ABSTRACTS OF REU FINAL REPORTS
The University of Toledo, Department of Physics & Astronomy
SUMMER 2008
(Faculty Mentor on parenthesis)

Astrophysics/Astronomy

Kyle Bednar, *PAH Emission, (*J.D.Smith)

Polycyclic Aromatic Hydrocarbons (PAHs) are ringed molecules responsible for up to 20% of the total infrared luminosity in galaxies, making them powerful diagnostics for probing star-formation, metal enrichment, and the presence of organic compounds at early epochs in the universe. PAH vibrational transitions produce broad emission bands in the mid-infrared (MIR) between 3-20 μm. However, the presence and behavior of PAHs in the distant universe is poorly understood. The goal of our research is to quantify both the relative PAH strength and band-to-band ratios over a large range of metallicity, radiation field intensity, and local gas density. For this, a sample of nearby galaxies with steeply varying radial gradients in gas phase oxygen abundance were mapped in the infrared using Spitzer's IRS spectrograph. These data are reduced using Cubism, an IDL-based software which constructs 3D spectral data cubes. The extracted spectra from the two instrument modules are then blended to produce a spectrum from 5-40 μm. Once completed, the data is resolved spatially; spectra extracted with Cubism are labeled by galactocentric radius. Finally, PAHFIT is used to decompose the data spectrally, determining the strength and form of PAH emission at a given radius. Future research will entail correlating these strengths and distances with radiation field intensity, gas density, and metallicity, in hopes of determining the extent to which PAH emission can be used to trace star formation and galaxy evolution at high redshift.

Molly Bittner, *Spectropolarimetry and the Study of Exoplanets*, (J. Bjorkman)

Spectropolarimetry can provide a powerful process through which the properties of planetary atmospheres may be determined. Careful calculations in radiative transfer, involving the simplest model of an isotropic star and a Lambert surface upon the planet, reveals comparisons for more realistic planetary systems. Both the ratio of the flux through the planet to that of the star and fractional polarization viewed from Earth can be shown to have phase angle dependence. This phase angle between the line of sight and the star, centered at the planet, allows the changes in brightness and polarization to be visualized. Specifically, the four Stokes' parameters measure intensity and linear and circular polarization, which may be dissected to reveal wavelength-dependent properties of planetary atmospheres. Because current technology cannot detect most magnitudes, studies tend to concentrate on systems involving hot Jupiters. These reflect more light back to Earth than do smaller planets, and have much hope for future research. Through modeling the theory behind spectropolarimetry and the motions of exoplanets, important properties of worlds beyond ours can be discovered.

Rachell Gestrich, The *Search For Stellar Clusters In NGC 4449 Position B*, (R. Chandar)

Little is known about starburst galaxies concerning how they form, how they die, and why they exhibit sudden, rapid star forming periods. Studying the stellar clusters within these galaxies can help us to understand why and how these events unfold. NGC 4449 is a starburst galaxy that has had little information published on it. Using images from the Hubble Legacy Archive my goal was to detect all of the clusters in position B of NGC 4449 and determine their properties such as age, velocity, and metallicity. Using procedures from a pre established

pipeline from NGC 1291 I was able to detect over 183,000 sources in position B of NGC 4449 and eventually narrowed down the number to a little more than 33,000 possible clusters.

Adam Gray, *Parallelization of a Microturbulence Code*, (L. Anderson-Huang)

Running a large code designed to calculate microturbulence in stellar atmospheres for multiple time steps and iterations can be a time consuming process when run on only one computer. However, if the code is run on multiple machines through the use of a Beowulf computer cluster, it has the advantage of allowing for the code to run much faster than if it were to be run only on one machine. Solving the code faster will leave less time wasted and more time to run the code again with new settings, thusly allowing for more work to be accomplished.

Lesley Simaton, *Extragalactic Star Formation*, (R. Chandar)

Photometry is used to determine many properties of astronomical objects such as brightness, age, metallicity, and mass. Finding these properties for star clusters in other galaxies can tell us about the formation and evolution not only of the star clusters, but also of the galaxies. This study focuses on establishing a procedure, or pipeline, for finding and taking photometric measurements on stellar clusters in galaxies outside of our local group. I worked on applying this method to the spiral galaxy NGC 1291's position 2 and to the starburst galaxy NGC 4449's position A

Atomic/Molecular/Optical Physics

C.David Bergman, *Longitudinal and transverse diffusion of Xe+ and Ne+ ions in the Xe/Ne Gas Mixture*, (C. Theodosiou, V. P.)

Ion swarm parameters such as longitudinal and transverse diffusion are found by Monte Carlo simulation of ion motion in the mixture of Xe/Ne gases with different concentrations of Xe over E/N range (where E is the electric field and N is the total gas density) from 10 to1000 Td. First we consider a simple model in which we vary ion and background gas masses and calculate the effect of the mass ratio on longitudinal and transverse diffusion coefficients. We also find the range of electric field where the atom temperature significantly affects the ion motion. The obtained results are applied to explain trends in the simulation data for Xe+ and Ne+ ions moving in gas mixture.

