

Houston Community College and the West Houston Center for Science & Engineering

Presents

The 2017 Research Experiences and Exploration in Materials Science (REEMS)

Research Experience for Undergraduates¹

Poster Presentation & Recognition Ceremony²



August 10, 2017

Held at the MD Anderson Cancer Center UT Health Graduate
School of Biomedical Sciences

¹ Funding for this event was provided by the National Science Foundation, Division of Materials Research, DMR 1460564 and the HCC West Houston Center for Science and Engineering. Special thanks to the administrators and staff at the Graduate School of Biomedical Sciences for providing the venue for this event.

² Second Revision, September 14, 2017

The 2017 Research Experiences and Exploration in Materials Science (REEMS): Research Experience for Undergraduates

Poster Presentation & Recognition Ceremony

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**The 2017 Research Experiences and Exploration
in Materials Science (REEMS):
Research Experience for Undergraduates**

Poster Presentations & Recognition Ceremony

August 10, 2017

Schedule of Events

| | |
|------------------------|---|
| <i>8:00 – 8:45 am</i> | <i>Student arrival and poster set-up</i> |
| <i>9:00 am</i> | <i>Judges Arrive</i> |
| <i>9:45 – 11:30 am</i> | <i>Poster presenters stand at posters for judging</i> |
| <i>Noon – 12:45 pm</i> | <i>Lunch</i> |
| <i>1:00 – 2:30 pm</i> | <i>Poster Awards and Recognition Ceremony</i> |

Houston Community College 2017 Summer Undergraduate Research Program in Materials Science

NSF REU: Research Experiences and Exploration in Materials Science (REEMS) for Houston Community College Science and Engineering Students (NSF DMR 1460564)

Bartlett (Bart) M. Sheinberg serves as the Principal Investigator for this award.

In 2015, The West Houston Center for Science and Engineering (WHC) was awarded funding from the National Science Foundation to develop an innovative materials science educational program and summer research program (REU) specifically for Houston Community College students.

The REEMS program, inclusive of the REU, provides a series of multidisciplinary learning experiences in chemistry, physics, engineering, the biological sciences, medicine, computational science, economics, and public policy. The Program experience includes individualized transfer guidance and academic advising to insure that each of the REEMS students transfer in a timely manner to complete their undergraduate education, an overview of graduate school as the next step in their academic careers, and student networking opportunities with materials professionals.

REEMS REU students represent diverse cultural, economic, educational backgrounds, and ages. While their backgrounds, and academic-career goals may vary, each student has an intense motivation to learn and a willingness to explore new challenges. Program evaluation data presents a strong correlation between student participation in the REEMS program with an enhanced appreciation of mathematical, physical & biological sciences, computer programming and engineering concepts discussed in their coursework. Students quickly grasp the importance and relevance of their coursework as they apply these concepts to solve research problems and begin to think about how their education and experiences in materials science can be applied to solving societal technology and material challenges.

The 2017 REEMS REU poster session provided the opportunity for students to share their summer research experiences with other students, university faculty, and the public. This book contains an overview of 2017 REEMS REU student profiles, research abstracts and posters; information on each of the REEMS Research faculty; profiles of the REEMS REU poster session judges; and recognition of the West Houston staff and Advisory Council members.

2017 REEMS REU Students

Yasaman Adel



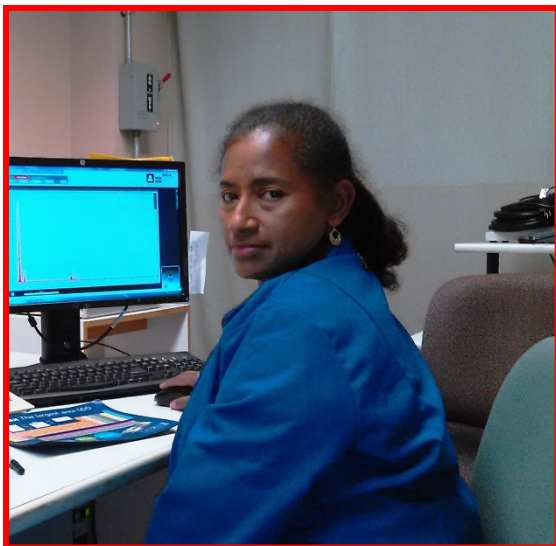
yasamanadel@gmail.com

REEMS REU Faculty Supervisor: Dr. Laura Smith Callahan, McGovern Medical School, UT Health Science Center – Houston

REEMS REU Mentor: Dr. Xi Lu

Transferring in fall 2017 to the University of Houston –Biological Sciences

Brenda Arceneaux



ba.arcen@yahoo.com

REEMS REU Faculty Supervisor: Dr. James K. Meen, University of Houston

REEMS REU Mentor: Dr. Karoline Müller

Returning to HCC in the Fall of 2017 to continue coursework in engineering and serving as an adjunct HCC instructor.

Andrew Michael Catalanotto



am.catala67@gmail.com

REEMS Faculty Supervisor Advisor: Dr. Zachary Cordero, Rice University

REEMS REU Mentor: Logan Ware

Transferring to the University of Texas – Tyler (Houston) in the fall of 2017 to study Electrical Engineering

Joshua Jackson



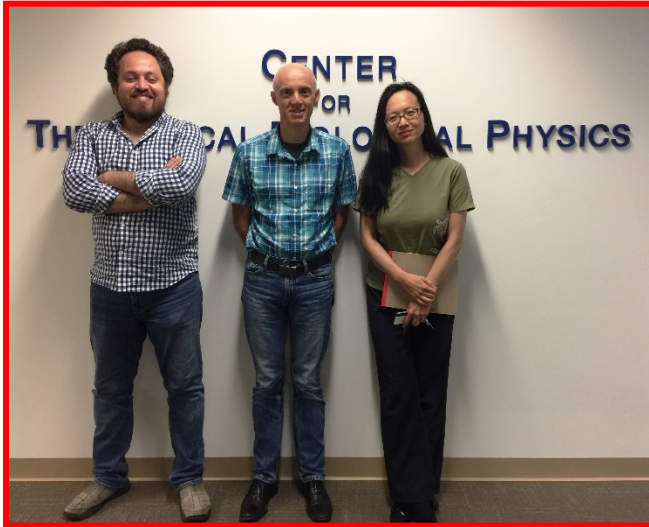
joshnm28@gmail.com

REEMS REU Faculty Supervisor: Dr. Rafael Verduzco, Rice University

REEMS REU Mentor: Jorge Wu Mok

Transferring to Prairie View A&M University in fall of 2017 to study electrical engineering

Frank Kornet



Frank Kornet (center), Margaret Cheung (right) & Millad Ghane (left)

frkornet@gmail.com

REEMS REU Faculty Supervisor: Dr. Margaret Cheung, University of Houston & Rice University

REEMS REU Mentor: Millad Ghane

Returning to HCC in fall of 2017 to prepare for graduate school.

Monica R. Martinez



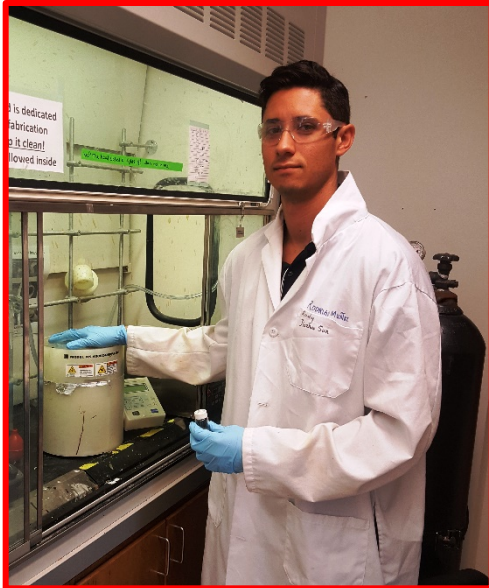
martinezhenriquez@hotmail.com

REEMS REU Faculty Supervisor – Dr. James K. Meen, University of Houston

REEMS REU Mentor: Dr. Karoline Müller

Transferring fall 2017 to University of Houston, Honors College, to study Mechanical Engineering

Rodrigo Munoz- Zarruk



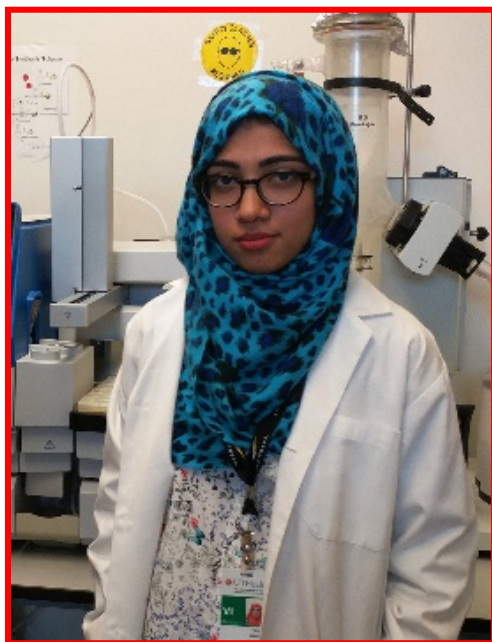
rodrigo.munozzarruk@mavs.uta.edu

REEMS REU Faculty Supervisor: Dr. Rafael Verduzco, Rice University

REEMS REU Mentor: Jorge Wu Mok

Transferring to the University of Texas - Arlington in the fall of 2017 to study mechanical engineering

Tasmia Nadeem



tasmia.nadeem27@gmail.com

REEMS REU Faculty Supervisor: Dr. Laura Smith - Callahan-McGovern Medical School, University of Texas Health Science Center –Houston

REEMS REU Mentor- Dr. Xi Lu.

Transferring fall of 2017 to attend the University of Texas MD Anderson School of Public Health, Bachelors Program in Molecular Genetics.

Gelareh Nobakht



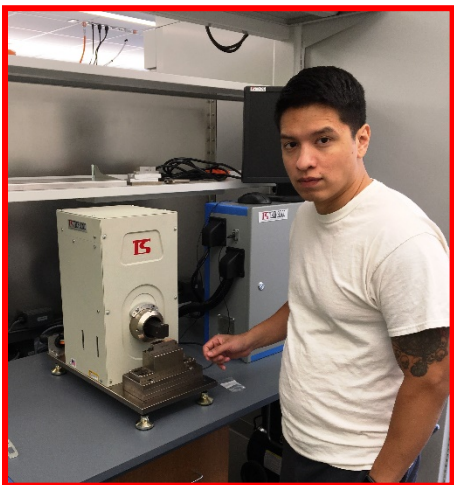
gelareh.no@gmail.com

REEMS REU Faculty Supervisor: Dr. Jakoah Brgoch,
University of Houston

REEMS REU Mentor: Aria Mansouri Tehrani

Returning to HCC in the fall of 2017 and transferring
to the University of Texas-Dallas, spring 2018 to study
computer science

Nathaniel Ocanas



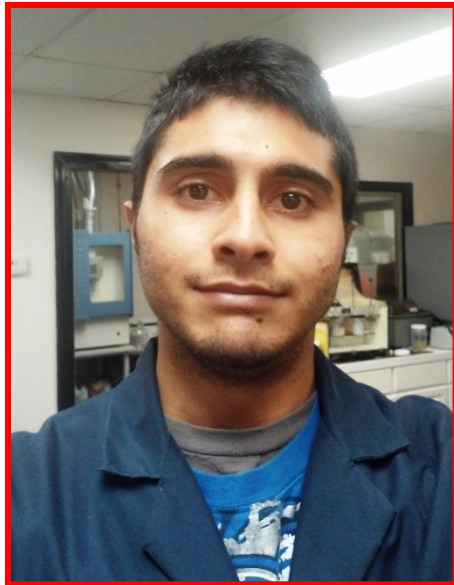
nathan_ocanas@yahoo.com

REEMS REU Faculty Supervisor – Dr. Zachary Cordero,
Rice University

REEMS REU Mentor: - Mr. Austin A. Ward

Transferring fall 2017 to study electrical engineering
at the University of Texas – Tyler (Houston)

Zeshan Rizvi



shanoo824@gmail.com

REEMS REU Faculty Supervisor: Dr. Jakoah Brgoch,
University of Houston

REEMS REU Mentor: A. Oliynyk

Transferring fall 2017 to Prairie View A&M University
to study chemical engineering

Kevin Scholtes



ktscholtes@gmail.com

REEMS REU Faculty Supervisor: Dr. Megan
Robertson, University of Houston

REEMS REU Mentor: - Dr. Wenye Ding

Fall Semester: Recipient of an internship at the
Department of Energy, Oak Ridge National Lab,
Center for Nanophase Materials Sciences

Transferring spring 2018 to study electrical
engineering at the University of Texas – Tyler
(Houston)

Brandon Vu



brandonvu00@gmail.com

REEMS REU Faculty Supervisor: Dr. James K. Meen, University of Houston

REU Mentor: - Dr. Karoline Müller

Returning to Houston Community College in the 2017/2018 academic year and transferring to Texas A&M University in the fall of 2018 to study electrical engineering. Brandon is a member of the Texas A&M Engineering Academy at Houston Community College.

2017 REEMS REU STUDENT ABSTRACTS

2017 REEMS REU POSTER PRESENTERS

| <u>STUDENT NAME</u> | <u>REEMS FACULTY SUPERVISOR</u> | <u>POSTER #</u> |
|-----------------------------|---------------------------------|-----------------|
| Gelareh Nobakht | Jakoah Brgoch | 1 |
| Zeshan Rizvi | Jakoah Brgoch | 2 |
| Yasaman Adel | Laura Smith-Callahan | 3a |
| Tasmia Nadeem | Laura Smith-Callahan | 3b |
| Andrew Catalanotto | Zachary Cordero | 4 |
| Nathaniel Ocanas | Zachary Cordero | 5 |
| Frank Kornet | Margaret Cheung | 6 |
| Brenda Arceneaux | James Meen | 7 |
| Monica Martinez | James Meen | 8 |
| Brandon Vu | James Meen | 9 |
| Kevin Scholtes | Megan Robertson | 10 |
| Joshua Jackson | Rafael Verduzco | 11 |
| Rodrigo Munoz Zarruk | Rafael Verduzco | 12 |

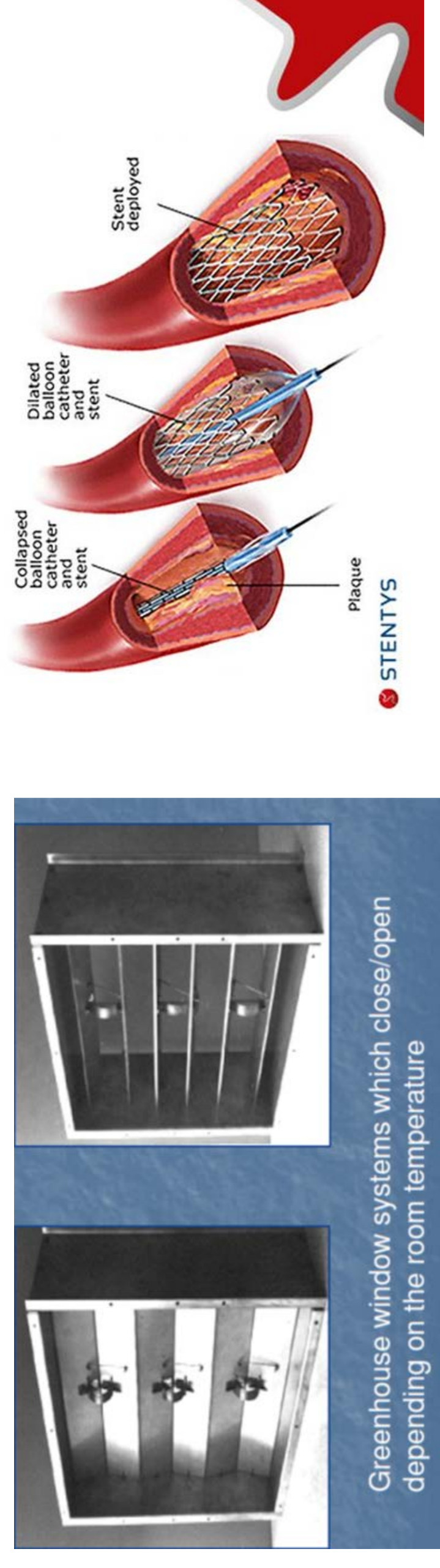
Temperature-induced Phase Transformation in NiTi – A Molecular Dynamics StudyG.Nobakht², A. Mansouri Tehrani¹, J. Brgoch¹¹Department of Chemistry, University of Houston, Houston, Texas²REEMS REU Program, West Houston Center for Science & Engineering, Houston Community College, Houston, Texas

Nickel-titanium (NiTi) shape memory alloys are widely used in medical and industrial fields. The shape memory behavior is due to a phase transformation between high temperature B2 and low temperature B19' phase. Here, the temperature-induced phase transformation in NiTi shape memory alloys is investigated by Molecular Dynamics (MD) simulation. The quality of MD simulations is substantially dependent on the used interatomic potential. Therefore, we compare the implementation of two most common interatomic potentials for NiTi MD simulations, EAM (Embedded Atom Method) and MEAM (Modified Embedded Atom Method). A series of simulations were performed using LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) software. The temperature was controlled using the Nose-Hoover thermostat while Parrinello-Rahman method was used for pressure. After the initial relaxation, the system was cooled to 200 K. During cooling, the phase transformation between cubic B2 (austenite) and B19' (martensite) phase occurs at 302.18 K using EAM and 261.8 K using MEAM potential. At high temperature (~400K), NiTi has austenite structure, by decreasing the temperature to ~200K, the system transforms to martensite phase with β of 95.30° and 95.47° for EAM and MEAM, respectively. The subsequent heating to ~400K, results in the recovery of the austenite phase (β =90°). This study shows that both EAM and MEAM potentials are capable of reproducing temperature-induced phase transformation in NiTi and they are in good agreement with experimental data. However, development of more accurate, versatile interatomic potentials for this intriguing alloy is further encouraged.

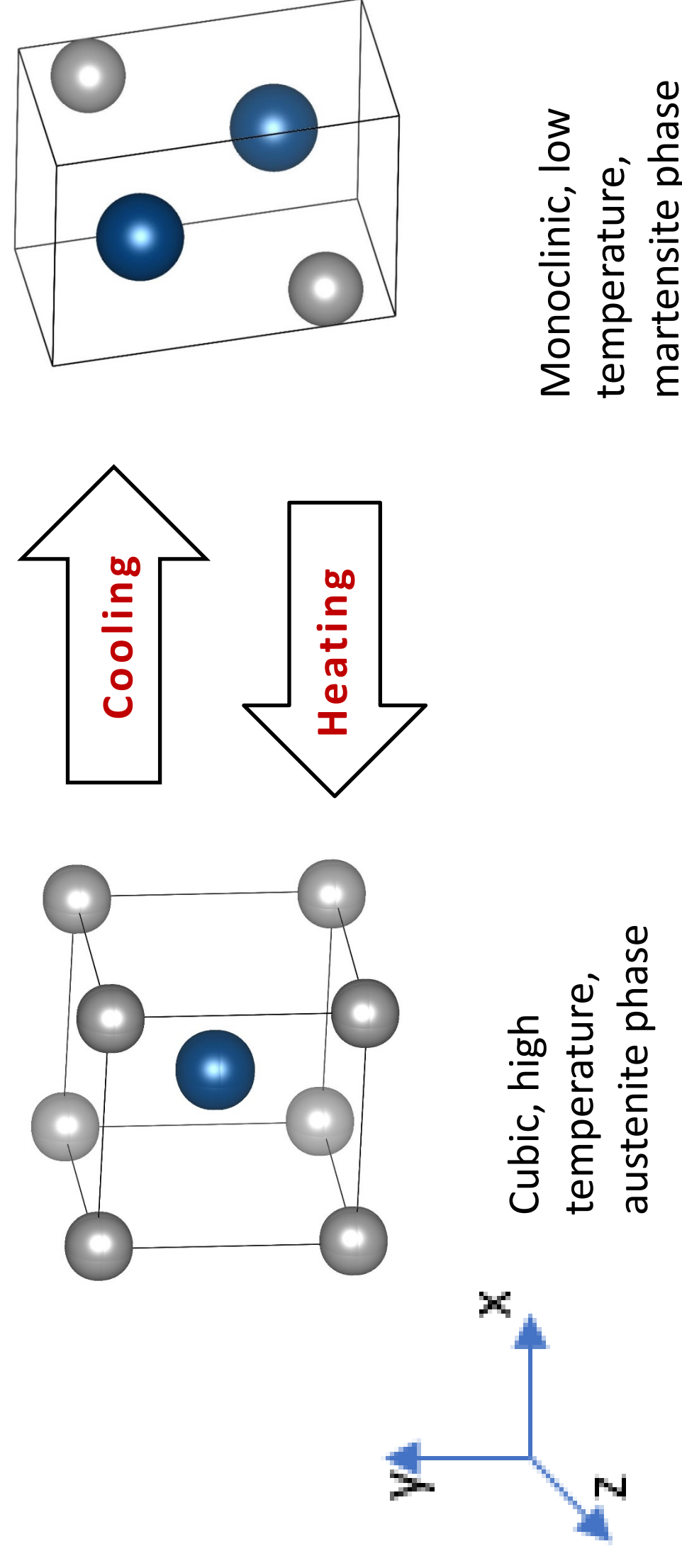
This work is supported by the American Chemical Society Petroleum Research Fund (55625- DNI10), the National Science Foundation Division of Civil, Mechanical & Manufacturing Innovation (NSF CMMI 15-62142), and National Science Foundation Division of Materials Research (NSF DMR 14-60564)

Introduction

A Shape Memory alloy (SMA) is an alloy that deforms to its pre-deformed shape when heated. Nickel-titanium (NiTi) is one of the main types of shape memory alloys. NiTi shape memory alloys are widely used in medical and industrial fields. The shape memory behavior is due to a phase transformation between high temperature (B2) and low temperature (B19') phase.



