## THE PENNSYLVANIA STATE UNIVERSITY SCHREYER HONORS COLLEGE

## DEPARTMENT OF CHEMICAL ENGINEERING

Study of the Dynamics of Glass Forming Liquids Using Molecular Dynamics Simulations

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A thesis submitted in partial Fulfillment of the requirements for a baccalaureate degree in Chemical Engineering with honors in Chemical Engineering

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### Abstract

The process that occurs as a glassy polymer transitions into an amorphous polymer is currently not well understood. In these materials, two distinct relaxation processes are observed: one of which is related to the glass transition and the other that is not. Previous research has hinted that if the strength of non-bonded interactions between atoms is increased, the relaxation times of the material respond like the relaxation process related to the glass transition, whereas if the torsional barriers of molecules are increased, the relaxation times respond like a completely different process unrelated to the glass transition. This connection of physical process like glass transition with relaxation behavior has not been clearly made. This experiment explored how different combinations of strengths of non-bonded and torsional forces affected the relation processes of the materials.

We have found that for simulations with non-bonded forces greater than two times chemically realistic values, the polymer transitioned from a fragile to a strong glass. This transition from a fragile to a strong glass with increasing non-bonded interaction strength implies that non-bonded interactions are responsible for this fragile to strong transition, which is important because the mechanics behind this transition currently are not understood well. We have also found that Boland's hypothesis holds true for the fragile glasses, and that changing non-bonded interactions and torsional barriers for fragile glasses results in the same effects on molecular behavior (via the diffusion coefficient) and segmental behavior (by the characteristic decay time). More research needs to be conducted investigating the effect of non-bonded interactions on the transition from fragile to strong glasses in order to investigate the mechanics behind the process.

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# Acknowledgements

The author would like to acknowledge Dr. Janna K Maranas for her unwavering support and assistance with the topic of this thesis as well as for providing an office where to work on the material. Thanks is also given to Kan-Ju Lin of Dr. Maranas's lab group for her assistance in teaching the use of C++ and the Linux shell as well as for providing some of the code that was used for analysis of the data in this report.

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## **Chapter 1 – INTRODUCTION AND MOTIVATION**

Researchers have made considerable advances on understanding the glass transition in the past decades. An extremely large amount of data now exists showing the dynamic properties of glasses over a wide range of materials and time domains, but the mechanisms underlying the glass transition of polymers are still not clearly understood or universally defined<sup>5</sup>. Traditional definitions of the glass transition include a marked increase in viscosity, an abrupt change in volume<sup>1</sup>, and a change in heat capacity of the material<sup>2</sup>. Many theories exist to explain this behavior, but no single theory addresses all the observed motions of polymers over all time scales<sup>3</sup>. Creating a universal theory to explain all experimental behavior of polymers is the ultimate goal of polymer physics.

One researcher, Dr. Erin Boland, has made an interesting discovery regarding molecular motions by using a seldom-explored feature of computer simulation. Typically, physical parameters of computer simulations are adjusted and tweaked to emulate experimental results best. However, computer simulations are not limited to recreating real-world results. While adjusting physical variables to unrealistic values may seem counterintuitive, it allows one to explore the effects that each of these variables has on molecular motions.

Boland's research<sup>4</sup> found that increasing the torsional barriers in simulations beyond real-world barriers, relaxation times increased linearly while when increasing the strength of non-bonded interactions in the simulations beyond realistic strengths, relaxation times increased in a Vogel mode. Since these linear and exponential increases in relaxation times mimicked the behavior of  $\beta$  and  $\alpha$  relaxation processes, respectively, to decreases in temperature, Boland hypothesized that non-bonded interactions contribute to the  $\alpha$  relaxation while torsional barrier heights contribute to the  $\beta$  relaxation process.