Jeremy Bancroft Brown, *Experimental and Semi-Empirical Branching Fractions of the $3s^2 3p^2 - 3s3p^3$ J=2 Transition Array in P II*, (L. Curtis and D. Ellis)

A semi-empirical method is used to characterize the $3s^2 3p^2 - 3s3p^3$ J=2 transition array in P II. In this method, Slater, spin-orbit, and radial parameters are fitted to experimental energy levels in order to obtain a description of the array in terms of LS-coupling basis vectors. The various IC and CI amplitudes resulting from this model are then used to predict the branching fractions of transitions within the array. Results close to LS-coupling values are presented, and these are compared to branching rations measured using beam-foil spectroscopy at the THIA laboratory. The work provides support for the hypothesis of Dr. Curtis that transition arrays with little upper state IC but significant upper state CI in atoms of low Z exhibit branching fractions close to LS-coupled values, although the data are inconclusive in this respect.

Biological, Health, and Medical Physics

Michelle Labrecque, *The Effect of Fluoride Varnish on the Caries of Pediatric Patients:Quantifying the Results*, (M. Dennis)

Currently, the most effective and commonly used treatment of dental caries is surgical intervention, which Involves drilling out the affected area of the tooth and replacing it with a filling. While no patient enjoys the operation, it is especially difficult and painful for children to endure the procedure. Several dentists at the University of Toledo Medical Center are interested in the effects of a fluoride varnish applied to the caries of pediatric patients. The subjects' radiographic films will be analyzed to find density changes in the teeth over time, indicating remineralization of the dental enamel or slower progression of the caries when compared to non-treated subjects. Typically, clinical dental research is reported using qualitative visual analysis of the x-ray films. However, this project will be focused on producing comparable images so that density changes can be evaluated quantitatively. This includes increased emphasis on the importance of the consistency of experimental set-up, film development and film digitization. To quantify density changes, the radiographic films will be shot with a constant reference object, digitized using the PACS system and then specific regions of interest of the tooth can be quantified and compared numerically as well as scaled to a common unit.

Condensed Matter Physics

Dante Amoroso , Motion *by Mean Curvature: The Phase-field Method, (J. Amar)*

The phase-field method is applied to the problem of motion by mean curvature. Simulations are performed doing motion by mean curvature explicitly on an initial sine wave, and analytical calculations are done for the effect of mean curvature governed evolution on an initial circle. The phase-field method is then used to solve the same situations and excellent agreement is found. The computation time of the phase-field method is then investigated, and a method involving Fourier transforms is implemented to speed up this computation. Error is introduced by this procedure, but two possible solutions are proposed. Due to time constraints, unfortunately, neither solution could be investigated. Lastly, the Fourier transform phase-field method is applied to a random initial condition and is seen to reliably produce domains which become more homogeneous with time, a result expected for any interface governed by mean curvature.

Casey Bennett, *Study of Ultra Thin CdTe Pv Cells*, (A. Compaan)

The decreasing avaiability of semiconductors grade silicon along with its high demand across multiple industries has caused silicon based solar cells to rise in cost. This gives other semiconductor materials a chance to advance. One of the most promising candidates is CdTe based collectors, unfortunately the scarcity of tellurium and toxicity of cadmium could present some problems for mass production. Additionally, CdTe hasn't yet attained the price/performance ratio of silicon based cells. One solution to these problems is to use less material per cell. However, this requires reoptimization of cell production and characterizations specific to ultra thin cells. Research on these new conditions was broken into three subprojects. The first involved determining the dependence of photovoltaic parameters on the thickness of the CdS and CdTe layers. This was done by measuring how varying thicknesses of cell layers and cadmium chloride treatment times effect the quantum efficiency and j-v measurements of the cell. The second was modeling the quantum efficiency of ultra thin cells by modifying a modeling spreadsheet to calculate the cells performance across the spectrum. The third involved

the optimization of $CdCl_2$ treatment times for ultra thin devices by calculating new treatment times and temperatures that exhibit similar chlorine diffusion profiles to circumvent uncertainties involved in shorter treatments.