Phase transition between the high temperature (austenite) and low temperature (martensite)



Embedded-atom method (EAM) VS Modified embedded atom method (MEAM)

EAM

$$E_i = F_\alpha \left(\sum_{\beta \neq i} \rho_\beta(r_{ij}) \right) + \frac{1}{2} \sum_{\beta \neq j} \phi_{\alpha\beta}(r_{ij})$$

- r_{ij} → distance between atom i and j
 - $\Phi_{\alpha\beta}$ → pairwise potential function
 - ρ_β → the electron charge density
 - F → an embedding function that represents the energy
- The embedded-atom method is describing the energy between atoms (interatomic potential). The energy is a function of sum of functions between the atom and its neighbors. The EAM is related to Finnis-Sinclair model, which is formulated for FCC metallic alloys.
- spherical symmetry

MEAM

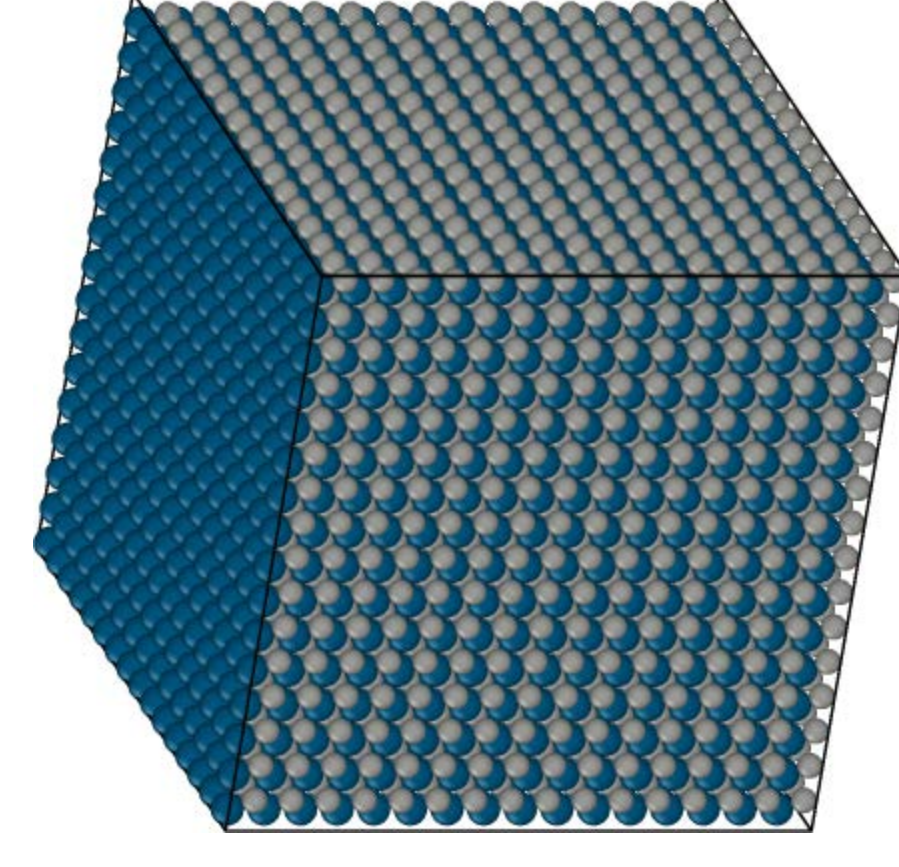
$$E = \sum_i \left[F_i(\rho_i) + \frac{1}{2} \sum_{j \neq i} S_{ij} \phi_{ij}(R_{ij}) \right]$$

- F_i → embedding energy as a function of ρ_i → electron density
 - S_{ij} → screening function between atoms i & j
 - $\Phi_{ij}(R_{ij})$ → pair interaction between atoms i & j, separated by distance R
- The MEAM potential behaves like the EAM potential but MEAM potential employs cubic splines instead of analytic functions.
- s, p and f symmetry.
 - Ideal for modeling fcc, hcp and diamond cubic.
 - MEAM = EAM + angular forces

Computational Details

NiTi phase transition between B2(austenite) and B19'(martensite) with EAM and 2NN MEAM potential

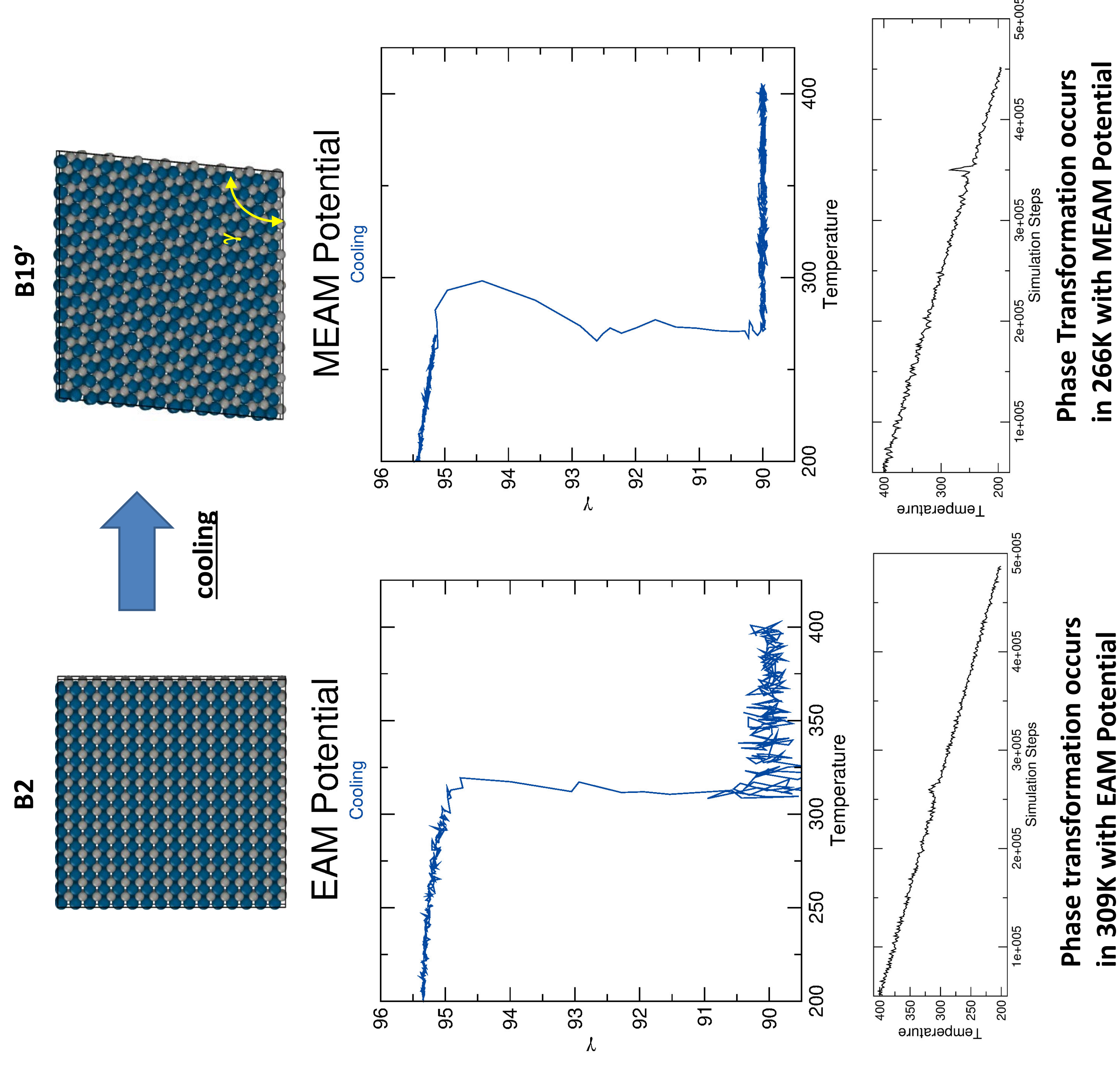
| | Potential | a [Å] | b [Å] | c [Å] | γ [°] |
|------|-----------|-------|-------|-------|--------------|
| B2 | MEAM | 4.82 | 4.81 | 4.81 | 90 |
| B19' | MEAM | 4.9 | 4.9 | 4.5 | 95.49 |
| B2 | EAM | 30.01 | 4.2 | 4.2 | 90 |
| B19' | EAM | 3.032 | 4.616 | 4.224 | 95.30 |
| B2 | MEAM | 3.016 | 4.265 | 4.265 | 90 |
| B19' | MEAM | 2.909 | 4.114 | 4.657 | 97.9 |



Periodic boundary conditions

Simulation step: 0.0005 Ps
During the process the system was isothermal and isobaric(NPT)

Phase Transformation



Conclusion

Shape Memory Alloys like NiTi have a phase transformation between 400 K to 200 K. Molecular dynamics helped to study the changes in the temperature. During cooling, the phase transformation between cubic B2 (austenite) and B19' (martensite) phase occurs at 302.18 K using EAM and 261.8 K using MEAM potential. At high temperature (400K), NiTi has austenite structure, by decreasing the temperature to ~200K, the system transforms to martensite phase with γ of 95.30° and 95.47° for EAM and MEAM, respectively. Studying phase transformation of NiTi using Molecular Dynamics simulations not only could provide a better understanding of the shape memory mechanism but also it can help design the applications more precisely.

References

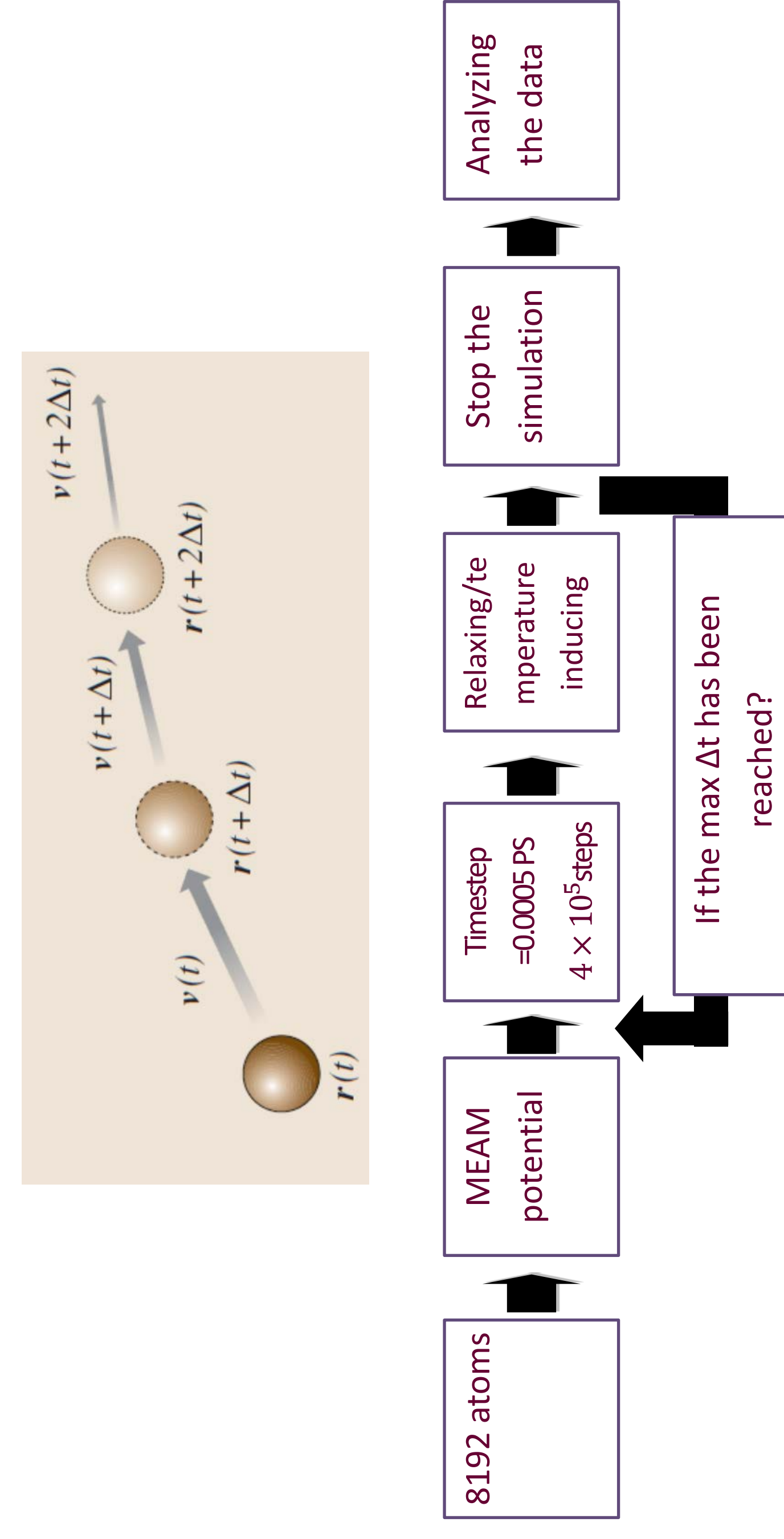
- Tehrani, A. M.; Shahrokhshahi, H.; Parvin, N.; Brgoch, J. *Journal of Applied Physics* 2015, **118** (1), 014901.
- Ko, W.-S.; Grabowski, B.; Neugebauer, J. *Physical Review B* 2015, **92** (13).

Acknowledgment

❖ The authors thank the Department of Chemistry and the Division of Research at the University of Houston. This work was also supported by the National Science Foundation, Division of Materials Research 14-60564.

MD simulation is a computer simulation method for studying physical movements of atoms and molecules.

MD algorithm



Machine-Learning-Driven Superhard Material Search: $\text{ReWC}_{0.8}$ and $\text{Mo}_{2-x}\text{W}_x\text{BC}$ **Rizvi, Z.,^{1,2} Oliynyk, A.,¹ Tehrani, A. M.,¹ Brgoch, J.¹**¹*Department of Chemistry, University of Houston, Houston, Texas*²*REU:REEMS Program, West Houston Center for Science & Engineering, Houston Community College, Houston, Texas*

Superhard materials are widely used in industry as abrasives and coatings, for polishing materials, as mechanical parts, as well as an array of other industrial uses.¹ The current materials used for these applications involve precious metals, often osmium, rhenium, and iridium, or require extreme synthesis conditions to make like high pressure and high temperature.^{2,3} This makes these materials costly and their production energy consuming. The development of new, alternative superhard materials that are not limited by resources, cost, or synthetic conditions has traditionally relied on searching for materials using traditional trial and-error-approaches. Recently, machine learning has shown promise as a tool for directing synthetic efforts towards materials with the most promising properties improving the chance of novel materials discovery. Unfortunately, hardness is a complex property and it is not currently possible to predict using machine learning directly. However, it is possible to machine learn a material's elastic constants, which are related to hardness, and are a fundamental for every material. This research employs machine learning to predict elastic constants and identify materials with high bulk and shear modulus to see if it indeed correlates with high hardness. The bulk and shear elastic moduli were predicted for $\approx 150,000$ potential candidates that are compiled from crystallographic databases. From this large set of materials two compositions, ternary ($\text{ReWC}_{0.8}$) and quaternary ($\text{Mo}_{2-x}\text{W}_x\text{BC}$) compounds were selected considering they had the highest predicted bulk modulus among three-component and four-component inorganic compounds, respectively. $\text{ReWC}_{0.8}$ and $\text{Mo}_{2-x}\text{W}_x\text{BC}$ compounds were synthesized using arc melting from stoichiometric mixture of the elements and their purity and crystal structure was confirmed using powder X-ray diffraction. The Vickers hardness was then measured using microindentation and demonstrated that $\text{ReWC}_{0.8}$ had a Vickers hardness of over 40 GPa (at 0.5 N applied load) whereas $\text{Mo}_{0.9}\text{W}_{1.1}\text{BC}$ showed a Vickers hardness of 42 GPa (at 0.5 N applied load). The study proves that the novel machine learning approach to search for materials with desired mechanical property is viable to produce new superhard materials

This work is supported by the American Chemical Society Petroleum Research Fund (55625-DNI10), the National Science Foundation Division of Civil, Mechanical &

Manufacturing Innovation (NSF CMMI 15-62142), and National Science Foundation Division of Materials Research (NSF DMR 14-60564)

References:

[1] R. K. Bogdanov, A. A. Shulzhenko, A. P. Zakora, A. M. Isonkin, V. G. Gargin, New Superhard Material for Drilling Tools, *Journal of Superhard Materials*, **2007**, 29, 56–63

[2] A. M. Terani, L. Ghadbeigi, J. Brgoch, T. D. Sparks, Balancing Mechanical Properties and Sustainability in the Search for Superhard Materials, *Integrating Materials and Manufacturing Innovation*, **2017**, 6, 1–8

[3] H. Tracy Hall, Ultra-High-Pressure, High-Temperature Apparatus: the “Belt”, *Review of Scientific Instruments*, **2004**, 31, 125–131

Machine Learning-Driven Superhard Material Search: $\text{ReW}_x\text{C}_{0.8}$ and $\text{Mo}_{2-x}\text{W}_x\text{BC}$



Zeshan Rizvi;^{1,2} Anton Olynyk;¹ Aria M. Tehrani;¹ Jakoah Brgoch¹
¹Department of Chemistry, University of Houston, Houston, Texas
²REEMS program, Houston Community College, Houston, Texas



Introduction: Industrial Need for Superhard Materials

Motivation

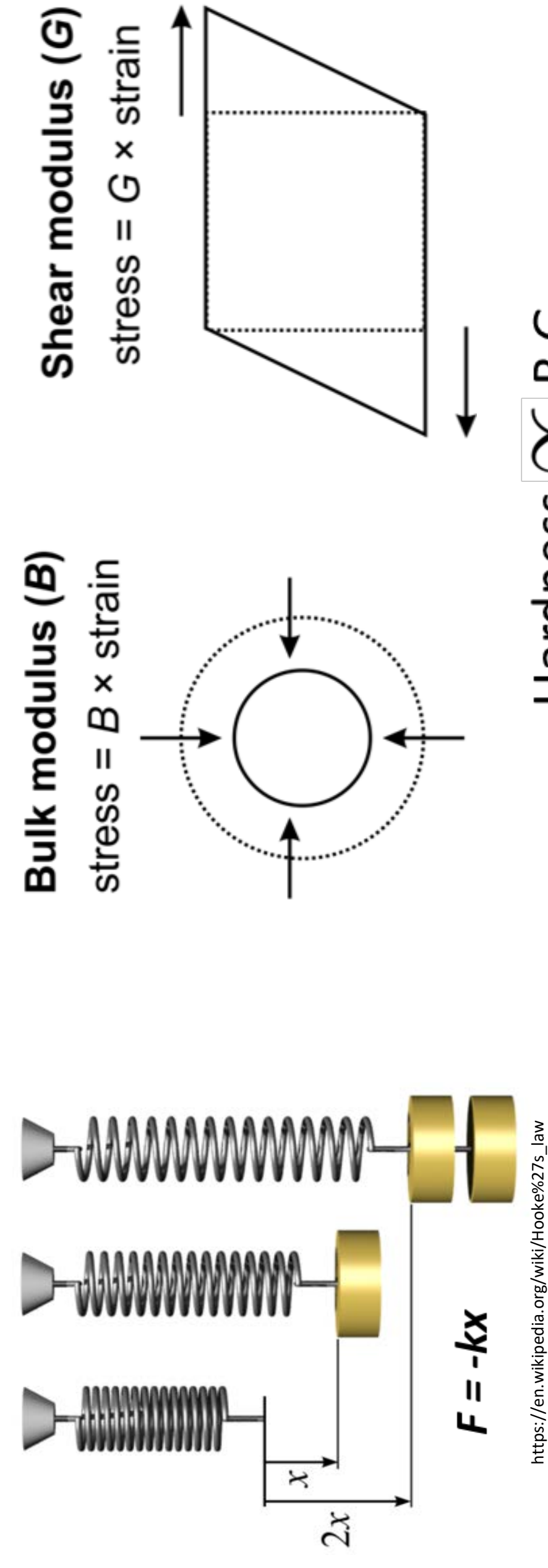
Superhard materials are widely used in industry as abrasives and coatings, for polishing materials, as mechanical parts.¹

Vickers hardness (H_v) measurement of over 40 GPa classifies a material as superhard.²

Current materials used for superhard applications involve precious metals or require extreme synthesis conditions, like high pressure and high temperature.¹

The long term sustainability precious metals remains unclear.

Employing machine learning predictions for potential superhard materials saves time and resources compared a traditional trial-and-error approach to synthesis.

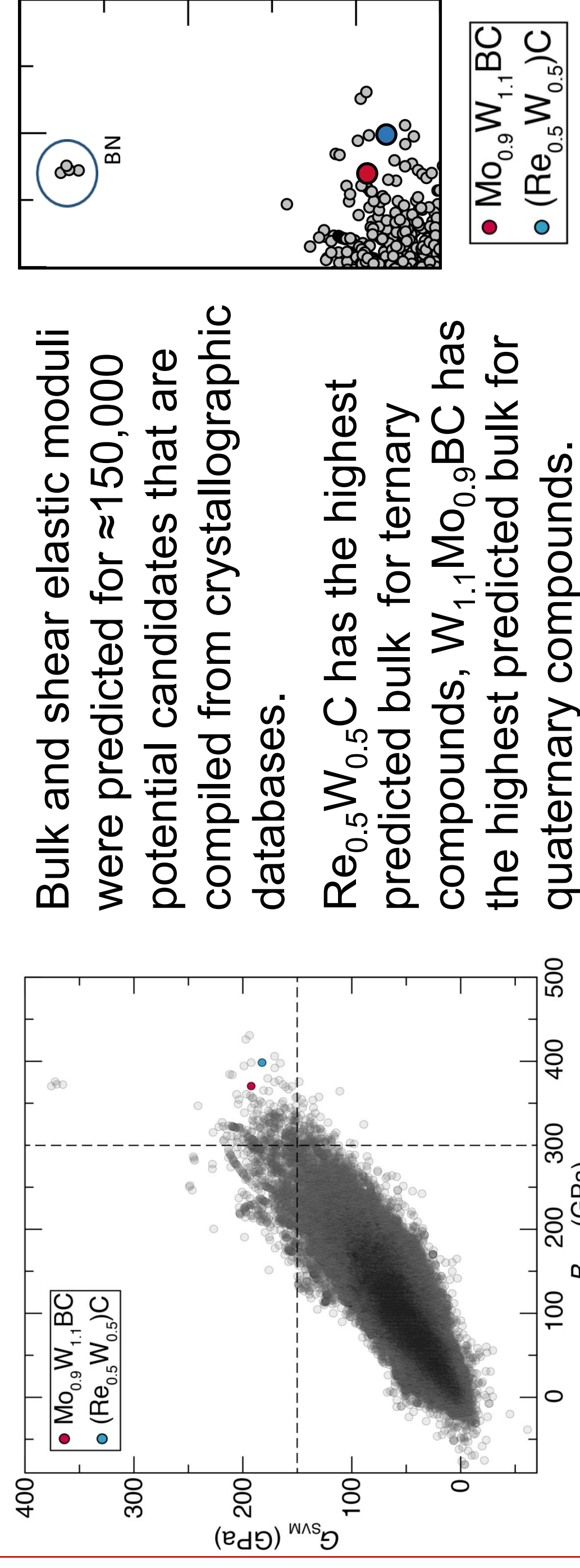


Research objectives

Use Machine Learning Simulations to predict promising Ternary and Quaternary compounds with highest predicted bulk moduli.

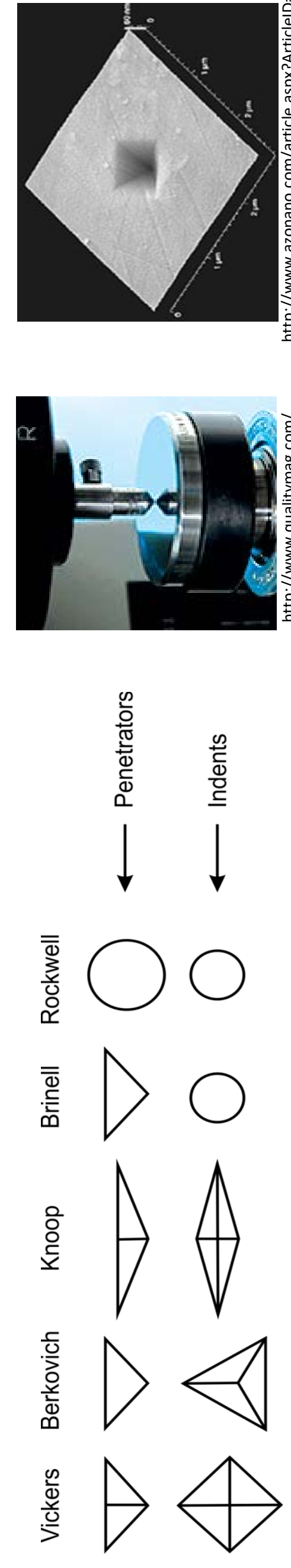
Investigate the hardness behavior of these intermetallic compounds, anticipated to have a Vickers hardness of over 40 GPa.

