Department of Physics
College of Arts and Sciences
Western Michigan University

Annual Research Report


Edited by
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1 INTRODUCTION

This is the thirty-seventh in a series of annual reports that summarizes the research activities of the members of the Department of Physics at Western Michigan University. The report includes research performed in this department as well as in collaboration with the faculty of other departments at Western, faculty at other institutions, and staff members of national and international laboratories.

Special thanks to Ms. Kerry Cochran for her invaluable assistance in the preparation and presentation of this document.

Thomas W. Gorczyca
Editor

Cover Design:

This image of Centaurus A shows a spectacular new view of a supermassive black hole's power. Jets and lobes powered by the central black hole in this nearby galaxy are shown by submillimeter data (colored orange) from the Atacama Pathfinder Experiment (APEX) telescope in Chile and X-ray data (colored blue) from the Chandra X-ray Observatory. Visible light data from the Wide Field Imager on the Max-Planck/ESO 2.2 m telescope, also located in Chile, shows the dust lane in the galaxy and background stars. The X-ray jet in the upper left extends for about 13,000 light years away from the black hole. The APEX data shows that material in the jet is traveling at about half the speed of light.

This is a dramatic illustration of one of several types of outflows that emanate from active galactic nuclei. Astronomer Kirk Korista studies another type of outflow, whose gas temperature is ~10,000 K and has flow speeds of a few to 10% of the speed of light. The plot (inset) demonstrates a means by which the gas density is measured in these latter outflows. Ultraviolet absorption lines (set against the powerful UV-X-ray spectrum emitted in the vicinity of the supermassive black hole) from several resonance lines of singly-ionized iron arising from a variety of lower levels within and near the ground term are observed and their column densities (absorber per m²) are then measured. The relative electron level populations are functions of gas density (colored curves), and these are compared to the measured values (points with error bars) indicating a consistent number density of \(10^{4.4} \text{ cm}^{-3}\). The photoionization calculations that produced the predicted relations rely on a vast array of atomic data, including some of those computed by atomic theorist Thomas Gorczyca.

It has been suggested that all this activity may have begun with the merger of a small spiral galaxy and Centaurus A about 100 million years ago. Such a merger could eventually trigger both the burst of star formation and the violent activity in the nucleus of the galaxy. The tremendous energy released when a galaxy becomes "active" can have a profound influence on the subsequent evolution of the galaxy and its neighbors. The mass of the central black hole can increase, the gas reservoir for the next generation of stars can be expelled, and the space between the galaxies can be enriched with heavier elements. Centaurus A is the nearest active galaxy, about 11 million light years away.
2 FROM THE CHAIRPERSON

Welcome to this latest issue in our continuing series of Physics Department Research Reports. I hope you will find the articles and statistics of some interest. It has been a very active and successful year for Physics research at WMU. Our recent moves to emphasize nuclear astrophysics, ultrafast science, nano-capillaries and other areas of applied physics are starting to reap results, as you will see in these pages. I am especially pleased that this report shows the high quality and quantity of research production by our cadre of excellent graduate students.

This productivity is continuing despite some shrinkage in our faculty numbers, and continuing budget restrictions in Michigan and the nation. This is a tribute to the dedication and efforts of our faculty, both those who are research active and those who help with the other jobs needed to keep a department like ours healthy, as well as to the rest of the staff who support our efforts.

We have some reasons to be optimistic for the near future. Some economic stimulus funding at the Federal level will apparently be used to boost basic research, and we have proposals and projects ready to take advantage of any such funding. In addition, we are now in the process of hiring a new faculty member, who will join us in the Fall of 2009.

As always, thanks are due to all who have contributed to this report, especially to the editor and the staff who actually put it all together. We very much appreciate what you have given us in this report.

Paul V. Pancella
Chair
3 ASTRONOMY

3.1 Physical Conditions in Quasar Outflows: Very Large Telescope Observations of QSO 2359-1241

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We analyze the physical conditions of the outflow seen in QSO 2359-1241 (NVSS J235953-124148), based on high-resolution spectroscopic VLT observations. This object was previously studied using Keck HIRES data. The main improvement over the HIRES results is our ability to accurately determine the number density of the outflow. For the major absorption component, the populations from five different Fe II excited levels yield a gas density $n_\text{H} = 10^{4.4} \text{ cm}^{-3}$ with less than 20% scatter. We find that the Fe II absorption arises from a region with roughly constant conditions and temperature greater than 9000 K, before the ionization front where temperature and electron density drop. Further, we model the observed spectra and investigate the effects of varying gas metallicities and the spectral energy distribution of the incident ionizing radiation field. The accurately measured column densities allow us to determine the ionization parameter $[\log U_H \approx -2.4]$ and total column density of the outflow $[\log N_{\text{H}}(\text{cm}^{-2}) \approx 20.6]$. Combined with the number density finding, these are stepping stones toward determining the mass flux and kinetic luminosity of the outflow, and therefore its importance to AGN feedback processes.

Based on observations made with European Southern Observatories Telescopes at the Paranal Observatories under program 078.B-0433(A).

Calculated level populations of excited levels of Fe II relative to the ground level vs.
hydrogen number density in the photoionization model. The points indicate the observed column densities of each level relative to the ground level. All five independent measurements are consistent with \( \log n_H \, (\text{cm}^{-3}) = 4.4 \) with less than 20% dispersion.
4 ATOMIC PHYSICS

4.1 Inner-Shell Double Photoionization: Coincident Energy and Angular Distributions in Xenon 4d_{5/2}

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Photo double-ionization (PDI), the emission of two electrons resulting from single photon absorption, has been intensively studied by many research groups over the past two decades since it is related to two important topics of modern atomic physics, namely electron correlations and the three-body Coulomb problem. Understanding the role of both effects in the PDI process can be achieved through a detailed description of the Triply Differential Cross Section (TDCS), which can only be carried out through coincidence measurements between two of the ionization fragments.

In sequential PDI, such as the 4d_{5/2} inner-shell ionization in xenon with subsequent N_5O_{2,3}O_{2,3} Auger decay, the singly-charged intermediate 4d core hole can decay via an Auger process into a doubly-charged final state. The two outgoing electrons are correlated via the intermediate state, and further through the final states under particular experimental conditions, such as both electrons having similar kinetic energy or ejection direction. Because electrons are indistinguishable, it is necessary to describe the Auger electron as a resonance embedded in the PDI continuum. The striking theoretical prediction within this model [1] of strong interference effects in the TDCS for the case when both free electrons have the same kinetic energies has caught researchers attention and was investigated experimentally in the valence outer-shell PDI of neon and xenon.

Earlier experimental work has also shown how the spin state determines the constructive or destructive nature of the interference, which is a consequence of a general selection rule [2] already verified in direct PDI of helium. With three charged particles in the final state, PDI requires in addition a detailed delineation of Coulomb interactions in the resulting few body system, also called Post Collision Interactions (PCI). The common manifestations of PCI in non-coincident measurements are significant shifts of the atomic lines whose tails also become asymmetric. While these effects disappear in photoionization experiments when the difference in velocities between photo and Auger electron is large, they are always present if the incident particle is charged. The influence of PCI on angular distributions of the emitted electrons and the dependence of the post collision interaction on the inter electron angle were studied separately, all requiring coincidence experiments for an accurate description.

We have carried out the first kinetic energy and angular distributions for the Auger decay from xenon 4d_{5/2} photoionization leading to ^3P_2 and ^1D_2 final states of the N_5O_{2,3}O_{2,3} Auger
We have also shown that it is possible to describe split infinitive adequately the coincident angular distributions using a two-step model approach. Furthermore, the angular distribution data allows one to extract some information about the amplitude and phases of the emitted Auger electron and photoelectrons [1].

We have used an instrument that consists of a set of four rotating electron time-of-flight (TOF) energy analyzers, well suited to perform coincident measurements. These detectors are ideal since they can detect easily the kinetic energy of the two emitted electrons which spreads out over a wide kinetic energy range. The four TOF analyzers are placed in a plane perpendicular to the direction of the incident light which crosses an effusive gas beam. Mechanical constraints (size of the vacuum vessel) limit the length of the drift tube of the analyzers to 12.5 cm.

We measured the triply differential cross section of previously unexplored doubly charged \( \text{Xe}^{2+} \) states \((^1D_2, ^3P_2)\) by coincident measurements of the \( N_5O_{2,3}O_{2,3} \) Auger electrons with the \( 4d_{5/2} \) photoelectron for the two final states \((^1D_2)\) and \((^3P_2)\) of the doubly charged ion as shown in Fig. 1. We found a very good agreement between our measurements and the theoretical models of the PCI effect given by both Kammerling et al. [3] as well as Sheinerman and Schmidt [4].

\[ \text{Figure 1} \quad \text{Polar plots of the angular distributions of the photoelectron or Auger electron. The light lines (blue in the colored version) are derived from using the best fit values for each set. The (red) dashed lines are the best common fit values for all 4 distributions used. The dark lines (black in the colored version) show the influence of the PCI effect and interchange effects. Top \((^3P_2)\) final state: (a) angular distribution of the photoelectron, Auger electron ejected at 0° with respect to the photon polarization direction. (b) angular distribution of the \((^3P_2)\) Auger electron. Both (a) and (b) show in general a very good agreement with the theoretical model given here. Bottom \((^1D_2)\): (c) angular distribution of the photoelectron, Auger electron ejected at 0°; (d) angular distribution of the Auger electron. Again, the agreement is very good. Thus, the two-step model is applicable for inner electron angles in the range of 35° to 180° if the energy separation between the two electrons is larger than the intrinsic level width of the intermediate state. Moreover, we measured the first angular distribution pattern of the TDCS for these two final states and were able to reproduce them by a semi-empirical model which describes the transitions populating these two states in the non-relativistic dipole approximation [1].}

Furthermore, the two-step model is applicable for inner electron angles in the range of 35° to 180° if the energy separation between the two electrons is larger than the intrinsic level width of the intermediate state. Moreover, we measured the first angular distribution pattern of the TDCS for these two final states and were able to reproduce them by a semi-empirical model.
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Acknowledgement:

All of the research work reported here is supported by the DoE, Office of Science, Basic Energy Sciences, Division of Chemical, Geosciences and Biological Science.

References:


4.2 New Multi-User Movable Ion-Photon Beamline Built by WMU

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We (Rene Bilodeau, WMU lead person with the help of ALS staff engineers and John Bozek) have designed and built a portable ion beamline, shown in Fig. 1. This instrument has been successfully commissioned in June of 2008.

The instrument will enable us (and any ALS user) to exploit the capabilities of other ALS beamlines, below 9 eV and above 600 eV photon energies (not available on BL10.0.1 with the presently fixed instrument), including tunable circularly polarized light for the study of negative and positive ions. In addition, the instrument can be used at any other facility such as the LCLS at SLAC, Stanford University.

This beamline will allow ions produced by the ion source to be accelerated between 2-10 keV and mass selected by the m/q magnet. The ion beam phase space is limited by two sets of four-jaw slits in the pre-merger section of the ion beamline which act as field stops. Two sets of steering plates are located before the electrostatic merger to allow the ion beam trajectory to be tuned for optimum ion-photon overlap. The ion beam will be merged counter-propagating against the photon beam in a collinear geometry using the electrostatic quadruple

---

**Figure 1** Schematic of the Movable Ion-Photon beamline (MIPB).
merger. The beam enters the interaction region after passing through electrostatic Einzel lenses. Two-dimensional spatial profiles of the merged ion and photon beams are monitored using 3 translating slit scanners located near the entrance, center, and exit of the 29-cm long energy-tagged interaction region as well as with rotating-wire beam profile monitors (BPMs). These allow fast feedback to facilitate the alignment of the ion and photon beams. The output from the scanners are digitized and recorded to determine the beam-overlap quality or form factor (for absolute cross section measurements). The merged path must be at an ultra-high vacuum of about $P=5\times10^{-10}$ Torr insured by three 270 l/s ion pumps and an 8” titanium sublimation pump, since previous experiments were limited by high background levels due to scattering of the ion beam by residual gases. For absolute cross-section measurements, the three translating scanners each with two slits at $45^\circ$ and $135^\circ$ from the horizontal axis, mounted on a linear-motion feed through/stepping-motor assembly, provide two-dimensional profiles at the center of the interaction region for more accurate form-factor measurements. The 29 cm long interaction region consists of an electrically-insulated wire-mesh cylinder (for effective pumping) with 13 mm diameter apertures on each end to define the interaction region for absolute cross-section measurements. Without bias on the cylinder, the interaction region extends to 120 cm, which is useful for spectroscopy experiments. After the interaction region, the beam enters the demerging magnetic field generated by a water cooled GMW 3473-70 dipole electromagnet magnet with 15-cm diameter pole pieces mounted for vertical beam dispersion. The magnet vacuum chamber contains faraday cups for the primary ion beams (positive or negative) and a channeltron single particle detector for the product positive ions. The resulting signals are normalized to the primary ion beam current and photon intensity.

In the case of negative ions, these merged experiments are a serious challenge since even if one achieves perfect overlap between the photon and ion beams, the background counts generated by stripping collisions with residual vacuum gas can easily exceed the photodetachment signal rate by up to 4 orders of magnitude (even though the background pressure in the interaction region is $\sim5\times10^{-10}$ Torr). In order to correct for background counts originating from collisional stripping and other background ionization, the photon beam is chopped at 1-10 Hz and the photodetachment signal is determined by subtracting the measured light-off signal from the light-on signal. The statistical error in the data is decreased by summing multiple sweeps of the photon energy of interest. The photon energies are separately calibrated using known resonance positions for neutral gases and are corrected for the Doppler shift. The photon beam is detected and recorded by a calibrated silicon photodiode, providing a measure of the photon flux.

We have produced a very strong C$^-$ ion beam current in the past [1,2] (> 1 µA) with our Cs sputtering ion source as well as produced C$_2$, C$_3$, and C$_4$ anions with similar ion currents. We used our June-July 2008 beamtime to test the new MIPB as well as to fix most of the problems found during the December 2007 commissioning beamtime. As can be seen from Fig. 2, we have successfully tested the MIPB by measuring the shape resonance just above the C$^-$ K-edge photodetachment threshold [1,2]. These raw preliminary data were collected with only approximately 15 minutes of total data collection time, while it took nearly 20 times longer to obtain data of slightly lesser statistical quality and fewer data points on beamline 10.0.1. Furthermore, we tested the photodetachment of C$_2^-$, as depicted in Fig. 3.
Complete photodetachment experiments in C\textsubscript{2}dimmer will be conducted in June of 2009.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{07030404.dat}
\caption{K-shell Photodetachment of C\textsuperscript{-} leading to C\textsuperscript{+} via Auger decay.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{07030531.dat}
\caption{K-shell Photodetachment of C\textsubscript{2}\textsuperscript{-} leading to C\textsubscript{2}\textsuperscript{+} via Auger decay.}
\end{figure}

Acknowledgement:

All of the research work reported here is supported by the DoE, Office of Science, Basic Energy Sciences, Division of Chemical, Geosciences and Biological Science. D. Rolles is indebted to the Alexander von Humboldt Foundation for a Feodor Lynen Fellowship.

References:

4.3 Ultrafast Research Using the Future Linac Coherent Light Source (LCLS)

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With the advent of a new ultrafast x-ray facility, the first of its kind in the world, we have added a new direction to our research program in the ultrafast domain. Specifically, we will study x-ray non-linear physics of atoms, molecules and clusters with intense ultrafast LCLS pulses. Lou DiMauro (OSU) and Nora Berrah (WMU) are the co-team leaders for the AMO community.

Our new program seeks to uncover the mechanisms of energy exchange among different degrees of freedom in systems ranging from diatomic molecules to large clusters such as the fullerenes. Specifically, this program will address fundamental questions concerning the ionization and fragmentation of molecules by intense, short pulses of x-rays from the LCLS. The study of short-time molecular dynamics that will be enabled by the LCLS is expected to provide new insight into fundamental aspects of molecular physics and chemistry.

