Atomic, Molecular, and Optical Physics

Travis Bean, *Characterizing the UNR Velocity Map Imaging System in the Photodetachment Experiments at the UNR-NIRF* (T. Kvale)

The Velocity Map Imaging System (VMI) has been implemented in a Laser Photodetachment Electron Spectroscopy (LPES) system to measure the electron affinities and the 3-D imaging of photoelectrons produced by photodetachment of negative ions. A weak electric field in the laser-negative ion beam interaction region directs the outgoing photoelectrons to a detector system. The intensity pattern of the image follows the relation: $I(\theta) = A(1 + \beta P_2 \cos \theta)$, where θ is the angle between the negative ion velocity vector and the photoelectron initial velocity vector, P_2 is the Legendre polynomial, and A is a constant. From the angular distribution of the image, the β parameter can be determined. The β parameter is important in that it carries with it information of the angular momentum of the photoelectron and the internal angular momentum of the negative ion and subsequent neutral atom states. Because the interaction region occupies an extended region and not just a point, the VMI system acts as a thick lens with spherical aberration. In order to obtain accurate values of β, the spherical aberration conditions need to be known so appropriate correction factors can be applied. This research involved using a numerical simulation program, SIMION, to accurately model the interaction region of the VMI system and thus obtain an understanding of the spherical aberration conditions of the VMI system.

Ace (Walter) Furman, *Measurement and Theoretical Calculation of the Radiative Meanlife of the 1433 Å Transition in Pb II* (R. Irving and D. Ellis)

The University of Toledo Heavy Ion Accelerator (THIA) was used to measure the radiative meanlife of the 1433 Å transition in lead II. Lead ions were accelerated into a carbon foil, where they excited and then de-excited, thus releasing photons. The photon intensity was measured as a function of time. After using an ANDC method to eliminate cascade effects, the mean lifetime was estimated from the experimental data to be 1.4 ± 0.1 ns. Moreover, an atomic simulation software, GRASP 2K, was used to calculate the theoretical mean life to be 1.6 ns. GRASP was also used to calculated mixing coefficients both in lead II and in other ions in its isoelectronic series to further explore the mechanisms behind these transitions.

Computational Physics

John Burt, *Community-Based Ceramics Database for High Performance Coatings* (S. Khare)

Estimates of available data in the scientific literature for structural, elastic, mechanical and electronic properties of solids related to coatings applications maybe conservatively placed in the 100,000 range. To make full use of this vast resource of computational knowledge, we have created such a platform, an open-access community-based ceramics database with an emphasis on high performance coatings. Our database handles large amounts of data with features of data selection tools and rapid search capabilities. It has active display features for generating a variety of formats of tables and graphs and has recently been beta-test/launched. Users can choose which fields to query corresponding to their computed or experimentally

measured properties of interest in a web-based user- friendly form. The resulting data can be brought in to tabular and graphic formats automatically displayed on demand to generate a visual representation of the dataset of choice. All entries are linked to the original papers on the web with full citation information through DOI or other identifiers. Participation and contribution from the coatings community is sought, encouraged and welcomed. The database is presently already populated with data from a few hundred materials and is expected to grow through the community's contributions. Being community-based, users can also be contributors, with the privilege to add/edit/delete entries from their own contributions. The names and contact

information of the contributors are displayed as an appreciation for their efforts, and also as a means to enhance peer reviewing. We hope this platform can attract the community's attention, usage and contribution, and fulfill its purpose to serve as an active and essential data hub in the field of coatings science and technology.

Plasma Physics

Luke Meech and **Christopher (Alex) Robinette**, *Characterization of X-ray emission during X-Pinch Shock Testing with Copper Target* (R. Irving, T. Kvale)

The goal of this experiment is to sample high energy photon emissions to determine the characteristics of the pulse created by an X-Pinch configuration in the Zebra located at the Nevada Terawatt Facility, University of Nevada, Reno (UNR-NTF). Due to the nature of the pulse, speed and energy, little is known about the shape or energy distribution of the emitted photons. These factors also create issues when attempting to directly measure the electron beam produced. Using Kodak BioMax MS film in a variety of container geometries, to limit low energy background, we attempted to find the shape of the pulse as well as the energy distribution of the photons. This information allows for an indirect measurement of beam intensity and energy. As well as give more information for safety personnel regarding radiation precautions. During these tests x-ray scattering was examined closely for any anomalous behavior. Using this data we observed an unknown scattering event involving the scatter angle from an Al backscatter plate. This will be further tested and analyzed in a future experiment.