However, Boland's result lacked robustness due to only testing the result in one specific set of simulation conditions. The primary goal of this thesis is to test the validity of this result by testing Boland's hypothesis in multiple scenarios with different combinations of torsional barrier heights and non-bonded interaction strengths. Through this research, we hope to gain more insight onto the connections between molecular forces and macroscopic properties of polymers.

## Chapter 2 – BACKGROUND

#### 2.1 The Importance of Simulation

Traditional experiments to explain the properties of crystalline polymers prove difficult. Isolating a specific variable that affects structural properties in an experimental setting is difficult due to the limited number of variables that a researcher can adjust. In addition, correlating experimental measurements with structural properties on the molecular level remains challenging due to the macro-scale nature of experiments. While experimental solutions to this problem have been proposed<sup>5</sup>, computer simulations present a straightforward solution to this problem. Computer simulations depict the individual positions of atoms and thus of molecules allowing a straightforward observation of molecular motions.

Molecular dynamics, one form of computer simulation, works by emulating molecular mechanics. As such, the total energy of interactions between atoms is computed and energy is conserved. Together, these interactions are knows as a force field.

While computer simulations do offer many advantages over pure experiment, they do have one very important limitation - scale. Macroscopic properties and motions can only be observed in simulations with very large numbers of molecules. While computational power has increased exponentially over the past decades, a modern, moderately sized supercomputer can still only handle simulating around 100,000 atoms at a time. Therefore, much focus has been put on improving computational performance through more efficient programming so that larger simulations can be created. One way to improve performance is to utilize a United Atom, or UA model. UA models cluster units of hydrogen atoms together with the carbon atom to which they are bonded. Thus, for example, a methyl group, normally containing 4 atoms, is treated as a single UA. Since in a UA model fewer atoms are simulated per molecule, more molecules can be put into a simulation and thus simulation results more closely resemble those of experiments.

The force field of a molecular dynamics consists of many components. Bond stretching potentials ensure that atoms bound to each other maintain the correct distance between each other. Angle potentials maintain bond angles between two bonds among three atoms. The improper torsional term is added to a prevent umbrella inversions of sp<sub>3</sub> bonds at tertiary carbon branches.

The torsional potential barrier in a force field regulates how difficult it is for a molecule to rotate along its bonds. The higher the torsional potential, the harder it is for a bond to pass through the torsional angle and thus the less likely that the bond is to rotate through the angle. Therefore, the bond is more likely to remain in a certain orientation, not having enough energy to pass over the torsional barrier. Logically, this would mean that the movement of molecules with higher torsional barriers would be slower.

The non-bonded parameters of a force field govern the inter-atomic attractions of united atoms not covalently bonded to each other. Any given atom resides in a "cage" formed by its nearest neighbors, some bonded and some not bonded to the atom. In order for the atom to move outside of this cage, it must break the non-bonded interactions holding it to other atoms. When non-bonded interaction strengths are increased, atoms require more energy to escape these interactions; therefore, the atoms would stay in the same cage longer thus meaning they move more slowly.

#### 2.2 Modes of polymer relaxation

In glassy materials, researchers have observed many motional processes that contribute to the unique properties of these glasses as they approach the glass transition. Two processes that dominate the research field are the  $\alpha$ - and  $\beta$ -relaxations. The  $\alpha$ -relaxation corresponds to movement of the entire molecule<sup>3</sup> and occurs on a relatively large time scale. The  $\beta$  relaxation, also known as the Johari-Goldstein process, is faster than the  $\alpha$ -relaxation. The  $\beta$  relaxation

corresponds to polymer backbone motion<sup>6</sup> and molecules exploring their conformational states<sup>7</sup>.

Researchers have observed that at high temperatures, the  $\alpha$ - and  $\beta$ -relaxations merge into one process. At a temperature just above  $T_g$  the  $\alpha$ - and  $\beta$ -relaxations split into motions on different time scales. This is known as the  $\alpha$ - $\beta$  bifurcation, and the temperature at which it occurs is known as the characteristic temperature<sup>8</sup>, usually abbreviated  $T_c$ .