We proposed to utilize the unprecedented LCLS peak power to study nonlinear and strong-field effects by carrying out excitation and ionization measurements of small molecules. Specifically, we will measure the relaxation mechanisms and Coulomb explosion subsequent to inner-shell ionization. Moreover, we plan to use the LCLS photon beam focused to a spot diameter of 1µm using KB mirrors to investigate multiple- and multi-photon-ionization processes, as well as the production of molecules with multiple core holes. We also plan to identify sequential/non-sequential many-photon multiple ionization. The understanding of such excitation and decay mechanisms will provide new information into the ionization and fragmentation dynamics of molecules, and into the correlated motion of the electrons remaining in the targets. In particular, fragmentation channels producing multiple heavy-particle fragments, subsequent to multiple ionization, will be measured using the AMO instrument ion detector simultaneously with electrons of all kinetic energies detected in five time-of-flight spectrometers.

The interaction of high-intensity x-rays with matter is somewhat different than the interaction of high-intensity infrared or optical photons with matter because the electron ponderomotive potential defined as \( U_p = e^2 \gamma^2 / 4m \omega^2 \) (quiver energy) is in general much weaker in the former case due to the much higher frequency of the x-rays. Unlike the case of lower frequency photons, x-rays couple strongly to inner-shell electrons, so we will observe new processes with the LCLS, including multiphoton processes involving core electrons, and sequential and
non-sequential ionization of inner-shell electrons. The LCLS will also enable the study of multiphoton ionization in the x-ray regime, that is, sub threshold ionization involving the use of multiple photons to ionize a single electron from a molecule.

Our proposed research will provide important information on damage mechanisms that will be important for the single bio-molecule imaging program. The damage mechanism for a single bio-molecule in a focused x-ray laser beam such as the LCLS is unknown. However, AMO physics can investigate the effect of nonlinear damage mechanisms, the effect of coherence and also find ways to diminish the radiation damage by varying the properties of the LCLS beam, such as shortening the duration of the LCLS pulse [1].

Acknowledgement:

All of the research work reported here is supported by the DoE, Office of Science, Basic Energy Sciences, Division of Chemical, Geosciences and Biological Science. M. Hoener is indebted to the Alexander von Humboldt Foundation for a Feodor Lynen Fellowship.

References:

4.4 Dielectronic Recombination of Al-Like Sulfur

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There has been much interest in measuring the oxygen-to-sulfur ratio in Jupiter’s plasma torus [1]. Calculations for total DR rate coefficients for all sulfur ions were done with an application to magnetic fusion plasma in mind, in which a single-configuration approximation to calculate energies and transition rates was employed. Also, a cutoff on the number of states was applied [2]. DR rate coefficients for $S^{q+}$ ($q=1-5$) ions have been calculated in the low density limit over the temperature range $T = 3 \times 10^4$ – $10^6$ K that is applicable to the Io plasma torus [3]. Cross sections and rate coefficients for $S^{3+}$ have been done using single-configuration and non-relativistic Hartree-Fock wave functions [4]. Photoionization cross sections and electron-ion recombination rate coefficients for $S^{3+}$ were calculated in the close coupling approximation using the R-matrix method [5]. Other DR calculations were done for $S^{3+}$ [6, 7]. All of these previous calculations for $S^{3+}$ were performed only within a non-relativistic LS-coupling approximation and at higher temperatures more suitable for collisionally-ionized plasmas but not at the lower temperatures appropriate for photoionized plasmas. Our calculations include both LS coupling and intermediate coupling (IC) using a multi-configuration Breit-Pauli (MCBP) approximation.

We have used the AUTOSTRUCTURE code to calculate energy levels and radiative and autoionization rates in LS- and IC-couplings, with non-relativistic radial functions [8, 9]. The autoionization rates are calculated in the isolated resonance approximation using distorted waves. This enables the generation of final-state level-resolved and total DR rate coefficients in the independent-processes approximation, i.e., we neglect interference between the radiative recombination (RR) and DR processes [10]. In our calculation, $n$ values were included up to 55 and a quantum-defect approximation for high-level values of $n$ up to 1000 was used, while $\ell$ values were included up to 13.

The DR rate coefficient, as a function of temperature, from an initial ground or metastable state $v$ to a final state $i$ is given by:

\[
\alpha_{vi}^{\rightarrow+}(T) = \left(\frac{4\pi a_0^2 I_H}{k_B T}\right)^{3/2} \sum_j \frac{g_j}{2 g_v} \exp\left(-\frac{E_c}{k_B T}\right) \sum_\ell \frac{A_{a j \rightarrow v, E_c} A_{r j \rightarrow i}}{A_{r j \rightarrow h} + \sum_m \frac{A_{a j \rightarrow m, E_c}}{A_{a j \rightarrow h}}},
\] (1)

where $g_j$ is the statistical weight of the $(N+1)$-electron doubly-excited resonance state $j$, $g_v$ is the statistical weight of the $N$-electron target state, and the autoionization rates, $A_{a\ell}$, and radiative rates, $A_{r\ell}$, are in inverse seconds. $E_c$ is the energy of the continuum electron with angular momentum $\ell$, which is fixed by the position of the resonance, $I_H$ is the ionization potential energy of the hydrogen atom, $k_B$ is the Boltzmann constant, and $(4\pi a_0^2)^{3/2} = \ldots$
6.6011 \times 10^{-24} \text{ cm}^3. \text{ For } \Delta n = 0 \text{ core-excitation, the resonance energies are empirically adjusted so that the series limits match the } 3 \rightarrow 3 \text{ excitation energies obtained from the NIST database [11].}

A study of the DR cross section for S^{3+} in LS- and IC-coupling schemes reveals that the dominant capture channel is via n = 3 target core excitations. One can see from Fig. 1 that, at higher energies, the strongest contribution to the DR cross section, and therefore to the DR rate coefficient, comes from the 3p \rightarrow 3d excitation. Also, the calculated DR cross section for S^{3+} using IC-coupling is lower than the corresponding LS-coupling result. This is in contrast to the general IC vs LS trend [13, 14], where IC-coupling effects increase the number of resonances, and the resulting cross section, by roughly 50%. But this is for the case of a pure ground state such as Li-like ions (1s^22s 2S_1/2). In our case, the ground state has a fine-structure splitting (3s^23p^2 \,^2P_{1/2},3/2) of around 0.118 eV.

The present reduction in the IC DR cross section is manifested in the DR rate coefficient, particularly in higher electron temperatures (see Fig. 2). At lower energies, the reason that the rate coefficient is higher using IC-coupling is due to additional contributions from the 3s^23p^2 [^2P_{3/2}]n\ell core-excited resonances that are forbidden in LS-coupling, and more additional core-excited autoionizing states are open. The RR calculations are also shown in Fig.2.

![Figure 1](image1.png)  
**Figure 1** DR cross section of S^{3+} using both LS and IC coupling schemes, convoluted with a FWHM Gaussian of 0.1 eV for illustrative purposes, indicating that the dominant contribution to the Maxwellian-averaged rate coefficient comes from both 3s3p^2n\ell and 3s3dnt\ell Rydberg series.

![Figure 2](image2.png)  
**Figure 2** DR IC, DR LS, and RR rate coefficients of S^{3+} using both LS coupling and IC schemes. PIE and CIE denote typical temperatures of photoionized and collisionally-ionized plasmas, respectively [16].

Accurate resonance energies are particularly important for the calculations of low-temperature DR rate coefficients. The radial wave functions are obtained by using the Slater-type-orbital model potential [12]. The 3s, 3p, and 3d radial scaling parameters, \lambda_{n\ell}, were determined by minimizing the equally-weighted sum of energies of the 40 lowest terms.
In an attempt to understand the suppression of the DR cross section in IC-coupling, calculations were carried out for the $3s \rightarrow 3p$ excitation ($e^+ + 3s^23p \ [2P_{1/2}] \rightarrow 3s3p^2 \ [2P_{1/2}, 3/2]n\ell$). The resulting DR cross sections for both $3s3p^2 \ [2P_{1/2}, 2P_{3/2}]n\ell$ series are convoluted with a full-width at half-maximum (FWHM) Gaussian of 1.2 meV (see Fig. 3). Both series begin to autoionize at principal quantum number $n = 31$. Also, the same calculations for the $3p \rightarrow 3d$ excitation ($e^+ + 3s^23p \ [2P_{1/2}] \rightarrow 3s^23d \ [2D_{3/2}, 5/2]n\ell$) were studied, and the resulting DR cross sections are plotted in Fig. 4. Again, the DR cross section drop occurs abruptly at $n = 31$. Thus, the reason for the reduction in the IC cross section is that the $3s3p^2n\ell$ and $3s^23dn\ell$ series autoionize to additional continua for $n \geq 31$, decreasing the resultant radiative branching ratio in Eq. 1 [15]. In Fig. 5, we present comparisons between our calculated LS-coupling and IC results and other available data for S$^{3+}$ [3, 5-7].

Figure 3 DR cross section for S$^{3+}$ in IC-coupling for the collision $e^+ + 3s^23p\ [2P_{1/2}] \rightarrow 3s3p^2\ [2P_{1/2}, 2P_{3/2}]n\ell$, convoluted with a FWHM Gaussian of 1.2 meV. A sudden drop in the cross section occurs for both series at $n = 31$.

Figure 4 Same as Fig. 3 but for the collision $e^+ + 3s^23p\ [2P_{1/2}] \rightarrow 3s^23d\ [2D_{3/2}, 5/2]n\ell$.

Figure 5 Comparisons between present and previously existing DR + RR rate coefficients for S$^{3+}$ [3, 5-7].
Our present investigation into the DR process of Al-like $S^{3+}$ has revealed that a sufficiently large atomic configuration basis leads to fairly accurate energies and transition rates for the target levels, and should yield reliable DR cross sections. With the inclusion of IC-coupling effects, additional radiatively-decayed states can autoionize, thereby decreasing the DR cross section. This occurs near the Rydberg limits and reduces the high-temperature rate coefficient that is more important for collisionally-ionized plasmas. On the other hand, IC effects open up additional core-excited autoionizing states, thereby increasing the low-energy DR cross section. This leads to a substantial increase in the low-temperature rate coefficient that is important for photoionized plasmas. These findings are a reminder that, as usually is the case, relativistic (i.e., spin-orbit) effects can have a profound effects even for low ionization. Despite the relative weakness of spin-orbit effects, which scale as $z^4$ and are expected to be least important for low ionization stages such as the present case of $S^{3+}$, even small energy shifts create additional autoionizing levels that greatly affect the resulting rate coefficient.

Acknowledgments:

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References:

4.5 Electron Capture by Ne\(^{6+}\) Ions from H\(_2\)O and CO\(_2\)

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Using translational energy-gain spectroscopy technique [1], we have measured the energy-gain spectra and absolute total cross sections for single- and double-electron capture in collisions of Ne\(^{6+}\) recoil ions with H\(_2\)O and CO\(_2\) at laboratory impact energies between 250 and 3000 eV. The translational energy-gain spectra show that only a few final states were selectively populated depending on the target and collision energy. In all collision systems studied here, the dominant reaction channels are due to non-dissociative single-electron capture into excited states of the projectile product. The final state populations were discussed on the basis of the reaction windows, which are calculated using the single-crossing Landau-Zener model [2] and the extended version of the classical over-the-barrier model [3].

Preliminary measurements of total cross sections for single-electron capture by Ne\(^{6+}\) ions from H\(_2\)O and CO\(_2\) are shown in Fig. 1 together with the predictions of the multi-channel Landau-Zener model [2] and the classical over-the-barrier (COB) model [3].

![Figure 1](image.png)

**Figure 1** Total cross sections for single-electron capture by Ne\(^{6+}\) ions from H\(_2\)O and CO\(_2\). –, present work; dotted curves; COB model; solid lines, MCLZ calculations.

For Ne\(^{6+}\) + H\(_2\)O collisions, the total cross sections increase with increasing impact energy, a pattern that is well documented for such collisions at low energies [4]. This can be understood by the reaction window, which broadens with increasing energies and therefore increases the
probability of capture channels with large Q-values. The energy dependence of cross sections is in direct contradiction with the MCLZ calculation which decreases with increasing energy, and the COB model over predicted the total cross section for capture by at least a factor of two. For Ne$^{6+}$ - CO$_2$ collisions, the total cross sections show no significant dependence on the collision energy. Our data are lower than those of the MCLZ model and about a factor of two smaller than the COB model predictions.

References:

4.6 Differential Cross Sections for Single-Electron Capture by Low-Energy O$_2^{2+}$ Ions with Ne and O$_2$

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A large variety of molecular ions have been identified in cold astrophysical environments and in planetary atmospheres. Molecular oxygen ions are of particular interest due to their potential influence on the properties of the ionosphere and their involvement in many atmospheric phenomena. Furthermore, electron capture involving multiply charged molecular ions has been proposed as a mechanism for generating ions in the earth’s upper atmosphere [1,2].

In the present work, a differential energy-gain spectrometer [3], capable of measuring simultaneously the scattering angle and the energy-gain of projectile products in ion-atom collisions, has been used for the study of state-selective non-dissociative single-electron capture in collisions of O$_2^{2+}$ recoil ions with Ne and O$_2$ at an impact energy 100 eV and scattering angles between 0° and 6°. Unfortunately, the peak of doubly charged molecular ion O$_2^{2+}$ coincides with the atomic ion O$^+$ peak in mass spectrum at m/q = 16. No attempt was made to estimate the fraction of O$_2^{2+}$ in the O$^+$ beam. However, we were able to easily separate the O$_2^+$ products resulting from electron capture by using an electrostatic analyzer (ESA) voltage which was double that required to transmit the elastically scattered ion beam. Following the nomenclature described by Kamber et al. [4], the observed reaction channels are denoted in the following fashion: the designations I, II, and III represent, respectively, the ground, first, and second electronically excited states of O$_2^{2+}$; a, β, γ, represent the ground and subsequent electronically excited states of O$_2^+$ ion; X, represents the ground state of the target product.

Figure 1 shows the translational energy-gain spectra obtained for single-electron capture by 100 eV O$_2^{2+}$ ions from Ne at different scattering angles. At 0° scattering angle, the energy-gain spectrum indicates that the dominant reaction channel is due to non-dissociative single-electron capture into the ground state (X 3Π$_g$) of the product O$_2^+$ from the ground state incident O$_2^{2+}$ (X 1Σ$^-_u$) ions with contributions due to capture from the low-lying metastable state (A 3Σ$^-_u$) of the O$_2^{2+}$ into the (A 2Π$_u$) state of O$_2^+$. There are smaller contributions due to capture into the a 4Π$_u$, A 3Π$_u$, and b 4Σ$^-_u$ states from the metastable states W 3Δ$_u$, B 3Π$_g$, and B' 3Σ$^-_g$ of the O$_2^{2+}$ ions via reaction channels IIβX, IIIγX, IIIβX, VδX, IVγX, IVβX, and VβX. A comparison with the measurements of Pederson [5] at 100 eV, and Hamdan and Brenton [6] at 6 keV shows good agreement with the present measurements.
As the scattering angle is increased, capture into the $X^2\Pi_g$ state (the $I\alpha X$ channel) remains dominant but contributions from reaction channels $II\beta X$, $III\gamma X$, and $V\delta X$, respectively, due to capture from the metastable states $W^3\Delta_u$ and $B^3\Sigma_g^-$ of the $O_2^{2+}$ ions into the $a^4\Pi_u$, $A^2\Pi_u$, and $b^3\Sigma_g$ states of $O_2^+$, increase with increasing the scattering angles. This indicates that the angular distribution for the $I\alpha X$ channel is more strongly peaked in the forward direction than for the reaction channels $II\beta X$, $III\gamma X$, and $V\delta X$. Figure 1 also shows our calculated reaction windows for 100 eV $O_2^{2+}$ - Ne collisions, using both a single-crossing Landau-Zener (LZ) model [7] and the extended version of the classical over-the-barrier (ECOB) model [8]. Calculated peak values have been normalized to our observed peak values in the energy spectrum. The reaction based on a single-crossing LZ model does not describe the position of the dominant reaction channel, while the reaction window based on the ECOB model maximizes at about 6 eV and underestimates the contribution of the $I\alpha X$ channel.