Machine Learning Prediction



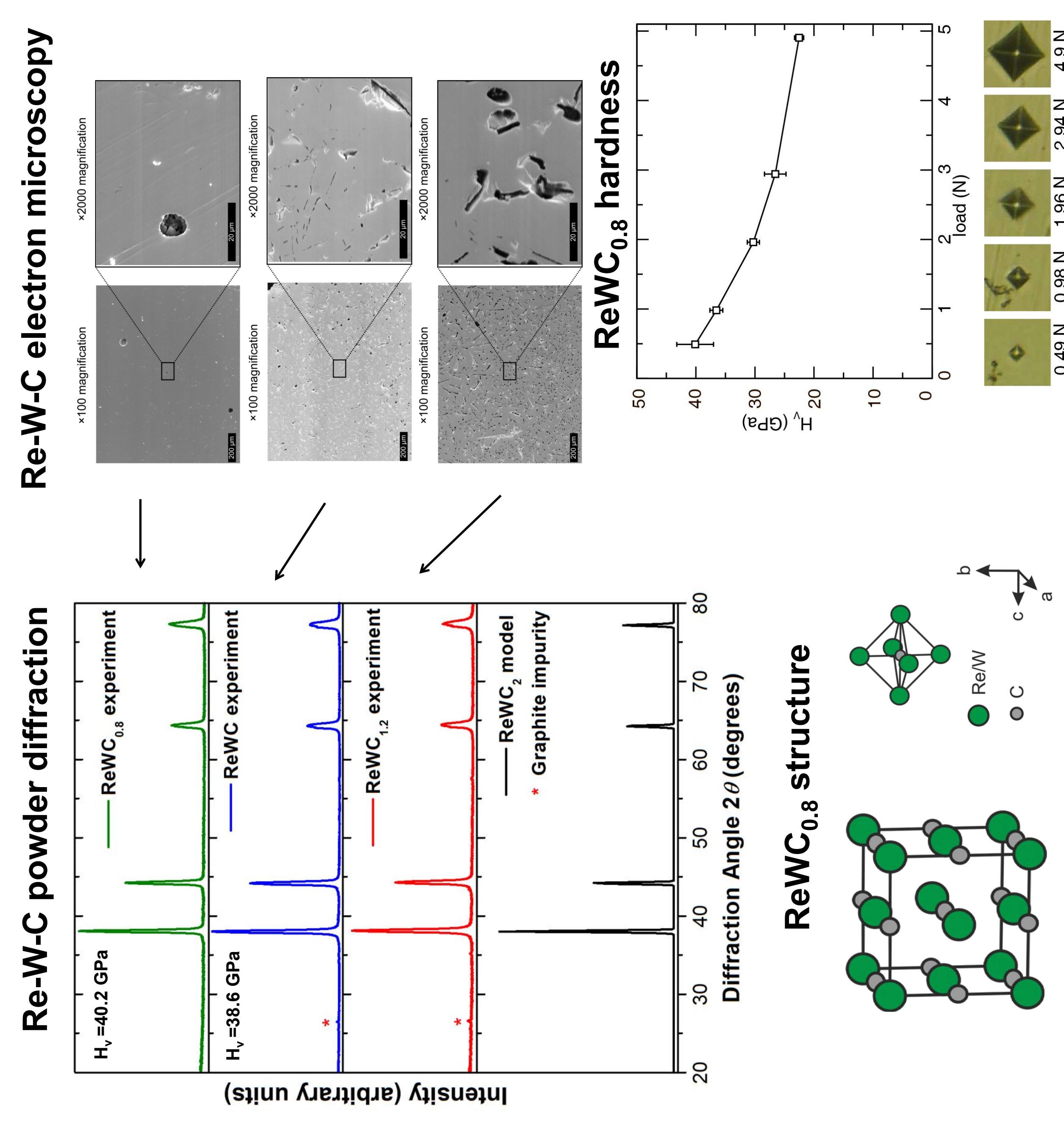
Samples were synthesized using arc melting from mixture of the elements. Purity and crystal structure was confirmed using powder X-ray diffraction.

Testing materials (Vickers hardness)

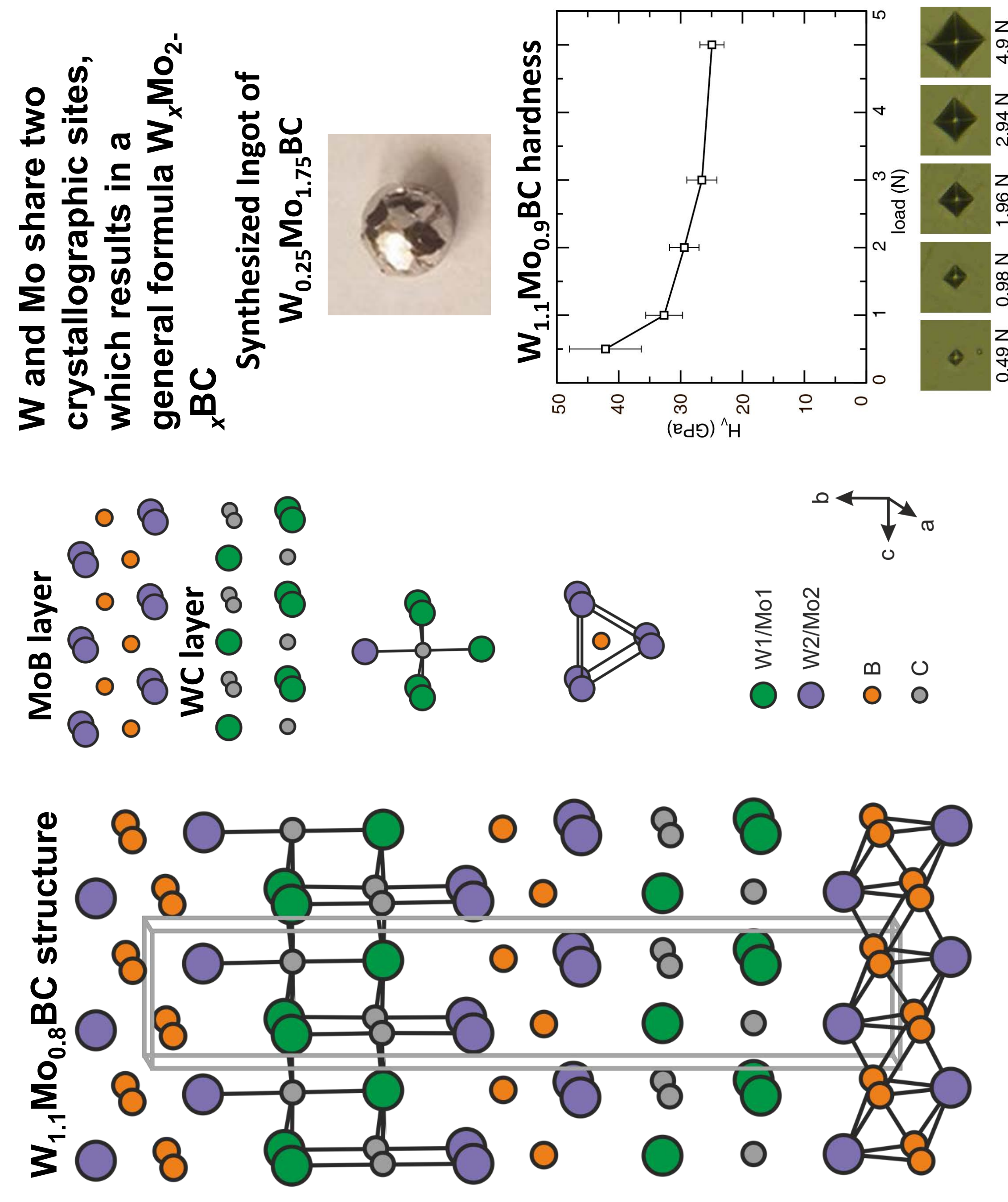


Ternary Compounds With the Highest Predicted Bulk and Shear Modulus

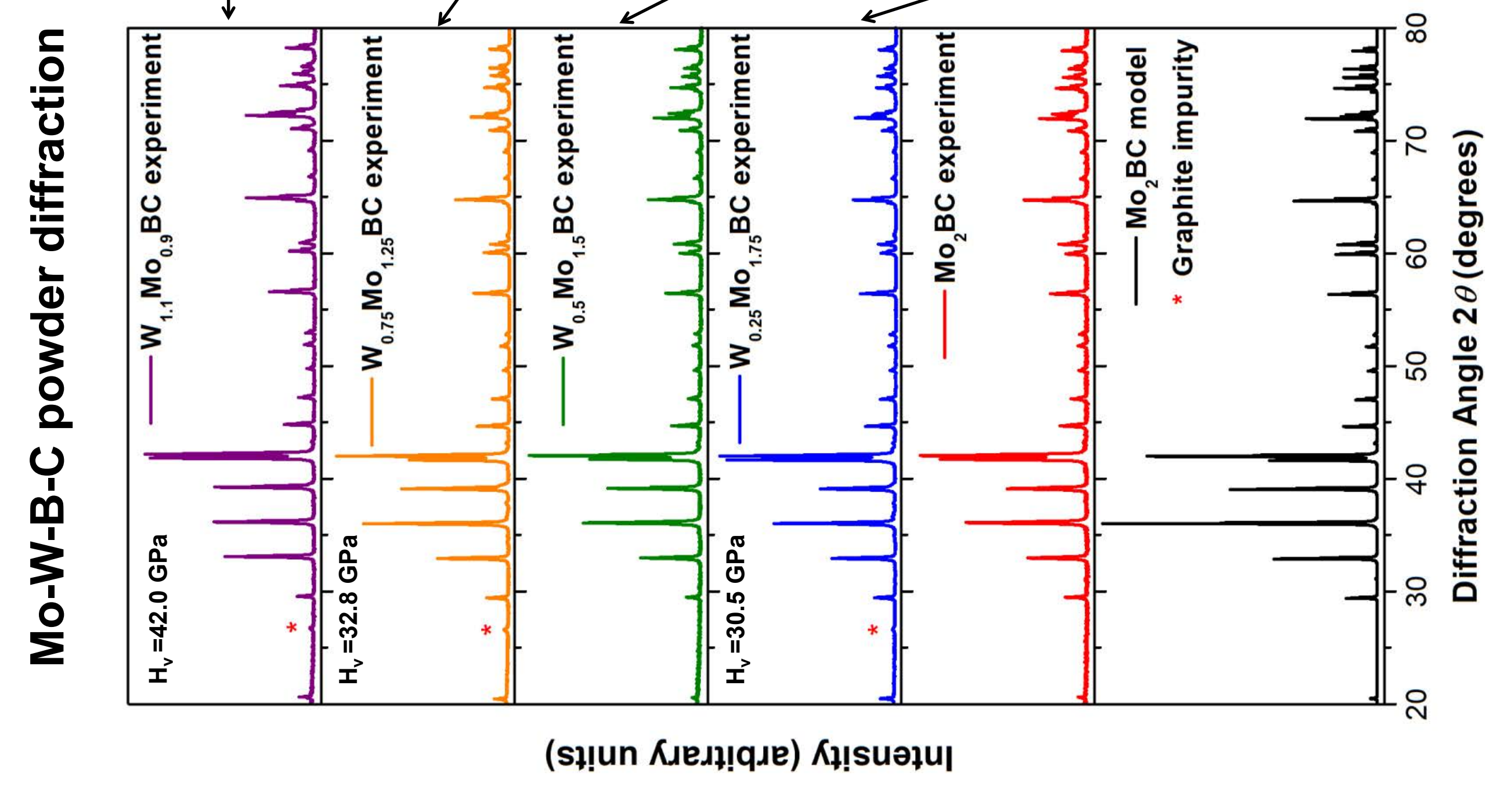
$\text{Re}_{0.5}\text{W}_{0.5}\text{C}$ has a deficient carbon site, which results in $\text{ReW}_{0.8}$ formula



Quaternary Compounds With the Highest Predicted Bulk and Shear Modulus



Compounds Formed From Tungsten-Doping of Mo_2BC



Conclusions

$\text{ReW}_{0.8}$ has a Vickers hardness of over 40 GPa (at 0.5 N applied load) whereas $\text{W}_{1.1}\text{Mo}_{0.9}\text{BC}$ shows a Vickers hardness of 42 GPa (at 0.5 N applied load).

The Vickers hardness of $\text{W}_x\text{Mo}_{2-x}\text{BC}$ series appears to increase as Tungsten concentration increases.

This study demonstrates that the novel machine learning method to finding materials with desired mechanical properties is a valuable approach to produce new superhard materials.

Future Work

Continue using machine learning method to synthesize and characterize new superhard compounds.

Explore new synthesis methods to better control desired phase formation.

Acknowledgements

We thank Gayatri Viswanathan, Amber Lim, and Shruti Hariyani (University of Houston) for assistance with experiments and data analysis. We are grateful to Bart Sheinberg and Dr. Gizzele Davis (Houston Community College) for administering the NSF Research Experiences and Exploration in Materials Science program. We thank the National Science Foundation (CMMI 15-62142 and DMR 14-60564) and American Chemical Society Petroleum Research Fund (55625-DN110) for funding.

[1] R. K. Bogdanov, A. Shulzhenko, A. P. Zakora, A. M. Isonkin, V. G. Gargin, New Superhard Material for Drilling Tools, Journal of Superhard Materials, 2007, 29, 55-63
[2] A. M. Tehrani, L. Ghaadbeigi, J. Brgoch, T. D. Sparks, Balancing Mechanical Properties and Sustainability in the Search for Superhard Materials, Integrating Materials and Manufacturing Innovation, 2017, 6, 1-8

Effects of Peptide functionalization on polyethylene glycol hydrogel and Biointeractions with oligodendrocyte progenitor cells

Adel, Y.,^{1,2} Nadeem, T.;^{1,2} Lu, Xi.;¹ Smith Callahan, L¹

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²REEMS REU program, West Houston Center for Science & Engineering, Houston Community College, Houston, Texas

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Spinal cord injury (SCI) leads to neuronal and axonal injuries along with significant oligodendrocyte death. The loss of oligodendrocyte and subsequent demyelination contributes greatly to the pathological process. Oligodendrocyte precursor cells (OPC) are potential source of cell therapy as they can respond rapidly to injuries, proliferate quickly and differentiate into myelinating oligodendrocytes. We fabricated and tested a polyethylene glycol (PEG) hydrogel functionalized with different concentrations of extracellular matrix protein (laminin1 and 2) based peptides to see whether the hydrogel would serve as a suitable OPC delivery system. To measuring the mechanical material, hydrogels were loaded with different concentrations of each peptides (0-1000 μ M). No significant differences in Young's modulus, swelling ratio, water content and mesh size were observed between the different concentrations or type of peptides. Rat derived OPC were embedded in laminin1 peptide hydrogels and cultivated for three days. Pico green DNA measurements showed that while the amount of DNA increased from day 1 to day 3. However, there was no difference in the increase between different peptide concentrations. Differentiation capacity of the OPCs in gels were assessed via imaging and counting myelin basic protein (MBP) positive stained cells. The data showed that 250 μ M of laminin1 peptide trended towards higher percentage of MBP positive oligodendrocytes compared to other peptide concentrations. All concentration of laminin2 peptide showed similar percentage of MBP positive cells. These results showed that the current work with these peptide functionalized hydrogels serve as a foundation for a delivery system for OPCs which may be a suitable therapeutic for

restoring myelination and motor function after spinal cord injuries.

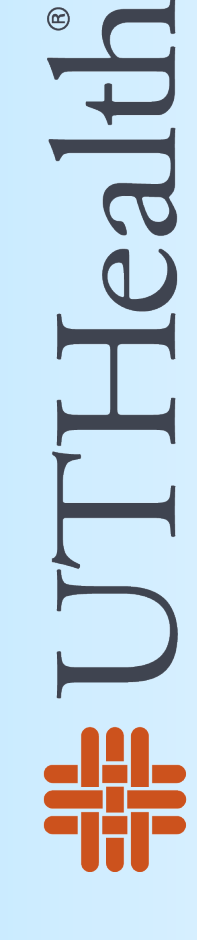
The authors gratefully acknowledge generous financial support provided by the National Science Foundation through NSF-DMR 1460564 and Ogilvie foundation.



Effects Of Peptide Functionalization on Polyethylene Glycol Hydrogel and Interaction with Oligodendrocyte Progenitor Cells

Tasmia Nadeem¹, Yasaman Adel¹, Xi Lu² and Laura Smith Callahan²

¹Houston Community College ; ²Department of Neurosurgery, University of Texas Health Science center, Houston, TX, USA.



The University of Texas Health Science Center at Houston



HOUSTON COMMUNITY COLLEGE
McCovern Medical School

Introduction

Spinal cord injury (SCI) leads to the death of neurons and glial cells which can then result in loss of motor functions and severely decrease patients' quality of life¹. Oligodendrocytes are a type of glial cells found in the central nervous system that are responsible for myelinating axons and secreting a variety of trophic factors necessary for neuronal function and survival. Loss of oligodendrocytes in spinal cord injury and subsequent demyelination are a major part of secondary injuries resulting from the primary insult/trauma. Re-myelinating surviving or regenerating axons is a crucial part of the recovery process and may potentially be facilitated by the delivery of progenitor stem cells in biomaterial scaffolds to the injury site. Oligodendrocyte progenitor cells (OPC) may be a useful source of cells for spinal cord therapy since they can differentiate into myelinating oligodendrocytes². In this work, we propose that by fabricating and testing polyethylene glycol (PEG) hydrogels containing peptides based on Laminin 1 or Laminin 2 domains, we can create a suitable system for insuring OPC survival and differentiation for use in treating SCI.

Methods

- Peptide functionalized PEG hydrogels were fabricated by crosslinking PEG (10%) in sterile phosphate buffer solution (PBS) with different concentrations (0-1000µM) of laminin 1 (peptide sequence: IKVAV) or laminin 2 (SYWYRIEASRTG), 3mM of MMP (KCGPQGIWGQCK) and 0.1% Irgacure 2959. The solution was passed through a 0.45µm filter and polymerized under UV light for 10 minutes.
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- To determine the water content, mesh size and swelling ratio, hydrogel samples after formation were weighted, swollen in PBS, weighed again, lyophilized overnight and then dry weight obtained.
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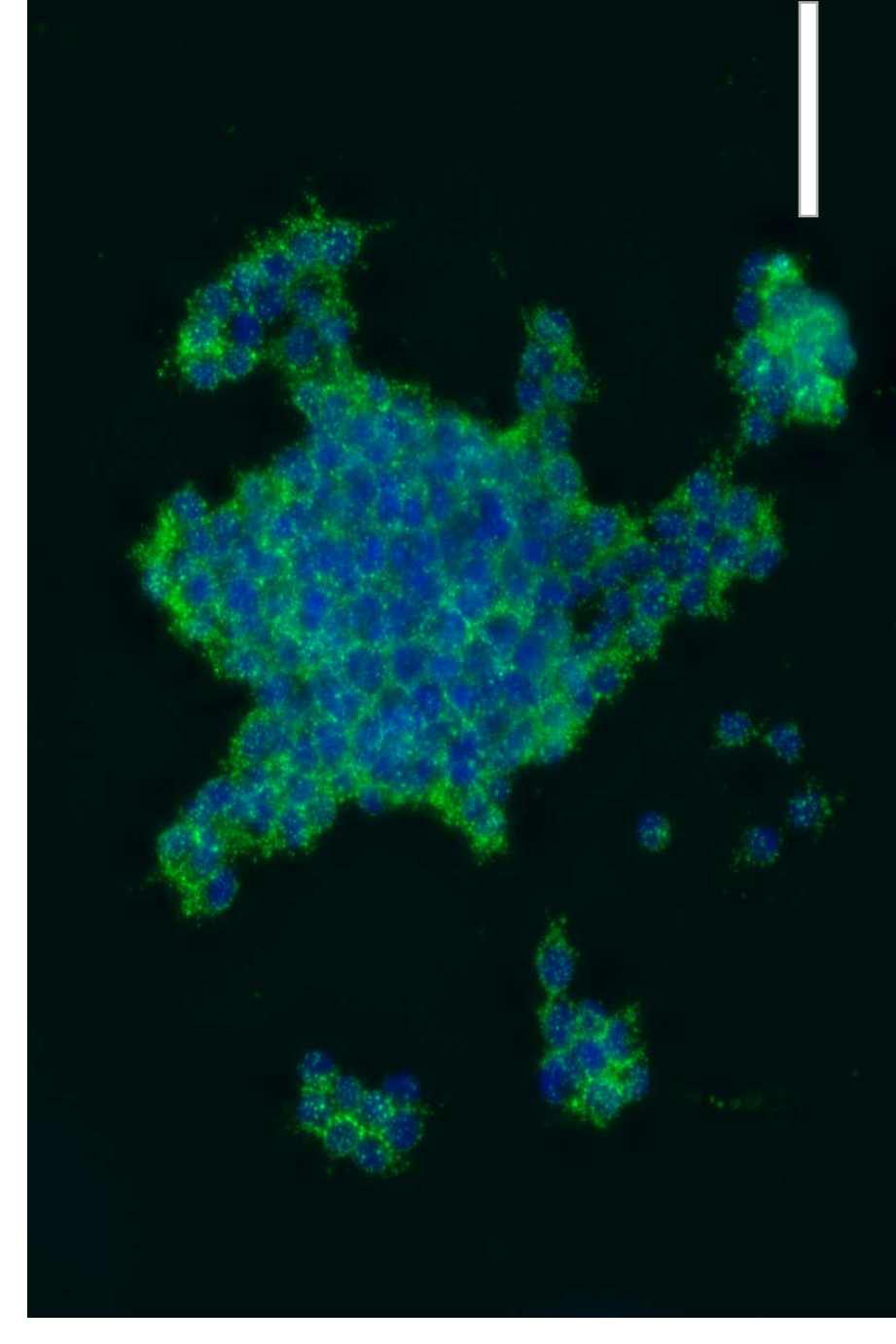


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| 100 | 50.9 | 2.7 | 75.86 | 17.2 |
| 250 | 36.3 | 6.3 | 52.1 | 7.7 |
| 500 | 67.3 | 16.2 | 56.1 | 31.02 |
| 750 | 67.6 | 18.9 | 82.6 | 30.8 |
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| 100 | 93.9 | 0.508 | 96.3 | 1.52 |
| 250 | 89.9 | 2.17 | 93.7 | 1.6 |
| 500 | 95.3 | 1.53 | 93.4 | 3.5 |
| 750 | 95.4 | 1.58 | 96.1 | 2.1 |
| 1000 | 93.01 | 4.74 | 93.6 | 1.5 |