Collaborative research project conducted at The University of Toledo and Nevada Terawatt Facility at The University of Nevada, Reno. Dr. Timothy Darling is the senior scientist for this experiment at UNR-NTF and was a co-mentor of L.M. and C.R.

Andrew (Drew) Polasky, *Localized Surface Plasmon Resonance in FeS_2 Nanocrystals* (R. Ellingson)

FeS_2 is, in many ways, an ideal candidate for a solar cell material. It is readily available, cheap to process, and non-toxic, with a bulk band-gap energy of 0.95 eV. However, the presence of a surface plasmon resonance in the material interferes with the absorption of sunlight, effectively reducing the surface band-gap energy to an unusable level. The plasmon peak of Iron sulfide nanocrystals in solution was found to vary consistently with the dielectric constant of the solvent. Oxidation of films of the nanocrystals showed an increase in the band gap, likely due to the presence of Iron Oxides or Iron Sulphate, which have band gaps around 2 eV, and could interfere with the plasmon resonance developing.

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Astrophysics

Daniel Kondratov, *Computer Simulation of Radiation Through a Stellar Atmosphere* (L. Anderson-Huang)

The project involved modeling electromagnetic radiation in a single atomic transition through a self-consistent stellar atmosphere. The stellar atmosphere was modeled on a three dimensional grid allowing for momentum transfer forward or back in six directions. The radiation was treated at frequency intervals throughout the Doppler line width of the scattered light. These parameters formed a linear matrix representing the numerical equations. Doppler shifts due to bulk motions are expected to enhance and/or redirect the radiation pressure on the fluid, resulting in an unstable turbulent medium. Preliminary results were presented.

Tyler Frey, *Discovery Channel Telescope U, B and I-band Observations of the Cep OB3b Cluster* (T. Megeath)

Cepheus OB3b is one of the two most massive young (< 5 Myr) clusters within 1 kpc in the Sun. We analyze Discovery Channel Telescope U, B and I-band imaging of this cluster designed to measure UV excesses from young stars due to accretion. The excesses measure the rate gas is accreted onto the stars from circumstellar disks. By measuring the rate of gas accretion for stars of different ages, we can trace the time evolution of the gas disks. More

specifically, the accretion rates provide an indirect measure of evolving gas surface density during the time these disks may be forming planets, and thereby provide constraints on the timescale for the formation of gas giants.

Condensed Matter Physics

Anna Barnes, *Optical Band Gap and Infrared Vibrational Modes for LSAT Single Crystal Obtained via Infrared to Ultraviolet Range Spectroscopic Ellipsometry* (N. Podraza)

$(La_{0.18}Sr_{0.82})(Al_{0.59}Ta_{0.41})O_3$ (LSAT) is a single crystal material commonly used as a substrate for epitaxial film growth. Optical properties of LSAT for the range of 0.033 to 5.887 eV were determined from spectroscopic ellipsometry measurements of the complex dielectric function, ε, and the complex index of refraction, N. The indirect band gap is determined to be 4.72 ± 0.01 eV and the lowest direct gap energy is found to be 5.70 ± 0.01 eV. Eleven transverse optical phonon infrared vibrational modes originating from tantalum oxide (Ta-O), lanthanum oxide (La-O), and aluminum oxide (Al-O) bonding in LSAT are identified over the range from 240 to 870 cm^{-1}.

Christopher Bisbee *Electric Field Distributions of Cylindrical Filament ReRAM Cells* (V. Karpov)

In order to investigate the switching characteristics of Redox Random Access Memory Cells (ReRAM) in terms of their energetic properties, I built a number of computer simulations that replicate these types of systems. Using Comsol Multiphysics software, I determined that when a fixed voltage is applied to each electrode in the electrode-filament system, we should not expect to see any should expect filament growth to occur spontaneously. I also explored the balance between establishing a fixed voltage between the electrodes quickly while still optimizing the switching time of these cells.

Alexa Van Hattum, *Effects of size-dependent island-edge barriers on submonolayer nucleation, utilizing a modified Union-Find-Delete algorithm* (J. Amar)