One other previous group of experimenters, Bedrov and Smith, has used simulations<sup>7,9,10,11</sup> to try adjusting torsional barriers outside of chemically realistic bounds. Such research is based on the premise that changing these barriers can cause the  $\alpha$ - and  $\beta$ -relaxations to bifurcate even above T<sub>c</sub>. Thus, the  $\alpha$ - and  $\beta$ -relaxations could be individually analyzed at these higher temperatures. This is especially useful because at temperatures below T<sub>c</sub>, the  $\alpha$ process occurs on such a slow time scale that it is difficult to measure.<sup>9</sup> In one experiment, Bedrov and Smith ran a simulation where the molecules had no torsional barriers<sup>10</sup>. They found that the  $\alpha$ -relaxation was unaffected while the  $\beta$ -relaxation sped up significantly. In further research with lowered (but not zero) torsional barriers, Smith and Bedrov suggested that the  $\beta$ relaxation is specifically related to dihedrals exploring all their conformational states<sup>7</sup>.

Boland's conclusion came from research to analyze force fields used to simulate polyolefins<sup>4</sup>. Boland noticed that, comparing three force fields to experimental results, the largest differences in the force fields' parameters involved the non-bonded and torsional potentials. Because of this, she decided to see exactly what effects these parameters had on the simulations. In one set of simulations, she increased the torsional barriers, and in the other set, she increased non-bonded interaction strength. Boland found in that when increasing the torsional barriers, relaxation times increased linearly while when increasing the strength of non-bonded interactions, relaxation times increased exponentially. These increases in relaxation times mimicked the behavior of  $\beta$  and  $\alpha$  relaxation processes to the Arrhenius and Vogel

dependences, respectively, to changes in temperature of a polymer. Due to this similarity, Boland concluded that the  $\beta$ -relaxation could be related to torsional barriers and the  $\alpha$ relaxation related to non-bonded interactions. However, since Boland's research was focused on determining a force field applicable to polyolefins, she only spent a small amount of time on this tangent, and thus she does not thoroughly verify the result. If we can run more simulations and verify these results, a new insight may be made into the relaxation behavior of glassy polymers.

## 2.3 Simulation Analysis

The raw data output by computer simulations consists solely of the coordinates of atoms – a data set that is both impossible for humans to interpret and is impossible to compare to experimental results. Therefore, methods to convert the simulations coordinates into useful data are needed.

The incoherent self-intermediate scattering function, S(q,t), is a self-correlation of particle motion and can describe segmental motion of the chain. When S(q,t) is close to one, the particle position is at time t is close to its position at time t0. When S(q,t) is close to zero, its position at time t is uncorrelated to its position at time t<sub>0</sub>. The equation used to calculate S(q,t) from atomic coordinates is presented below. N is the total number of atoms in the system, q is the wave vector,  $x_i(t)$  is the x coordinate of atom i at time t, and  $x_i(t_0)$  is the x coordinate of atom i at the initial time.

$$S(q,t) = \frac{1}{N} \langle \sum_{i=1}^{N} \cos(q \cdot |x_i(t+t_0) - x_i(t_0)|) \rangle$$

The incoherent self-intermediate scattering function is fit to Boland's equation below. The equation includes terms for the fast relaxation ( $\tau_{fast}$ ) and of the slow relaxation ( $\tau_{slow}$ ). It also includes an elastic incoherent structure factor, which partitions the decay between the two processes.

$$S(q,t) = \left\{ EISF_{fast} + \left(1 - EISF_{fast}\right) \cdot \exp\left[-\frac{t}{\tau_{fast}}\right] \right\} \cdot \exp\left[-\left(\frac{t}{\tau_{slow}}\right)^{\beta}\right]$$

Instead of plotting all fitting parameters independently, an overall characteristic decay time ( $\tau_c$ ) is created that accounts for the contributions from both relaxations.