Figure 2 shows the translational energy-gain spectra for single-electron capture by 100 eV $O_2^{2+}$ ions from $O_2$ at different projectile laboratory scattering angles. The observed spectra clearly indicate that non-dissociative single-electron capture into the $O_2^+$ ($c^4\Sigma_u$) state from the low-lying metastable state ($A^3\Sigma_u$) of the $O_2^{2+}$ is the predominant channel, although
Figure 2 Translational energy-gain spectra for single-electron capture by 100 eV O2\(^{2+}\) ions from O\(_2\) at different projectile laboratory scattering angles. Also shown are reaction windows calculated on the basis of a single-crossing LZ model (dotted curve) and the ECOB model (dashed curve). Smooth lines are drawn to guide the eye.

capture by the ground state (X \(^1\Sigma\)) of O\(_2\)^{2+} ions into b \(^4\Sigma\)\(_g\), and B \(^2\Sigma\)\(_g\) states are also significant. As the scattering angle is increased, a relative shift of about 0.45 eV in the energy gain of the \(\Pi\zeta X\) channel is observed going from scattering angle of 0\(^\circ\) to 6.71\(^\circ\). This is attributed to the energy given to the target and is in accordance with energy and momentum conservation rules. The reaction windows favor Q values smaller than those observed and are positioned near the \(\iota eX\) channel.

The experimental total differential cross sections (d\(\sigma/d\Omega\)) for single-electron capture by 100 eV O\(_2\)^{2+} ions from Ne and O\(_2\) are shown in Figure 3. The general features of the distributions are qualitatively explained in terms of semi-classical model based on Coulomb potential curves which have been described in detail by Andersson et al. [9]. The traditional two-state model has been used to estimate the critical angle \(\theta_c\), which corresponds to capture at an impact parameter equal to the crossing radius, by assuming that capture occurs at a localized curve crossing between the potential energy curves for entrance and exit channels. For small angles, \(\theta_c = Q/2E\), where Q is the exoergicity of the collision and E is the collision energy. This angle separates the events scattered at smaller angles due to capture on the way-out of the collision and events scattered at larger angles due to capture on the way-into the collision.

For O\(_2\)^{2+} - O\(_2\) collisions, the distribution is peaked in the forward direction inside the critical angle \(\theta_c = 1.32^\circ\), which corresponds to the \(\Pi\zeta X\) capture channel. This distribution represents contributions from electron capture that takes place on the way-out of the collisions. For O\(_2\)^{2+} - Ne collisions, the measurements show that the projectile products which correlate with capture into the (X \(^2\Pi\)) state are distributed forward inside the critical angle \(\theta_c = 0.8^\circ\), indicating that capture takes place on the way-out of the collision.
Figure 3 Experimental differential cross sections for single-electron capture by O$_2^{2+}$ ions from Ne and O$_2$. Spline lines are drawn to guide the eye.

References:

4.7 State-Selective Electron Capture by O\(^{3+}\) Ions from Atomic and Molecular Targets

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State-selective electron capture processes in low-energy collisions of O\(^{3+}\) recoil ions with He, Ar, D\(_2\), O\(_2\), H\(_2\)O and CO\(_2\) at impact energies between 0.3 and 1.2 keV and scattering angles between 0º and 6º have been studied using a differential energy-gain spectrometer [1], capable of measuring simultaneously the energy-gain and the scattering angle of projectile products in ion-atom/molecule collisions. The energy-gain spectra showed that the dominant reaction channels were due to capture into excited states of the projectile product O\(^{2+}\). In this work, no clear evidence of the processes involving long-lived metastable state O\(^{3+}\) (2s 2p 2 4 P) was observed. The energy-gain spectra were interpreted qualitatively in terms of the reaction windows, which are calculated using the single-crossing Landau-Zener (LZ) model and the extended version of the classical over-the-barrier (ECOB) model.

The experimental total differential cross sections (d\(\sigma\)/d\(\theta\)) for single-electron capture by 300 eV O\(^{3+}\) ions from He, D\(_2\) and H\(_2\)O are shown in Figure 1. The differential cross sections were determined using the translational energy-gain technique, by calculating the area under the peaks in the energy-gain spectra at different projectile laboratory scattering angles using a curve fitting program. The general features of the distributions are qualitatively explained in terms of semi-classical model based on Coulomb potential curves, which have been described in detail by Andersson et al. [2]. The traditional two-state model has been used to estimate the critical angle \(\theta_c\), which corresponds to capture at an impact parameter equal to the crossing radius, by assuming that capture occurs at a localized curve crossing between the potential energy curves for entrance and exit channels. For small angles, \(\theta_c = Q/2E\), where Q is the exoergicity of the collision and E is the collision energy. This angle separates the events scattered at smaller angles due to capture on the way out of the collision and events scattered at larger angles due to capture on the way into the collision. The critical angle for each dominant channel is indicated by an arrow in Fig. 1.

For 300 eV O\(^{3+}\) - He collisions, the distribution contains a broad peak lying slightly outside the critical angle \(\theta_c = 1.21^o\) for capture into the excited state 2s2p\(^3\)3\(^3\)P of the O\(^{2+}\) ion. This distribution represents contributions from electron capture that takes place on the way into the collisions. For 300 eV O\(^{3+}\) - D\(_2\) collisions, the spectrum shows a smooth rise to a broad maximum around 2\(^o\) outside \(\theta_c = 0.61^o\), assuming that electron capture occurs into 2p 3s of the O\(^{2+}\) ion. The distribution is due to capture on the way into the collision. For 300 eV O\(^{3+}\) - H\(_2\)O collisions, the distribution contains a peak slightly greater than \(\theta_c = 0.59^o\), which corresponds to the 2p 3p capture channel, indicating that capture takes place on the way into the collision.

The measured total cross sections for single-electron capture by O\(^{3+}\) ions from He, D\(_2\), H\(_2\)O and CO\(_2\) are shown in Fig. 2 together with other available measurements and calculations.
For O$^{3+}$ - He collisions, the total cross sections show no significant dependence on the collision energy. Our data are in reasonably good agreement with the experimental results of Bangsgaard et al. [3] and Ishii et al. [4]. The data presented in this study, however, are considerably higher than the recommended cross sections of Janev et al. [5] and found to be 60% higher than the multi-channel Landau-Zener calculations [6], based on the Taulberg expression for the coupling matrix $H_{12}$ [7]. The measured cross sections are about a factor of 2 smaller than the classical over-the-barrier (COB) model [8] prediction of $10.737\times10^{-16}$ cm$^2$ assuming the capture probability $A = 0.5$. An average value for $A$ of 0.253 is found experimentally, by dividing the measured total cross section by the classical cross section ($\pi R_C^2$). This small value of $A$ is probably due to the population of core excited states. The responsible coupling matrix element ($H_{12}$), which couples the incoming channel with the outgoing reaction channels leading to these core excited states, is small and thus will yield measured cross sections smaller than $\pi R_C^2$.

For O$^{3+}$ + D$_2$ collisions, the total cross sections slowly decrease with increasing collision energies. Our data are in good agreement with the measurements of Phaneuf et al. [9], and the recommended cross sections of Janev et al. [5] for O$^{3+}$ + H$_2$ collisions, but are a factor of 2 higher than the results of Beijers et al. [10]. The present measurements are in good agreement with the COB model prediction of $27.24\times10^{-16}$ cm$^2$ with $A = 0.5$, and MCLZ calculations at low energies ($\leq 900$ eV) and show similar behavior (cross sections slowly decrease with increasing collision energies). Recently Wang et al. [11] performed a nearly complete $ab\ initio$ study of single-electron capture in collisions of ground state O$^{3+}$ ($2s^2(1S)2p^3P$) ions with molecular hydrogen using a fully quantum-mechanical, molecular-orbital (QMO) coupled-channel method, adopting the so-called infinite order sudden approximation (IOSA), the vibrational sudden approximation (VSA), and the electronic approximation (EA). The data presented here is considerably lower than those of EA calculations by a factor of 1.35, and found to be on average 1.42 and 3.33, respectively, higher than VSA and IOSA predictions.

**Figure 1** Experimental differential cross sections ($d\sigma/d\theta$) for single-electron capture by 300 eV O$^{3+}$ ions from He, D$_2$, and H$_2$O. Spline lines are drawn to guide the eye.
For $\text{O}^{3+} + \text{H}_2\text{O}$ and $\text{CO}_2$ collisions, the total cross sections increase with increasing impact energy, a pattern that is well documented for such collisions at low energies [7,12]. This can be understood by the reaction window, which broadens with increasing energies and therefore increase the probability of capture channels with large Q-values. For $\text{O}^{3+} + \text{H}_2\text{O}$ collisions, the energy dependence of cross sections is in direct contradiction with the MCLZ calculation which decreases with increasing energy, and the COB model over predicted the total cross section for capture by at least of a factor of 1.2. For $\text{O}^{3+} + \text{CO}_2$ collisions, The MCLZ results are at least a factor of 2 smaller than the experimental results and show the same energy dependence, whereas, the prediction of the COB model lie about 30 – 40% below the experimental results.

![Figure 2](image)

**Figure 2** Total cross sections for single-electron capture by $\text{O}^{3+}$ ions from He, $\text{D}_2$, $\text{H}_2\text{O}$ and $\text{CO}_2$. • present work; □, Ishii et al. [4]; ▲, Bangsgaard et al. [3]; ▽, Janev et al. [5]; Δ, Phaneuf et al. [9]; ○, Beijers et al. [3]; dotted curves; COB model; dash-dot, EA – Wang et al. [11]; dash-dot-dot, IOSA – Wang et al. [11]; dash, VSA – Wang et al. [11]; solid lines, MCLZ calculations.

References:

4.8 Suppression of Primary Electron Interferences in the Ionization of N$_2$
by 1 – 5 MeV Protons

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It is well known that electrons have both particle and wavelike properties similar to photons. A manifestation of this duality has recently been shown to occur in the ejection of electrons from H$_2$ impacted by fast ions [1]. Whereas electron ejection from an atom gives rise to a single outgoing ionization “wave”, corresponding ejection from H$_2$ occurs simultaneously from both atomic centers, resulting in coherent ionization waves that can interfere. This phenomenon of interference associated with electron ejection from molecules is analogous to Young’s two-slit experiment with the atomic centers acting as “slits”, and was considered already more than forty years ago in the photoionization of molecules [2,3]. Prior to recognition of this Young-type interference involving simultaneous emission from two atomic centers, Kronig [4] attributed oscillatory structures in the K-shell ionization spectra of heteronuclear molecules to intramolecular scattering. In the latter case, the ionization wave originating at one nucleus is scattered from the adjacent nucleus causing subsequent interference between the original and scattered waves. This phenomenon is related to the well-known EXAFS (extended x-ray absorption fine structure) technique [5,6] used in solid-state physics to study the structure of materials. Hence, while atomic ionization is generally well understood [7,8], more subtle effects arising from coherent electron emission distinguish molecular ionization from its atomic counterpart and consequently reveal the wavelike aspects of the ejected electrons.

In the present work, interferences associated with electron ejection are investigated for N$_2$ impacted by 1 – 5 MeV H$^+$ ions (see Ref. [9] for details). For diatomic molecules such as N$_2$ ionization can occur from several molecular orbitals, as opposed to the single K-shell orbital in H$_2$. However, the probability for ionization of the valence L-shell orbitals in N$_2$ is about three orders of magnitude larger than for the K-shell orbitals [7,8], which are not expected to contribute significantly to any interference effects. To compare the experimentally observed oscillatory structures with the expected Young-type interference structures, theoretical calculations were performed for the ionization of N$_2$ obtaining molecular to atomic cross section ratios using a formulation similar to that developed by two of the present authors for H$_2$ [10]. The main difference is that N$_2$ has several molecular orbitals giving different interference patterns.

From measurements conducted at Western Michigan University using the 6-MV tandem Van de Graaff accelerator, experimental molecular N$_2$ cross sections were divided by the theoretical atomic N cross sections, giving the ratios shown in Fig. 1. The cross section ratios, normalized to about unity for convenience, show clear evidence of oscillatory behavior with no significant dependence on the electron observation angle or collision velocity, in contrast to earlier results for Kr$^{33+}$ [1,11] and H$^+$ [12] + H$_2$ for which there was a strong dependence of
the primary interference structures on the observation angle and a smaller but definite dependence on the collision velocity. Thus, the observed oscillatory structures for N\textsubscript{2} suggest an origin other than primary Young-type interferences, and are suggestive of previously observed secondary interferences that have been attributed to interference of the primary ejected electron wave with the secondary wave that results from scattering at the other atomic center [13].

To quantitatively characterize the oscillatory structures and frequencies for N\textsubscript{2}, the normalized cross section ratios of Fig. 1 were parameterized according to the function

\[ f(k) = A[I + \sin(kcd - w)] + B, \]

where \( k \) is the electron momentum (velocity), \( d \) is the internuclear separation, \( c \) is a fitting parameter representing the oscillation frequency, \( w \) allows for a phase shift, and \( A \) and \( B \) are normalization constants. Allowance for a phase shift was also utilized in Refs. [12,13] to describe the secondary interference structures attributed to intramolecular scattering.

The values obtained for \( c \) and \( w \) from the fitting are shown in Figs. 2a and 2b, respectively. The frequency parameter \( c \) (Fig. 2a) shows only a small dependence on the electron observation angle (note the suppressed ordinate) and the collision velocity in sharp contrast to results for the primary interferences in H\textsubscript{2} [11,12]. On the other hand, the second-order oscillations for these same collisions gave values for \( c \) in the range \( \sim 2.5-3 \) that were nearly independent of the observation angle. Regarding the phase shift \( w \), Fig. 2b shows this parameter to have a maximum around 45° and a minimum at 90°, with little dependence on the collision velocity. The presence of this shift can be seen already by careful examination of the cross section ratios in Fig. 1. On the contrary, the second-order oscillations in Kr\textsuperscript{33+} + H\textsubscript{2} [13] and H\textsuperscript{+} + H\textsubscript{2} [12] exhibited a constant phase shift of \( w \sim \pi \). The exact reason for the
angular dependence of this phase shift is presently unknown, but is likely contained in the amplitude factors governing the secondary interferences (see Ref. [13]).

If the observed oscillatory structures in Fig. 1 are indeed secondary interferences, then the underlying mechanism for their production must be understood. It might be argued that secondary interference occurs when an L-shell electron undergoes large momentum transfer in a relatively “hard” binary encounter, causing the electron to scatter off the adjacent nucleus, leading to interference between the initial L-shell ionizing event and the subsequent secondary scattering event. Such scattering is similar to that resulting from the core ionization of heteronuclear molecules discussed by Kronig [4], and also to that observed in EXAFS studies [5,6], for which oscillations occur in the energy region just above the threshold for core ionization.

The present results can also be compared to those for photoionization of N$_2$. In the case of K-shell photoionization [14], the localized nature of the K electrons suppresses Young-type interferences because the ejected electron is not coherently emitted from both centers. On the other hand, ionization of the valence electrons produces modulations in the resulting cross sections that have been attributed to Young-type interference [2,3]. The fact that there are several L orbitals delocalized over the molecule might be the reason that primary Young-type interferences are strongly suppressed for ionization of N$_2$ by fast ions.

Similar measurements for other diatomic molecules such as O$_2$ shed additional light on the observed oscillatory structures (see next report). The differences in the structures observed for H$_2$ and heavier molecules such as N$_2$ further highlight the unique character of molecular ionization compared to atomic ionization.

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References:

4.9 Interferences in Electron Emission from O$_2$ by 30 MeV O$^{5,8+}$ Impact

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As discussed in the preceding report, investigations of electron interferences for 1-5-MeV H$^+$ + N$_2$ exhibit mainly secondary oscillations resulting from intramolecular scattering [1]. Strong suppression of the primary Young-type interferences is attributed to cancellation of the contributions from the symmetric and anti-symmetric L orbitals of N$_2$. The present work extends the experimental studies for N$_2$ to 30 MeV O$^{5,8+}$ impact with O$_2$ (see Ref. [2] for details).

The 30 MeV O$^{5,8+}$ ion beams were obtained from the tandem Van de Graaff accelerator at Western Michigan University. After collimation, the ion beam was directed into the scattering chamber onto an O$_2$ target supplied by a gas jet with a flow rate set to maintain single collision conditions. The energy spectra of electrons emitted from the target were measured with a parallel-plate analyzer equipped with a channel electron multiplier for angles of 30º, 60º, 90º, 120º, and 150º with respect to the incident beam and ejected electron energies of 15 - 400 eV.

