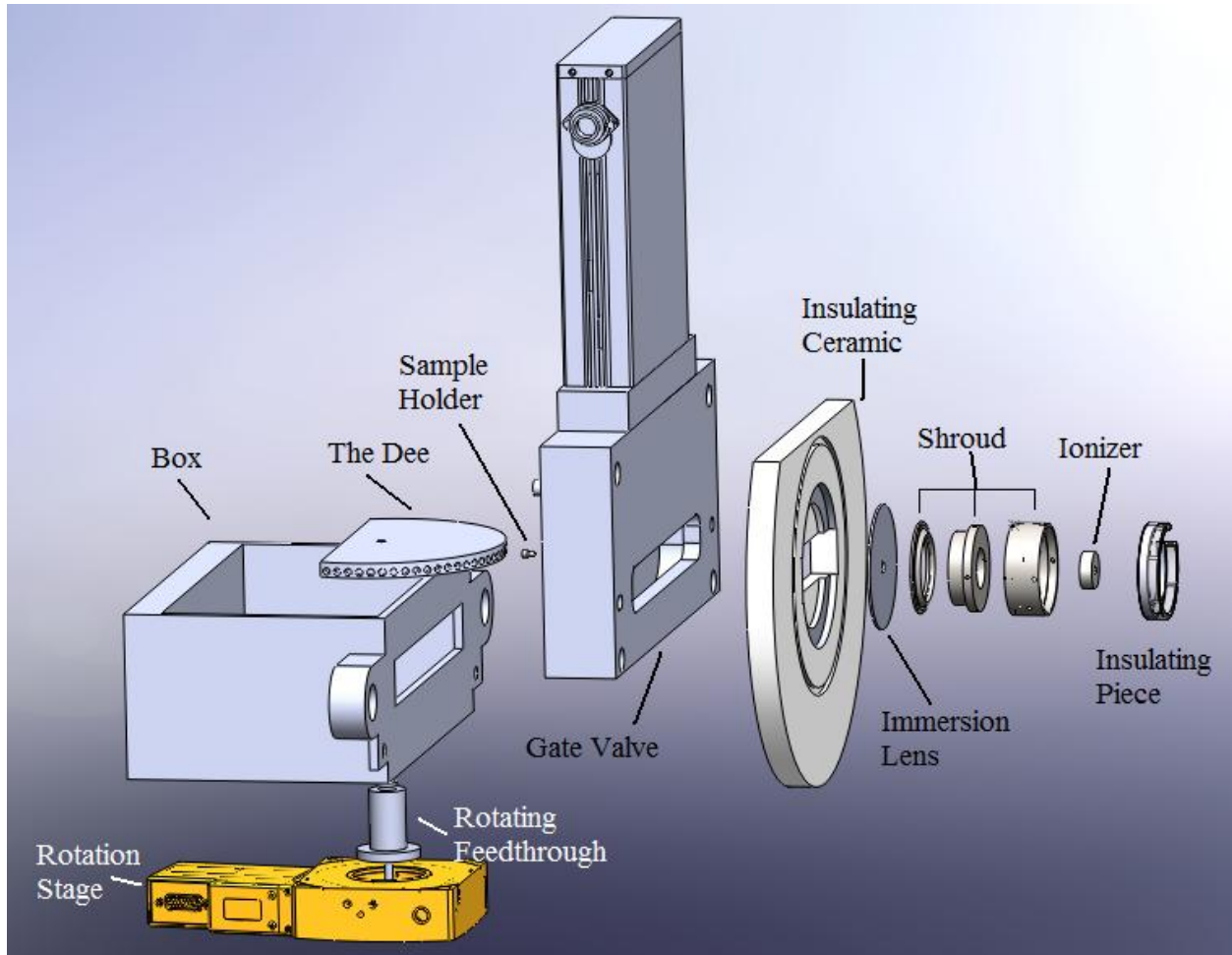
Victoria Yu, Rutgers University; Daniel Pinghero, Clarkson University; Simon Freedman, Illinois Institute of Technology; Richard Lefferts, THOMAS K. HEMMICK, Department of Physics & Astronomy, Stony Brook University.

The primary goal of this project is to design a high-intensity, sample-changing negative ion source for future research in Accelerator Mass Spectrometry (AMS). This type of ion source is needed because AMS research requires rapid sample-changing and precise positioning without vacuum disruption in order to conserve similar conditions between trials.

In this design, we achieve a significantly more efficient sample-changing mechanism by utilize a computer-controlled and rotating, semi-circle-shaped sample-holding “Dee” which contains forty holding slots arranged along its radii, the precision of which brings each sample to the desired position within the system. The Dee is placed into a lidded, vacuum-sealed box that is connected to a rectangular gate valve. After the sample slots on the Dee are loaded, the system is pumped to vacuum and the Dee can be pivoted to bring any sample into the measurement position. When all of the intended trials on one Dee have been completed and new samples are to be placed into the system, the whole Dee can be rotated out through the gate valve and into the box, after which the gate valve will close behind it. The box can then be opened without compromising the vacuum state of the system on the other side of the gate valve. This design saves time between trials because only the volume of air in the box will need to be pumped out to re-attain a vacuum instead of the entire system.

In a negative ion source, the electrically neutral Cesium atoms gain a positive charge through contact with the heated ionizer, causing them to be propelled towards a highly negative cathode. The resulting impact releases negative ions that are accelerated by Coulomb repulsion. The ion optics, which refers to the paths of the Cesium ions and the negative ions, are both crucial to the intensity of the beam source. These paths are determined by the potential levels and distances between the ionizer, immersion lens and the cathode. SIMION 8.0 was used to model the ion optics. The most efficient combination of voltage levels, shapes and distances of all the beam steering elements was obtained. With the results from SIMION simulations, the sample changing mechanism and building onto some existing parts of an old ion source, various pieces of the ion source were designed and drawn using SolidWorks; including modifications to a commercially bought spherical ionizer, a shroud surrounding the ionizer that guides the Cesium beam to a better focus, insulating pieces to separate the different voltage levels, extraction electrode, the Dee, and the box that contains the Dee and cooling systems. More computer aided research has been conducted to make sure that this ion source would be structurally sound and achieve its desired performance once physically fabricated. A picture of some parts in the design in shown in Figure 1. The design was successfully completed and an ion source test stand was built to be used for testing when the ion source is successfully assembled.

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