The effects of size-dependent island-edge barriers on submonolayer nucleation are studied via kinetic Monte Carlo simulations of a simplified model of epitaxial thin-film growth. Standard nucleation theory predicts an exponent $\chi = i/(i+2)$ (where i is the critical island size) relating the island density N at a fixed coverage q to the ratio between diffusion rate D and the deposition rate F, $N \sim (D/F)^{\chi}$. In contrast, Attachment Limited Aggregation (ALA) assumes that a barrier to attachment to islands leads to a higher prediction of $\chi = 2i/(i+3)$. The viability of ALA as an explanation for recent experimental values of χ greater than 1 is examined. Regimes with a critical island size, i, of 1 and 3 are simulated, along with two cases of a barrier to monomer attachment. In the first case, a size-independent barrier for attachment of a diffusing monomer to another monomer or island is assumed, while in the second case, there is only a barrier for attachment to islands larger than a given size S. Our results support a previous conjecture that barriers to island attachment extend the transient regime of island nucleation. Additionally, it appears that size-dependent barriers lead to the onset of island coalescence at a lower coverage q as well as a shortened aggregation regime. However, our results do not indicate that barriers to monomer attachment increase the value of χ. In the first case, corresponding to a island-size independent monomer attachment barrier, we find that the exponent χ is seen to decrease with the inclusion of a barrier to any attachment. With a size-dependent barrier to attachment, there is no clear observed trend in the values of χ with varying S. These results do not support ALA alone as the explanation for the unusually high values of χ observed experimentally.

Ryon Michalak, *Electron Transport at Low Temperatures in Single-Walled Carbon Nanotubes* (M. Heben)

Several proposals for quantum computing devices are based on individual or thin films comprised of single-wall carbon nanotubes. In this project, single-wall carbon nanotubes were synthesized by pulsed laser vaporization, purified, and formed into thin-films by a spray deposition process. The current transport mechanisms were studied as a function of temperature

using a closed-cycle helium refrigerator, customized software, and Keithley source meter. Several approaches were taken to modify the tunneling barriers between tubes in the film in an effort to create delocalized electronic states. These included evaporation of metallic species, and inclusion of organometallic compounds. In all cases, tube-tube connectivity was limited, as indicated by a thermally activated transport process.

Medical Physics

Julianna Pfadt, *"Monte Carlo Simulation of Ionization Chamber Energy Response Function"* (D. Shvydka)

Determination of photon beam spectra is often conducted through transmission measurements, which are relatively simple to implement, but fairly difficult to analyze. A recently published article describes an advanced approach to data collection and analysis for MeV photon spectra restoration, where one of the steps requires energy response functions for different build-up caps used in measurements. Calculation of such response functions is possible only through Monte Carlo (MC) simulations. My goal was to obtain the energy response function for brass build-up cap used by the Department of Radiation Oncology for transmission measurements. In order to validate my MC simulation geometry, the first step was to recreate the published response function for an ion chamber with a water-mimicking acrylic (PMMA) cap. After that was successfully accomplished, I was able to modify the input files to obtain a

response function for the brass cap; data for this material does not exist in the literature. In the course of this project I learned MCNP5, a radiation transport software package, which allowed me to create input files that include the geometry, materials, source, and tally specifications necessary to simulate 21 different energies ranging from .1 MeV to 10 MeV. I have also created input files modeling the transmission measurement geometry setup; these simulation results will be used to compare with the measured data.

Other students conducting research in Summer 2014 supported mainly by other sources

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Astrophysics

Sarah Burkhart, *An Investigation into Interstellar Dust: PAHs vs. Large Grains* (Adolf Witt)

Interstellar dust exists everywhere in the Milky Way but can be seen most easily in the galactic plane, as the dust grains absorb starlight and cause reddening and extinction. There is a wide range of sizes of dust grains, but we are focusing on PAHs (polycyclic aromatic hydrocarbon molecules), about 1 nm in linear size, and larger dust grains of about 100 nm in linear size. Our goal in conducting this research was to look at the PAH/large dust grain emission intensity ratio in different environments to see how PAHs are affected by supernova remnants, optical thickness, and variations in the UV radiation field.

Mainly supported by the UT Physics and Astronomy with minor funding (Travel & Housing) from REU but fully participated in the REU program.

Condensed Matter Physics

Brooke Paquin*, *Zinc Phosphide Thin Films Grown by Close Space Sublimation* (Y. Yan)

Zinc Phosphide (Zn_3P_2) thin films are grown by close-spaced sublimation and fabricated into Mg Schottky Diodes. Zinc Phosphide of varying thickness (6-10μm) is grown on silver coated Soda Lime glass. A thin layer of thermally deposited Mg is then added to aid in the junction, followed by a thick top contact of Mg. Devices were then annealed. JV displayed a profound amount of shunting and no photo reactive behavior possibly due to undesired doping of Na from Soda Lime glass or MgO from the surface of the device. Doping of Na using thermally deposited NaF as well as Bromine etches are used to test these possible contributing issues to making a working Zinc Phosphide device. Results concluded that these are not the key issues

causing shunting and further investigation is needed.

*Supported by the UT Physics and Astronomy but fully participated in the REU program.