The measured molecular cross sections were divided by theoretical molecular O$_2$ cross sections calculated using one-center wave functions following the methods developed in [3]. The resulting ratios, shown in Fig. 1, exhibit oscillations that do not change significantly with observation angle, a behavior expected for primary Young-type oscillations [4,5]. To quantify the oscillatory structures, the ratios were fit to the phase shifted sinusoidal function [6]:

$$f(k) = A \sin(kcd - w) + B$$  

(1)

where $k$ is the electron velocity (in a.u.), $d$ is the internuclear distance (2.28 a.u.), $c$ is an adjustable frequency parameter, $w$ is an adjustable phase shift, and the constants $A$ and $B$ represent the interfering and non-interfering cross-section fractions, respectively.

The frequency parameter $c$ shown in Fig. 2 for 30-MeV O$^{5,8+}$ + O$_2$ is indeed found to be nearly constant for all angles and both incident charge states, a behavior similar to that observed for 1-5 MeV H$^+$ + N$_2$ collisions [1], and the phase parameter $w$ also follows a pattern similar to that reported for H$^+$ + N$_2$ with an apparent minimum near 90º. The independence of $c$ on the electron observation angle is suggestive of secondary interferences as found previously for ~ 60 MeV/u Kr$^{34+}$ + H$_2$ [6] and 1-5 MeV/u H$^+$ + H$_2$ collisions [5]. Furthermore, no obvious evidence for primary interferences is seen as was the case for H$^+$ + N$_2$ [1]. On the contrary, the oscillation interval of $\Delta k$ ~ 4 a.u. for O$_2$ has a value two times larger than the $\Delta k$ ~ 2 a.u. found for N$_2$. The reason for this difference in $\Delta k$ for O$_2$ and N$_2$ is not known and is presently being explored.
Figure 1 Experimental-to-theoretical cross section ratios for 30 MeV O^{5+} + O_2 at the indicated observation angles. The smooth curves are the results of fitting the phase-shifted sinusoidal function given by Eq. 1 to the ratios.

Figure 2 Frequency $c$ and phase shift $w$ parameters determined from fitting Eq. 1 to the cross section ratios of Fig. 1.

References:

4.10 Nonstatistical Enhancement of the 1s2s2p 4p State in Electron Transfer in 0.5-1.0 MeV/u C4,5+ + He and Ne Collisions

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Nonstatistical enhancements for formation of the metastable 1s2s2p 4P state compared to the similarly configured 1s2s2p 2P- and 1s2s2p 2P+ states were observed following single electron transfer to C 4+(1s2s 3S) and double electron transfer to C 5+(1s) ions, respectively. In our previous work, similar enhancements were observed in the population of the 4P metastable state resulting from electron transfer in ~1 MeV/u F 7,8+ + He and Ne collisions [1]. The enhancements were attributed to a dynamical Pauli exchange mechanism involving projectile and target electrons having the same spin alignment [1].

More recently, it was suggested that, in addition to the Pauli exchange mechanism, cascading following electron transfer to (1s2s 3S)nl 4L states with n ≥ 3 can lead to 4P enhancement [2]. In such a scenario, capture to an nl 4L state is followed by successive prompt radiative transitions with Δl = 1 until the captured electron reaches the 1s2s2p 4P from which it cannot decay radiatively, and which has a long Auger lifetime as well.

To further understand the observed enhancement of the 4P state, new investigations of Auger emission spectra in collisions of 0.5-1 MeV/u C4,5+ with He and Ne targets were undertaken [3]. Experimental ratios of the resulting 4P intensities to the sum of the 2P- and 2P+ intensities, i.e., R = 4P/(2P- + 2P+), for the collision systems studied give values three to four times larger than the expected value of two based solely on spin statistics [4] for single transfer to C4+(1s2s 3S) and double transfer to C5+(1s). Detailed theoretical calculations of the effect of electron cascading on the measured value of R indicate that cascade feeding due to capture into n≥3 levels does indeed play an important role, but explains only about half of the observed enhancement as shown in Fig. 1. Consequently, Pauli exchange during electron transfer of similarly aligned target and projectile electrons, as originally proposed in Ref. [1], is still deemed to be a viable mechanism for selectively populating the 4P state. Nevertheless, quantitative calculations are needed to better assess its significance.
Figure 1 Calculated and measured ratios of the $1s2s2p$ $^4P$ intensities to the sum of the $1s2s2p$ $^2P_+$ and $1s2s2p$ $^2P_-$ intensities as a function of the incident projectile energy for single transfer in $C^{4+}(1s2s^3S) + He$ collisions. Dashed line: calculation including cascades from all relevant states up to $n=3$, dash-dotted line: calculation including cascades from all relevant states up to $n=4$, dash-dot-dot line: calculation including cascades from all relevant states up to $n=5$, full line: extrapolation to $n\to\infty$ (see text). The observed $^4P$ intensities were corrected for contributions from the $C^{4+}(1s^5)$ ground state and for lifetime effects (see text). The horizontal short dashed line at $^4P/(^2P_+ + ^2P_-) = 2$ represents the value expected from spin statistics.

References:

4.11 Guiding of Electrons through Insulating PET Nanocapillaries

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The interaction of highly-charged ions (HCI) with surfaces has been the subject of extensive research both experimentally and theoretically not only because of its potential application in the field of nanotechnology but also from the point of view of fundamental understanding [1,2]. In recent years attention has centered on the transmission of HCI through nanocapillaries with the reported guiding of slow positive ions (3 keV Ne$^{7+}$) through insulating nanocapillary foils of polyethylene terephthalate (PET) by Stolterfoht et al. [3]. Surprisingly, ion transmission with negligible energy loss or charge change was observed for foil tilt angles up to 20$^\circ$ with respect to the incident beam direction, indicating only distant encounters with the capillary walls. These observations have been attributed to a self-organizing charge-up of the walls of the capillaries [3] that, after a characteristic charging time, deflects the traversing ions causing them to be “guided” through the sample along the capillary axis. In subsequent work by these authors additional properties of slow ion guiding in PET foils were investigated [4].

Experimental and theoretical works by other investigators have been conducted for slow (~1-10 keV) positive ions [5,6,7,8,9], including in addition to PET nanocapillary samples of SiO$_2$ [6], alumina [8] and tapered glass [9]. In all cases, the surfaces of the insulating nanocapillary foils were coated with a thin conducting layer, e.g., gold, to prevent charging of the sample during the measurements. More recently, guiding for 200-350 eV electrons in Al$_2$O$_3$ nanocapillary foils has been reported [10].

In this work, the transmission and guiding of 500 and 1000 eV electrons through insulating PET nanocapillaries of diameter 200 nm and aspect ratio 50 have been investigated [11]. The experiment was performed at Western Michigan University. The sample was mounted in a goniometer that allowed precise two-dimensional positioning with respect to the incident beam. The electron beam was produced from a simple filament source and collimated to a diameter of ~1.5 mm. The transmitted electrons were energy analyzed with a parallel-plate spectrometer located a few centimetres behind the sample and counted with a channel electron multiplier (CEM).

Fig. 1 shows the angular distributions of the transmitted electrons for 500 and 1000 eV. The transmitted intensity was normalized to the incident beam current on the sample and all data were taken after the guiding had reached its equilibrium (~ 15 minutes). From Fig. 1 we observe that electron guiding depends strongly on the foil tilt angle $\psi$ and the incident electron energy. Specifically, the transmitted intensity decreases exponentially with tilt angle and with incident electron energy (for 500 eV guiding was observed up to $\psi = 11^0$, whereas for 1000 eV only up to $\psi = 7^0$). Furthermore, a plot of the centroids of the angular distributions of the
observation angles vs. foil tilt angles, displayed in Fig. 2, shows a linear relationship, agreeing with results observed for HCIs.

**Figure 1** Angular distributions of the integrated normalized transmitted electron intensities as a function of observation angle $\theta$ for the indicated foil tilt angles $\psi$ for (a) 500 eV and (b) 1000 eV incident electrons.

**Figure 2** Plot of the centroids $\theta_{cent}$ of the angular distributions vs. foil tilt angle $\psi$ for 500 and 1000 eV electrons incident on PET. The linear dependence demonstrates guiding.

These results show that electron transmission and guiding depend strongly on the capillary foil tilt angle as well as the incident electron energy. It is seen that the transmission intensity at zero degree tilt angle increases with increasing energy, while the relative transmission intensity decreases with increasing tilt angle. The observation angle and the tilt angle show a linear relationship, demonstrating that electrons are guided through nanocapillaries in a manner similar to positive ions. These studies are ongoing to determine additional properties of electron guiding in insulating capillaries.

**References:**


4.12 Dissociative and Non-Dissociative Charge-Changing Processes in 1.0-2.0 MeV/u O5+ + O2 Collisions

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Interactions of molecular oxygen in collisions with charged particles are relevant to many fields of study including astrophysics, atmospheric physics, and the life sciences. These interactions are especially relevant to the life sciences as both atomic and molecular oxygen are abundant in most living matter, as well as being one of the essential components of many organic molecules. The generation of ion-radiation induced reactive oxygen and how it affects surrounding cellular tissue is a primary example [1]. Within the field of atomic physics results for the ionization of molecular oxygen by fast ions are important for analyzing the fragmentation of H2O and other molecules. Similar work has been the subject of recent attention for protons, neutral hydrogen, and carbon projectiles [2,3] colliding with H2O. In an effort to gain additional understanding of such interactions, dissociative and non-dissociative products of O2 associated with single electron capture, single electron loss, and direct ionization have been measured for 1.0, 1.5, and 2.0 MeV/u O5+ + O2 collisions.

These measurements were conducted at Western Michigan University using the tandem Van de Graaff accelerator. Time-of-flight techniques were used to detect coincidences between target ion fragments and individual outgoing projectile charge-state components. A collimated O5+ beam interacted with O2 contained within a differentially pumped target gas cell, in which the pressure was kept below 2.0 mTorr. In all cases, spectra were measured for several target pressures to check for single-collision conditions. Recoiling target ions were extracted by an electric field transverse to the beam direction and detected with a set of coupled microchannel plates. Following interaction with the target gas, the projectile beam was magnetically analyzed and the individual charge-changed components were counted with silicon surface-barrier detectors. To ensure the validity of the data, spectra for He and Ne were collected and the ratios for multiple ionization were compared with previously measured values [4,5], as well as the measured yields for total single electron capture and loss [4,6]. These latter yields also provided the calibration factor to determine absolute cross sections for the O2 data.

Fig. 1 shows the target ion products associated with projectile electron capture in 1.0 – 2.0 MeV/u O5+ + O2 collisions compared with the corresponding spectrum for 2 MeV/u O5+ + Ne. Both non-dissociative molecular and dissociative atomic products are formed with charge states up to 4+. In the figure the total integrated beam current is the same for each spectrum, indicating a strong decrease in the relative cross sections as a function of projectile energy. The spectra for projectile electron loss and direct ionization (not shown) gave similar results. From these spectra, absolute cross sections can be determined, as well as the relative yields for dissociative and non-dissociative ionization of O2, to obtain information on the mechanisms for the molecular fragmentation of O2. Additional measurements for incident oxygen charge states 6, 7, and 8+ are planned to determine the charge-state dependence of the various processes.
Figure 1 Target ion fragments associated with projectile electron capture for 1.0, 1.5, and 2.0 MeV/u O5+ + O2 collisions compared with the corresponding spectrum for 2.0 MeV/u O5+ + Ne.

References:

4.13 Zero-Degree Electron and Ion Spectrometer for the Shanghai EBIT

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A tandem parallel-plate electrostatic energy analyzer has been constructed for use at the Shanghai electron-beam-ion trap (EBIT) [1]. The spectrometer is similar to the one used at Western Michigan University and is designed for use at zero degrees, i.e., for electron or ion emission along the beam direction. It is of the same type as that used successfully by Stolterfoht and co-workers for studies of high-resolution electron spectroscopy for many years [2]. At WMU, the spectrometer has been used for making high-resolution Auger measurements [3,4] and forward-going continuum (i.e., cusp) electron measurements [5].

To date, the EBIT facility in Shanghai has been used for spectroscopic and dynamical measurements of collisions taking place inside the trap region [6]. A schematic of the EBIT is shown in Fig. 1. Work is presently underway to extract ions from the EBIT, and it is anticipated that this capability will be accomplished within the next year. Following vertical extraction the ions will be deflected electrostatically into a horizontal plane and a magnetic analyzer will be used to select beams of the desired species and charge state and direct them into the experimental beamline. The extracted beam will be used for spectroscopic and dynamical studies of collisions between the slow highly-charged ions and atomic or molecular targets. Beam intensities are expected to be about $10^5$ ions per pulse.

A major component in the extracted beam studies is a recoil-ion momentum spectrometer and its associated supersonic “cold” target, constituting a so-called COLTRIMS apparatus [7]. This instrumentation permits detailed investigations of collision dynamics by simultaneously recording the momenta of the recoiling target ions and electrons. Construction of this instrument is nearly complete.

To further enhance the capabilities of the beamline and to enable an even wider range of investigations, the zero-degree spectrometer will be installed immediately following and in close proximity to the COLTRIMS apparatus. A schematic of the spectrometer is shown in Fig. 2. With this spectrometer, two principal areas of investigation are presently envisioned:
(1) high-resolution Auger emission from highly-charged high-Z ions [3,4], and (2) transmission and guiding of ions through insulating nanocapillary foils [8].

Following the zero-degree spectrometer an electrostatic state analyzer will be installed so that the outgoing projectile charges states may be determined. This latter capability will enable the detection of specific outgoing projectile charge states in coincidence with forward ejected electrons detected in the spectrometer, or in coincidence with recoiling target ions or electrons observed in the COLTRIMS apparatus. Moreover, electrons detected in the spectrometer can be recorded in coincidence with these same recoiling target products.

The combined capabilities of the COLTRIMS apparatus and the zero-degree spectrometer will constitute a powerful and unique facility not presently duplicated elsewhere.

References:

5 CONDENSED MATTER PHYSICS

5.1 Entanglement Perturbation Theory for the Quantum Ground States in Two Dimensions

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To calculate the partition functions and to solve the Schrödinger equations for macroscopic quantum systems are undoubtedly the most fundamental problems in theoretical physics. It would not be an exaggeration to say that the history of the development of quantum theory is primarily that of a pursuit of a variety of methods for this problem. Methods are roughly categorized into two, a variety of mean field theories and otherwise. The essence of mean field theories is to make truncations of correlations [1]. The merit of mean field theories lies in an essential simplification of calculations. When the systems of interest are very complex with many local degrees of freedom, such as involving electrons of orbital degeneracy and phonons, mean field methods are currently the only methods available. The penalty is, nevertheless, conceptually huge: if we don't know the importance of those neglected correlations, we are not sure how good the results of mean field approximations are. This is precisely the starting point and motivation of non-mean field theories. Here we currently have roughly three methods. First are rigorous methods such as Bethe Ansatz [2-8]. In spite of its remarkable success over the last several decades, a major drawback of rigorous methods is that they are mostly limited to 2D classical or 1D quantum systems of rather special structures. Second are numerical simulations such as exact diagonalization and Monte Carlo [9]. With an ever-increasing computer power and a steady supply of various ingenious ideas in algorithm, they provide a solid starting point often with a superb accuracy, but the finite size problem continues to be a serious issue. The negative sign problem is yet another serious problem in Monte Carlo. Third is the method of NRG (numerical renormalization group), initiated by Wilson [10], developed further first by White's DMRG (density matrix RG) [11] and most recently by Vidal's ER (entanglement renormalization) [12]. However, the inability of DMRG for two dimensions is now clear and one still needs to see how much that inability of DMRG can be improved by ER. Indeed, a deep question remains, namely how far one can go with the very idea of the Hilbert space truncation.

In recent papers, one, two and three of us (SGC) started a novel many-body method to calculate partition functions for dimensional macroscopic classical systems and the ground states of macroscopic quantum systems in one dimension [13,14]. We call this method EPT (entanglement perturbation theory). The key point of EPT is that it does not truncate the Hilbert space (no RG), and it does not have the finite size problem. Of particular interest among many possible extensions and applications of the EPT is how the EPT handles the fermion anticommutation algebra leading to infinite range correlations among fermions. Let us call this problem simply the sign problem in a wider sense [15]. No existing non-mean-field methods can handle this sign problem satisfactorily.
We here formulate the EPT for the quantum ground states in two dimensions. Our preliminary calculations on the 2D Heisenberg antiferromagnet and the Hubbard model show that EPT is computationally feasible [16]. A fortunate situation for EPT is that, due to the fact that it is based on the local basis, the free electron gas is most challenging but of course soluble by hand. Moreover, the fermion sign problem can still be handled by EPT: An essential difference from spins and bosons is that we need to calculate the excited states of an 1D infinite object but with an essential simplification that only the excited states with the same translational symmetry as the ground state need to be calculated, making the EPT calculation highly executable. We thus recognize the following issues for EPT: (1) to establish a stable and converging numerical procedure, and (2) to treat 2D fermions on a rigorous footing. It is also known that Monte Carlo encounters a negative sign problem not only in fermions but also in spins on a frustrated lattice such as Kagomé. EPT is free from this difficulty, and the quantum spin liquid issue offers an excellent testing ground for EPT.

