Fibril Formation in a Model of Polyglutamine

C. Nadia Buckles, Jason Haaga, James Gunton

We study, through a coarse grained model of spherical particles with implicit solvent, the kinetics of aggregation in polyglutamine. These kinetics are studied via a molecular dynamics simulation and we show that the model used reproduces a recent experimental result[1] for the growth of fibrils in polyglutamine. Funding for this project was provided by the NSF REU program, via grant PHY-1359195.

References:

[1] C. Stanley, T. Perevozchikova, and V. Berthelier, Structural Formation of Huntingtin Exon 1 Aggregates Probed by Small-Angle Neutron Scattering. *Biophysical Journal 100 (2011): 2504-2512*

Comparison Between Saturated and Sub-Saturated Atomic Layer Deposition

Meredith Cohen, Dr. Strandwitz, Rod Marstell

Atomic Layer Deposition (ALD) is a method for creating thin films by sequential self-limiting chemical reactions. During their creation, they are specially treated with precursors in order to cause this very regulated and exact growth of reactions. In this experiment, two samples were made, one normal, and one deliberately undersaturated with a lower dose of the precursors. The two samples were then compared. There was no significant difference in their densities (2.96 g/cm^3), roughnesses, atomic concentrations, optical constants, and effective dielectric constant (~6). However, their growths per cycle, fixed charges, and trap densities, all show dramatic differences.

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Transfer and Raman Characterization of Graphene

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The transfer of CVD-grown graphene from its metal growth substrate to a desired target substrate may introduce mechanical damage or contamination to the graphene. A method of optical and chemical characterization is necessary to ensure quality graphene. Raman spectroscopy has proved to be a useful, non-invasive method for determining the number of layers and presence of defects in graphene. Here we show that this technique can also be used for not only detecting, but also quantifying strain and chemical impurities. Using statistical analysis, strain and doping can be measured and mapped at each pixel. This information may give insight to how such defects affect the properties of graphene.

This work received support from National Science Foundation grant PHY-1359195, CREF grant by Lehigh University, and CORE grant by Lehigh University.

Spherulite Growth in Thin Film Rubrene

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Rubrene thin films are created by heating rubrene molecules, resulting in vapor deposition that should create an amorphous film on a substrate. However, in reality smaller sections of the amorphous film orient, creating nanocrystal structures called spherulites. Varying the amount of rubrene used, the substrate material, and whether or not the film was annealed following the deposition resulted in physical differences between the six samples created. Particular attention was paid to the small areas of crystallized rubrene, called spherulites. The primary goal of the research was to vary aspects of the deposition process and observe the physical and optical changes in the spherulites present on the films. Replacing the glass substrate with sapphire reduced these regions by 35%. Doubling the deposition time and the amount of rubrene in the crucible reduced the spherulite diameters by a third. Annealing the sample had the unexpected effect of decreasing the spherulite size by almost 60%. Photoluminescence spectra revealed little change between peak wavelength emissions. This research would not have been possible without the support of the NSF (grant PHY-1359195).

Identifying Variable Stars in the Alpha Persei Cluster

Sabrina DeSoto and Joshua Pepper

The Kilodegree Extremely Little Telescope (KELT)-North survey is a wide field survey that observes millions of stars over many years, designed to detect transiting exoplanets around bright stars. We used data from KELT-North to calculate rotational periods for the determination of a gyrochronological age of the Alpha Persei star cluster. Alpha Persei was a good candidate cluster because its members are not too widely spread on the sky, it is located close to Earth (185pc) and has an age determination as a younger cluster (approximately 70 Myr) by other means. We extracted light curves for 756 potential cluster members, and searched for rotational variability with period-finding algorithms. We report the results of our search for rotationally variable cluster stars, and the discovery of 4 detached eclipsing binary stars.

Acknowledgments:

This research was supported by the National Science Foundation grant PHY-1359195 as part of the Research Experience for Undergraduates summer internship program. I would additionally like to thank Lehigh University for hosting this internship along with a special thanks to Professors Josh Pepper and Ginny McSwain for all of their help through out the project.

Shock heating of stellar nanoparticles

Todd Elder, Georgia State University

Adviser: Professor Yong W. Kim, Lehigh University

Abstract.

The $21\mu m$ emission spectra found in protoplanetary nebulae and supernovae has no identified source. In this paper we prepare for an experimental solution to this mystery through the scope of supernovae using theoretical calculation of the dissociation of nanoparticles which are approximated to be spherical nanocrystallites.