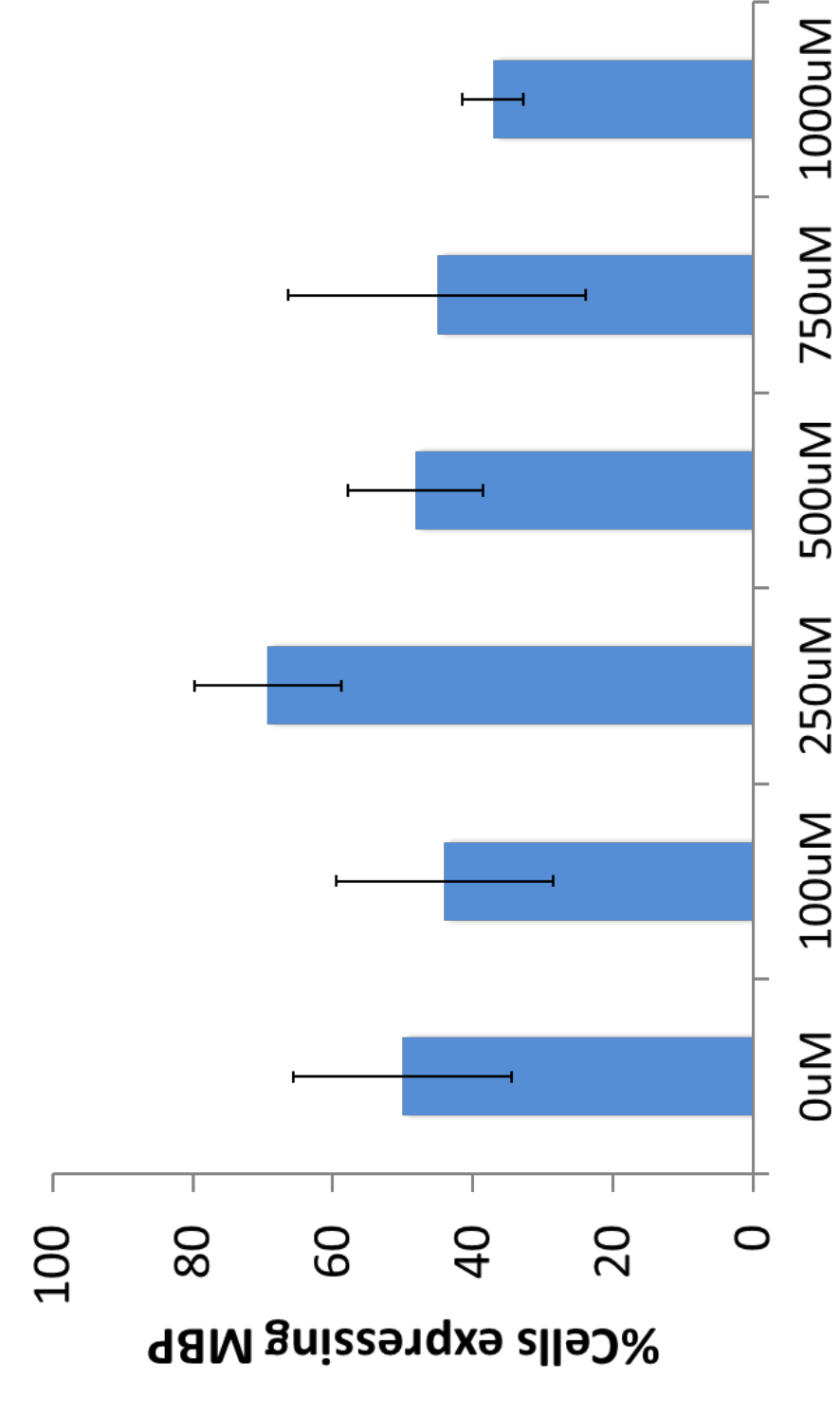


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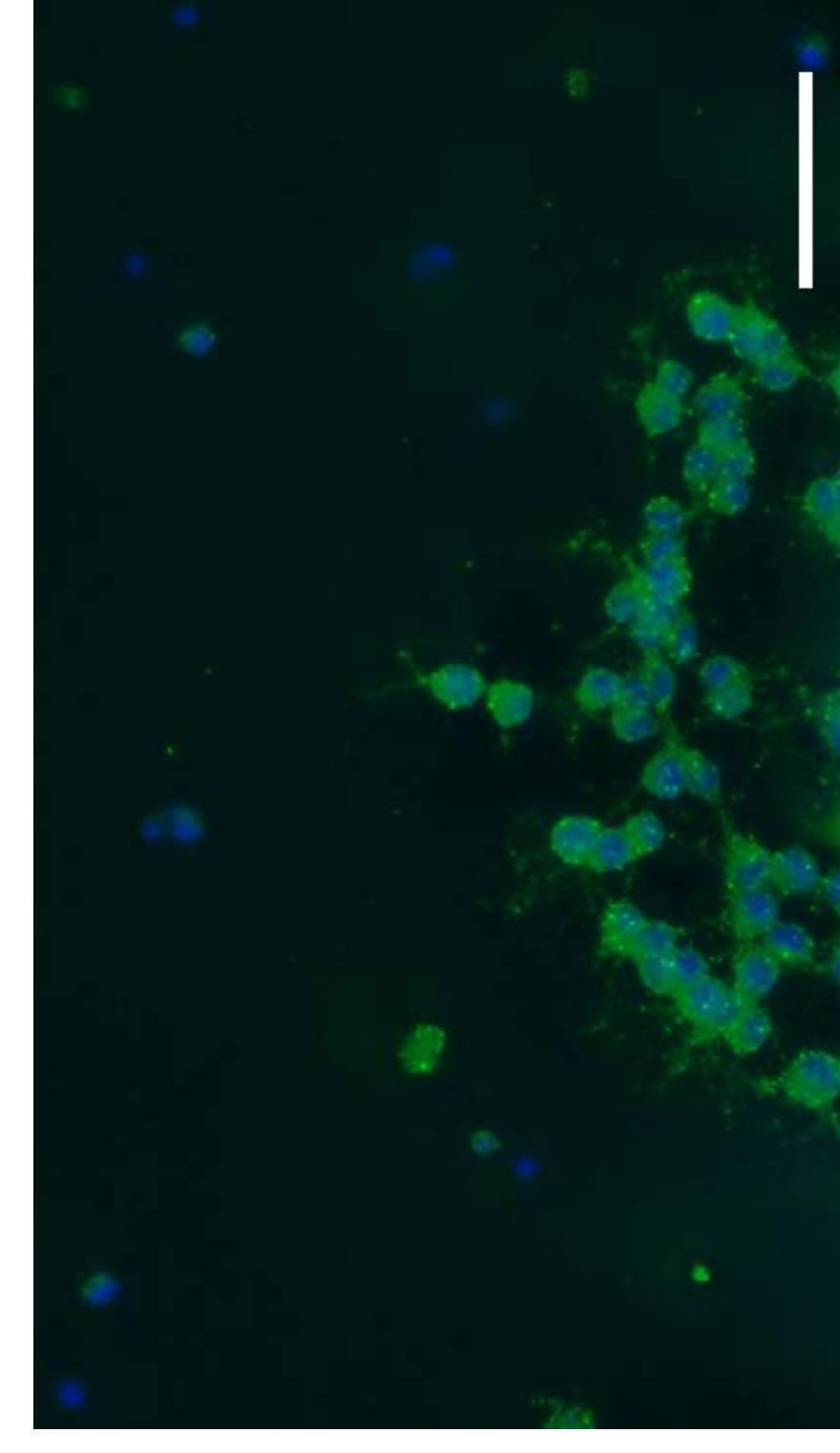


Fig 6: r-OPC survived and differentiated into oligodendrocyte (myelin basic protein (MBP) in green, DAPI in blue) by day 3. Scale bar indicates 100 µm.

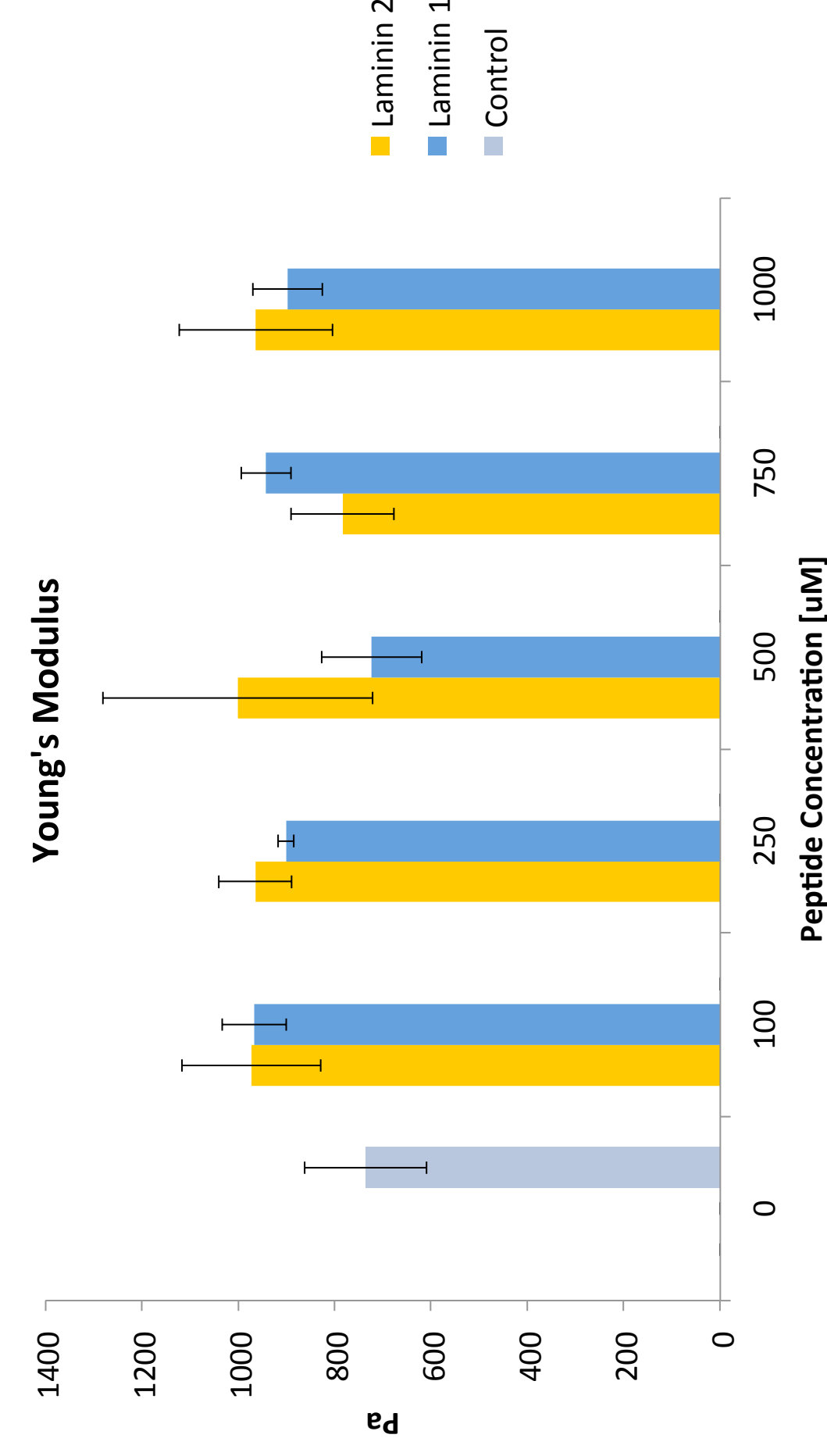


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| 500 | 23.3 | 8.61 | 20.4 | 15.2 |
| 750 | 24.16 | 10.27 | 30.7 | 14.04 |
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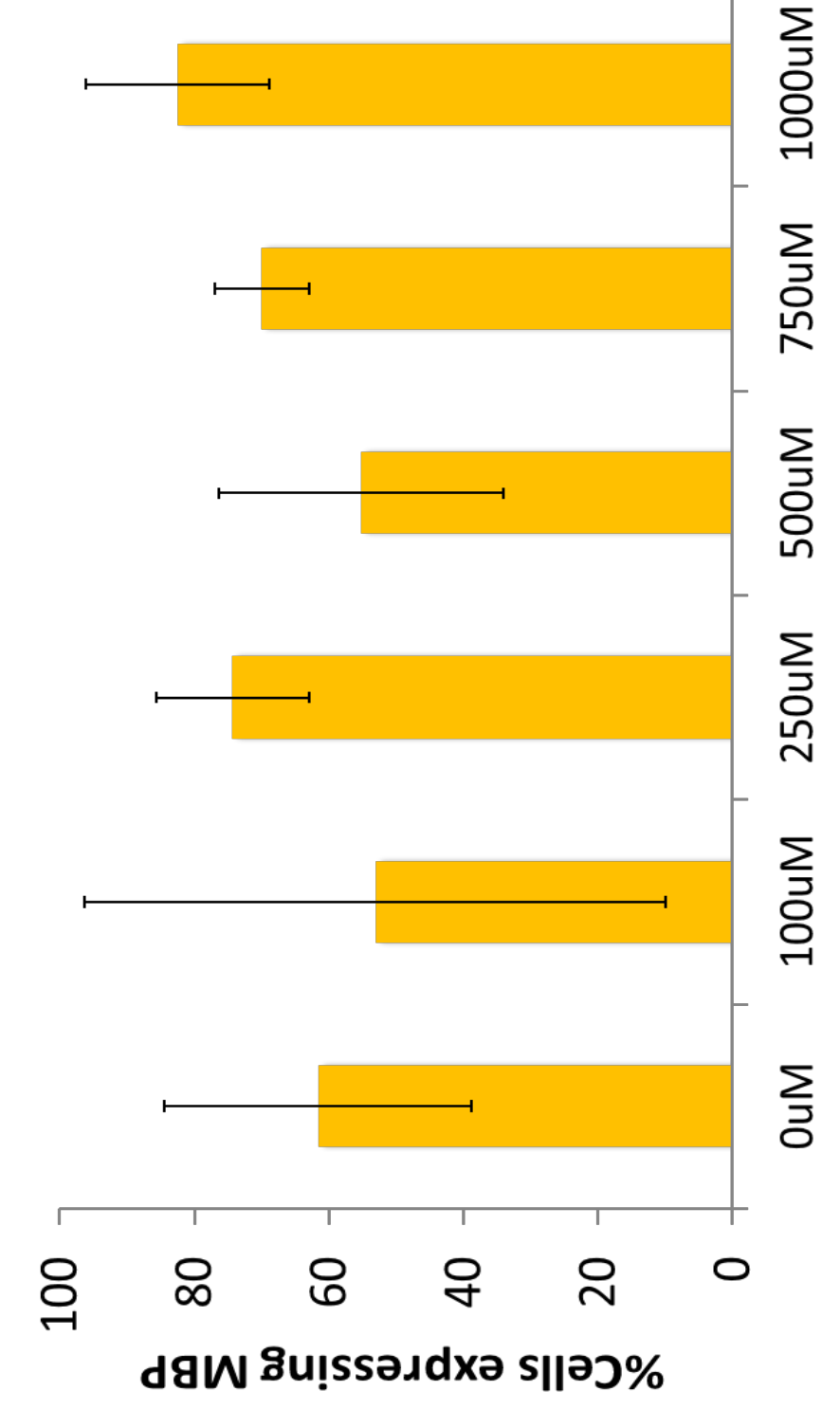


Fig 5: Quantification of r-OPC differentiation in laminin 2 gels. Cells positive for MBP is expressed as a percentage of the total number of cells. ~300-400 total cells counted per gel were counted for each concentration of peptide laminin 2 (n = 2 gels per group).

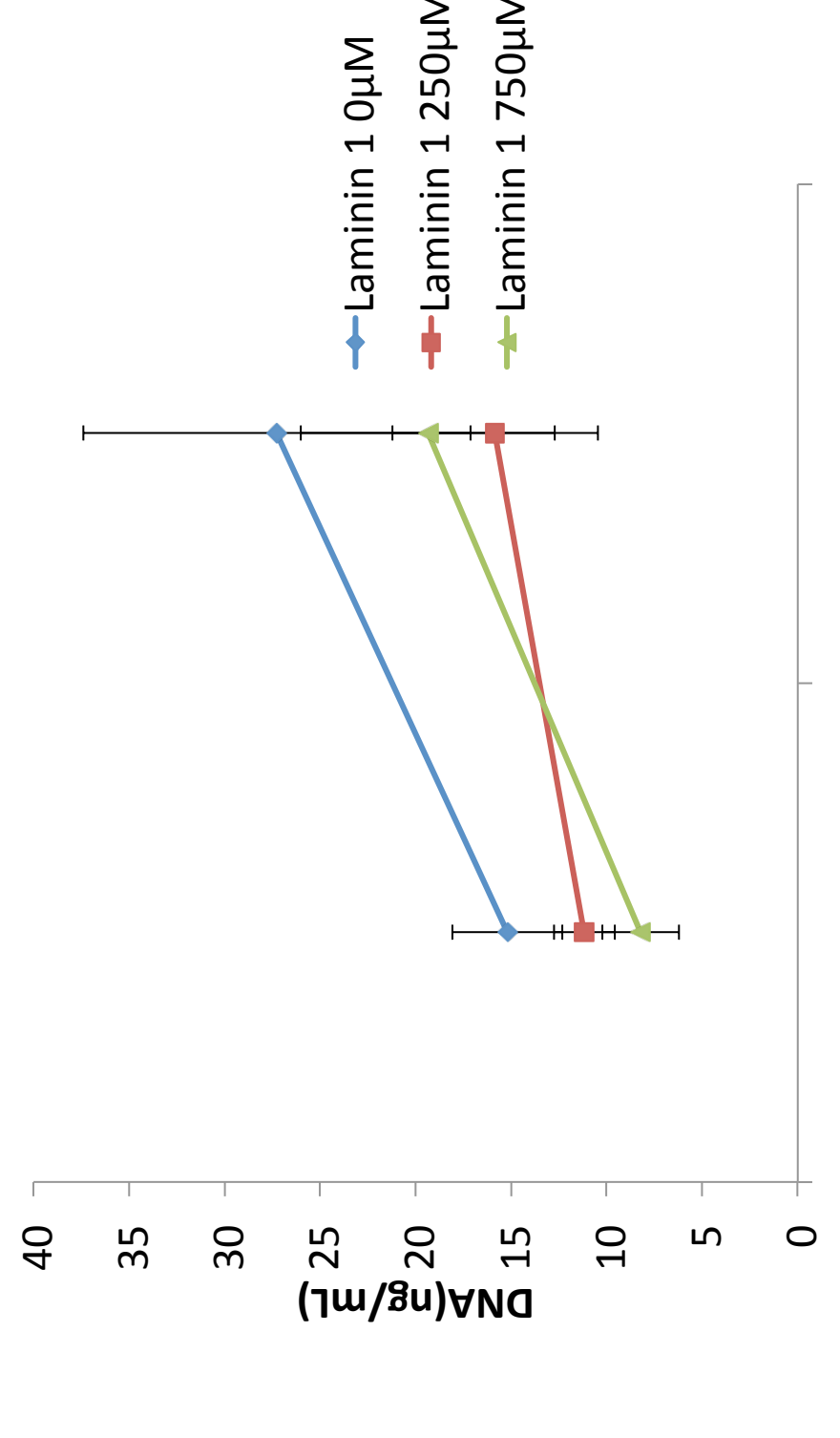


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Discussion

Synthetic PEG hydrogel offers a flexible, easily modifiable, and controllable base for developing cell delivery systems³. Proteins found in the extracellular matrix such as laminin 1 and 2 are known to affect OPC survival and function such as by enhancing myelin membrane formation. Peptides based on the functional domains of the proteins are easily tethered to the hydrogels and may mimic the biological function of the original proteins. We found that adding peptides to the hydrogels did not affect the major mechanical properties of the hydrogels such as Young's modulus, mesh size, and swelling ratios which suggests that whatever biological effects that occur would then be due to the addition of the peptides and their concentration. Counting the MBP positive cells showed the percentage of differentiated r-OPC's was approximately 50-60% for both of the peptides. While 250µM concentration of laminin 1 trended higher percentage of differentiated OPCs compared to other laminin 1 concentrations, there were no significant differences. One reason may be that the concentration of each peptide may not have been optimized to cause the greatest levels of cell differentiation. Additional concentrations should be tested. It would also be interesting to see whether combinations of laminin 1 and 2 in the same gel will affect cell function.

Conclusion

- Embedding up to 1000µM of Laminin 1 or Laminin 2 peptides into 10% PEG hydrogel did not cause significant changes to mechanical properties of the gels
- Within these hydrogels, OPCs can survive, proliferate and differentiate into oligodendrocytes
- Future studies will continue to optimize these gels for human OPCs and involve animal studies to test the viability of these system for restoring myelination and motor function after SCI.

Acknowledgment

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Effects of Peptide Functionalization on Polyethylene Glycol Hydrogel and Biinteractions with Oligodendrocyte Progenitor Cells.

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¹REEMS REU Program, West Houston Center for Science & Engineering, Houston Community College, Houston, Texas

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Spinal cord injury (SCI) leads to neuronal and axonal injuries along with significant oligodendrocyte death. The loss of oligodendrocyte and subsequent demyelination contributes greatly to the pathological process. Oligodendrocyte precursor cells (OPC) are potential source of cell therapy as they can respond rapidly to injuries, proliferate quickly and differentiate into myelinating oligodendrocytes. We fabricated and tested a polyethylene glycol (PEG) hydrogel functionalized with different concentrations of extracellular matrix protein (laminin 1 and 2) based peptides to see whether the hydrogel would serve as a suitable OPC delivery system. To measure the mechanical and material properties, ten percent PEG hydrogels were loaded with different concentrations of each peptides (0-1000 μ M). No significant differences in Young's modulus, swelling ratio, water content and mesh size were observed between the different concentrations or type of peptides. Rat derived OPC were embedded in laminin 1 peptide hydrogels and cultivated for three days. Pico-green DNA measurements showed that the amount of DNA increased from day 1 to day 3. However, there was no difference in the increase between different peptide concentrations. The differentiation capacity of the OPCs in hydrogels were assessed via fluorescence imaging and counting the number of cells positive for myelin basic protein (MBP) staining. The data showed that 250 μ M of laminin 1 peptide trended towards higher percentage of MBP expressing oligodendrocyte compared to other peptide concentrations. All concentration of laminin 2 peptides showed similar percentage of MBP positive stained cells. These results showed that the current work with these peptide functionalized hydrogels serve as a foundation for a delivery system for OPCs,

which may be a suitable therapeutic for restoring myelination and motor function after spinal cord injuries.

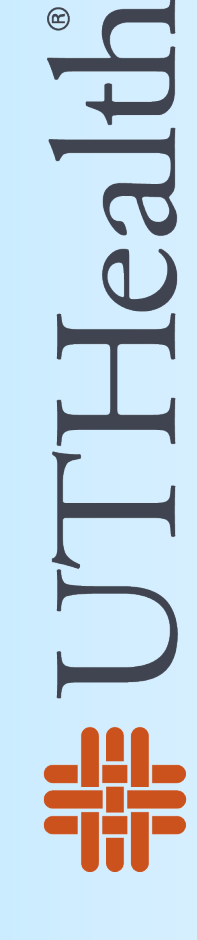
The author gratefully acknowledges support from Houston Community College REEMS REU Program and generous financial support from National Science Foundation Division of Material Research through NSF-DMR 1460564 and Ogilvie foundation.