References:

5.2 High Temperature Thermal Stability and Oxidation Resistance of Magnetron-Sputtered Homogeneous CrAlON Coatings on 430 Steel

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Current energy crises and fuel prices have made Solid oxide fuel cells (SOFC) increasingly attractive as a way of converting chemical energy into electrical energy by means of the electrochemical combination of hydrogen and oxygen via an ion-conducting solid oxide electrolyte. The operational requirements of high ionic conductivity and good catalytic performance in the fuel cell must be balanced against the practical requirements of low cost and high-temperature corrosion resistance for components in the fuel cell stack [1]. Of particular interest in our work is the bipolar plate serving as the current collector or interconnect between adjacent cells of the SOFC stack. The interconnect must not only retain low electrical resistivity throughout the operating lifetime of the fuel cell, but must also have good surface stability, necessitating that thermal expansion and other physical properties be compatible with the materials in the stack [2]. Doped LaCrO$_3$ plates have worked well for cells operating at 1000°C, but suffer from high cost as well as difficulties in fabrication. A thorough evaluation of several heat-resistant alloys with a variety of compositions led to the conclusion that it would be difficult for most traditional alloys to meet the material requirements of long-term operation above 700°C [2]. Alloys of bcc, ferritic stainless steels appear to have thermal expansion coefficients that are well matched to other components in the stack, but do not possess the high electrical conductivity needed for required operation. The authors conclude that for improved oxidation resistance and electrical conductivity, either new alloys need to be developed, or surface engineering of existing alloys is required [3]. The present work falls into the latter category of surface engineering, namely, the use of coatings to improve oxidation resistance while maintaining acceptably low resistivity values. Related research on surface engineering includes the use of conducting oxide coatings and thermal nitridation [4].

Chromium nitride is a good oxidation resistant material with anti-corrosive properties. Its uses include applications in metal forming and plastic molding [5,6]. It is presently known that exposing CrN to oxygen at elevated temperatures leads eventually to loss of nitrogen and the formation of Cr$_2$O$_3$ [7] a semiconductor with sufficient low resistivity for use in interconnect applications at an operating temperature of 800°C [8]. In our study, using an RF and DC magnetron sputtering technique, we deposited coatings of varying Cr/Al ratios onto a 430 stainless-steel plate sample substrate. For this particular study balanced magnetron heads were used to deposit CrAlN coatings. For analysis of sample elemental composition and oxidation resistance, Rutherford backscattering spectrometry (RBS) and Non-Rutherford scattering were used. The films were annealed at 800°C in air for up to 25 hrs, and subsequently analyzed.
After the each oxidation period, samples were removed from the tube furnace and were placed in a vacuum chamber for ion beam analysis (IBA) measurements. For the present measurements a beam of 1.1 MeV deuterium ions (D+) and 3.0 MeV protons (p+) were incident on the samples at an angle of 0° from the surface normal. Reaction products were detected at a scattering angle of 170°. Proton beam was used mainly to determine the Cr and Al concentration, whereas, deuterium beam was used to measure the oxygen and nitrogen concentrations. Nuclear reaction analysis (NRA) using D+ can be quite useful in this case because the spectral peaks originating from O and N typically sit on a very low or zero-background signal [9]. Using the SIMNRA program, the set of target composition profile parameters was adjusted until a single set of parameters could be used to accurately simulate both the proton and deuteron spectra of the as deposited samples [10]. The spectra obtained using D+ are shown in the figures 1, 2, 3 and 4, which are the overlapped spectra of the

![Figure 1](image1.png)

**Figure 1** Overlapped spectra of sample A5, taken after each oxidation period, with 1.1 MeV D+ beam at 170 degree scattering angle. Reactions shown are protons from the ^16O(d,p)^17O, ^14N(d,p)^15N and alpha from ^16O(d,α)^13C

![Figure 2](image2.png)

**Figure 2** Overlapped spectra of sample AC1, taken after each oxidation period, with 1.1 MeV D+ beam at 170 degree scattering angle. Reactions shown are protons from the ^16O(d,p)^17O and ^14N(d,p)^15N.

![Figure 3](image3.png)

**Figure 3** Overlapped spectra of sample AC5, taken after each oxidation period, with 1.1 MeV D+ beam at 170 degree scattering angle. Reactions shown are protons from the ^16O(d,p)^17O and ^14N(d,p)^15N.

![Figure 4](image4.png)

**Figure 4** Overlapped spectra of sample C5, taken after each oxidation period, with 1.1 MeV D+ beam at 170 degree scattering angle. Reactions shown are protons from the ^16O(d,p)^17O and ^14N(d,p)^15N.
samples, taken after each oxidation period. Oxygen and nitrogen have several nuclear reactions with the D+ beam. The detected particles for these measurements shown in the figure 1, were protons from the $^{16}$O(d,p)$^{17}$O, $^{14}$N(d,p)$^{15}$N and alpha from $^{16}$O(d,$\alpha$)$^{13}$C. The broader peak is from the nuclear reaction $^{16}$O(d,$\alpha$)$^{13}$C because of energy straggling of the emitted $\alpha$-particle in the coating. This means that the coating has a higher stopping power for $\alpha$-particle than for protons. The peaks shown are the most prominent nuclear reaction, but there are other small satellite peaks which are also reactions with nitrogen. Not shown in these figures is a nuclear reaction with carbon.

To determine oxygen and nitrogen concentrations, only $^{16}$O(d,p)$^{17}$O reaction for oxygen concentration and $^{14}$N(d,p)$^{15}$N reaction nitrogen concentration were modeled. As shown in the figures 1, 2, 3 and 4, notice the N loss and O gain in each of the samples as the oxidation of the samples were carried out. In some cases there is a rapid decrease in N content following the initial one-hour heat treatment, which is attributed to the transformation of CrN to Cr$_2$N [11,12]. Moreover, a more gradual loss of N during subsequent annealing is attributed to the transformation of Cr$_2$N to Cr$_2$O$_3$. Formation of Cr$_2$O$_3$ could have formed a barrier layer for the subsequent oxygen to diffuse into the sample. The area specific resistivity (ASR) studies for uncoated and coated stainless steel samples for CrAl nitride coatings have shown that the values for both coated and uncoated samples reached a minimum of below 10 mohm-cm$^2$. However, the ASR value of the uncoated sample rose relatively fast compared to that for the coated sample, indicating reduced oxidation rate and increased electrical conductivity for the coated samples [13].

Nitrogen was lost with the gain of oxygen in the first 5 hours followed by relative stability. As shown in figure 1, the sample that performed the worst was A5. In first five hours of oxidation, A5 lost most of its nitrogen to oxygen. AC1, shown in figure 2, had a similar Cr/Al ratio as that of A5 and was also similar in performance. The performance of sample AC5, shown in figure 3, and sample C5, shown in figure 4, was almost the same and their Cr/Al ratios were similar as well. These two samples retained most of their nitrogen and therefore are better oxidation resistant samples. The low Cr/Al ratio samples performed poorly, while the high Cr/Al ratio samples were better. The sample that performed the best was C5 with a Cr/Al ratio of 0.9 which correlates with our earlier study [8].

References:

5.3 Ion Beam Analysis of the Thermal Stability of Hydrogenated Diamond-Like Carbon Thin Films on Si Substrate

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Diamond-like carbon (DLC) films have attracted a great deal of attraction because their properties are closely related to diamond. The properties of diamond like carbon films depend upon the growth conditions i.e. ion energy and substrate temperature. Ion beam deposition of diamond like carbon was first carried out by Aisenberg and Chabot [1]. They were able to produce films exhibiting many of the properties of diamond and called them diamond like. Incorporation of hydrogen in the carbon films deposited by PECVD or sputtering system appears to be generally required in order to modify their optical and electrical properties.

An accessible and generally used method to determine the total hydrogen content in a thin film is elastic recoil detection Analysis (ERDA) [2]. In DLC, total hydrogen content critically determines film structure at the atomic level, and therefore the physical properties of the films. Hydrogen content is also a key to obtaining a wide optical gap and high electrical resistivity [3]. Raman studies on these films show that heating DLC in ambient air at temperatures above 300°C, significant conversion of DLC to nano-crystalline graphite takes place. This conversion is complete at 600°C [4]. The loss of hydrogen through annealing at high temperatures generally causes a collapse of the structure to a graphite-like phase dominated by sp² bonds [5].

DLC films are typically transparent in the infrared, with the exception of the CHₓ bonds, which are weakly absorbing in the visible spectrum, and are increasingly absorbing with decreasing wavelength in the UV. The hydrogen content is critical in controlling the optical properties, and removal of hydrogen from DLC films causes the loss of IR transparency [6]. A wide range of optical gap values (E_{opt}), spanning the range from 0.38 to 2.7 [7] were reported for DLC films prepared under presumably similar conditions, indicating the dependence of the property on the deposition conditions. For otherwise similar deposition conditions, E_{opt} was found to decrease strongly for DLC films deposited above 250°C [8]. This behavior reflects the role of hydrogen in stabilizing the structure of DLC layers.

Films deposited at lower temperatures (in the range 25-250°C) contain significant concentrations of hydrogen; most of the sp³ coordinated carbon atoms, as well as a substantial fraction of the sp² coordinated carbons are bound to at least one hydrogen atom. The index of refraction is also affected by the hydrogen concentration in the DLC films. It generally increases with decreasing hydrogen content [9]. A higher index of refraction usually indicates DLC with higher hardness, and better wear resistance. The most substantial structural and property changes occurred at temperatures higher than 400°C [10].
Characterization of the samples is carried out using ion beam analysis (IBA) techniques, which include Rutherford backscattering spectroscopy (RBS), Forward Elastic Recoil detection analysis (ERDA) and Nuclear reaction analysis (NRA). Ion beam analysis of these samples was performed using a 6 MV tandem Van de Graaff accelerator at the department of physics, Western Michigan University, Kalamazoo, MI. Rutherford backscattering spectra (RBS) and Nuclear reaction analysis (NRA) were recorded using 2.5 MeV beam of $\text{H}^+$ ions, incident at 67.5° from the normal to the sample surface. Proton beam was used mainly to determine the C and O concentration in the film. The non-Rutherford enhancement in the cross section of C and O at this energy of protons is useful to precisely measure the concentration of the two elements, especially when these elements are sitting on heavier background like Si. Recoil spectra of the samples was obtained using 16 MeV O$^{5+}$ beam, incident at 67.5° from the normal to the sample surface.

The onset temperature for hydrogen release for all of the samples was found to be around 400° C, as shown in the figure 1. We have shown a qualitative means of comparing the thermal stability of thin films of DLC, deposited on silicon substrates using ion beam analysis techniques. The results from ion beam analysis are both qualitative and quantitative and do not depend on the stoichiometry. From our results, we conclude that hydrogen evolution from DLC films takes place around 400° C. No significant bias effect on the deposited sample was observed. Future measurements will extend the annealing time to better simulate the samples. Also element diffusion process will be investigated quantitatively using He$^+$ beam.

**Figure 1** Hydrogen content (at %) with the annealing temperature for the samples 0-50, 25-50 and 50-50.

**References:**

5.4 Shifts in the Melting Temperature of the Vortex Lattice in 9 MeV Proton Irradiated YBCO

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We compare the effects of low doses of 9 MeV proton irradiation on the first order melting transition temperature with theoretical predictions [1]. Three different single crystals were studied in this investigation. All were characterized before irradiation and after successive 9 MeV proton irradiations ranging from $0.25 \times 10^{15}$ p/cm$^2$ to $2 \times 10^{15}$ p/cm$^2$. The superconducting transition temperature was determined from the peak in the temperature derivative of the electrical resistivity curve, $\frac{dT}{d\rho}$. The width of the transition was defined as the difference between $T_c$ and the temperature where the resistance dropped to zero. The first crystal YBA285 had dimensions of 440 $\mu$m x 880 $\mu$m and a thickness of 40 $\mu$m along the crystallographic c-axis. The zero field superconducting transition temperature $T_{co}$ before irradiation was 92.8K and $\Delta T_{co}$ = 0.4 K. The second crystal, YBA256, had dimensions of 680 $\mu$m x 630 $\mu$m (ab-plane) x 150 $\mu$m (c-axis) with a $T_{co}$ = 93.0 K and $\Delta T_{co}$ = 0.44 K. The final crystal WYB005 had dimensions of 750 $\mu$m x 660 $\mu$m (ab-plane) x 80 $\mu$m (c-axis) with a pre-irradiation $T_{co}$ = 93.4 K and $\Delta T_{co}$ = 0.4 K.

The 9 MeV proton irradiations were performed at Western Michigan University’s tandem van de Graff accelerator at room temperature with the beam directed parallel to the crystallographic c-axis. A low flux of $6.25 \times 10^{10}$ p/cm$^2$sec was used in order to minimize heating during irradiation. This resulted in a temperature increase less than 20°C above ambient temperature during irradiation. Calculations using TRIM [2] simulations give the range of 9 MeV protons in YBCO as 280$\mu$m, which is much larger than the thickness of the crystals used in this investigation. Simulations using the SRIM program with the default lattice energies of 3 eV for all the ions yield vacancy- displacement defect pairs with the following relative concentrations: 7.7% Y: 15.4% Ba: 23.1% Cu: 53.8% O.

Figure 1 shows the normalized first order melting temperature as a function of dose in an applied magnetic field of $H = 6$T applied parallel to the crystallographic c-axis. For all three crystals investigated, the normalized melting temperature decreases roughly linearly with dose at a rate of $6.3 \times 10^3$ per $10^{15}$ p/cm$^2$. This corresponds to a downward shift of 0.58 K for each 1 x $10^{15}$ p/cm$^2$ dose. This downward shift is of the same order of magnitude as predicted by Nonomura and Hu [3] who performed simulations based on a three dimensional frustrated XY model.
Dasgupta and Valls [1] used a numerical minimization of the Ramakrishnan-Yussouff [4] free energy to study the effects of strong random point pinning on the melting transition. They perform their calculations for a concentration of $1.36 \times 10^{-4}$ defects per 100 units cells of the crystal lattice. This corresponds to 1 defect out of every $7.35 \times 10^5$ unit cells. In comparison, Transmission Electron Microscopy and SRIM calculations [5] show that the doses used in our experiments correspond to approximately one defect in $2.9 \times 10^4$ (for the $0.25 \times 10^{15}$ p/cm$^2$) to $3.6 \times 10^3$ (for $2.0 \times 10^{15}$ p/cm$^2$) unit cells of the crystal.

The results of Dasgupta and Valls [1] predict that the transition should cross over to a first order transition between a liquid and a vortex slush at intermediate concentrations of defects. The slush would consist of well defined crystalline domains separated by domain boundaries. However, our previous results have shown that the melting transition does not broaden with increasing defect density. Imry and Wortis argue that this lack of broadening indicates that the energy of creating domain walls in this systems is not energetically favourable [6].

References:

6 NUCLEAR PHYSICS

6.1 Effects of $\beta$-Decays of Excited State Nuclei on the Astrophysical $r$-Process


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The solar system $r$-process abundances act as the canonical constraint to $r$-process theories as well as the prime indicator of the success of $r$-process models. Several $r$-process sites have been proposed; the hot-bubble region of a type II supernova (SNII) has been modeled fairly successfully. The composition of the environment in which the $r$-process occurs might be expected to have a profound effect on the final abundance distribution. Observations indicate that the $r$-process site is primary [1] and further evidence may suggest that the $r$-process is also unique [2], it may occur in a single site or event. The uniqueness of the $r$-process site, however, remains a subject of study [3].