The stellar atmosphere is heated by the fusion reaction of hydrogenic nuclei. As a star ages, heavier nuclei are fused until the production of iron, the most stable nuclei. As more iron nuclei are produced, the outer stellar environment begins to cool relative to the core of the star. This leads to the formation of clouds of nanoparticles. If the star is sufficiently massive, a supernovae is produced. In current models of supernovae, the core collapses and a powerful shock wave is generated. The shock wave is then believed to instantaneously heat gases in the outer atmosphere of the star, thereby heating the nanoparticle clouds and causing their dissociation, which ostensibly produces the $21\mu m$ emission spectra.

The dissociation of a spherical nanocrystallite may be represented $C_N \rightarrow C_{N-1} + A$, where C_N, C_{N-1} are spherical nanocrystallites of $N, N-1$ atoms and A represents a dissociated atom.The dissociation of a spherical nanocrystallite of N atoms may occur $N-1$ times until there are N dissociated atoms in a system. The dissociation of a nanoparticle may be described using the Law of Mass action. Specifically, a quantity known as the degree of dissociation, $\alpha_{N,i}$ may be introduced to measure the percentage of nanoparticles which have experienced the ith step of dissociation. Thus an N-atom nanoparticle will have $N-1$ degrees of dissociation, which yields a system of coupled linear equations which may be solved iteratively.

Before the system of coupled linear equations may be solved, the dissociation potential of an $(N-i)$-atom spherical nanocrystallite must be known.

The dissociation potential of an $(N-i)$-atom spherical nanocrystallite is the energy necessary to move a surface atom infinitely far away from the surface of the spherical nanocrystallite. The dissociation potential of a spherical nanocrystallite may be found using the Lennard-Jones interaction potential, which is a model of the interaction potential between two non-bonded neutral atoms, and is dependent upon the Lennard-Jones parameters which are specific to atomic species. Explicitly, we may find the dissociation potential by summing the Lennard-Jones interactions between the dissociating atom and every atom within the spherical nanocrystallite as it leaves the surface. By calculating the dissociation potential of each atom on the surface of an $(N-i)$-atom spherical nanocrystallite we may find the average dissociation potential of an $(N-i)$-atom spherical nanocrystallite.

In this paper we present an example calculation of the dissociation potential and dissociation equations for a nanoparticle composed of the copper-gold alloy $AuCu_3$ in a heat bath of argon gas. We find that the number of dissociated atoms in the system increases as a function of temperature, and utilizes the energy of the argon heat bath to dissociate $(N-i)$-sized spherical nanocrystallites.

This example calculation has laid out a framework for future calculations of arbitrarily sized and composed nanoparticles which will aid in the experimental effort at Lehigh University.

Lehigh University Physics REU 2016, NSF Grant PHY-1359195

Polarization in the Emission-Excitation Spectroscopy of Erbium Doped Lithium Tantalate

Alexander Ferencin, Andrew Helbers, Volkmar Dierolf

With the goal of trying to further understand how the symmetry present in rare earth doped crystals affects the strength of different transitions, we set out to develop a method to observe different angles of polarization for the excitation and emission beams while performing excitation-emission spectroscopy on such materials. We also varied the angle of the magnetic field relative to the sample. This was used to preliminarily test the symmetry present in a sample of erbium doped lithium tantalate.

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Degenerate Four-Wave-Mixing Interferometry Setup to Measure the Phase of Third-Order Susceptibilities

Holly Hamlin, Wheaton College, MA

Advisor: Ivan Biaggio, Lehigh University

August 5, 2016

Abstract

A setup for interferometric analysis of the phase of a degenerate four wave mixing signal was characterized in terms of stability and reproducibility. Clear, stable interference fringes between the four wave mixing signal and each of the pump beams were successfully obtained and recorded. The simplicity of the setup, due to minimal amounts of optical mirrors, allows for stability of the interference fringes over a period of at least 10 minutes. The dependence of the shift of the fringes was confirmed to follow the predicted mathematical dependences on the phase of each pump beam. Lastly, the stability of the setup was confirmed over multiple cycles of removing and replacing the nonlinear sample in its cell holder. All these components of stability allow for degenerate four wave mixing experiments to be performed using this setup, in order to obtain the phase of the third-order susceptibility of the material as a function of concentration. This research was funded by the National Science Foundation grant PHY-1359195.