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The University of Texas Health Science Center at Houston



HOUSTON COMMUNITY COLLEGE
McCovern Medical School

Introduction

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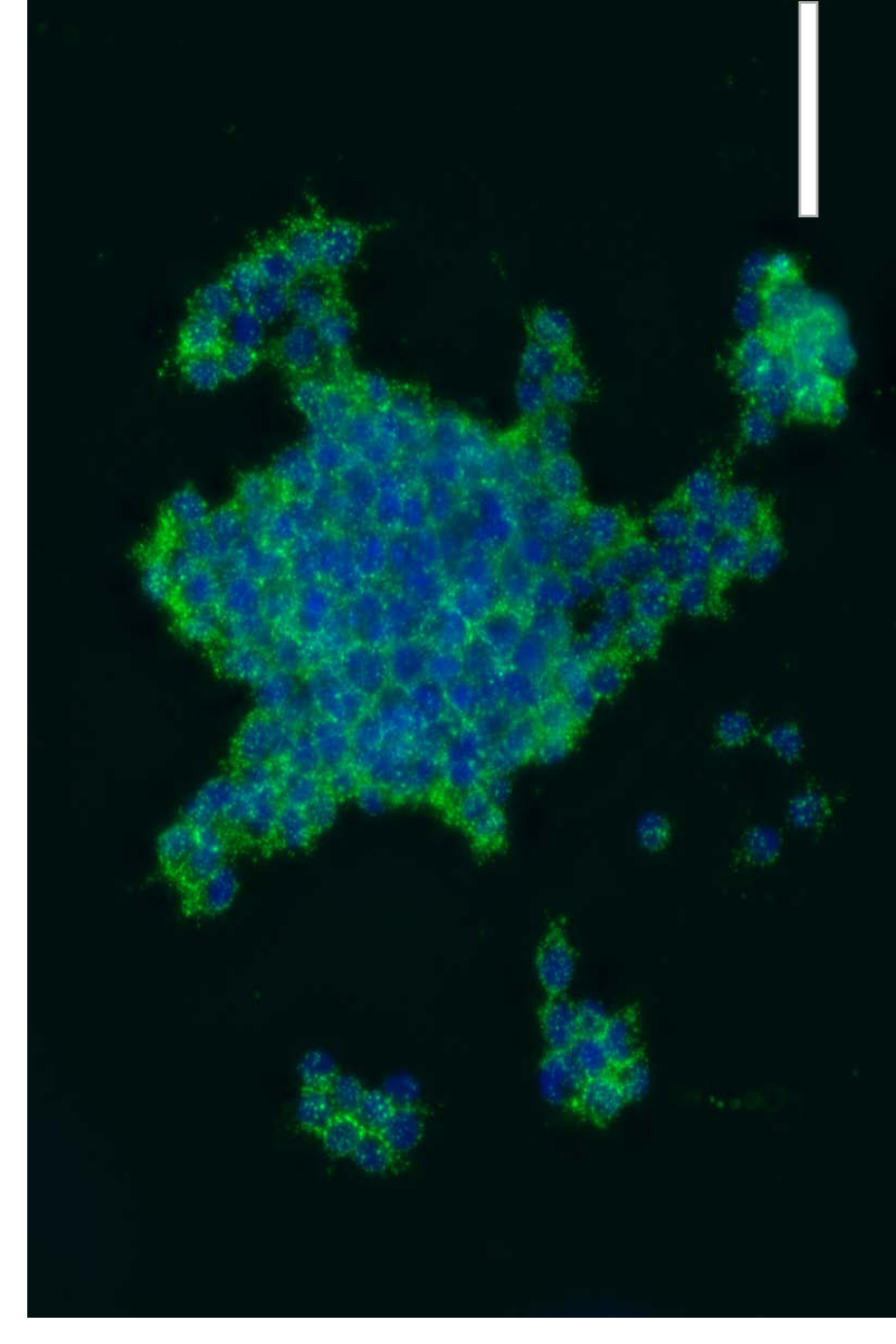


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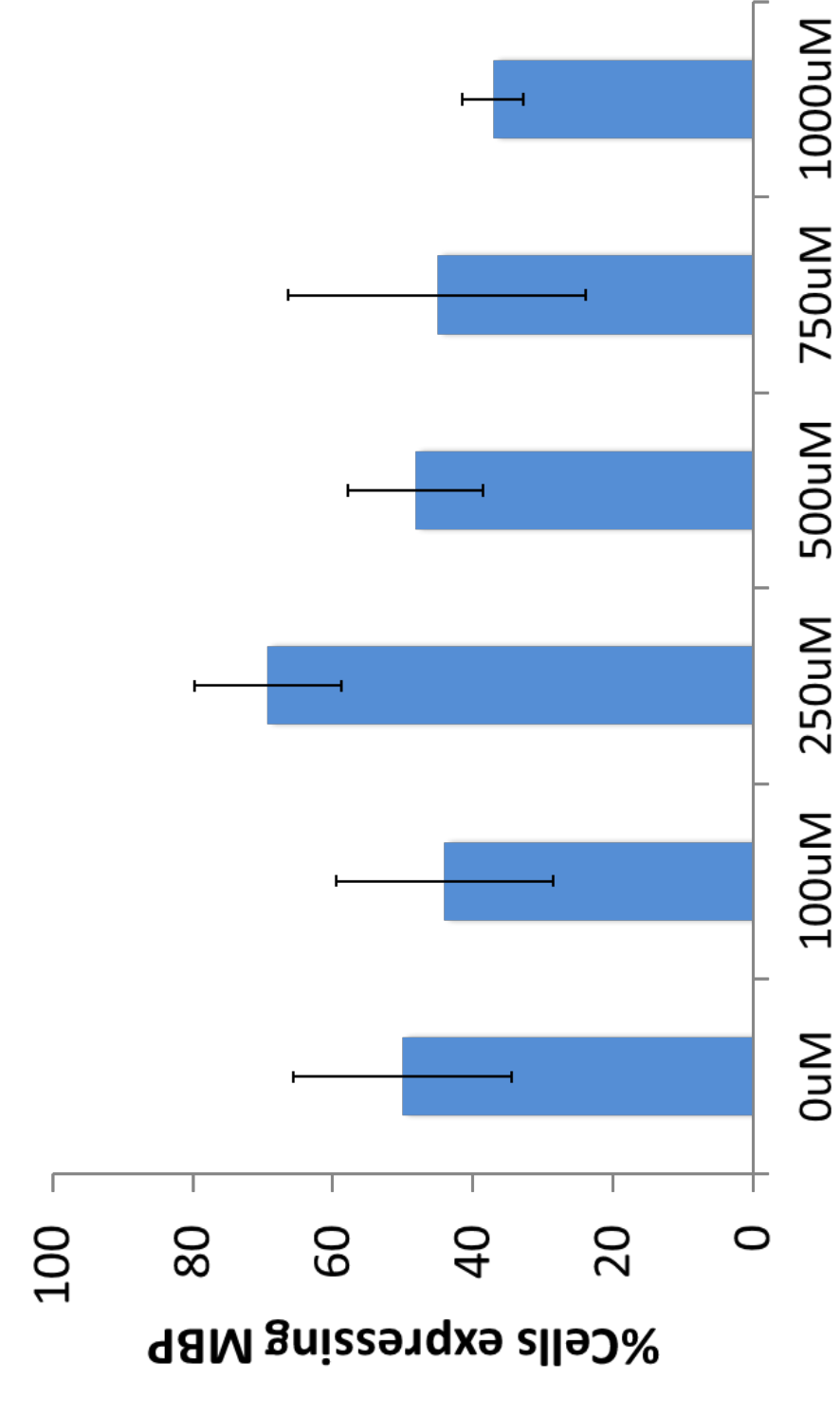


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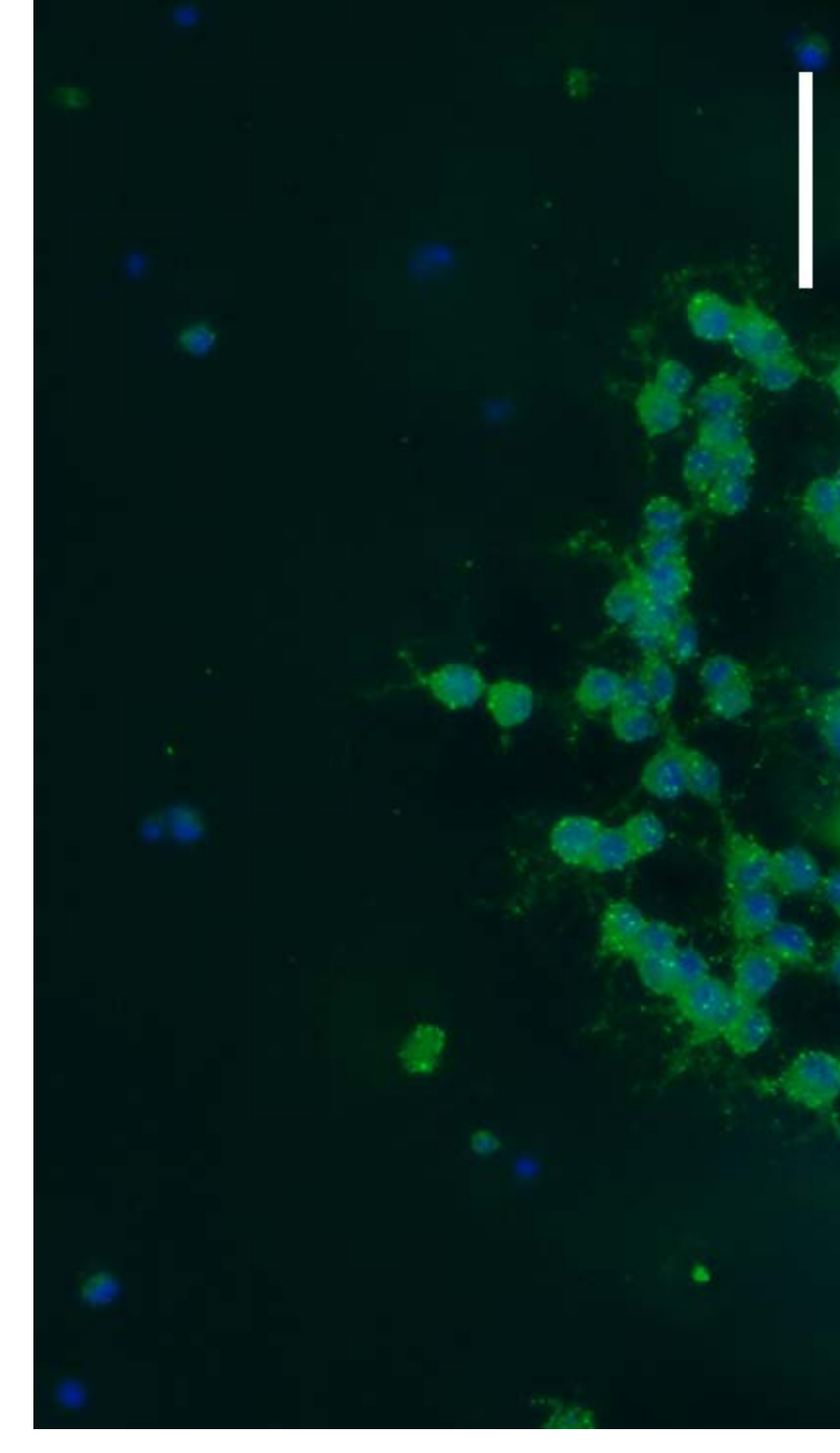


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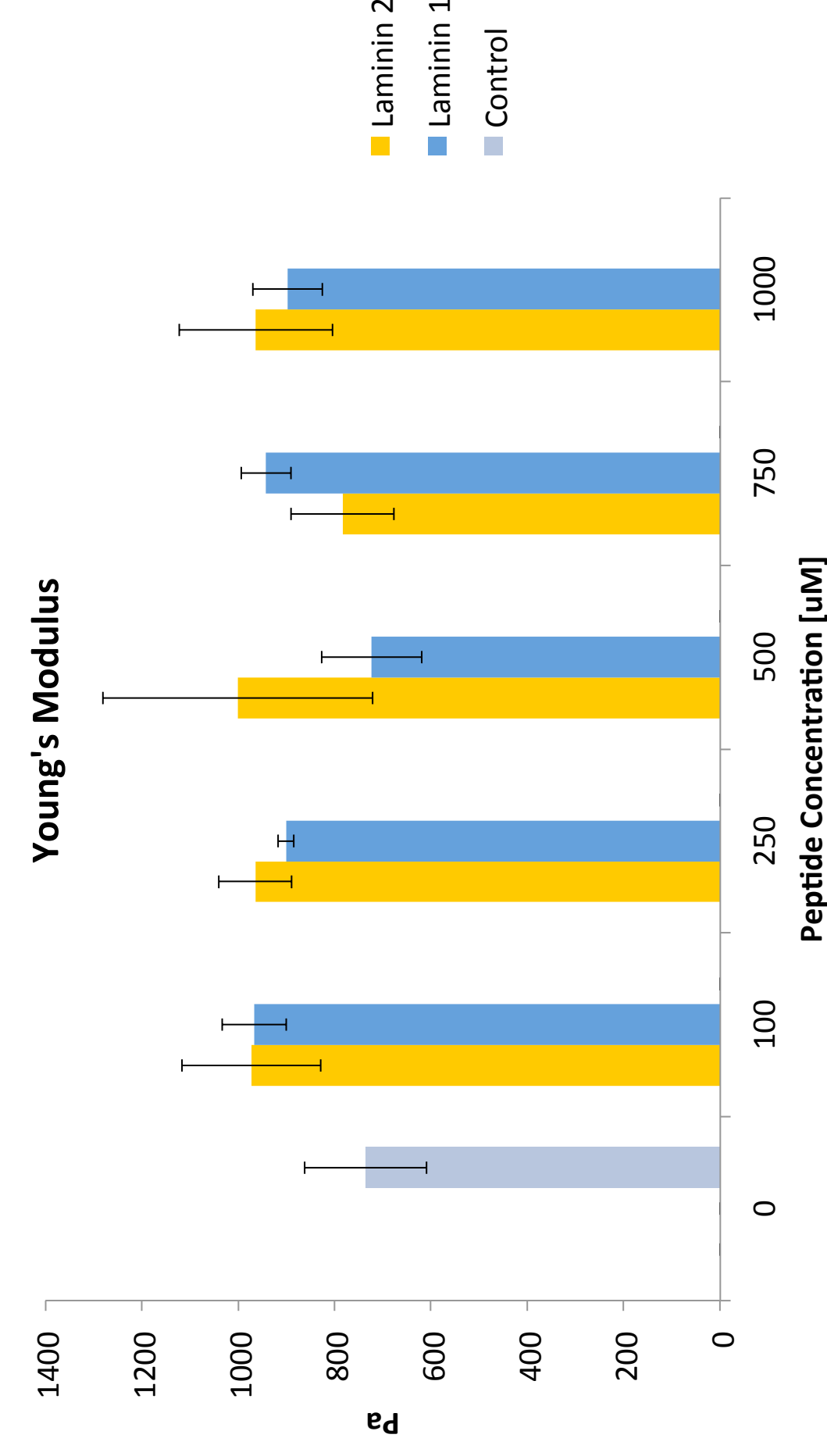


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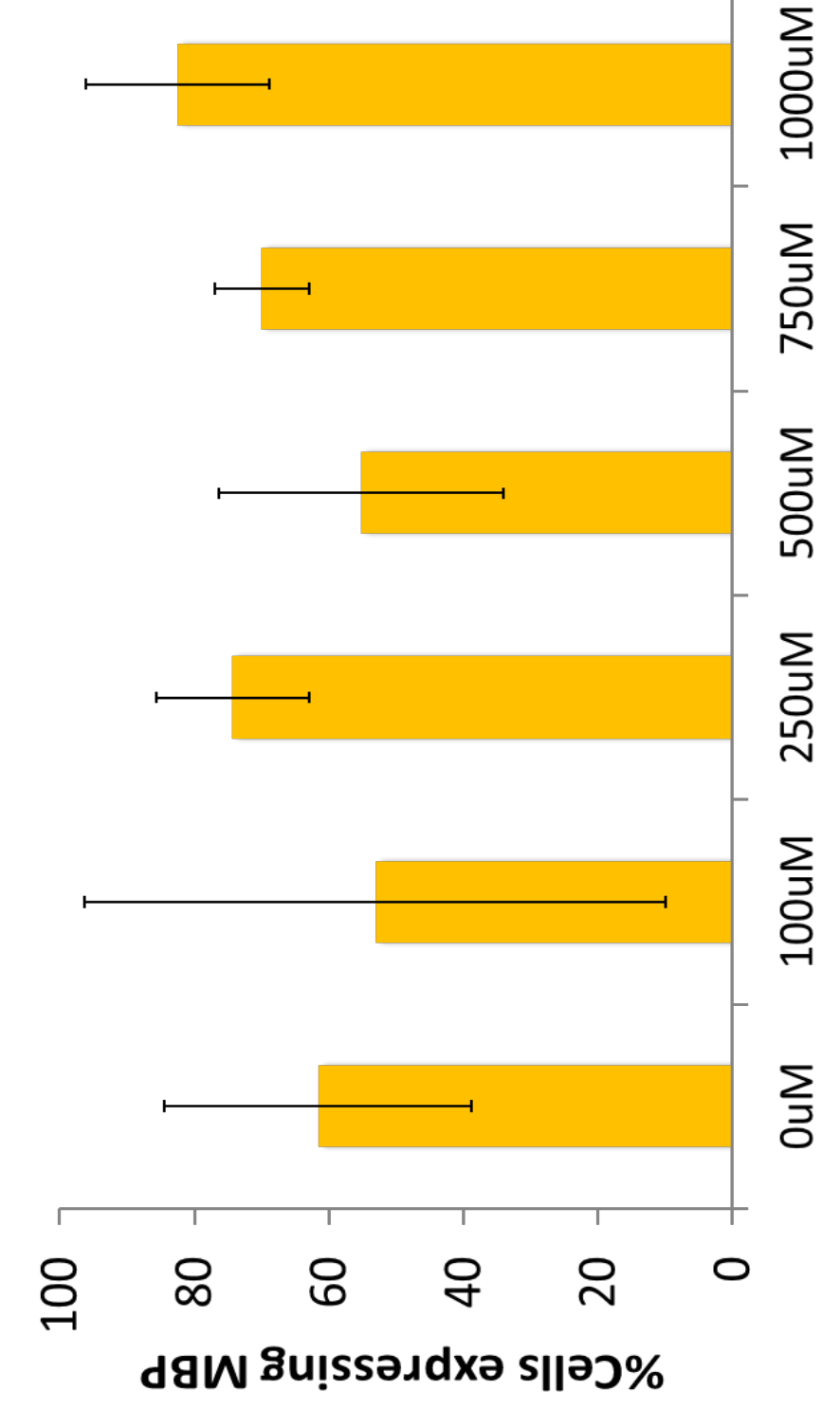


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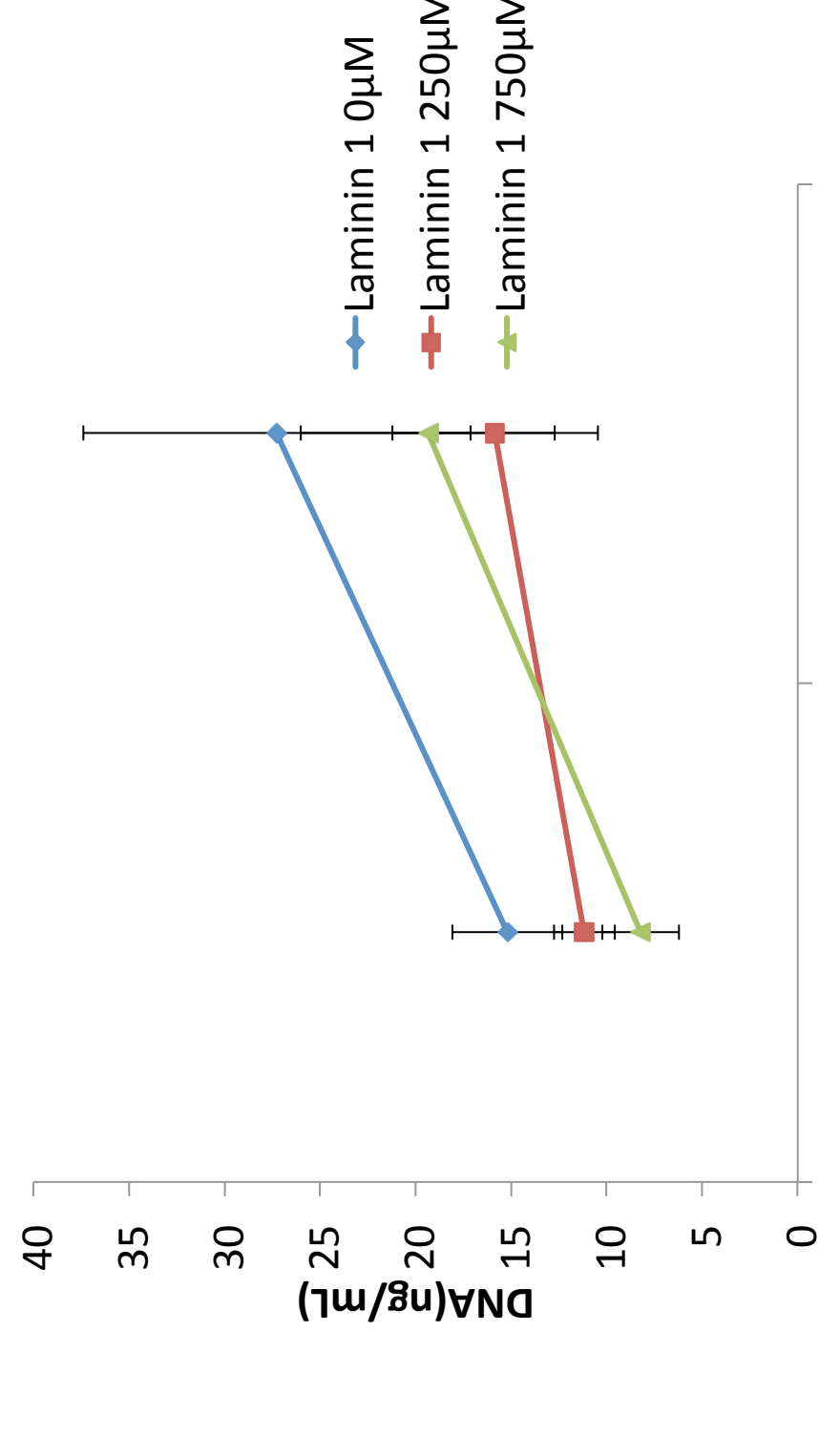


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Solidification Front Velocity and Temperature Gradient in Metal Crystals Grown from the Melt

Andrew Catalanotto¹, Daniel Suzuki², Logan Ware², Zachary Cordero²

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² Department of Material Science and Nano Engineering at Rice University, Houston TX

Directional solidification of single crystals and bicrystals requires a steep temperature gradient in the liquid phase to maintain a planar solid-liquid interface perpendicular to the growth direction. Knowledge of the thermal profile in the metal charge during growth can help guide the selection of optimal process variables (e.g., growth velocity). In this study, we directly measured the thermal profile during the directional solidification of a tin bicrystal using thermocouples sheathed in glass and placed in the center of the specimen. We then analyzed our measurements and determined the temperature gradient and solidification front velocity along the length of the specimen. Our experimental results help explain the physics of the crystal growth method under development, and confirm the benefit of incorporating the chill rod.

This work is supported by the National Science Foundation (DMR-1460564) and the Houston Community College District.

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Directional Solidification & The Bridgman Method

Directional solidification is the process of cooling metal castings by freezing the metal progressively from one end of the casting to the opposite end. Various methods of directional solidification are used to eliminate cavities, remove impurities from metals, and grow large single crystals and bicrystals.