Nuclear properties also constrain the $r$-process, and the purpose of this work is the examination of one particular characteristic - $\beta$-decay - as it relates to the $r$-process. The $\beta$-decay inputs, and other nuclear physics inputs, have been shown [4,5] to have important effects on the success or failure of $r$-process models. This is somewhat unfortunate, as properties of only a few nuclei on the neutron closed shells closer to stability have been experimentally determined, while data for the rest are relegated to calculation. Of paramount importance is the determination of nuclear masses and $\beta$-decay rates. Nuclear mass formulae based on the microscopic properties of nuclei are slowly replacing the empirical droplet models, and these can change resulting reaction rates by factors as large as $10^3$ [6]. As well, the $r$-process path is affected by the choice of mass formula, since the path roughly follows a line of constant $S_n$ [6].

For the purposes of this study, the most recent semi-gross theory of $\beta$-decay [7] has been adapted to neutron-rich nuclei relevant to the $r$-process. The ability of this model to determine decay properties of an extremely wide range of nuclei with reasonable accuracy and speed makes it ideal for this preliminary calculation. In particular, the semi-gross theory has good agreement for very neutron-rich nuclei [8,9]. It has also been used to improve the accuracy of decay rates for astrophysical calculations by incorporating first-forbidden transition strengths [10]. In its original form, the gross theory of $\beta$-decay assumed that the energy states of a nucleus consist of a smoothed distribution with transition strengths that peak at or near the
energy of the isobaric analog state[11]. Subsequent evolutions of the gross theory incorporated strength functions allowing for transitions of higher forbiddenness[12], as well as improvements over the original theory to include odd-odd effects[13], sum rules[14], even-odd mass differences[15], and improvements on the strength functions[16].

The results from several hydrodynamic parameter sets, as well as electron fraction parameter values $Y_e$, were examined. For each parameter set, the core mass in solar masses, core radius, neutrino luminosity, initial electron fraction, and whether or not $\beta$-delayed neutron emission is included are listed. Using these parameters and the calculations of reference [17] the dynamic timescale and the entropy in the expansion are constrained. Though still in agreement with current predictions, the dynamic timescales in these calculations are shorter than average. However, the entropy is lower, and no artificial increase in the entropy (as is often assumed) was required [3].

Each simulation is run until several seconds beyond freezeout. While this time is sufficient to gauge the gross features of the r-process abundance distribution, a longer simulation may have resulted in more post-processing, allowing for smoother abundance distributions. One notes some residual even-odd effects in the calculated distribution as the effects of smoothing may not be complete, though the gross features of the distribution are noted.

Results from two representative models are displayed in Figure 1 for both the hot (i.e., including excited-state decays, solid line) and cold (i.e., not including excited state decays, dotted line) models[18]. The A~195 peak is most profoundly affected, along with the nuclei just below this mass region. From the relationship between the decay rates and temperature, it can be seen that decay rates of the nuclei in the region just below the A~195 peak (and - to a lesser extent - the region just below the A~130 peak) are quite sensitive to changes in temperature even at low temperatures. This is expected due to the high level densities of these nuclei (lying just below the N=126 and N=82 closed shells). Shell quenching has not been

![Figure 1](image)

Figure 1 Comparison of r-process freezeout abundance distributions for two models (a) and (b) [19]. The dots correspond to the solar abundance distribution. The dashed line corresponds to a freezeout distribution assuming excited-state $\beta$-decays, and the solid line corresponds to a model using only ground-state decays.
included in this calculation, though the effect is noted, and no conclusions can be drawn from this study to evaluate the effects of quenched closed shells far from stability. Other rates, however, are not as sensitive to temperature changes at low temperatures and, as the r-process progresses, these rates would drop to their ground-state values before those of the nuclei in the regions below the abundance peaks. The decay rates of nuclei in this region would increase relative to those of nuclei in other regions of the path, selectively depleting the abundances of nuclei in this region.

References:

6.2 Mass Measurements of Astrophysically Interesting Nuclei:
Commissioning of the Zero Degree Spectrometer

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The rapid proton capture process, or rp-process, has seen a great deal of attention as the source of heat and light in X-ray bursts [1]. The rp-process is thought to occur in hot (T~10^9) environments in which the nuclei involved are far from stability. In the case of the rp-process, many of these nuclei lie close to the proton drip line [2]. Theoretical descriptions of the rp-process rely on nuclear reaction network calculations involving hundreds of nuclei and thousands of reactions for the simplest networks. While progress continues in studying important reaction rates and nuclei involved, there is still much to be learned.

A successful model of the rp-process site depends heavily on knowledge of nuclear masses, decay rates, and proton capture rates. These nuclear properties dictate the environment necessary for a successful rp-process. However, because of the expected low level densities of the nuclei involved in the rp-process, statistical rate calculations such as those based on the Hauser-Feshbach formalism are not as accurate as in the cases of the neutron-rich nuclei. For many cases, theoretical predictions of Q-values vary by amounts greater than the temperature of the rp-process environment [3-5], and – though progress is being made - experimental masses of several of the rp-process nuclei are still unknown, and many experimentally determined masses still have large uncertainties. (See, for example, references [6-8].) Likewise, mass models, such as the FRDM and the HF(+BCS), which are used to predict masses of the exotic nuclei, disagree in many cases by several hundred keV near the drip line [9,10]. Experimental validation of the rp-process nuclei is necessitated by these uncertainties [11].

Nuclear reactions from the rp-process are thought to drive the explosive hydrogen burning in X-ray bursts from accreting neutron stars, and the interdependency of the nuclear properties of rp-process nuclei and conditions on the surface of the accreting neutron star has been explored [2]. The light curve of the associated X-ray burst is directly determined by heating from the nuclear reactions within the burst. The burst luminosity and it ensuing evolution are both dictated by the initial amount of hydrogen accreted onto the neutron star and the rate at which it is consumed. Calculations predict that processing to A~100 may be responsible for bursts with timescales of several hundred seconds. Additionally, the shape of the light curve is determined by the rate of processing. Processing dominated by β-decay due to low (p, γ) rates along the rp-process path will cause a “bottleneck” or “waiting point” in the processing, directly affecting the X-ray burst luminosity and lengthening the burst in time. Understanding the luminosity of the burst and the nuclear physics involved will permit a better understanding of the dynamics of the neutron star crust, its composition, rotation, and magnetic field [2,12]. The composition of material produced in the burst is also important, as it has been recently
shown that at least 1% of the p-nuclei in the solar system may have been produced in X-ray bursts [13].

For reasonable analyses of the rp-process environment, Q-values and masses should be known to within roughly kT~100 keV. Widely used mass formulae may suffer disagreements greater than this value. Mass measurements of rp-process nuclei, especially those near the waiting points and out to the proton drip line are extremely useful for not only constraining the rp-process path and pace, but also in constraining mass parametrizations of exotic nuclei. Recent experimentation has been conducted by the spokesperson at the National Superconducting Cyclotron Laboratory to explore the (p, γ) Q-values of the nucleus \(^{69}\text{Br}\) – a possible rp-process waiting point nucleus, and analysis is underway [14]. Other recent measurements have either measured for the first time or reduced the uncertainty in masses of some of the nuclei in the \(^{65}\text{As}/^{70}\text{Br}\) region using TOF techniques [15]. A reduction in the uncertainties of the previous mass measurements along with the measurements of new masses will help to further constrain uncertainties in the mass models used while providing experimental data for current network calculations. Nuclei around this waiting point may include \(^{60-64}\text{Ga}\), \(^{62-65}\text{Ge}\), \(^{64-67}\text{As}\), \(^{66-69}\text{Se}\), and \(^{70-72}\text{Br}\), as the rp-process path is thought to pass through these nuclei. The accuracy of current mass models at the proton-drip line would also be tested in a study of these nuclei. Finally, measurements of these nuclei would present new experimental challenges as good statistics can now be obtained for mass measurements using TOF techniques with the RIBF facility, pushing the limits of studied masses towards the proton drip line.

The masses of several nuclei near the \(^{68}\text{Se}\) waiting point will be measured directly using the TOF-Bρ technique [1,15]. The nuclei studied include, but are not necessarily limited to, \(^{60}\text{Ga}\), \(^{62,63}\text{Ge}\), \(^{64-66}\text{As}\), \(^{66,67}\text{Se}\), \(^{70,71}\text{Br}\). Some of these nuclei have been studied before using the TOF-Bρ or other techniques, and the current experiment seeks to verify the previous measurements with high statistics provided by the RIBF. The masses of most of these nuclei have never been measured, and will represent a first measurement. The accelerator settings used to produce the studied nuclei will also produce nuclei for which masses are already well known. These nuclei will be used as reference masses to calibrate the TOF experiment.

Using this technique, the time-of-flight (TOF) of a nucleus between two points in the accelerator is related to its mass:

\[
\frac{\gamma m}{Q} = \frac{B\rho t}{L}
\]

where a nucleus of mass m, charge Q, Lorentz factor \(\gamma\), and rigidity Bρ takes a time t to travel a distance L along the beamline. The travel time for two nuclei, one of well-known mass, can be compared using this technique. It is expected that masses of individual beam particles can be measured to an accuracy of \(~10^{-4}\) with average mass measured to an accuracy of about \(2\times10^{-6}\). The expected lifetime limit for nuclei studied in this experiment is about 445 ns.

In addition to an accurate mass measurement of new proton-rich nuclei, the accuracy of mass formulae in this region can be gauged [1-3].

Phase I of an experimental program to measure the masses of exotic nuclei is now in progress with the completion of the commissioning of the RIBF zero-degree spectrometer. This
commissioning includes the operation and testing of the spectrometers in various optics modes. Of particular interest is the rigidity resolution of the spectrometer (A/Q) in these modes. Preliminary particle identification is shown in Figure 1 for a $^{238}$U primary beam, and the resulting A/Q resolution has been measured to be as low as 0.1% for the full acceptance mode of operation. For modes with a much tighter acceptance, this resolution can be improved dramatically.

![Figure 1](image.png) Preliminary PID plot for the ZDS commissioning corresponding to the full acceptance optics mode of the ZDS.

References:

6.3 Constraining the Nuclear Equation-of-State

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Collisions involving 112Sn and 124Sn nuclei have been calculated with the Improved Quantum Molecular Dynamics transport model. The results of the calculations reproduce the data from two isospin diffusion measurements and the ratios of neutron and proton spectra. By comparing these data to calculations performed over a range of symmetry energies at saturation density and different representations of the density dependence of the symmetry energy, constraints on the density dependence of the symmetry energy at sub-normal density are obtained. These constraints are compared to existing constraints from other recent analyses.

The nuclear symmetry energy, which describes the difference between the binding energy of symmetric matter, with equal proton (Z) and neutron (N) numbers, and that of neutron rich matter, governs important properties of nuclei and neutron stars [1,2]. In nuclei, the symmetry energy and the Coulomb energy define the binding energy minimum where nuclei are stable against beta decay [3,4]. In neutron stars, the symmetry energy and its density dependence influence strongly the nature and stability of the phases within the star [5], the feasibility of direct URCA cooling processes within its interior [6], the composition [5] and the thickness of its inner crust, the frequencies of its crustal vibrations [7], as well as its radius, and mass [7].

The sum of the symmetry energy and the energy per nucleon of symmetric matter, \( E(\rho, \delta) = E_0(\rho, \delta=0) + E_{\text{sym}} \), provides the total energy per nucleon (i.e. the Equation of State (EoS)) of cold matter. The average symmetry energy per nucleon in uniform matter can be written as \( E_{\text{sym}} = S(\rho)\delta^2 \), where the asymmetry \( \delta = (\rho_n - \rho_p)/\rho \) where \( \rho_n, \rho_p, \) and \( \rho \) are the neutron, proton and nucleon number densities, and \( S(\rho) \) describes the density dependence of \( E_{\text{sym}} \). Both symmetry and total binding energy terms in the nuclear semi-empirical binding energy formulae reflect averages of \( E_{\text{sym}} \) over the densities of nuclei [3]. The values of surface and volume symmetry energy terms obtained over fits of such formula to measured masses provide some sensitivity to the density dependence of \( S(\rho) \) near saturation density [3,4]. Giant resonances, low-lying electric dipole excitations and the difference between neutron and proton matter radii may also provide sensitivity to the density dependence of \( S(\rho) \) near saturation density [8-11].

We have preformed a series of ImQMD calculations at \( b=6 \) fm with different values of \( \gamma_i \) with \( S_0 \) between 25 to 40 MeV to locate the approximate boundaries in the \( S_0 \) and \( L \) plane that satisfy the 2\( \sigma \) criterion in the \( \chi^2 \) analysis of the isospin diffusion data where the slope parameter \( L=3p_d S(\rho)/d\rho \approx [3/\rho_0]p_0 \). Even though the sensitivity of constraints on \( S_0 \) and \( L \) to differences between \( m_n \) and \( m_p \) and to the in-medium cross-sections have not been fully
explored, BUU calculations indicate that their sensitivities to these are weaker than their sensitivities to $S_0$ and $L$.

Initially, neutron/proton double ratio data have been calculated using the ImQMD model [12]. This observable derives its sensitivity to the symmetry energy from the opposite sign of the symmetry force for neutrons as compared to protons [13]. First experimental comparisons of neutron to proton spectra in ref. [14] used a double ratio to reduce sensitivity to uncertainties in the neutron detection efficiencies and to relative uncertainties in energy calibrations of neutrons and protons. This double ratio

$$DR(Y(n)/Y(p)) = \frac{R_{n/p}(A)}{R_{n/p}(B)} = \frac{dM_n(A)/dE_{CM}}{dM_p(A)/dE_{CM}} \cdot \frac{dM_n(B)/dE_{CM}}{dM_p(B)/dE_{CM}}$$

is constructed from the ratios of energy spectra, $dM/dE_{CM}$, of neutrons and protons for two systems $A$ and $B$ characterized by different isospin asymmetries. The star symbols in the left panel of Figure 1 show the neutron-proton double ratios measured at $70^\circ \leq \theta_{CM} \leq 110^\circ$ as a function of center-of-mass (C.M.) energy for nucleons for central collisions of $^{124}$Sn+$^{124}$Sn and $^{112}$Sn+$^{112}$Sn [14].

We have performed calculations for two systems: $A=^{124}$Sn+$^{124}$Sn and $B=^{112}$Sn+$^{112}$Sn. About 60,000 events are simulated for each impact parameter. Within the statistical uncertainties, the double ratio observable, $DR(Y(n)/Y(p))$, is nearly independent of impact parameter over a range of $0 \leq b \leq 5$ fm. The lines in the left panel of Figure 1 show double ratios vs. the C.M. energy of nucleons emitted at $70^\circ \leq \theta_{CM} \leq 110^\circ$ for $\gamma_i=0.35, 0.5, 0.75, 1$ and 2. The computation uncertainties in Figure 1 are statistical. To increase the statistics for high energy nucleons, the double ratios are averaged over $b=1, 2, 3$ fm.

Despite the large experimental uncertainties for higher energy data, these comparisons definitely rule out both very soft ($\gamma_i=0.35$, dotted line with closed diamond points) and very
stiff ($\gamma_i=2$, dotted line with open diamond symbols) density-dependent symmetry terms. The right panel shows the dependence on $\gamma_i$ of the total $\chi^2$ computed from the difference between predicted and measured double ratios. We determine to within a 2$\sigma$ uncertainty, $0.4 \leq \gamma_i \leq 1.05$ corresponding to an increase in $\chi^2$ by 4 above its minimum of near $\gamma_i$=0.7.

In summary, the ability of QMD models to reproduce both isospin diffusion and double ratio of neutron and proton spectra data is an important step forward in obtaining information about the symmetry energy in heavy-ion collisions. All three observables examined here provide consistent constraints on the density dependence of the symmetry energy. Some shifts in the boundaries of the constraints can be expected with improvements in the precision of the experimental data and in the understanding of transport calculations. Nevertheless, the consistency between the different probes of the symmetry energy suggests that increasingly stringent constraints on the symmetry energy at sub-saturation density can be expected.