Using Digital Micromirror Devices to Spatially Modulate Light's Phase and Amplitude

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It is of great interest to simultaneously and independently modulate light's phase and amplitude for applications in microscopy and holography such as aberration correction in imaging. A method is presented to do such with fewer optical elements and higher accuracy than existing methods by use of a digital multimirror device. The method was tested and phase and intensity modulation was achieved with 4x4 superpixels on the DMD and using an aperture as a frequency filter in the Fourier plane of a 4F setup.

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Atsou Koudonou Advisor: Volkmar Dierolf

Creation and Optical Characterization of Femtosecond Laser Induced Single Crystal Lines in $LaBGeO_5$ Glass

Abstract

All modern electronic devices contain integrated circuits where billions of transistors are printed in a dense configuration, allowing for high speed data processing and low power consumption of the device. The creation of these circuits helps companies reduce the size and cost of their devices considerably. However, since the beginning of the 1980's, a promising technology has emerged: the photonic integrated circuit (PIC). Very similar to the electronic integrated circuit, PICs use photons instead of electrons for data transmission with the potential for higher data transmission rates. A lot of progress has been made in this technology; however, the photolithographic processes suitable for planar geometries that are used to make these integrated circuits does not allow for higher density of components. To solve this problem, we used a femtosecond laser to create single crystal waveguides imbedded in $LaBGeO_5$ glass, allowing for 3D integrated optics. We then constructed a setup to optically characterize the waveguides. We prepared a glass sample in which we created a series of crystal lines using a special laser writing set-up. For the femtosecond laser we used a wavelength of 1027 nm, a power of 1300 mw, and scanned the laser focus within the glass at a speed of 30 μm/s. Then we optically characterized the waveguides with our setup using a 532 nm green laser and 1570 nm infrared laser. Additionally, we measured the mode profile image of the waveguides at each wavelength. We also calculated the power lost inside the waveguides. The average power lost in the waveguides was estimated to be 6.69 dB/cm using the green light and 2.74 dB/cm using the infrared laser. The system that we built will help us improve the waveguides which will be used to create high density 3D photonic integrated circuits.

We are grateful for the funding provided by the National Science Foundation through NSF Grant PHY-1359195 and GOALI Award DMR – 1508177.

Background subtraction from $X_{J\gamma}$ and photon+jets in p+p collisions at $\sqrt{S_{NN}}$ =200 GeV

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Aug. 5, 2016

Lehigh University, Bethlehem. PA

Abstract

Photon jets have been lauded as "golden probes" of the quark-gluon plasma (QGP) as photons do not have a QCD color charge and therefore do not interact with the QGP. Thus, photons can give us a good idea of the in-medium energy loss by hard partons traversing the QGP that fragment into jets. Although they have been held up as highly useful, only recently have we recorded enough statistics to run a thorough analysis on photon+jets created in high-energy nuclear collisions. This paper analyzes data taken from PYTHIA simulations of p+p collisions at $\sqrt{S_{NN}}$ =200 GeV with 5 GeV $\leq p_{T,min} \leq$ 50 in 5 GeV increments. A detailed look at the usefulness of unfolding and FastJet's subtractor class to reduce a randomly inserted background are presented for data at varying jet radii and $p_{T,min}$. For events collected with 20 GeV $\leq p_{T,min} \leq$ 50 GeV and 0.2 $\leq R_{Jet} \leq$ 0.3, a combination of unfolding and FastJet's subtractor class returned $X_{J\gamma}$ significantly similar to $X_{J\gamma}$ for the PYTHIA data with no background. For data taken with R=0.4 or $p_{T,min} \leq$ 15 GeV, our analysis failed to recover a similar $X_{J\gamma}$ and a different approach is needed.

LEHIGH UNIVERSITY PHYSICS REU 2016, NSF GRANT PHY-1359195

Biooil catalytic upgrading using solid acid catalysts

Eric Nelson, Dr. Jonas Baltrusaitis

The importance of sustainable energy sources continues to rise as natural fossil fuels are quickly being depleted. Biooil made by hardwood pyrolysis can be used as a renewable fuel once it is upgraded using solid acid catalysts. This biooil starts off being crude and high in acidity. It can be upgraded by reacting with ethanol and a solid acid catalyst. We used a high temperature, high pressure stainless steel reactor to perform this task. The solid acid catalysts used in this research were $SiO_2H_2SO_4$ (SSA), WO_3/ZrO_2, and $NiO\text{-}WO_3/ZrO_2$. These catalysts have varying surface structures and acidity that produce different resulting upgraded biooil. The upgraded biooil is analyzed by gas chromatography-mass spectrometry (GC-MS), which is a method that identifies the present compounds. We are currently interested in producing biooil that has lower amounts of acidic compounds, such as: ketones, acids, and aldehydes, and higher amounts of esters and other long carbon chain molecules. We found that the SSA catalyst had the largest increase in esters and decrease in acidic compounds. Additionally, the $NiO\text{-}WO_3/ZrO_2$ can be synthesized with the most variation in acidity. Understanding the structure of the catalysts along with the reaction mechanisms can greatly increase the production and quality of fuel created from biooil.