$$\tau_c = \frac{\tau_{slow}}{\beta} \Gamma\left(\frac{1}{\beta}\right)$$

The diffusion coefficient is a molecular property and is chain length dependent. It is measured using the following equation

$$D = \frac{1}{6N} \sum_{i=1}^{N} \left[ \lim_{t \to \infty} \frac{d}{dt} \langle (r_i(t) - r_i(t_0))^2 \rangle \right]$$

 $r_i(t)$ - $r_i(t_0)$  is the distance vector of molecule i defined by

$$[r_i(t) - r_i(t_0)]^2 = x_i^2(t) + y_i^2(t) + z_i^2(t) - x_i^2(t_0) - y_i^2(t_0) - z_i^2(t_0)$$

where x(t), y(t), and z(t) are the centers of mass of the molecule in the x-, y-, and z-axes. Centers of mass of each axis is calculated by

$$x_i(t) = \frac{\sum_{j=1}^M m_{x,j} \cdot x_j(t)}{\sum_{k=1}^M m_k}$$

 $m_i$  is the mass of atom j, and  $x_i$  is the x coordinate of atom j at time t.

## **Chapter 3 – EXPERIMENTAL METHODS**

#### **3.1 Simulation Parameters**

Simulation methods practiced by Boland were followed as closely as possible for the research. All simulations used the OPLS force field specified in Appendix A. The Lennard-Jones constant  $\varepsilon_0$  was multiplied by a constant in order to increase or decrease non-bonded interaction strengths. The torsional constants  $\alpha_0$ -  $\alpha_3$  were multiplied by a constant in order to increase or decrease torsional barrier heights. In total, 42 simulations were run consisting of all the combinations of torsional multipliers 0.25, 0.5, 1.0, 1.5, 2.0, or 3.0 and non-bonded multipliers 0.25, 0.5, 1.0, 1.5, 2.0, and 4.0. The LAMMPS simulation package was used in place of Boland's own simulation code due to the increased computational speed afforded by multiprocessing available in LAMMPS. Due to LAMMPS not including support for the RATTLE algorithm used by Boland, simulations used harmonic bond stretching potentials adapted from Rappe et al.<sup>12</sup>. These potentials maintain the 1.54 Å bond distance specified by Boland.

All simulations were run at 423K. 25 atactic polypropylene chains with 40 backbone units each (aPP40) were inserted into the simulation box, with each chain initially spaced the non-bonded cutoff length - 10 Å - from each other. The simulation box was shrunken to the desired box length of 35.86Å over 200ps in 0.05fs time steps. This box length was determined by dividing the total mass of molecules in the box (25 x 828 g mol<sup>-1</sup>) by the density of the polymer (0.7542 g cm<sup>-3</sup>) and taking the cubic root. After shrinking to the desired density, the simulations were run using 5fs time steps.

## **3.2 Simulation Analysis Parameters**

Equilibrium was determined using Boland's criteria. When three consecutive S(q,t) snapshots of the same simulation spaced 3ns apart were determined to look the same and were no longer shifting to longer decay times, the simulation was declared equilibrated. A wave vector of q=0.99 Å<sup>-1</sup> was used for all S(q,t) calculations in order to enable comparison of results directly to Boland's.

## **Chapter 4 – RESULTS AND DISCUSSION**

The first goal was to verify the integrity of the experiment by comparing the data to previous data obtained in the same conditions, so the results were compared to Boland's results in figure 1. It is immediately apparent that the  $\tau_c$  for the NB=3.0 results is about two orders of magnitude shorter than the results obtained by Boland.