References:

6.4 The $p$-Shell $\Lambda$-Hypernuclei with the Nijmegen ESC04 Baryon-Baryon Potential

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Beginning in 1998 a series of experiments using the Hyperball detector [1] attempted to measure gamma rays from $p$-shell $\Lambda$-hypernuclei. The experiments ended in 2005 with KEK 566. Data from this last experiment are still under analysis, but the energy and yield of the measured gamma rays from all experiments have provided valuable information on the structure of seven nuclei. These experiments were motivated by the work of Refs. [2] and [3]. It was shown in Ref. [2] that the five $p_{N\Lambda}$ two-body matrix elements depend on the radial integrals associated with each component of the standard interaction, $V_{AN}(r) = V_0(r) + V_\sigma(r)S_N S_\Lambda + V_\Lambda(r)S_N + V_N(r)S_N + V_T(r)S_{12}$. The radial integrals are conventionally denoted by the parameters $\bar{V}, \Delta, S_J, S_N$, and $T$. The energy splitting of spin partners can be related to these parameters and, therefore, to the spin-dependent components of the $\Lambda N$ interaction. Hence, calculations for the $p$-shell nuclei provide a test of these components. This test is applied to the new Nijmegen ESC04 potentials [4].

Effective interactions were generated via the Brueckner-Hartree procedure with $^4$He and $^{16}$O cores for the four ESC04 potentials. Structure calculations were then performed for the seven nuclei in the RCCSM formalism and with the Cohen and Kurath (6-16) [5] $NN$ interaction. This formalism allows expansion of the $\Lambda$ wave function in a series of oscillators as measured from the center of mass of the core. It also allows use of the $\Lambda$ mass, and yet still allows no spurious components. The results for $^7_{\Lambda}$Li with the $^4$He core interaction are shown in Fig. 1. From the results of Ref. [6], one expects to see overbinding from the ESC04 potentials. However, one sees that ESC04B gives excellent values for the two splittings. The $1/2^+ - 3/2^+$ splitting depends almost entirely on the spin-spin parameter $\Delta$. One cannot calculate a value of $\Delta$ for realistic interactions like those from ESC04 because they have different even and odd components. However, one can extract an effective $\Delta$ by turning off all components of the interaction except the triplet and singlet central terms and then compare the calculated splitting with the formula in Ref. [7], $1/2^+ - 3/2^+ = 1.461 \Delta$. With the $^4$He core interaction one extracts an effective $\Delta$ value of 0.428. This compares favorable with that obtained from fits with the standard interaction, $\Delta = 0.430$. The standard interaction requires a smaller $\Delta$ from the middle to the end of the $p$-shell [7]. Figure 2 demonstrates that this requirement arises very naturally as the Pauli operator changes from the $^4$He core to the $^{16}$O core and weakens the spin- spin interaction. The ESC04B interaction continues to do very well on the structure throughout the $p$-shell. ESC04A also does well until $^{16}_{\Lambda}$O. ESC04C and ESC04D do miserably. The refit NSC89 is slightly worse than ESC04A. The primary difference between the pair A,B and the pair C,D is the spin-spin interaction. This can be seen in the ratio of the
relative g-matrix elements $^1S_0^2S_1$ for $n=0$. For A, B, C, D, and the refit 89, this value with the $^4$He core is 1.65, 1.48, 1.06, 1.18, and 1.50, respectively.

Clearly, any new $YN$ interaction must have a value close to those of A and B.

References:

6.5 The Structure of $^7$He


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Although the resonance corresponding to the ground state of $^7$He has been known for over three decades, the properties of excited states of this exotic, very neutron-rich system have remained uncertain. With only seven nucleons, this system is one in which modern theories of nuclear structure such as the Quantum Monte Carlo (QMC) approach can be readily applied. This technique can predict not only the spins, parities, and excitation energies of states in light nuclei with A<12, but also can be used to calculate the spectroscopic factors for nucleon transfer reactions. In $^7$He, the low-lying excited states are predicted to be populated very selectively by neutron stripping (adding one neutron to $^6$He) or proton pickup (removing one proton from $^8$Li) reactions. Previously, we have studied the neutron-stripping reaction $^6$He(d,p)$^7$He, and identified a likely candidate for the $J^π=1/2^-$ first-excited state. More recently, we have used the proton-removal reaction $^8$Li(d,3He)$^7$He to produce $^7$He in a complementary fashion, using a radioactive $^8$Li beam produced with the in-flight facility at the ATLAS accelerator at Argonne National Laboratory. The $^3$He ejectiles, and the $^6$He and $^4$He residual nuclei left from the decay of $^7$He, were detected using a set of silicon detectors. Theory predicts that this second reaction should populate the ground and second-excited 5/2$^-$ of $^7$He. Figure 1 shows excitation-energy spectra from these two reactions, where the excited states in $^7$He are identified by their decay properties. The first excited state decays by single-neutron emission (Fig. 1b) and experimentally is produced only in neutron transfer. The second-excited state populated in the (d,$^3$He) reaction decays by 3-neutron emission (Fig. 1f).

![Figure 1](image)

Figure 1 Excitation-energy spectra for the $^2$H($^6$Li,3He)$^7$He and $^2$H($^6$He,p)$^7$He reactions. The $^3$He particles in (a-c) and protons in (d-f) are detected in coincidence with $^6$He and $^4$He, $^6$He, and $^4$He ions, respectively.
The QMC calculations, combined with a distorted-wave Born approximation (DWBA) of the scattering reaction can predict the cross sections for the $^8\text{Li}(d,^3\text{He})^7\text{He}$ reaction. Figure 2 shows angular distributions for this reaction (Fig. 2d, Fig. 2e) as well as for $(d,t)$ and $(d,^3\text{He})$ reactions with a stable $^7\text{Li}$ beam as a calibration reaction. The theoretical results are in quite reasonable agreement with the data, giving confidence in the predictions from the modern nuclear-structure calculations even for the exotic, unbound neutron-rich $^7\text{He}$.

**Figure 2** Angular distributions for various transitions in $^7\text{Li}+d$ and $^8\text{Li}+d$ interactions. The curves are described in the text.
6.6 The $^2\text{H}(^{11,12}\text{B},p)^{12,13}\text{B}$ Reactions and the Influence of $^{11,12}\text{B}(n,\gamma)$ on the r-Process Abundance of Light Elements

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The rapid neutron capture process, or r-process, is a set of neutron-capture and beta-decay reactions thought to occur in violent, explosive astrophysical environments such as Type II supernovae, neutron-star mergers, or gamma-ray bursts. The r-process is responsible for the production of many heavy elements, but recently the success of the neutrino-driven wind model for core-collapse supernova have suggested that light, neutron-rich nuclei should also be considered. To determine the possible reaction paths and predict the abundance of nuclei produced in this particular r-process, it is important to understand the properties of the nuclei involved. Two reactions that could influence the r-process are the neutron-capture reactions on $^{11,12}\text{B}$. The $^{12}\text{B}(n,\gamma)$ neutron-capture reaction cannot be performed in the laboratory, however it is possible to study some of the relevant aspects of the residual nucleus $^{13}\text{B}$ using the neutron-transfer reaction $^{12}\text{B}(d,p)^{13}\text{B}$. We have studied this reaction using a radioactive $^{12}\text{B}$ beam produced at the In-Flight facility at the ATLAS accelerator laboratory at Argonne National Laboratory. In the same experiment, the $^{11}\text{B}(d,p)^{12}\text{B}$ reaction was also studied with a stable $^{11}\text{B}$ beam that was used as calibration. The protons from the (d,p) reactions were detected using an array of segmented silicon detectors, and the $^{13}\text{B}$ and $^{12}\text{B}$ ($^{12}\text{B}$ and $^{11}\text{B}$) fragments from bound and unbound states in $^{13}\text{B}$ ($^{12}\text{B}$) were detected in a set of silicon $\Delta E-E$ telescopes to provide particle identification.

The most important state in $^{11}\text{B}$ for the r-process is the 3.389 MeV state that lies just above the neutron-decay threshold in $^{12}\text{B}$. For this level, we have determined the neutron-decay branching ratio $\Gamma_n/\Gamma_\gamma$ to be 94±5 compared to a previous estimate of 124 from Raucher et al [1]. This result increases the resonance strength $\omega_\gamma$ by approximately 50% over previous estimates, and the reaction rate of $^{11}\text{B}(n,\gamma)^{12}\text{B}$ increases by approximately the same amount. For $^{13}\text{B}$, the important states above the neutron-decay threshold in the vicinity of 5 MeV excitation energy were previously thought to have negative parity; the present results suggest positive parity instead and the influence of resonant neutron capture through these levels is currently being assessed.

Reference

6.7 HELIOS: The HELical Orbit Spectrometer

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The HELIOS device is a novel new spectrometer, based on a large-volume high-field magnetic solenoid, designed to study nucleon transfer and other reactions in inverse kinematics. A detailed technical description of the device and its expected capabilities are contained in Ref. [1]. HELIOS plays a prominent role in the future Strategic Plan for the ATLAS facility, as it is well matched to the ongoing CARIBU radioactive beam source development project.

Over the past year, major progress has been made in the HELIOS project, and the spectrometer is complete in its prototype form. The magnetic solenoid, obtained from Siemens, is installed at the ATLAS facility at Argonne National Laboratory, and the mechanical elements that transform the bore of the magnet into an evacuated reaction chamber are complete and installed. The HELIOS beam line has also been constructed and is now ready to accept both stable, and unstable beams from the ATLAS accelerator. Commissioning experiments that will demonstrate the functionality of the device are scheduled for 2008 and 2009, using stable, and unstable beams, respectively. Figure 1 shows the upstream end of the spectrometer with detector electronics installed.

The heart of the spectrometer is an array of position-sensitive silicon detectors constructed at WMU (Fig. 2). The energy and position resolutions of the detectors used in the array were previously evaluated using proton beams from the WMU tandem accelerator. The silicon array is now installed in the magnet (See Fig. 3), and the performance of the device has been evaluated using alpha particles from a radioactive source. The performance of the silicon array was excellent, and should provide the resolution necessary to identify closely spaced excited states populated in inverse-kinematic transfer reactions that will make up a significant fraction of the physics program that will utilize the unstable beams from the CARIBU source.

Reference:

Figure 1 Completed HELIOS spectrometer at the ATLAS facility at Argonne National Laboratory.
Figure 2 Assembled HELIOS silicon-detector array ready for installation in the HELIOS chamber.
Figure 3 Silicon-detector array installed in HELIOS chamber.
7 PHYSICS EDUCATION

7.1 Facilitating Change in Undergraduate STEM: Initial Results from an Interdisciplinary Literature Review

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Introduction

Recent decades have seen increasing calls for fundamental change in the teaching of Science, Technology, Engineering, and Mathematics (STEM) based, in part, on the concern that the United States will lose its role as a leader in science and technology fields due to outdated and inappropriate instructional practices [1]. The resulting significant expenditures of time and money focused on improving teaching and learning have met with only modest success [2].

We see three distinct research communities involved in this endeavor to improve undergraduate instruction in STEM disciplines. Disciplinary-based STEM Education Researchers (SER) are particularly interested in studying student learning within their discipline and developing discipline-specific curricular materials to improve this learning. Faculty Development Researchers (FDR) often focus on providing faculty with more general pedagogical skills or motivation and tools for self-improvement. Higher Education Researchers (HER) often study how cultural norms, organizational structures, and state and national environments and policy influence higher education practices.

We see a need for interdisciplinary research on STEM instructional improvement that draws from the knowledge and experiences of all of these research communities. The initial analysis of the peer-reviewed literature presented here is one of the early steps in this agenda. The research questions are:

1) What strategies do change agents use to promote change in undergraduate STEM teaching practices?

2) How do change strategies described by authors relate to the disciplinary background of the authors?

3) What evidence is available to support the effectiveness of these strategies?

4) How do authors connect their work with other change literature (e.g., individual and organizational change theories)?
Methods

We identified journal articles that describe efforts by change agents to improve instructional practices used in undergraduate STEM education. For this initial review, we examined 130 randomly chosen articles from the set of 295 articles identified. An inductive analysis process led to the emergence of four categories of change strategies. In a second analysis round, we selected 10 articles from each of the four categories for further qualitative examination. Additional details about the methodology and results can be found in Ref. [3].

Analysis and Results

The four proposed categories of change strategies are based on the answers to two fundamental questions. The first question was, “What is the primary aspect of the system that the change strategy seeks to directly impact: individuals or environments and structures?” The second question was, “To what extent is the intended outcome for the individual or environment known in advance: prescribed or emergent?”

Four Categories of Change Strategies

Based on the possible combinations of responses to the two guiding questions, we developed a four-square typology of change strategies (Figure 1). Of the 130 articles, 15 were not relevant to our analysis and were removed. Four articles could not be classified in a single category. The remaining 111 articles fit into one of the four core categories.

Individual/Prescribed: Focus on Disseminating Curriculum and Pedagogy. (39 articles, 30%).

The emphasis of this type of intervention is on communicating the change agent’s vision of good teaching to individual instructors. The prominent aspects of the interventions typically include curricular materials, instructional strategies, and/or associated instructor knowledge/conceptions.

Individual/Emergent: Focus on Developing Reflective Teachers. (40 articles, 31%). The emphasis of this type of intervention is on encouraging teachers to use their own knowledge, experience, or skill to improve their instructional practices. Information about various instructional strategies and materials may be provided, but this is not the main focus.

Environments/Prescribed: Focus on Developing Policy. (18 articles, 14%). The emphasis is on developing appropriate environments (e.g., rules, reward systems, reporting requirements, investments in support structures) to facilitate instructors’ engaging in specific or desired activities.
Environments/Emergent: Focus on Developing Shared Vision. (6 articles, 5%). The emphasis is on developing a new collective vision for the department, institutional unit, or institution that supports new modes of instruction. The change agent uses stakeholders to develop a shared vision and design new environments that are consistent with this vision.

**Conclusions**

1. **Change Strategies Used.** Change strategies described in the articles were much more likely to focus on changing individual faculty (61% of all 130 articles) than on changing environments or structures (19%). The articles were more evenly divided between working towards prescribed outcomes (44%) and emergent outcomes (36%). We conclude that change agents frequently work at the individual level, rather than at extra-individual levels.

2. **Use of Different Change Strategies by Different Disciplines.** We proposed that the three different disciplines (SER, FDR, and HER) each operate more or less independently of one another and that each has their own distinct perspectives and strategies about change. The literature classification supports this proposition.

3. **Evidence of Effectiveness of Change Strategies.** Of the 43 articles analyzed, 13 did not present a specific change strategy warranting evidence of success. Of the 30 remaining, we judged 12 (40%) to have at least moderate evidence supporting their assertions of success (or lack thereof) of a change strategy. Five articles were judged to offer weak support, and 11 offered little or no support. No articles offered strong evidence supporting the success of a change intervention.

4. **Connections with Other Change Literature.** Fewer than half (20/43) of the articles cited literature that we could label “change literature.” Those that did not fit within our assessment of using change literature typically not only failed to ground their selected change strategy in the change literature, but also failed to justify their choice of change strategy. This trend was consistent across the four change categories.

**Discussion**

We plan to continue with the analysis. An important trend thus far is that it appears to be possible to use two relatively simple criteria to usefully categorize articles about STEM instructional change into a small number of meaningful categories. In addition, the categories presented here support our supposition that the three disciplines operate independently and use largely different strategies for promoting change. This finding supports our expectation that interdisciplinary work involving researchers from SER, FDR, and HER might be productive since each group can bring different sets of knowledge. There is no evidence that we have missed an important disciplinary community. Finally, an important trend is the presence of common weaknesses across all four change categories and all three research communities. Many of the articles did not present convincing evidence to support the conclusions drawn and many articles did not build arguments and change strategies from the
research literature. This finding suggests that there is substantial need for synthesis work such as the work represented by this project.

Acknowledgements:

We wish to thank the National Science Foundation for their support of this project (SES-0623009, DRL-0723699) as well as participants at the June 2008 Facilitating Change symposium for their valuable feedback on this work.

References:


8 PUBLICATIONS

8.1 Papers Published


D. Strohschein, D. Rührbein, T. Kirchner, S. Fritzsche, J. Baran, and J. A. Tanis, Nonstatistical Enhancement of the 1s2s2p 4P State in Electron Transfer in 0.5 – 1.0 MeV/u C^{4,5+} + He and Ne Collisions, Phys. Rev. A 77, 022706 (2008).


8.2 Papers in Press


### 8.3 Papers Submitted


### 8.4 Books Published

9 DISSERTATIONS

9.1 Ph.D


9.2 Masters
10 PRESENTATIONS

10.1 Research Talks at Professional Meetings and Other Institutions

10.1.1 Invited


C. A. Burns, *Electronic Interactions in the Strongly Correlated Liquid Metal Li-NH₃*, IXS Workshop, APS Users Meeting, Argonne, IL May 6, 2008.