This project was funded by the National Science Foundation grant PHY-1359195.

The Role of Charge Transfer Excitons in High-mobility Polymers

Jacob Parker and Heather Jaeger

Polymers with high hole mobilities often have rigid backbones and ordered macroscopic structures. The two polymers, PBTTT and IDTBT, have hole mobilities of $1cm^2V^{-1}s^{-1}$ and $2cm^2V^{-1}s^{-1}$, respectively. PBTTT is semi-crystalline, while the stable thermodynamic phase of IDTBT is amorphous. To understand why an amorphous polymer exhibits a higher mobility than a semi-crystalline polymer, we turn to the microscopic properties of the polymer. From the view of the donor-acceptor pairs that underlie electronic transport, backbone rigidity and macroscopic order facilitate strong donor-acceptor coupling and increase the rate of adiabatic transfer. Expanding the view of electronic transport to a manifold of Born-Oppenheimer electronic states, low energy excitons couple to ground state and affect the rate of nonadiabatic transfer. The presence of low energy charge transfer (CT) excitons can only increase the overall transfer rate, by way of nonadiabatic coupling. Using linear-response TDDFT, we identified the sub-band-gap excitons of the two polymers. The charge transfer character of these excitons was determined from a density-based analysis, forgoing the need for a simplified orbital picture. The analysis shows that the lowest energy excitation of PBTTT does not involve charge transfer, while the lowest energy excitation of IDTBT transfer charge over an average distance of 4.55 Å. Similar trends are found for higher energy excitons. The nonadiabatic coupling between ground and excited states are expected to be significant but must be assessed, in order to unequivocally demonstrate the relationship between low lying CT excitons, thermal transfer rates, and transport properties. With this work, we recognize that molecular-level properties are responsible for high-mobilities in polymers and demonstrate a correlation between charge transfer excitons and ideal transport characteristics.

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Cell growth and characterization on transferred graphene: Towards development of continuum sensing

Destiny Pounds, Slava Rotkin, and Sabrina Jedlicka

Abstract

Graphene, a nanomaterial with unique material properties, is being evaluated for use in cell culture as a method of continuum force sensing. This project seeks to evaluate graphene as a cell culture substrate. To do so, materials involve in the transfer of graphene were evaluated for cellular toxicity, and cell microstructures associated with cell force were examined. Data was taken over a 10-week period. The methods used in this analysis were immunocytochemistry, fluorescence microscopy, and Image J software. This research was supported by the following grants: REU NSF # PHY-1359195, CORE by Lehigh University, and NSF ECCS-1509786.

In Search of Stellar Music: Finding Pulsators for the TESS Mission

Tyler Richey-Yowell and Joshua Pepper

In December 2017, the Transiting Exoplanet Survey Satellite (TESS) will launch for the start of its two-year mission to detect transiting exoplanets. One of the additional objectives of TESS is to observe oscillating variable stars to precisely measure these stars' masses, radii, and internal structures. Since TESS can observe only a limited number of stars with high enough cadence to detect these oscillations, it is necessary to identify candidates that will yield the most valuable results. Using data from the Kilodegree Extremely Little Telescope (KELT), we searched for bright stars to be top candidates for TESS observation. We found 3,486 variable blue stars with a B-V color < 0.5 and 192 red stars with color > 0.5. Further analysis will be carried out on the blue stars to establish final candidates. This project was funded by the National Science Foundation grant PHY-1359195 to the Lehigh University REU program.