Figure 1 - Comparison of our results (A) to those of Boland (B)

Figure 2 shows the presumptive reason for this lower  $\tau_c$  value. The S(q,t) plot shows the characteristics of super exponential decay, meaning that in order to generate a reasonable fit to the data, the exponent  $\beta$  must be greater than one. In our fits,  $\beta$  is restricted to less than one because the theoretical meaning of  $\beta$ >1 is unclear. From conversation with Boland, it was determined that Boland only ran the simulations 80ns. Due to the short length of the simulations, Boland could not observe the entire S(q,t) plot and thus could not determine that the fitting equation did not fit the plot properly . Fitting the equation to only the first 80ns of simulation, shown in Figure 3, creates a  $\tau_c$  of 2.7 x 10<sup>7</sup> ps, which is in line with Boland's data, supporting this hypothesis.





Figure 2 – T=1.0 NB=3.0 S(q,t) plot and best fit



Figure 3 - T=1.0 NB=3.0 S(q,t) plot and fit to only the first 80ns of data

Because the behavior of figure 1 is completely unexpected, we try to determine what is actually occurring.  $\tau_c$  is increasing with a Vogel fit with NB until NB=2, after which point it continues more of an Arrhenius fit. The Vogel fit of NB<2 is characteristic of the  $\alpha$ -relaxation of a fragile glass while the Arrhenius fit of NB>2 is characteristic of the  $\alpha$ -relaxation of a strong glass. This is very similar to the type of fragile to strong transition what occurs when temperature is raised<sup>13</sup>, so this behavior seems to indicate that a fragile to strong glass transition is occurring around NB=2.

The S(q,t) plot of NB=3.0 T=1.0 also supports this transition theory. The plot displays a two stage decay – an immediate beta relaxation, a plateau S value for a while, then a rapid, super-exponential alpha decay until S=0. This two-stage decay has previously been observed in the fragile to strong transition of boron oxide by Fullerton and Maranas<sup>14</sup>. Fullerton and Maranas also observed that the strong glass of boron oxide displayed an oscillation around the plateau S value, a characteristic that is also present in the S(q,t) plot of T=1.0 NB=3.0.

Decay plots of all the simulations are presented in figure 4, grouped by NB and in figure 6, grouped by T. One can see that the behavior of the T=1.0 NB=3.0 simulation is not limited to that case. Instead, it occurs in all the simulations when NB=3.0 and in the simulations where NB<3.0 but T is high. All simulations decay to S=0 by  $5 \times 10^6$  ps. This decay likely corresponds to the relaxation time of the entire molecule rather than segmental relaxation of a part of the molecule.



Figure 4 - S(q,t) decay plots grouped by NB strengths



Figure 5 - S(q,t) plots grouped by T barrier heights

Looking at these plots, we can divide the simulation set into three categories. The first category, the "true" fragile glasses, occur at NB<3 and at low T. These can be fit nearly perfectly to Boland's equation to calculate characteristic decay time. The second category is the "transition glasses." This category encompasses the simulations at NB<3 and high T. These simulations display characteristics between fragile and strong glasses. They still have a stretched decay but they do not have a slope that approaches 0 as S approaches 0. The final category is the "true" strong glasses. These occur at NB>2 as well as at NB=2 and T>3. These simulations display super exponential decay and lack a stretched exponential plot. Figure 6 shows which simulations were fit into which category.





For all the glasses, a fit is applied to each simulation using Boland's equation, and the characteristic decay time is determined. In figure 7, the decay times of the fragile glasses are plotted against T with constant NB in plot A and against NB with constant T in plot B. We test the validity of Boland's original hypothesis by applying an Arrhenius fit in plot A and a Vogel fit in plot B. Figure 7 confirms that Boland's conclusion holds true and increasing NB causes  $\tau_c$  to increase in a Vogel manner while increasing T causes  $\tau_c$  to increase in an Arrhenius manner for the fragile glasses. The data points where T<1 and NB<1 show significant fluctuation in  $\tau_c$  thus preventing a perfect fit to the data, but  $\tau_c$  for all four of these simulations is within the same order of magnitude.