C. Henderson, A. Beach, N. Finkelstein, and R. S. Larson, *Preliminary Categorization of Literature on Promoting Change in Undergraduate STEM*, Facilitating Change in Undergraduate STEM Symposium, Augusta, MI, June 17, 2008.


J. A. Tanis, *Nonstatistical Enhancement of (1s2s2p) 4P and (2p 5 3s3p) 4D Metastable States in Electron Transfer*, Symposium at the Institute of Modern Physics, Fudan University, Shanghai, China, November 21, 2007.


A. H. Wuosmaa, HELIOS at ATLAS – A New Tool for Inverse-kinematic Reactions, Nuclear Chemistry Department, Washington University at St. Louis, March 2008.

A. H. Wuosmaa, Insights into the Structure of $^7$He, Heavy-Ion Discussion Group, Physics Division Argonne National Laboratory, March 2008.

10.1.2 Contributed


N. Finkelstein, C. Henderson, A. Beach, and R. S. Larson, *Considering Change in STEM Education: A Research-Based Perspective on Initiating and Sustaining Change*, Physics Teachers Education Coalition National Meeting, Austin, TX, February 29, 2008.


A. Beach and C. Henderson, *Identifying Connections within the Literature on STEM Instructional Change Using a Historiographic Approach*, Facilitating Change in Undergraduate STEM Symposium, Augusta, MI, June 17, 2008.

C. Henderson and M. Dancy, *Science Faculty and Educational Researchers: Divergent Expectations as Barriers to Instructional Change*, Facilitating Change in Undergraduate STEM symposium, Augusta, MI, June 17, 2008.


G. Turri, B. Lohmann, B. Langer, G. Snell, U. Becker and N. Berrah, *Spin Polarization of the Ar*\(^+\) 2p\(^{1/2}\)4s, and 2p\(^{1/2}\)3d Auger Decay*, 15\(^{th}\) International Conference on Vacuum Ultraviolet Radiation Physics, p. 107, Berlin, Germany, July-August (2007).


10.2 Research and Public Lectures at WMU

The Department of Physics sponsors lectures on physics research intended mainly for graduate students and faculty. These talks inform faculty and students at Western of research efforts here and at other institutions as well as acquaint visiting speakers with our research and academic programs at Western. The Department of Physics also sponsors public lectures on physics topics of general interest. These talks are intended for faculty, physics graduate students, physics undergraduate students, and non-physicists. The research and public lectures are listed below.


**Smashed Atoms Tamed - Thermalized Rare Isotope Beams from Projectile Fragmentation for Mass Measurements and Other Precision Experiments**, Georg Bollen, National Superconducting Cyclotron Laboratory, Michigan State University, October 1, 2007.

**Shell Evolution and Structure of Exotic Nuclei in the sd-pf Shell Region**, Utsuno Yutaka, Japan Atomic Energy Research Institute, October 8, 2007.

**Educational Outreach in Physics**, Elizabeth Simmons, Michigan State University, October 15, 2007.


**Big-Bang and Stellar Nucleosynthesis Studied in the Laboratory**, Fred Becchetti, University of Michigan, October 22, 2007.


Network-Based Manipulation of Complex Systems, Adilson E. Motter, Northwestern University, November 12, 2007.

Thermal Lens Shaping: A New Modality for Diode-Pumped Solid-State Lasers, W. Andreas Schroeder, Department of Physics, University of Illinois at Chicago, November 19, 2007.


Acoustic Birefringence in Superfluid $^3$He, William P. Halperin, Department of Physics, Northwestern University, December 3, 2007.

Quasars and the Birth and Evolution of Galaxies, Kirk Korista, Department of Physics, Western Michigan University, January 14, 2008.


Gas Phase Physics and the Evolution of Galaxies, J. Christopher Howk, Department of Physics, University of Notre Dame, February 4, 2008.


The Fascinating World of Exotic Nuclei, Werner Richter, University of the Western Cape, South Africa, February 13, 2008.

Predicting the Properties of Atomic Clusters when Every Atom Counts, Koblar Alan Jackson, Department of Physics, Central Michigan University, February 18, 2008.

The Tevatron and the CDF Experiment – A Year in Review, Robert Roser, Fermi National Accelerator Laboratory, February 25, 2008.

Spartan Infrared Camera, High Resolution Imaging for the Soar Telescope, Ed Loh, Department of Physics and Astronomy, Michigan State University, March 10, 2008.

Reflections of AGN Outbursts in the Hot Gas in Galaxies and Clusters, Christine Jones, Center for Astrophysics, Harvard University, March 24, 2008.

Reflections from Outbursts of Supermassive Black Holes at the Centers of Galaxies, Christine Jones, Center for Astrophysics, Harvard University, March 25, 2008.

Using X-rays to Probe Biomolecular Interfaces, Andrew Richter, Valparaiso University, March 31, 2008.

The Role of Language in Learning Physics, David Brookes, Postdoctoral Research Associate, Illinois Physics Education Research Group, University of Illinois at Urbana-Champaign, April 7, 2008.

Hans Bethe – Master Calculator and Gentleman of Science, Robert Manweiler, Valparaiso University, April 14, 2008.
11 PROPOSALS AND GRANTS

N. Berrah (PI), Department of Energy, Office of Science, BES, Division of Chemical Sciences, Geosciences and Biosciences grant. Project title: Probing Complexity using the ALS and the LCLS, funded $590,000 for period March 2008-2011.


N. Berrah (Co-PI), and Subra Mural (Co-PI), WMU Chemistry Department, Presidential Innovation Fund, WMU to establish a Center for Nano-Enabled Instrumentation and Nanofabrication (CNIN), awarded $383,000, for the period 03/06-02/08.

N. Berrah (PI), Artie Bienenstock, Stanford University and Judy Franz, APS (Co-Pis), Gender Equity: Strengthening the Physics Enterprise in Physics Departments and National Laboratories, NSF, awarded $90,000 for the period 2006-2008.

N. Berrah (PI), Artie Bienenstock, Stanford University and Judy Franz, APS (Co-Pis), Gender Equity: Strengthening the Physics Enterprise in Physics Departments and National Laboratories, DOE, Office of Science, awarded $90,000 for the period 2006-2008.

N. Berrah (PI), Gender Equity: Strengthening the Physics Enterprise in Physics Departments and National Laboratories, NSF and DOE funded, supplement, $10,000 for Fall 2007.

N. Berrah (PI), applied for 12% of beamtime, every six months, for three years on undulator beamline 10.0.1 of the Advanced Light Source, Lawrence Berkeley National Laboratory, CA, beamtime to carry out research experiments was granted for 2008-2011.

N. Berrah (PI), applied for beamtime at a higher energy undulator beamline, (8.0.1) at the Advanced Light Source, beamtime granted for 3 weeks (2007-2008).

N. Berrah (PI), NSF, Project title: PROMISE: Providing Resources, Opportunities, and Mentoring In Science and Engineering for Women Faculty at Western Michigan University, $3,912,516 requested, not funded.

S. Chung, National Science Foundation, Entanglement Perturbation Theory for Strongly Correlated Condensed Matter Systems, requested $499,502, not awarded.

S. Chung, National Science Foundation SU of Teragrid Cobalt Supercomputer at the University of Illinois at Urbana-Champaign, A Novel, Many-Body Method in Condensed Matter Physics, awarded $10,000 to February 28, 2009.


C. Henderson (PI) and M. Dancy, (Co-PI), Understanding Instructor Practices and Attitudes Towards the Use of Research-Based Instructional Strategies In Introductory College Physics, National Science Foundation, $331,143 awarded for the period 1/1/08 to 12/31/10.

A. Beach (PI), C. Henderson and N. Finkelstein, (Co-Pls), STEM Educational Change Efforts in Higher Education: A Meta-Synthesis of Activities, Strategies, Concepts, and Theories across Disciplines, National Science Foundation, $198,379 awarded for the period 9/15/07 to 9/14/09.


A. N. Kayani (PI), M. A. Famiano (co-PI), E. Y. Kamber (co-PI), J. A. Tanis (co-PI), and A. H. Wuosmaa (co-PI), MRI: Equipment Acquisition for WMU Accelerator Lab Upgrade, National Science Foundation – Major Research Instrumentation program, requested $284,101, declined.


J. A. Tanis (PI), *Travel Grant for US-Based Student and Postdoctoral Participants to Attend ICPEAC XXV*, National Science Foundation – Atomic and Molecular Dynamics Program, awarded $7500 for the period 06/15/07-05/31/08.

J. A. Tanis, *Visiting Lecturer/Researcher*, Institute of Modern Physics, Applied Ion Beam Physics Laboratory, Fudan University, Shanghai (China), awarded $7,500 for two visits of one month duration each during the period 11/01/07-12/30/08.

J. A. Tanis (PI), *Guiding of Fast Electrons and Positive Ions in Nanocapillaries*, Research Corporation, awarded $50,000 (sponsor) + $25,000 (required matching) for the period 6/30/07-06/29/09.


J. A. Tanis (PI) and C. Whelan (co-PI), *Collaborative Research: Atomic Collision Physics at Extreme Velocities and Field Strengths*, National Science Foundation – Atomic and Molecular Physics program, requested $544,815 for the period 06/01/08-05/31/11.


A. H. Wuosmaa (PI), Argonne National Laboratory, *Research in Nuclear Physics*, awarded $8,000 for the period 7/1/07-12/31/07.

A. H. Wuosmaa (PI), Argonne National Laboratory, *Research in Nuclear Physics*, awarded $14,841 for the period 9/1/07-12/31/07.
12  SCHOLARLY ACTIVITY


N. Berrah, member, ALS, LBNL, UC, Berkeley, Science Advisory Committee (SAC), 2007-2010.

N. Berrah, member, SSRL, SLAC, Stanford University, Science Advisory Committee (SAC), 2006-2009.

N. Berrah, co-team leader (with Lou Dimauro), for Atomic and Molecular Science at the femtosecond Linac Coherent Light Source (LCLS) at SLAC, Stanford, CA, 2004-present.

N. Berrah, chair, Local Committee, International Conference on Photonic, Electronic, and Atomic Collisions, ICPEAC09.


N. Berrah, member, APS, DAMOP, Nominating Committee, 2008-2010.

N. Berrah, member, Executive Committee of the Division of Atomic, Molecular, and Optical Physics (DAMOP) of the American Physical Society, 2005-2008.

N. Berrah, member, Executive Committee of the APS Topical Group on Few-Body Physics (GFB).


N. Berrah, member, review committee of the FOCUS NSF Laser Center, University of Michigan, 2007-2009.


C. Burns, member of Executive Board for Inelastic X-ray Scattering Collaborative Development Team (IXS-CDT).

C. Burns, member of Beamline Advisory Committee for Sector 30, Advanced Photon Source, Argonne National Laboratory.
C. Burns, chair of the Beamline Advisory Team (BAT) for the Ultra-high Resolution Inelastic X-ray Scattering Beamline under construction at NSLS-II, Brookhaven, NY.

C. Burns, co-organizer of the Workshop on Inelastic X-ray Scattering at NSLS-II, Feb. 7-8, 2008, Brookhaven National Laboratory, Upton, NY.

C. Burns, book reviewer for the American Association for the Advancement of Science.


M. A. Famiano, reviewed 2 DOE grant proposals.

M. A. Famiano, refereed for Proceedings of Science.

M. A. Famiano, member of the Michitoshi Soga Japan Center Faculty Advisory Committee, May 2007 - Present.

T. W. Gorczyca, reviewed two manuscripts for Physical Review Letters and one manuscript for Journal of Physics B.

T. W. Gorczyca, served on a 2-day panel review for the NASA Solar and Heliospheric Research and Technology Program (4/08 in Washington, D. C.).


C. Henderson, reviewed 22 grant proposals for i) National Science Foundation; ii) US Department of Education, Fund for the Improvement of Post Secondary Education (FIPSE); iii) National Research Foundation, International Science Cooperation Grants (Swedish Research Collaboration Programme)

C. Henderson, chair, American Association of Physics Teachers Committee on Research in Physics Education.

C. Henderson, president, Michigan Chapter of the American Association of Physics Teachers.

C. Henderson, member, Physics Education Research Leadership and Organizing Council.

C. Henderson, external evaluator, Physics and Astronomy New Faculty Workshop.

E. Y. Kamber, reviewed two papers for Physical Review A.


A. R. McGurn, elected a Fellow of the Optical Society of America.

A. R. McGurn, cited by the American Physical Society as an Outstanding Referee of the American Physical Society.

A. R. McGurn, awarded the distinguished Faculty Scholar Award at Western Michigan University.

L. M. Paulius, refereed 4 proposals for the National Science Foundation and 1 proposal for the Research Corporation.

D. Schuster, Referee for Physics Education Research Conference proposals and papers.

D. Schuster, Referee for the National Association for Research in Science Teaching proposals and papers.

D. Schuster, Physics textbook reviewer for John Wiley & Sons.

J. A. Tanis, selected as one of the inaugural group of 534 Outstanding Referees by the American Physical Society.


J. A. Tanis, served as ad hoc Divisional Associate Editor for Physical Review Letters.

J. A. Tanis, chair, Local Committee, XXVI International Conference on Photonic, Electronic, and Atomic Collisions (ICPEAC) to be held in Kalamazoo, July 22-28, 2009.


A. H. Wuosmaa reviewed 2 DOE Phase I SBIR/STTR grant proposals, 1 DOE Phase II SBIR/STTR grant proposal, 2 proposals for the UK Science and Technologies Facilities Council, 1 proposal for the South African National Research Foundation.

A. H. Wuosmaa, served on Review Panel of DOE visiting committee for the Texas A&M University Cyclotron upgrade project.

A. H. Wuosmaa, served on Review Panel of DOE visiting committee for the Holifield Rare Isotope Beam Facility (HRIBF) Scientific and Technical Review.

A. H. Wuosmaa WMU representative to Central States Universities Incorporated, Secretary and Board Member.
## 13 PERSONNEL

### Faculty
- Berrah, Nora
- Burns, Clement
- Chung, Sung
- Dobbin, Donya (Part Time)
- Famiano, Michael
- Gorczyca, Thomas
- Halderson, Dean
- Hadie, Gerald (Assistant Chair)
- Henderson, Charles
- Kaldon, Philip (Part Time)
- Kamber, Emanuel
- Kayani, Asghar
- Korista, Kirk
- McGurn, Arthur
- Miller, Mark (Part Time)
- Pancella, Paul (Chair)
- Paulius, Lisa
- Rosenthal, Alvin
- Schuster, David
- Tanis, John
- Wuosmaa, Alan

### Staff
- Cochran, Kerry
- Gaudio, Benjamin
- Kern, Allan
- Krum, Lori
- Scherzer, Bob
- Welch, Rick

### Post-Docs
- Bilodeau, René
- Hoener, Matthias
- Nikolić, Dragan
- Pesic, Zoran
- Rolles, Daniel
- Said, Ayman

### Graduate Students
- Abdel Naby, Shahin
- Adams, Betty
- Adams, Dan
- Al-Amar, Mohammad
- Al Faify, Salem
- Ayyad, Asmá
- Baran, Jamie
- Bedoor, Shadi
- Cassidy, David
- Das, Susanta
- Dassanayake, Buddhika
- Dumitriu, Ileana
- Durren, Michael
- El Kafrawy, Tamer
- Ganapathy, Subramanian
- Gao, Xuan
- Garratt, Elias
- Ghannam, Talal
- Giacherio, Brenna

### Adjunct Faculty
- Stolterfoht, Nikolaus

### Faculty Emeriti
- Bernstein, Eugene
- Kaul, Dean
- Soga, Michitoshi
- Poel, Robert
- Shamu, Robert

### Graduate Students (cont.)
- Goodman, Nicholas
- Grineviciute, Janina
- Hamam, Khalil
- Hasoglu, Muhammet Fatih
- Ihrig, Caleb
- Kodikara, Ravin
- Lagha, Rahmah
- Li, Chengyang
- Li, Shujun
- Lighthall, Jonathan
- Marley, Scott
- Moore, Andrew
- Nandasiri, Manjula
- Rai, Buddhi
- Stefanick, Trevor
- Vyas, Anjali
- Wang, Lihua
- Wang, Xue
- Winkworth, Melike
- Zhang, Huai Zhien
- Zhang, Yingfa