Kinetics of Actin Networks with Distributed Polymerization and Depolymerization

Vedant Sachdeva and Dimitrios Vavylonis

Cellular protrusions and other changes of cell shape are driven by a dynamic actin filament network that assembles near the membrane. The Arp2/3 complex promotes the formation of branched (dendritic) actin networks by nucleating side branches off of pre-existing actin filaments. In this work, we explored the behavior of a phenomenological model by Lewalle et al. on actin network growth in the lamellipodial protrusions at the leading edge of motile cells [1]. This model accounts for actin filament polymerization, Arp2/3 complex-mediated branching, capping of barbed ends, severing by cofilin and depolymerization at or near the pointed filament end; the model does not keep track of filament lengths. A unique feature of this model is that it accounts for these processes occurring distributed in space and allows for an exponential steady state solution. We further explored the implications of this model by determining values for some of the rate constants from experimental works and tuning the branching, severing and depolymerization rate such that they provide a length scale for the lamellipodium width of order a few μm. Using the Euler method, we numerically evolved the system and verified the steady state predicted by Lewalle et al. However, this solution requires that the concentration boundary conditions at the leading edge match the exponential profile. We found the model allows for other steady state behaviors depending on the values of the concentrations of barbed ends, capped ends, and branches at the leading edge. This includes solutions with a peak of actin filament density away from the leading edge (similar to prior experimental measurements) and solutions with network vanishing at a finite distance from the leading edge. The existence of multiple steady state solutions suggests further study on the effect actin network priming at the leading edge boundary. We also propose an extension to the model proposed by Lewalle et al. which considers variable filament length using the method of Edelstein-Keshet and Ermentrout [2]. This work was made possible by NSF grant PHY-1359195.

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Stu Synakowski

Programming DNA-Mediated Interactions to Control Colloidal Self-Assembly

DNA coated particles (DCPs) can be self-assembled into novel functional materials. The ability to manipulate pair interactions between particles, specifically through the number of DNA strands, length of the DNA, and number complementary nucleotides, can be used to engender a desired material. The correlation between these intrinsic properties of DCPs and their particle to particle interaction has been increasingly known. Quantifying the interaction between two DCPs is best described with a pair potential. When one perturbs the intrinsic properties of each DCP, they manipulate their according potential well, which greatly influences the crystal structure. Understanding the relationship between pair potentials and crystal structure is pivotal in exploring design strategies that control the self-assembly of DCPs into desired structures. Through manipulating pair potentials of a system of particles, it is found that non-close packed structures can be created. In addition, the crystal structure of a system can be tuned by temperature .

This research could not have been achieved without the invaluable members of the Lehigh University Biophysics and Soft Matter Group. A special thanks to Jeetain Mittal and Hasan Zerze for their insight and guidance in this project. The project would not have been possible without sponsorship from the National Science Foundation grant PHY-1359195, U.S. Department of Energy, Office of Basic Energy Science, Division of Material Sciences and Engineering under Award (DE-SC0013979), the Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by National Science Foundation grant number ACI-1053575, and Lehigh University's Physics Department

Computational Simulations of Excitonic Fission and Fusion Processes in Rubrene Single Crystals

Ian Trauffer, Ivan Biaggio, Vinnie Zoutenbier

The dynamics of exciton fission and fusion in rubrene crystals were modeled using a set of rate equations for the different excitonic species involved in the fission and fusion processes. Since the equations contain terms scaling quadratically with exciton density, the solutions are sensitive to the initial conditions, such as crystal depth, as the energy of the incident pulse is attenuated exponentially during propagation through the crystal. By integrating the solutions obtained at different depths, we obtained a full time-dependence for depth-integrated excitonic densities, and determined the resulting integrated photoluminescence. Another project focused on the analysis of excitonic diffusion patterns which depend on a second-order nonlinear diffusion equation. The presence of a quadratic term which accounts for interparticle interaction in the diffusion equation leads to unique instabilities when attempting a solution. Different approaches to stabilize a numerical solution have been explored. The material is based upon work supported by the National Science Foundation under Grant Numbers DMR-1408862 and PHY-1359195.

Surface Raman Studies of Reduced Strontium Barium Niobate*

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The vibrational spectra of $Sr_xBa_{1-x}Nb_2O_{6-\delta}$ (SBN, x = 0.61) are studied on the surface of single crystals for $\delta = 0$ (unreduced) and $\delta > 0$ (reduced) using Raman confocal microscopy. The surface spectra are compared with the bulk spectra measured using conventional Raman spectroscopy.A good overall agreement is found between the surface and bulk measurements for the unreduced samples; however, the reduced samples show agreement between bulk and surface measurements only in particular configurations and not in others. We find that for light polarized along one crystal axis, the spectra of the reduced crystals resemble those of the unreduced crystals, with a greater degree of internal disorder, while for light polarized along the other are indicative of a more ordered internal structure.

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