Modified Bridgman Method

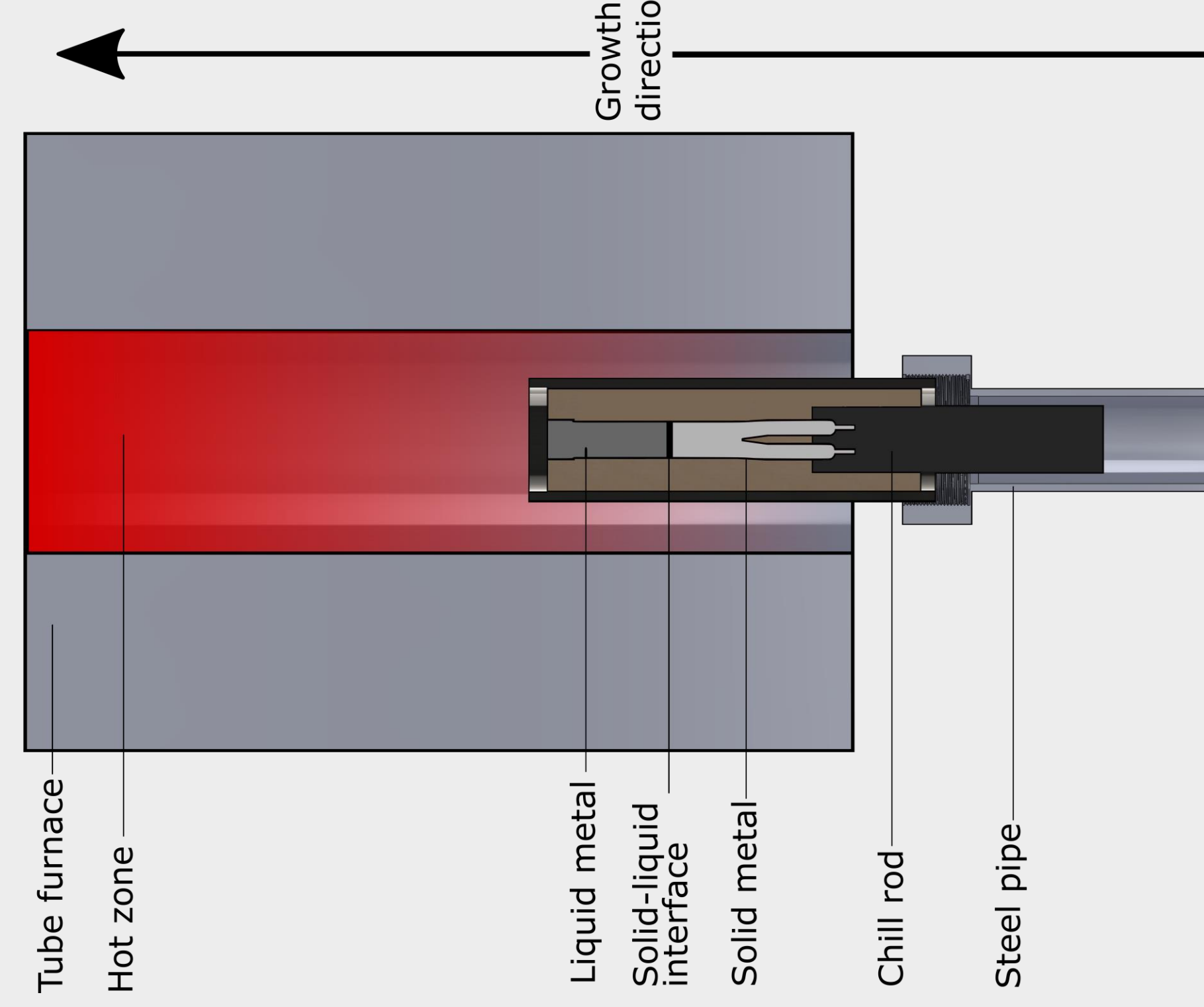


Figure 1. Cross section diagram of modified Bridgman setup with moving furnace directionally solidifying a stationary metal casting. The graphite chill is inserted into the steel pipe at room temperature to act as a heat sink, increasing the temperature gradient along the vertical axis.

In this work we fabricate molds capable of measuring the thermal profile during growth, then analyze the profile to explain why our growth conditions are in the optimal range.

Thermal Measurement Specimen

Fabrication of specialized molds to measure the thermal profile during growth is necessary due to the mold geometry, which prevents direct probing of the metal along its axis as the crystal is grown. Glass tubing is invested in the plaster,

Thermal Measurement Molds

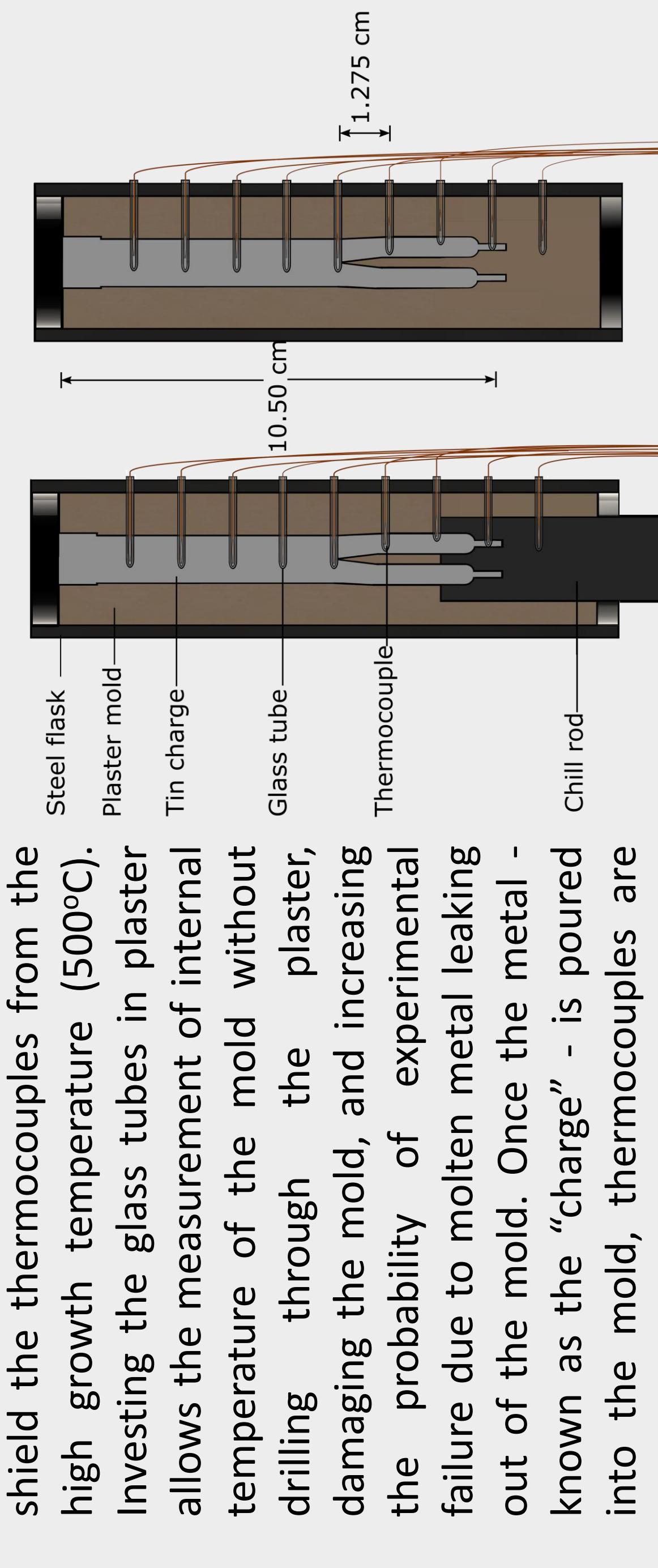


Figure 2. Cross section diagram of molds used to measure the thermal profile during crystal growth with a chill rod (left) and without a chill rod (right).

Solidification Front Velocity

To calculate the solidification front velocity, the position of each thermocouple within the charge is plotted against the time at which the surrounding metal (tin) freezes. Figure 3 shows a ~25% decrease in growth velocity with the addition of the chill. By conducting latent heat away from the metal, the chill initiates freezing earlier in the growth and leads to a less steep, more controlled growth velocity.

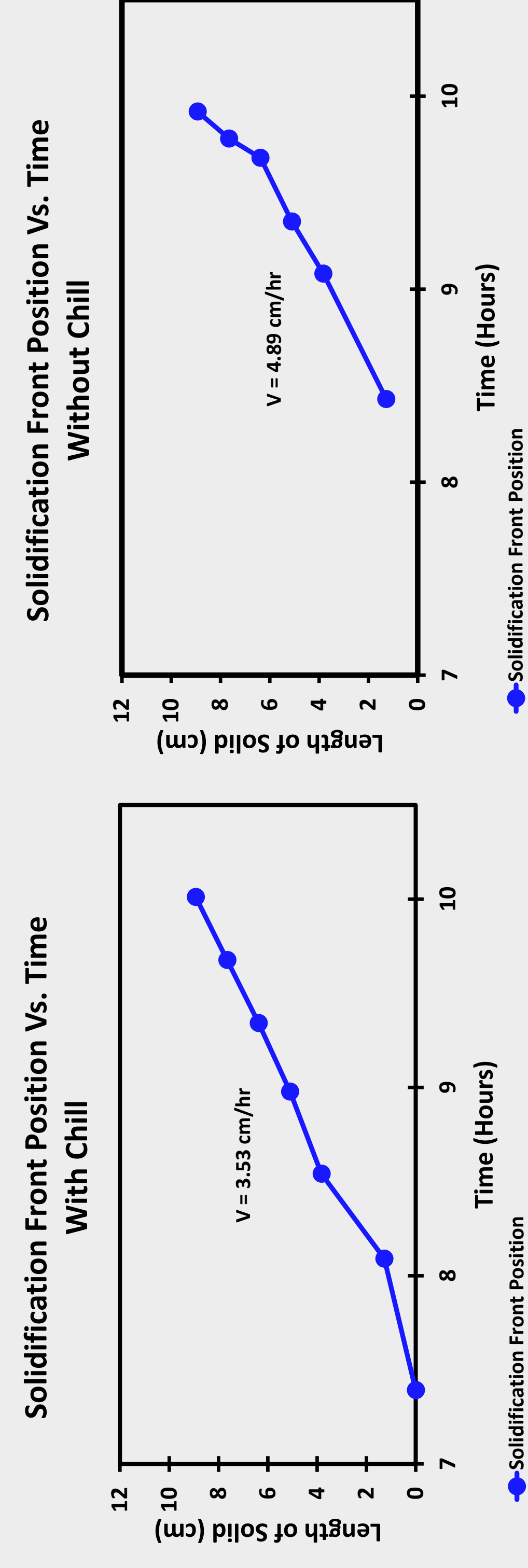


Figure 3. Graph of the length solidified vs. time for a specimen both with (left) and without (right) a chill. Each point represents the time metal freezes around a thermocouple and its position along the length of the charge. The slope of the lines represents the growth velocity.

Temperature Gradient

To calculate the temperature gradient (G), the temperature of the metal around each thermocouple is plotted against its position along the length of the charge each time the metal surrounding a thermocouple freezes. Figure 4 shows a plot during solidification, when the solid is ~5.1 cm long. Figure 5 shows the temperature gradient at each thermocouple as the solidification front passes it against the length of the solid. The graphs show that the gradient in the liquid (G_L) with the chill is approximately double that with no chill throughout the growth.

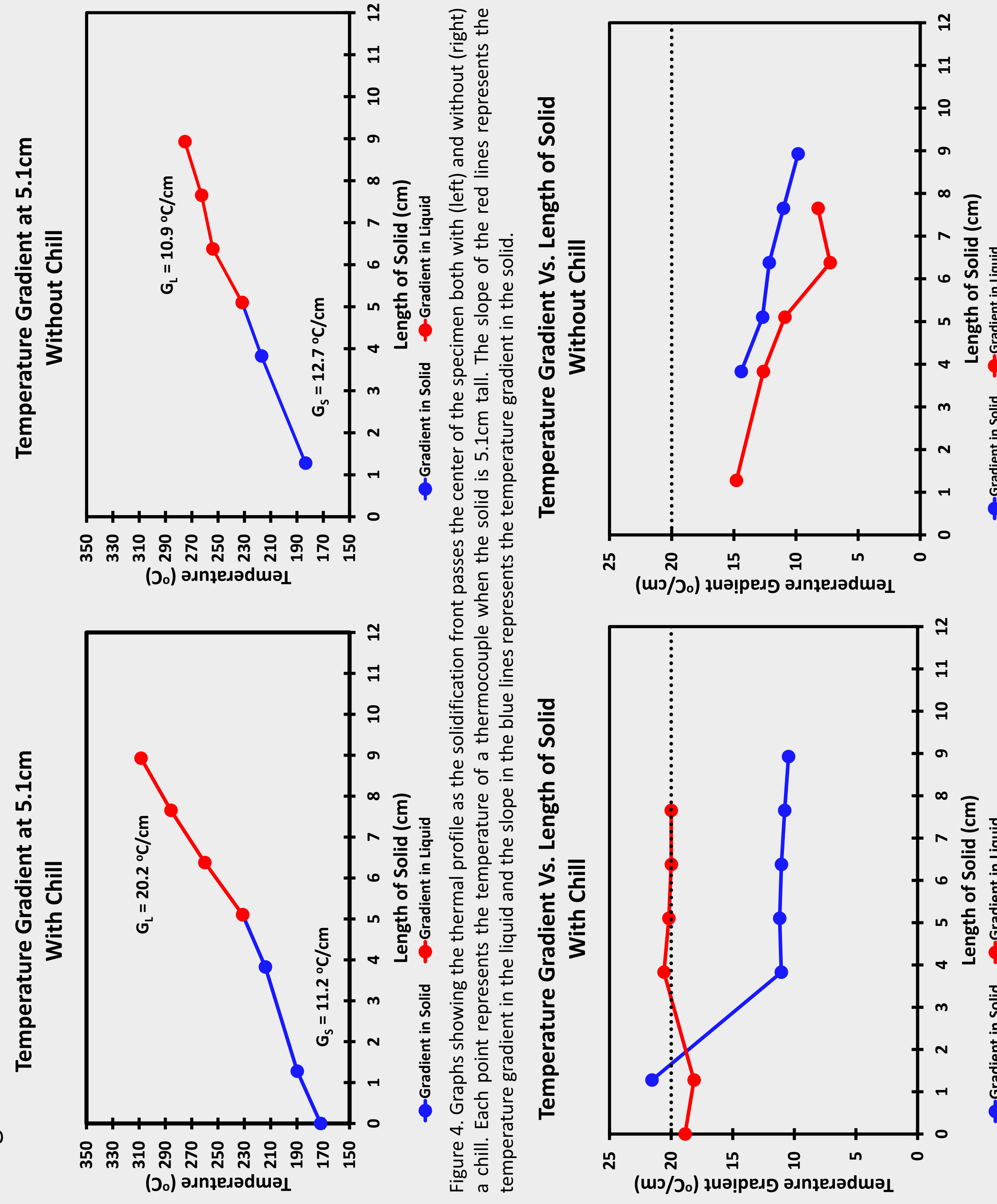


Figure 4. Graphs showing the thermal profile as the solidification front passes the center of the specimen both with (left) and without (right) a chill. Each point represents the temperature of a thermocouple when the solid is 5.1cm tall. The slope of the red lines represents the temperature gradient in the liquid and the slope in the blue lines represents the temperature gradient in the solid.

Figure 5. Graph showing the temperature gradient as the solidification front passes each thermocouple in the specimen with a chill (left) and without a chill (right). The dotted black line represents the target gradient in the liquid phase. Each point represents the temperature gradient as the solidification front passes a different thermocouple within the charge.

Discussion

These results clearly demonstrate that the experimental configuration in Figure 2 can be used to analyze the effect of process variables on our modified Bridgman method. Analysis of the data in Figure 3 shows the chill rod decreases the growth velocity by approximately 25% and produces a more uniform growth rate of the solid over time. Figure 4 shows a 2X increase in the temperature gradient in the liquid phase near the middle of the growth. Figure 5 shows that this increased gradient is seen throughout the growth, and is within ~2 °C/cm of the target value for the temperature gradient in tin [3].

Low temperature gradient and high growth velocity are factors that increase the likelihood of parallel solidification, nucleation of stray crystals, and migration of grain boundaries in directionally solidified crystals [2]. Thus, the increase in temperature gradient and reduction in growth velocity help explain the success of our modified Bridgman method with the chill rod.

Future Works

Finite element analysis:

Thermal profile measurements can take up to 4 days to perform. The plaster, glass, and graphite are all very fragile and prone to failure. In order to rapidly and reliably test a variety of geometries and growth conditions, finite element analysis software can be used to simulate the thermal profile during crystal growth.

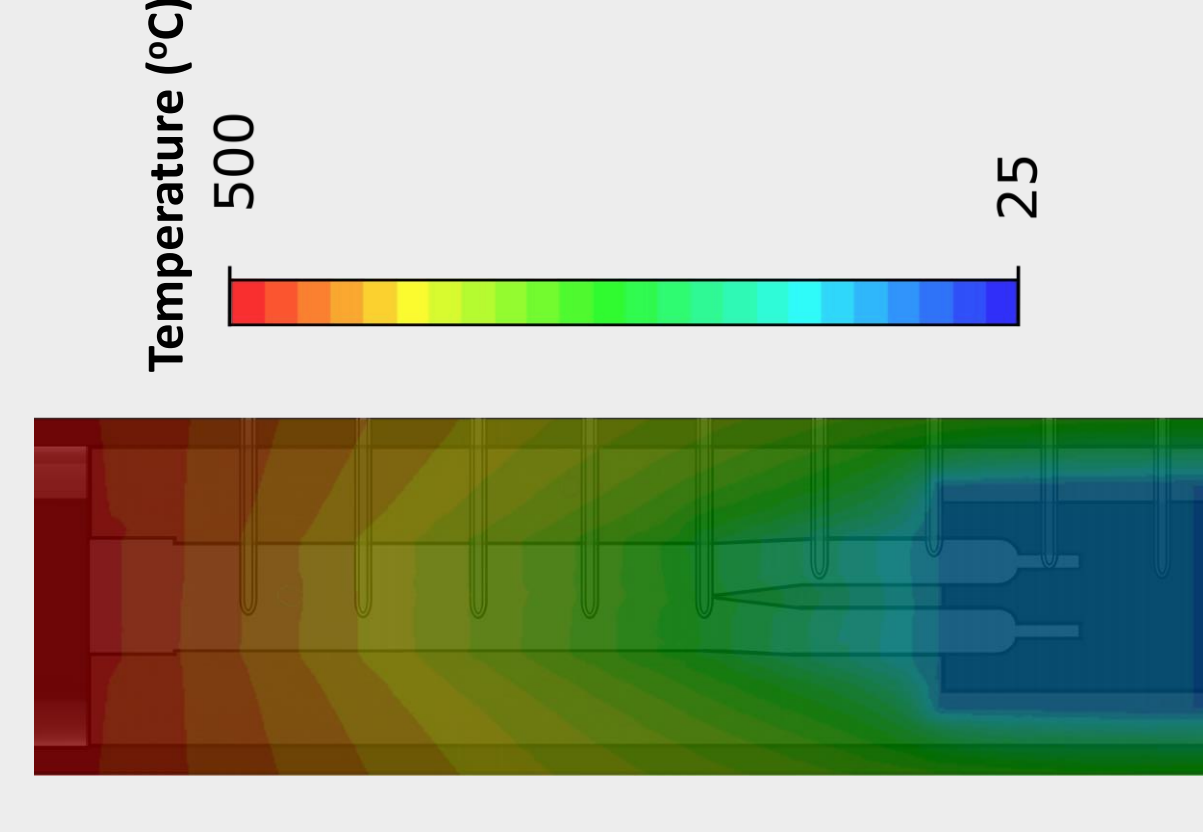


Figure 6. Sinusoidal, helical, and "helioidal" bicrystal geometries currently being explored using our method.

Testing complex geometries:

Thermal profile measurements and analysis have so far been performed using only a traditional bicrystal geometry. Analysis of more geometrically complex crystal molds will help us understand how geometric variation affects the growth process.

Acknowledgement

I thank the National Science Foundation Division of Materials Research Grant DMR 1460564 for this research opportunity. I would also like to thank Daniel H. Suzuki, Logan G. Ware and Dr. Zachary C. Cordero for their support and guidance during my research experience at The Additive Lab this summer.

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- [2] B. Chalmers, Canadian Journal of Physics 31 (1953) 132-146.
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Fabrication of Bulk Nanocrystalline Alloys Using Ultrasonic Powder Compaction

Nathaniel Ocanas¹, Raquel Torres³, Austin Ward², Zachary Cordero²

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²Department of Material Science and Nano Engineering at Rice University, Houston TX

³NSF Research Experience for Teachers, Rice University, Houston, Texas

Nanocrystalline alloys have high strengths, high hardness values, and excellent wear resistance, making them attractive materials for use in numerous structural applications. However, it remains a challenge to reliably fabricate bulk nanocrystalline materials because the most straightforward synthesis method, powder consolidation, involves the densification of nanostructured powder at high temperatures. This approach presents challenges because nanocrystalline materials exhibit rapid grain growth at elevated temperatures, resulting in the loss of their unique properties, attributed to fine grain sizes. One low-temperature method that could be used to consolidate nanocrystalline powders without significant coarsening is ultrasonic powder compaction. In this process, a punch compresses feedstock powder in a die and then shears the powder at ultrasonic frequencies transverse to the loading axis. This combination of normal pressure and oscillating shear stresses disrupts the native oxide on the feedstock powder particles, resulting in metallurgical bonding. Although elevated temperatures are not required for ultrasonic powder compaction, they can result from frictional heating. Therefore, to optimize the grain size and mechanical properties of our compacts, we have identified the set of ultrasonic powder compaction variables (e.g., uniaxial compaction pressure, compaction time, oscillation amplitude) that will cause minimal heating, but still produce a fully dense compact. Ultimately, this work will inspire future work on the fabrication of bulk nanocrystalline materials and improve our understanding of the mechanical properties of nanocrystalline materials.

This work is supported by the National Science Foundation (DMR-1460564), the Houston Community College District, and Rice University.

Nanocrystalline Materials

Nanocrystalline materials have many unique properties because of their small grain size (< 100 nm). For example:

Advantages

- High strength [1]
- High hardness [2]
- Strong magnetic properties [3]
- Excellent wear resistance [4]
- Good thermoelectric properties [5]

Disadvantages

- Unstable at high temperatures
- Difficult to synthesize in bulk

Motivation for Project

1. The superior properties of nanocrystalline materials make them ideal for applications in the aerospace, biomedical, and automotive industries among other structural applications.
2. The fabrication of bulk nanocrystalline specimens would enable scientific work on the behavior of nanocrystalline materials which is currently impossible.

Solid State Bonding

Rather than synthesizing large quantities of nanocrystalline materials, we attempt to consolidate small amounts of previously synthesized nanostructured material into bulk components.

Because nanocrystalline materials can not be joined with traditional high temperature welding techniques, such as arc welding, we examine using solid-state bonding techniques. We use ultrasonic powder compaction to densify bulk material once nanocrystalline powder is milled to a desired particle size.

Experimental Details

To synthesize our feedstock powder, we milled 99.9% metals basis Cu powder in a SPEX high energy ball mill for 5 hours with 0.8% stearic acid added as a process control agent.

Ultrasonic Powder Compaction Process

1. A punch (sonotrode) compresses the feedstock powder in a die.
2. The sonotrode shears the powder at ultrasonic frequencies transverse to the loading direction.
3. The combination of normal pressure and oscillating shear stresses disrupts the native oxide on the feedstock powder particles, resulting in metallurgical bonding when the particles deform and are brought within close contact.