Figure 7 – Characteristic decay time of the fragile glasses plotted by constant NB and by constant T

In figure 8, the characteristic decay time data is presented for all the glasses but in a different manner. In each graph, one data set has T held constant at one value while NB is varied by X, and the other has NB held constant at that same value while T is varied by X. We apply a Vogel fit to the constant T fragile glasses and an Arrhenius fit is applied to the constant NB fragile glasses (solid lines). An Arrhenius fit is applied to the strong and transition glasses - both for constant T (dashed line) and constant NB (dotted line). There are not enough data points to confirm the Arrhenius fit for the strong and transition glasses with NB<1.5. The fits are simply a guide as for what trend the data would be expected to take.





One immediately notices that the  $\tau_c$  of the strong and transition glasses with NB>1.0 increase very little with respect to T;  $\tau_c$  for all these simulations is around 10<sup>6</sup> ps. This behavior is possibly due to the short length of the polymer chain. The relaxation time of the chain in these simulations is likely shorter than the segmental relaxation time. Increasing the length of the chain would lengthen the molecular relaxation time and would make  $\tau_c$  represent the segmental relaxation time, which should increase with increasing T. Another behavior to note regards the fragile glasses. As the series of charts progresses, the same X goes from having  $\tau_c$  higher for NB than for T to having  $\tau_c$  higher for T than for NB. One would suspect that this would apply for all values of X should the progression of charts be continued. This is an interesting trend, although its implications are unclear.

We now analyze the diffusive behavior of the molecules. The diffusion coefficients of all the strong glasses are around  $5 \times 10^{-17} \text{ m}^2/\text{s}$ , regardless of T or NB. This indicates that, once the fragile to strong transition has been reached, the glass reaches a maximum viscosity.

In contrast, the fragile glasses simulations' diffusion coefficients vary significantly with T and NB. These diffusion coefficients are plotted in figure 9. Interestingly, the diffusion coefficients seem to follow an inverse Arrhenius behavior with respect to T just like the characteristic decay times. To further investigate this, the inverse of the diffusion coefficients are plotted against T and NB in figure 10. The inverse of diffusion is taken to match units with the characteristic decay time – time will be in the numerator in both the inverse diffusion coefficient and the characteristic decay time. From this plot, we see a repetition of Arrhenius behavior with respect to T. In figure 10–B, we would expect to see a Vogel fit with respect to increasing NB, but a clean Vogel fit does not occur. This is most likely due to experimental error in the data rather than a new result.



Figure 9 - Diffusion coefficients of the fragile glasses with respect to T



Figure 10 - Inverse diffusion coefficients plotted against T and NB

To further confirm that the segmental and diffusive behaviors of the fragile glasses are the same, the inverse diffusion coefficients and characteristic decay times are plotted on the same graph in figure 11.  $T_c$  is plotted on the left axis and represented by solid points while inverse diffusion coefficients are plotted on the right axis and are represented by hollow points. The axes are adjusted in scale, and the points are found to overlap confirming this hypothesis.



Figure 11- Inverse diffusion coefficient and  $\tau_c$  plotted against T

## **Chapter 5 – CONCLUSION**

It was found that at high NB, the simulation transitions from a fragile to a strong glass. This is an important discovery as the exact reason behind this transition is currently unknown and this result indicates that non-bonded interactions are responsible for this transition. More research is needed to determine the exact NB strength at which this transition occurs as well as the exact dynamics of this transition. It also was found that Boland's original conclusion - the Arrhenius increase in  $\tau_c$  with respect to T and the Vogel increase in  $\tau_c$  with respect to NB - holds true for all conditions where the glass is fragile. Finally, it was found that the segmental and molecular behavior of the fragile glass with respect to increasing T and NB are the same. As T is increased, both  $\tau_c$  and 1/D increase in an Arrhenius fashion while as NB is increased both  $\tau_c$  and 1/D increase in a Vogel manner.