Allison Fink, *Structural, Mechanical and Electronic Properties of WS_xSe_{1-x} (x = 0, 0.25, 0.5, 0.75, 1), Using Ab Initio Computations*, (S. Khare)

My objective was to use the *ab initio* method to theoretically calculate properties of the tungsten sulfide selenide systems W_2S_3Se, $W_2S_2Se_2$, and W_2SSe_3, of hexagonal 6-atom crystal structure. The properties of WS_2 and WSe_2 (composed of two atoms of tungsten and four respectively of S and Se) were already calculated and used to compare the results of mixtures of sulfur and selenium. I ran a computer program that calculates the ground state energy of one unit cell in a crystal from first principles by approximating the solutions to the many body Schrödinger equation given the specific atoms and their positions for a unit cell in a crystal lattice. I used output data from this program to calculate structural, electronic, and mechanical properties for the three materials: lattice constants, density of states, band structure, and elastic constants, from which the coefficient of friction could be determined. My advisor and the graduate student that I worked with aim to publish my results in a scientific journal, on which I may later collaborate.

Kellen McGee, *Guidelines for Improving the Reflectivity of Silver [Ag] Back-reflectors through the Use of a Zinc Oxide [ZnO] Thin Film*, (R. Collins)

This paper seeks to calculate the extent to which the absorption of an Ag back reflector, (using a pure Drude model) may be minimized by a thin film of ZnO (using a pure Cauchy model with k = 0). Starting with the basic Fresnel Equation, in which theta = 0, expressions for the reflectivity of an Ag-ZnO-Air stack are developed, as are expressions describing the periodicity of the maxima and minima of reflectivity as a function of thickness. All models are then plotted to demonstrate the change of optical properties of the stack as thickness of the ZnO layer and the incident light wavelength varies. Suggestions are then made for the direction of future research in this area, based on this report's findings.

Nathan Reaver, *Accelerated Degradation of CdTe Solar Cells on Flexible Substrates*, (A. Compaan)

CdTe solar cells are second-generation thin film cells and have typically been fabricated on glass substrates/superstrates. Researchers at the University of Toledo have been fabricating CdTe cells on flexible polymer substrates. One such polymer used in cell fabrication is DuPont™ Kapton® polyimide film. This project focuses on the degradation of CdTe solar cells on Kapton® substrates vs. similar cells on glass substrates. Cells fabricated on both glass and Kapton® were soaked in continuous one-sun conditions to accelerate the degradation of the cells' performance. The degradation of the cells' performance was determined through the measurement of each cell's open circuit voltage, short circuit current, efficiency, and fill factor over time on a logarithmic timescale. Degradation of each of the cell's attributes over time was studied to determine correlations between type of substrate and degradation of the cell's performance.

Sam Spencer, *RF Sputter Deposition of In_2O_3-Fe_2O_3 as a TCCR Layer for Immersion-type Solar Cells*, (B. Ingler)

This experiment attempted to identify the conditions under which the transparency, conductivity, and corrosion resistance of a thin film of In_2O_3-Fe_2O_3 may be maximized, for use as a protective outer layer of an immersion-type solar cell. The best sample was produced at 275 °C, 100W Fe_2O_3 and 30W In sputter powers, 6% oxygen gas, 11 sccm total gas flow, at 6.0 mTorr for two hours of deposition, and had an increasing current density at 1.6V of 4.32 mA/cm2 after 28 cycles of cyclic voltammetry from -1V to 3V.

Rosa Zartman, *Anti-reflective Coating for Photovoltaics*, (S. Marsillac)

This research focuses on using magnesium fluoride (MgF_2) to make an anti-reflective film for copper indium gallium diselenide (CIGS) photovoltaic solar cells. To accomplish this feat, the employment of a thermal evaporator with a baffled boat is the method of application. The baffled boat is essential to insure that no spitting of magnesium fluoride happens on the substrate. The test substrates of soda lime glass, indium tin oxide (ITO), and CIGS showed great improvement from before the application of MgF_2 to after that application. On the soda lime glass, the percent reflection went from 9% to 1.7%, which is a decrease of 18% in reflection. The results for ITO were even better with a decrease of at least 35% in reflection. After applying magnesium fluoride to copper indium gallium diselenide solar cells, the tests were done mainly on reflection and quantum efficiency. The reflection decreased up to 40% and quantum efficiency complemented this decrease by increasing at the same wavelength no matter the thickness of the MgF_2. The complementation has sparked an ongoing process to understand this relationship and find a way to predict the optimal thickness for each individual cell to obtain the peak performance. Magnesium fluoride is heavily used in the manufacture industry today, so it will be easy to make this research application work well in that industry.

Ryan M Zeller, *A Simple Precise Optical Thickness and Temperature Monitor*, (A. Compaan, K. Wieland)

In order to achieve maximum efficiency and performance in a photovoltaic solar cell module, optimal thickness of semiconductor layers must be controlled. Thickness of thin film layers determines key properties of cell performance. In order to optimize the performance of a RF magnetron sputtering chamber, an Optical Thickness Monitor (OTM) was built to better understand and to monitor the deposition process in real time. The OTM utilizes laser light reflected off the growing sample, which is detected with a photodiode. With LabVIEW software, the monitor outputs real-time film thickness and material growth rate. It also allows determination of substrate temperature.