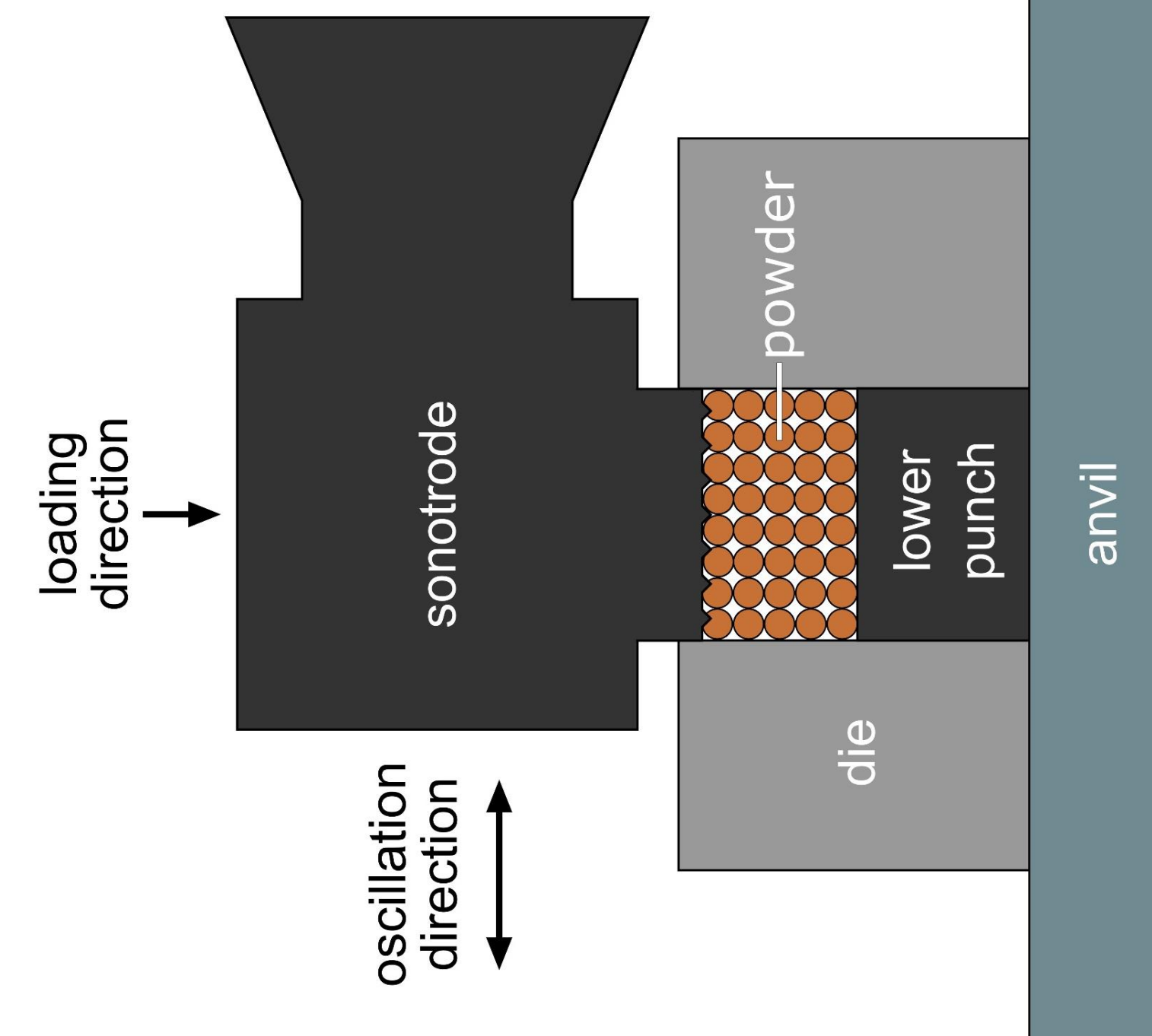


Figure 1. Schematic of the ultrasonic powder consolidation apparatus using an instrumented ultrasonic welder.

Theory & Modelling

Powder Densification

Eq 1 gives the density (ρ) of a powder compact with yield stress σ_Y due to plastic yielding under an applied uniaxial pressure (σ) [6]. However, Eq 1 dramatically underestimates the density of our compacts because it does not account for the ultrasonic vibrations which aid in densification.

$$\rho = 1 - \exp\left(\frac{-3\sigma}{2\sigma_Y}\right) \quad (1)$$

Grain Size Strengthening

Eq 2, the Hall-Petch equation, relates the yield stress of polycrystalline materials to their grain size (D). In this work, we use Eq 2 to estimate the grain size of our compacts by measuring their hardness, which is $3\sigma_Y$, and using material constants $\sigma_0 = 40$ MPa and $k = 110$ MPa $\cdot \mu\text{m}^{1/2}$ found in literature [7].

$$\sigma_Y = \sigma_0 + \frac{k}{\sqrt{D}} \quad (2)$$

Powder Densification Results

Figure 2 shows experimental density measurements for compactions performed at different amplitudes. Generally, density scales up with increasing amplitude.

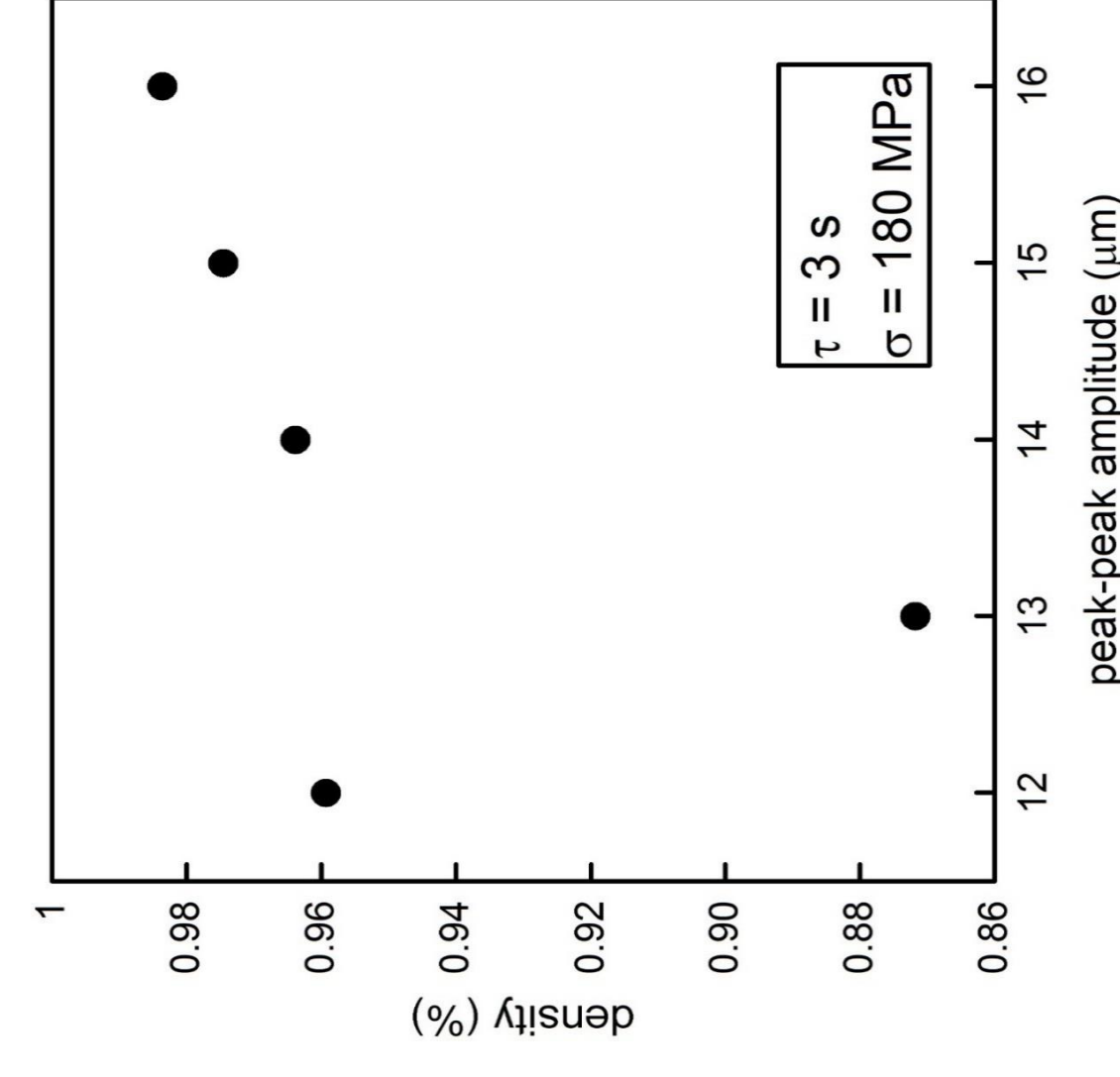


Figure 2. Density as a function of peak-peak amplitude

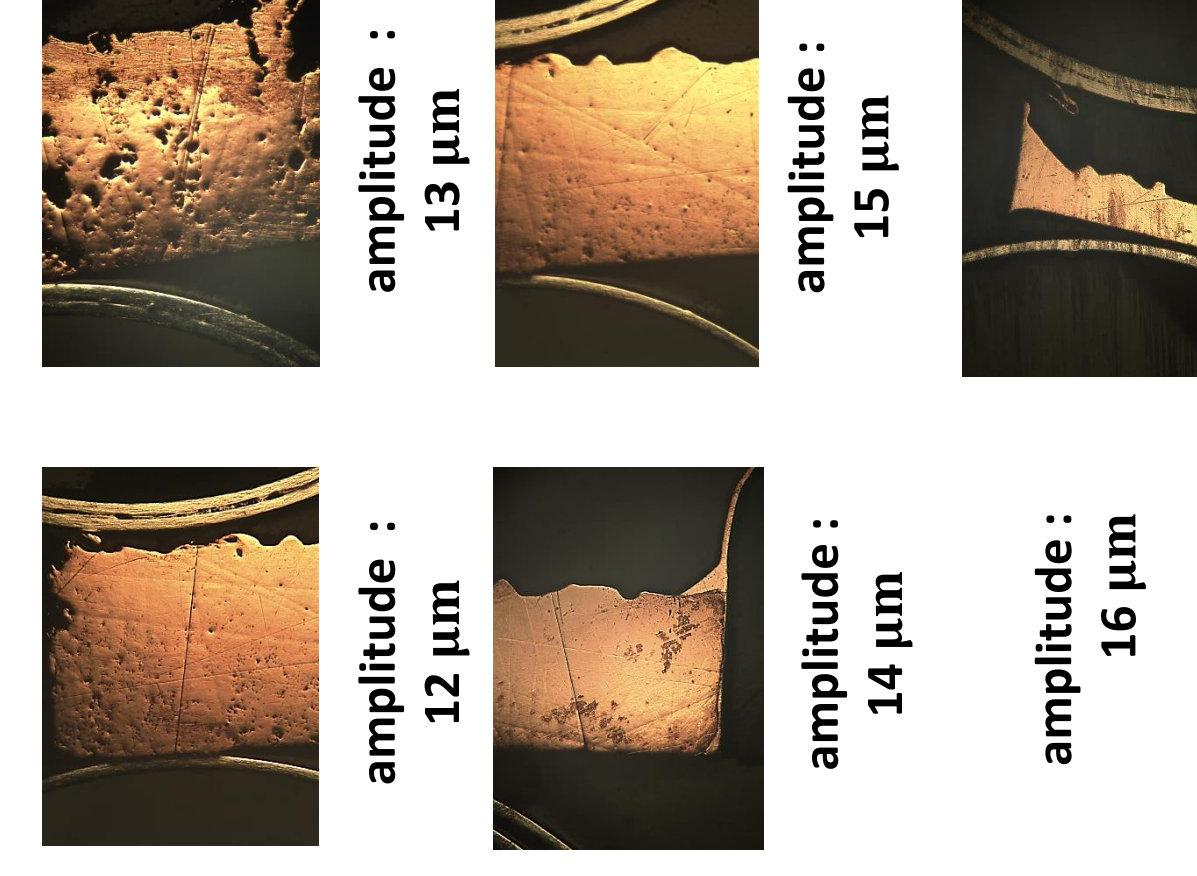


Figure 3. Nanocrystalline Copper Micrographs of increasing Amplitude



Figure 4. Nanocrystalline Copper micrographs of Vickers Hardness test

Figure 5 shows experimental hardness measurements and grain size predictions by Eq 2. We found higher pressures put out compacts with lower hardness values.

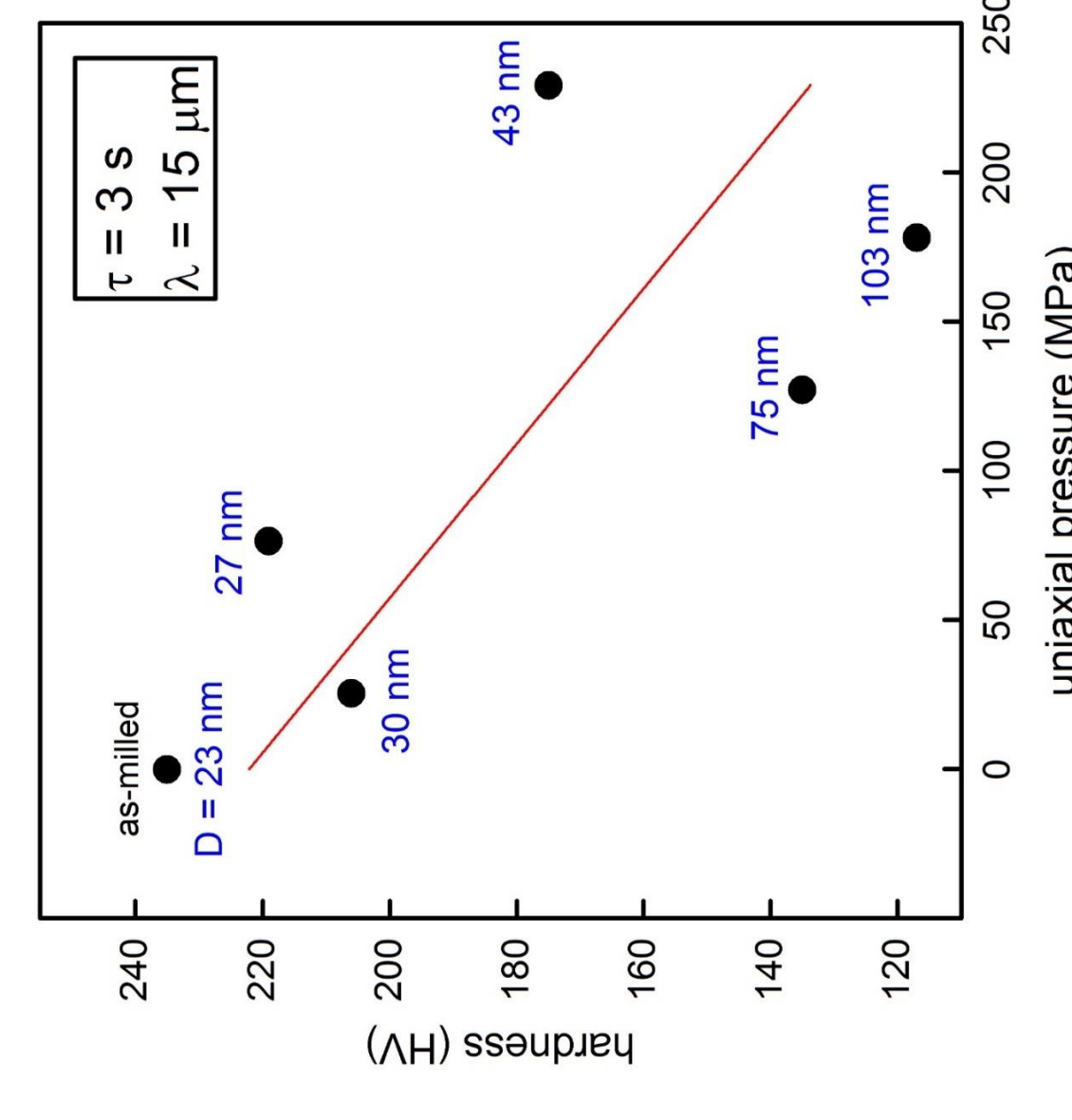


Figure 5. Hardness as a function of uniaxial pressure

Conclusions & Future Work

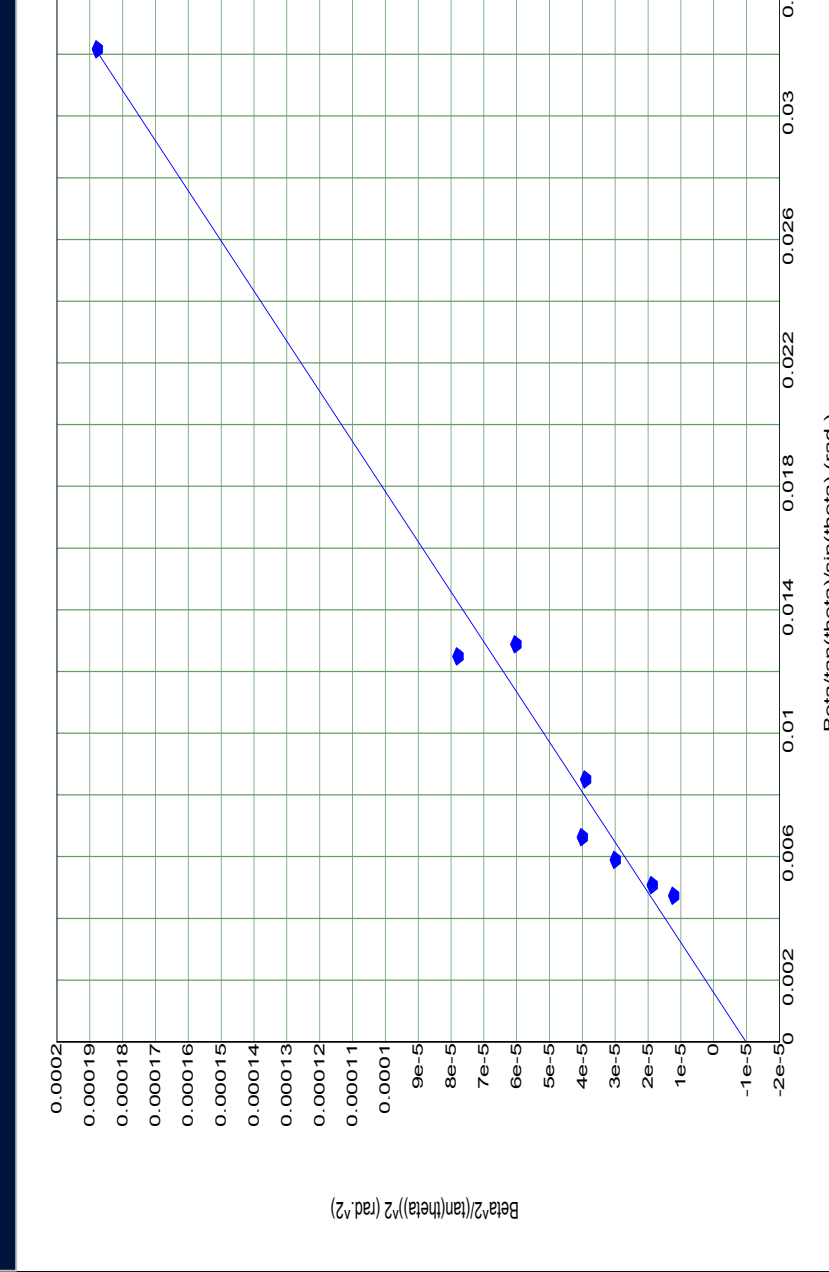


Figure 6. X-ray Diffraction results from densified nanocrystalline Copper

These findings clarify the effect ultrasonic vibrations have on nanocrystalline powder densification and the mechanical properties of the compacts.

- Ultrasonic vibrations aid the densification of powders. Compact density scales with ultrasonic oscillation amplitude.
- Compact hardness decreases with increasing applied uniaxial pressure. The Hall-Petch equation predicts that these compacts retained their nanostructure.

Next, we will explore the effect of the process parameters and temperature on the structure of the feedstock powder. We will:

- Create an analytical model which relates the process parameters to the temperature change thus the final structure in the compact

These next steps will enable us to preserve compact nanostructure during densification.

Acknowledgements

I thank the National Science Foundation Division of Materials Research Grant DMR 1460564 for this research opportunity. I would also like to thank Austin A. Ward, Dr. Zachary Cordero and Raquel M. Torres for their support and mentorship during my research experience as well as my development as both a researcher and engineer.

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Investigating Portability of Molecular Dynamics Applications⁽¹⁾
Frank Kornet⁽²⁾, Millad Ghane⁽³⁾, Pengzhi Zhang⁽³⁾ and Margaret S. Cheung⁽³⁾

Most scientific applications will have to be revisited to run on Graphic Processor Units (GPUs) to obtain speedup with modern architectures. Compute Unified Device Architecture (CUDA) is widely used within the scientific community as the proprietary NVIDIA GPU programming standard. OpenACC is the open, standard alternative. A careful comparison between the two is lacking in terms of productivity, portability and performance.

CoMD, a proxy for molecular dynamics applications developed by national laboratories, is exploited to assess abovementioned criteria. A partial OpenACC and a full CUDA version of CoMD exists that try to investigate capabilities of each programming model. The partial OpenACC version is modified by porting one of the remaining functions to OpenACC. We evaluated the performance of both implementations on a single computer node with two NVIDIA K80 GPUs.

Experiences with the porting show that OpenACC is learned in about two weeks. The lines of code show that OpenACC is more productive than CUDA (3,704 vs. 6,781) and in terms of portability, CoMD runs successfully on multiple architectures. After applying different strategies on the partial OpenACC code to improve performance, OpenACC speedup over serial CoMD reaches 7.2x while CUDA speedup still dominates (61.1x). Investigations show that changes have been made to the underlying CUDA CoMD algorithm. A firm conclusion regarding performance cannot be drawn at this stage as the two algorithms are different.