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**APPENDIX A: Force Field Parameters** 

Table 1 - Force Field Parameters. Torsional barriers and non-bonded forces are normal.

Bond Bending:
$$U_{bend} = k_b (\theta - \theta_0)^2$$
Angle Identity $k_b$   
(kcal/mol rad²) $CH_X-CH_X-CH_X$ 62.09114

Bond Torsion: 
$$U_{dihedral} = \sum a_i cos^i \varphi$$

Dihedral Identity	$a_o$	$a_1$	$a_2$	$a_3$
	(kcal/mol)	(kcal/mol)	(kcal/mol)	(kcal/mol)
CH <sub>x</sub> -CH <sub>x</sub> -CH <sub>x</sub> -CH <sub>x</sub>	0.814	1.792	0.389	-3.673

Improper Torsion:	$U_{improper \ torsion} =$	$= k_{improper torsion}(\varepsilon)$	$(-\varepsilon_0)^2$
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	$k_{improper\ torsion}$	ε
Improper Identity	(kcal/mol)	(degrees)
all	40	27.25

Lennard-Jones:  

$$U_{L-J} = 4\varepsilon_{ij} \left[ \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{6} \right]$$

$$\varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j}, \quad \sigma_{ij} = 0.5 (\sigma_i + \sigma_j)$$

UA Identity	σ	ε		
	(Å)	(kcal/mol)		
CH <sub>3</sub>	3.910	0.160		
CH <sub>2</sub>	3.905	0.118		
СН	3.850	0.080		

# Bond Stretching $U_{stretch} = k_{stretch}(r - r_0)^2$

Bond Identity	k <sub>stretch</sub> (kcal/mol)	r <sub>0</sub> (Å)
CH <sub>X</sub> -CH <sub>X</sub>	700	1.54

**APPENDIX B: Experimental Data** 

τ <sub>c</sub> (ps)		Non-bonded multiplier					
	0.25	0.5	1	1.5	2	3	
	0.25	11.6	7.1	5.0	23.7	261.4	1008219.4
Torsion multiplier	0.5	11.2	9.4	7.7	46.7	743.3	588997.7
	1	7.1	10.7	19.7	923.2	101834.4	449179.5
	1.5	8.4	22.8	119.9	13304.3	1143818.0	686177.2
	2	16.8	51.9	431.2	257120.8	486430.1	709378.5
	3	36.2	233.1	4538.1	531734.0	497042.8	1004975.7
	4	256.2	1305.7	495452.0	495452.0	1134552.9	612331.7

 Table 2 - Characteristic decay times (including bad fits)

**Table 3 - Diffusion Coefficients** 

<b>D</b> (m <sup>2</sup> )	/s)	Non-bonded multiplier					
X 10 <sup>15</sup>		0.25	0.5	1	1.5	2	3
	0.25	57210	57085	32162	5668	936	0.0224
Torsion multiplier	0.5	71395	30112	21115	3647	198	0.0686
	1	28478	20125	13947	162	2.05	0.0574
	1.5	30602	11954	3932	52.1	0.0259	0.0381
	2	15687	9667	433	0.333	0.0960	0.0471
	3	10911	3377	156	0.0883	0.0691	0.0391
	4	7089	862	1.05	0.0794	0.0453	0.0453

### ACADEMIC VITA of Christopher Henry Sokolowski

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Education: Bachelor of Science Degree in Chemical Engineering, Penn State University, Fall 2010 Honors in Chemical Engineering Thesis Title: Study of the Dynamics of Glass Forming Liquids Using Molecular Dynamics Simulations Thesis Supervisor: Janna K. Maranas

## Work Experience:

Summer Semester 2009 Title: Undergraduate Research Assistant Description: Programmed molecular dynamics simulations on Linux platform and C++

## Awards:

Dean's List Schreyer Scholar

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Windows XP, Vista, 7 Linux C and C++ programming languages Microsoft Office HYSYS Plant Simulator ICARUS Economic Evaluator