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³University of Houston

Parallel Programming

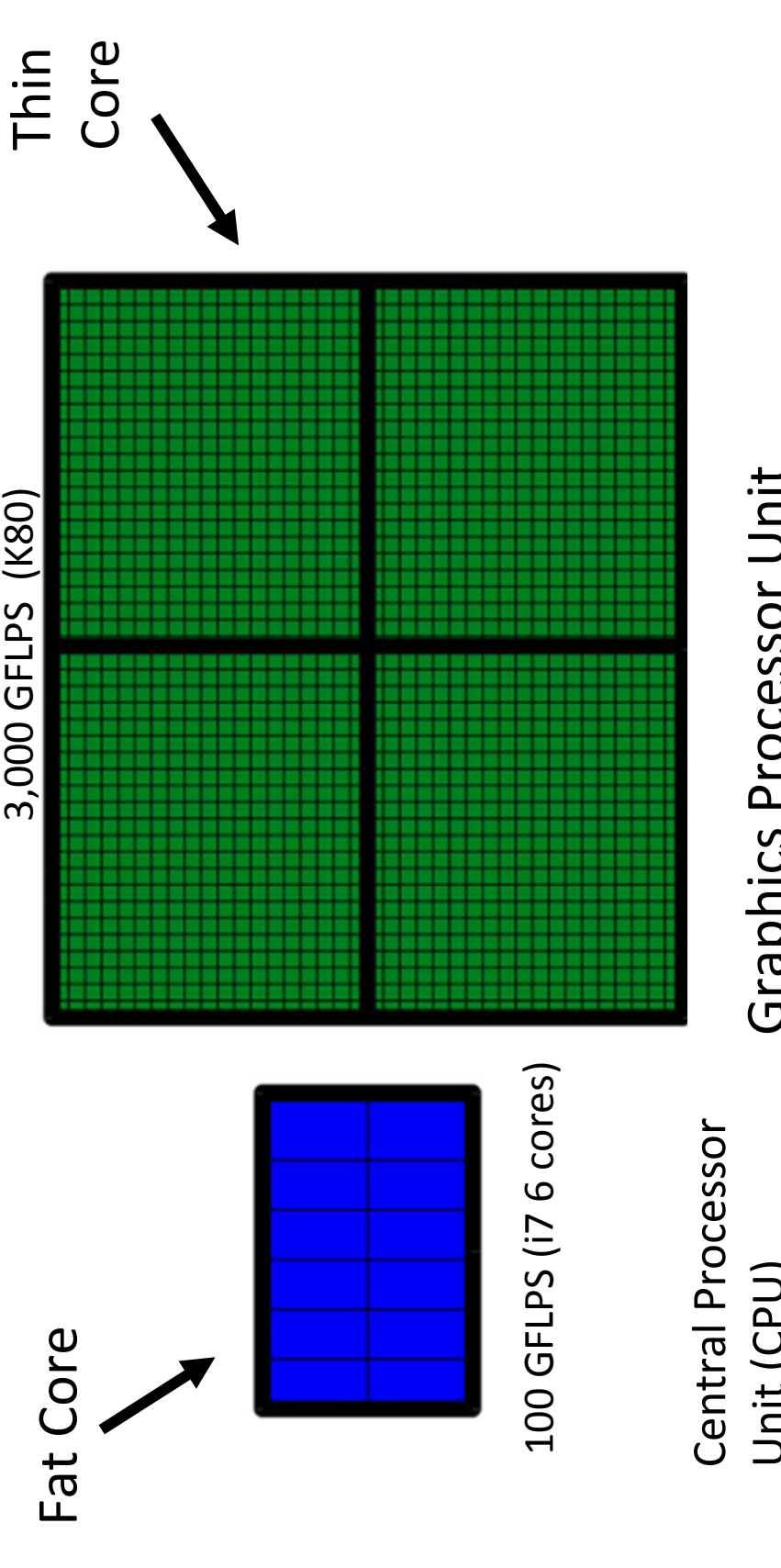
```
#pragma acc parallel loop
for (int i=nLocalBoxes;
    i < nTotalBoxes;
    ++i)
    s_boxes_nAtoms[i] = 0;
```

Example of OpenACC compiler directive.

Why Parallel Programming?

- Moore's law running out of steam and scientific applications will no longer get an automatic performance boost
- Scientific applications need to run ever larger simulations. To do so, they need to become faster
- The only realistic way to make scientific applications faster is by writing parallel programs running on (massively) parallel platforms

CPU and GPU Cores



Source: <http://www.nvidia.com/object/what-is-gpu-computing.html>

CUDA vs OpenACC

| | CUDA | OpenACC |
|-----------|-------------------|--------------------|
| Platforms | NVIDIA GPUs only | CPUs and GPUs |
| Languages | Fortran and C/C++ | Fortran and C/C++ |
| Usage | Function call | Compiler directive |
| Level | Lower | Higher |

Hypothesis:

- OpenACC is easier to use and more productive than CUDA
- OpenACC is more portable than CUDA
- OpenACC performs at similar levels as CUDA

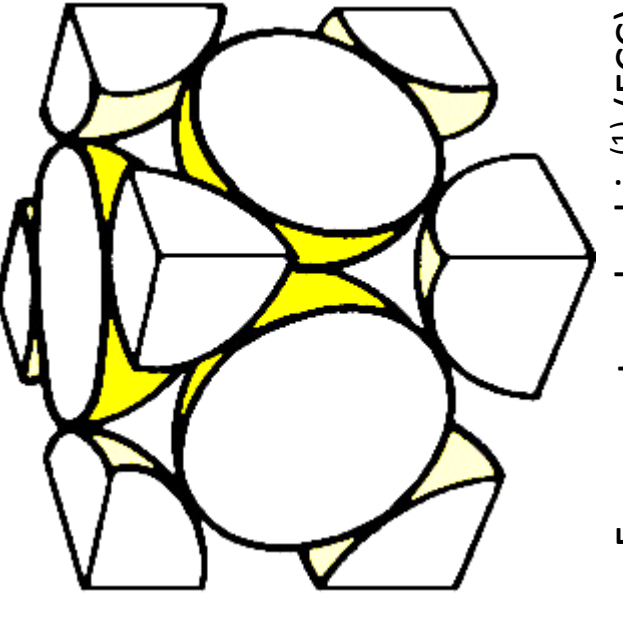
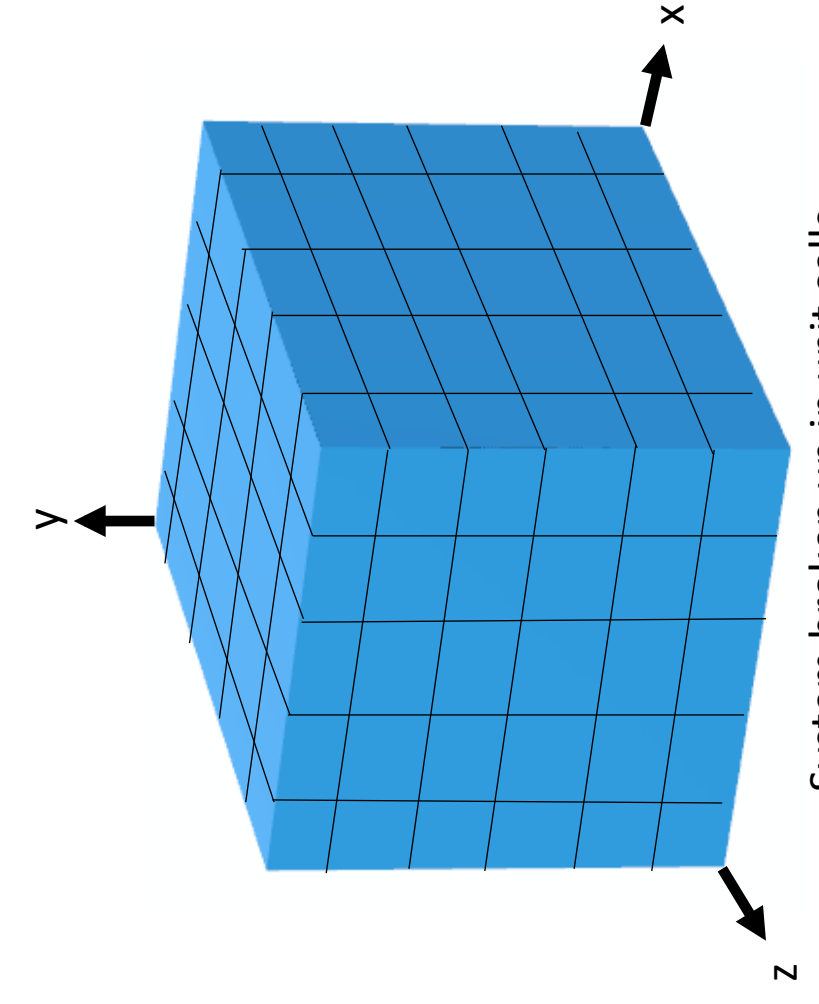
NB: conventional view is that OpenACC performs at CUDA levels only when algorithm is very easy to run in parallel or is embarrassingly parallel.

Objectives

- Demonstrate that OpenACC is easier to use and more productive than CUDA
- Demonstrate that OpenACC is more portable than CUDA
- Demonstrate that OpenACC's performance is within 10 – 20 per cent of CUDA's performance

Use CoMD as Proxy

Molecular dynamics (MD) is the method of simulating the kinetic and thermodynamic properties of molecular systems using Newton's equations of motion and represents an important class of scientific applications. CoMD is used as it is both small and representative of this class. It carries out a microcanonical ensemble simulation (NVE) and is developed by DoE Co-design Center for Materials in Extreme Environments (ExMatEx).



Number of Atoms
 $4 * X * Y * Z$

Force Calculation
Neighbor Cells

Force Model
Lennard-Jones & EAM⁽³⁾
(pair-wise with cutoff)

Sample Screen Output

| # | Loop-Time (fs) | Total Energy | Potential Energy | Kinetic Energy | Temperature | Performance | Variable | Constant |
|-------|----------------|--------------|------------------|----------------|-------------|-------------|----------|----------|
| 0 | 0.00 | -3.46052323 | -3.53807922 | 0.07755599 | 600.0000 | 0.0000 | 0.0000 | 0.0000 |
| 32000 | 1.0 | 10.00 | -3.46052263 | -3.52992415 | 0.06940451 | 536.9142 | 0.9557 | 0.9557 |
| 32000 | | | | | | | | |

Total Energy = Potential Energy + Kinetic Energy

CoMD implements an O(N) Verlet algorithm. For large simulations, CoMD will split the system and distribute cells over participating nodes. A partial OpenACC version and a full CUDA version are available on GitHub and are used in the study. Please note that CoMD results provide an upper bound of what is achievable with GPUs in practice $O(N) \rightarrow O(N^2)$.

(1): <http://chebzi.website/pages/face-centered-cubic-unit-cell/> (2): https://www.etsy.com/listing/288728381/real-copper-cube-periodic-table-element?utm_campaign=shopping_us_geoevo_sfc_osa (3) Embedded Atom Model (EAM)

Change Made

| Function | CPU | GPU |
|----------------------|-----|-----|
| main | X | X |
| timestep | X | X |
| sumAtoms | X | X |
| printThings | X | X |
| advanceVelocity (*) | X | X |
| advancePositions (*) | X | X |
| redistributeAtoms | X | X |
| updateLinkCells | X | X |
| haloExchange | X | X |
| sortAtomsInCell | X | X |
| computeForce (*) | X | X |
| advanceVelocity (*) | X | X |
| kineticEnergy | X | X |

(*) Basic Momentum Verlet algorithm (2nd version) as described in <http://www.chem.utoronto.ca/~jmschofi/simulation/partmd.pdf>

Ease and Productivity

- OpenACC basics can be learned in 1-2 weeks. Once learned, developers can start to optimize their applications.
- OpenACC needs fewer lines of code than CUDA, but different algorithm overstates CUDA part

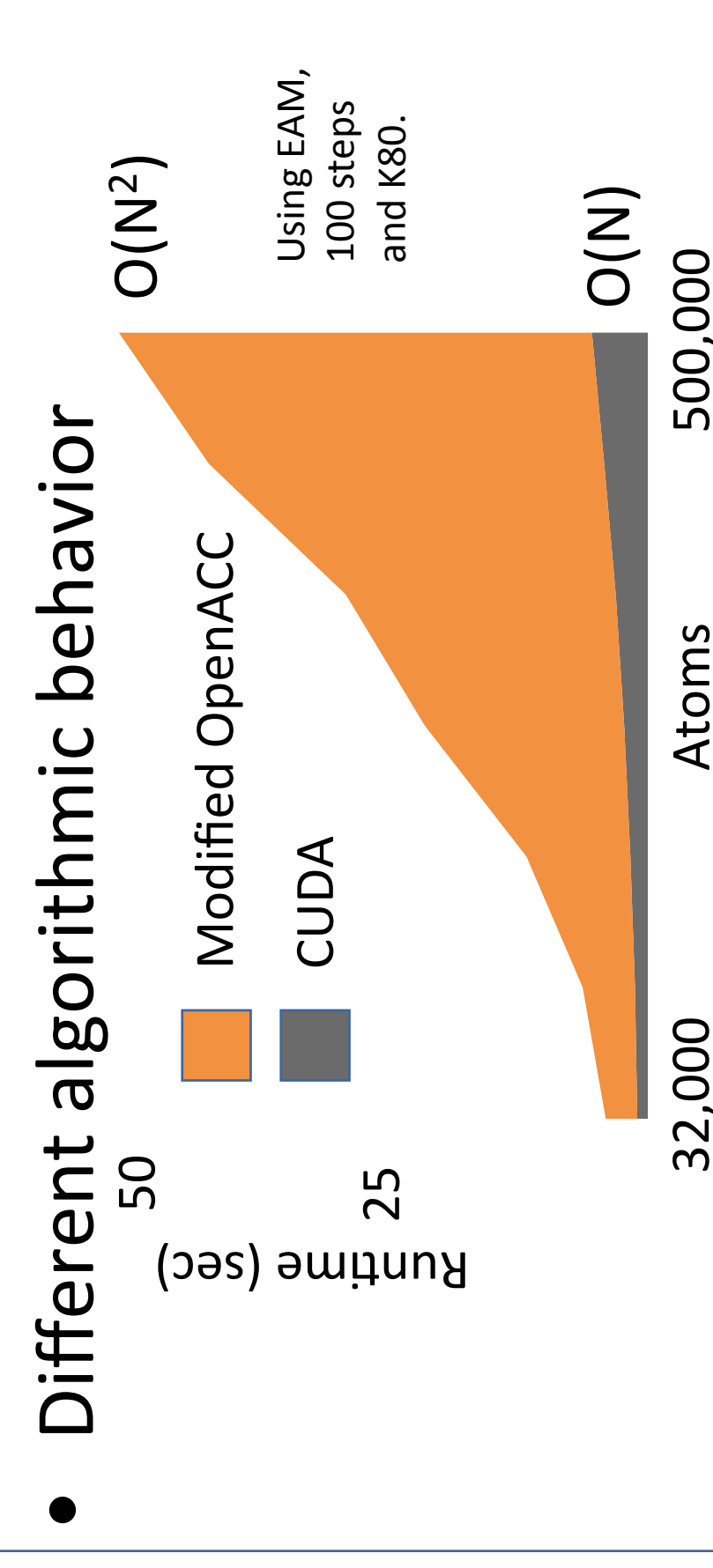
| | Serial | OpenACC | CUDA |
|---------------|--------|---------|-------|
| Lines of Code | 3,407 | 3,704 | 6,781 |

NB: the lines of code have been counted using the 'lincod' tool.

Portability

- CoMD was successfully tested and run on NVIDIA Quadro 600 and K80
- Non-NVIDIA GPUs were not tested as part of this study

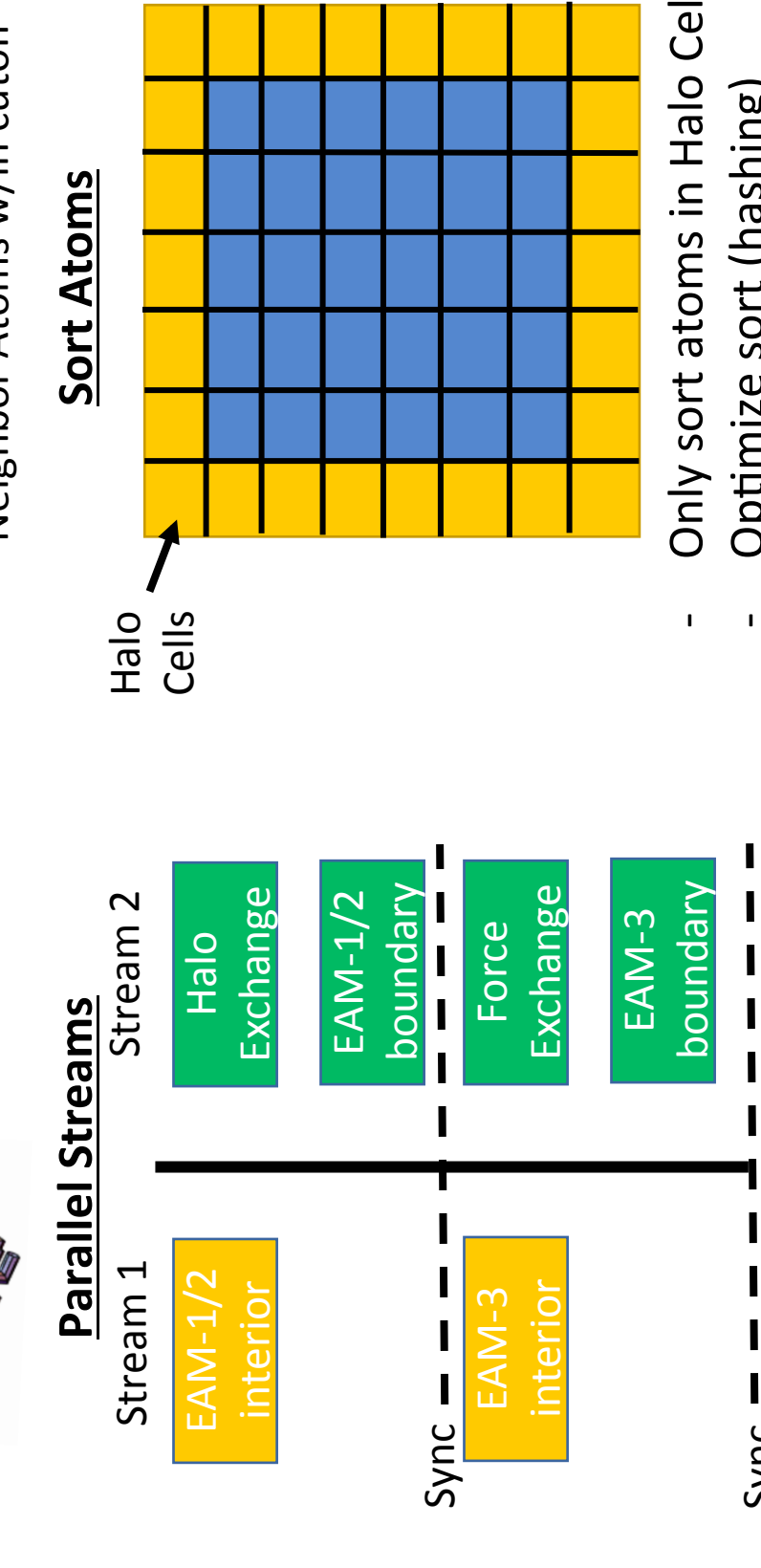
Performance



- Different algorithmic behavior
- CUDA made changes⁽¹⁾, but unclear which of the changes result in different behavior



Hilbert Curve to improve texture caching



- Only sort atoms in Halo Cells
- Optimize sort (hashing)

- So, it is too early to assess performance
- Near future work: migrate haloExchange to GPU and in parallel investigate what truly drives the CUDA algorithm

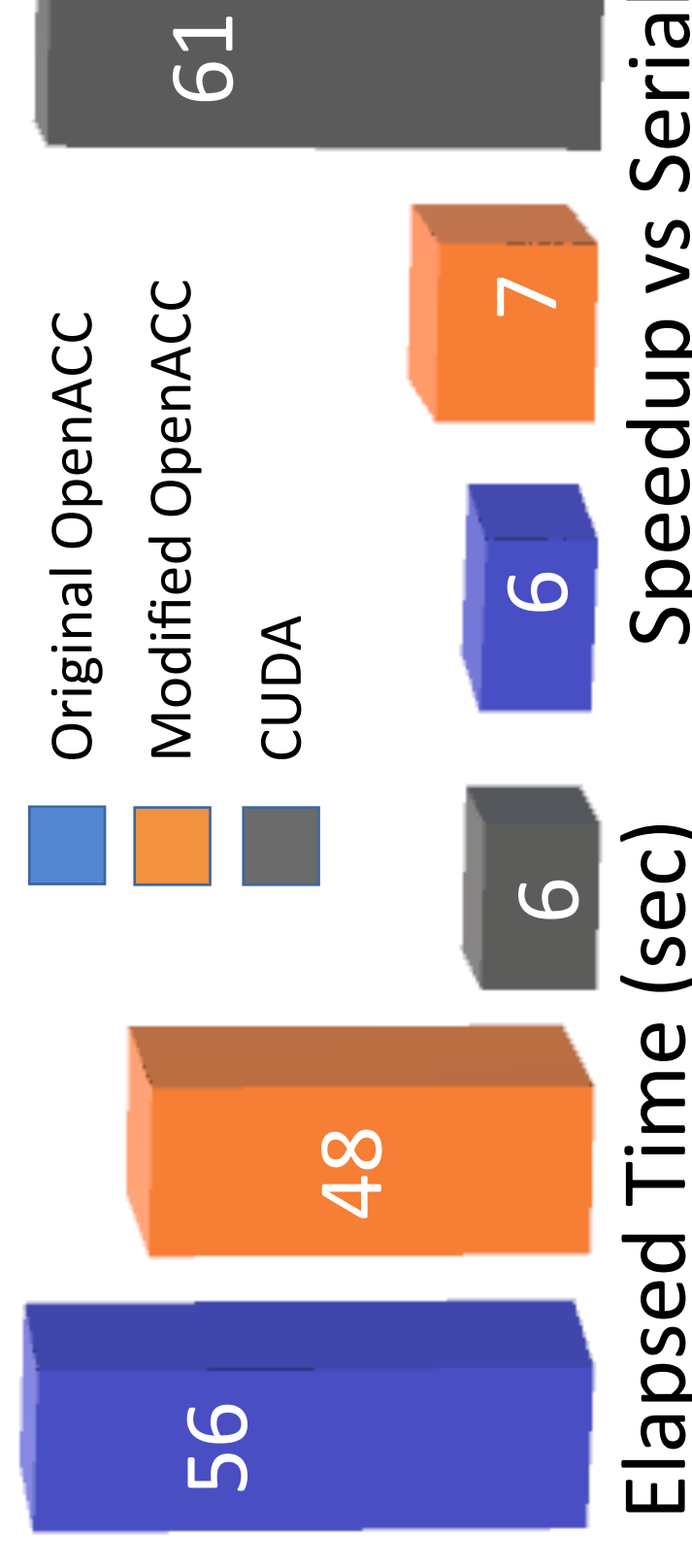
(1): <http://on-demand.gputechconf.com/gtc/2014/presentation/54465-optimizing-cuda-molecular-dynamics.pdf>

Acknowledgement

Frank Kornet would like to thank Millad Ghane, Pengzhi Zhang, Bart Sheinberg, Sunita Chandrasekaran and Margaret S. Cheung for providing him the opportunity and helping him along the way. Frank would also like to thank National Science Foundation (NSF) for providing funding for the project.



Why is the gap so big?



Elapsed Time (sec) Speedup vs Serial algorithms?

Force model: EAM. Simulating 500,000 atoms (100 steps) on single node with 2 x K80.

Synthesis of Magnesian –Iron Silicate Phases by the Solid State Method

Arceneaux, B.^{1,2.}, Martinez, M.^{1,2.}, Vu, B.^{1,2.}, Meen, J.^{2.}, Müller, K.^{2.}

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Many magnesian silicates have extensive solid solutions with iron substituted for magnesium and properties of the solutions vary with Mg:Fe. We have synthesized bulk compositions that should crystallize $(\text{Mg,Fe})_2\text{SiO}_4$ (olivine) and $(\text{Mg,Fe})\text{SiO}_3$ (pyroxene) by grinding together suitable pure powders (MgCO_3 , SiO_2 , Fe_2O_3) and sintering them. The sintered pellet was broken and reground three times and then pressed onto a platinum loop which was held in a vertical tube furnace at temperatures between 1300 and 1400 °C. Experimental changes were first studied by scanning electron microscope to determine phase assemblages and then, after polishing, by electron microprobe analyzer to determine precise atomic compositions of phases. Results of selected experiments will be shown and principles of the kinetics of these systems discussed.

This work is supported by REEMS (NSF DMR 1460564) and by funding from the State of Texas to JKM through the Texas Center for Superconductivity.

Synthesis of Magnesium-Iron Silicate Phases by the Solid State Method

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INTRODUCTION

ABSTRACT

Many magnesium silicates have extensive solid solutions with iron substituted for magnesium and properties of the solutions vary with Mg:Fe. We have synthesized bulk compositions that should crystallize (Mg,Fe)₂SiO₄ (olivine) and (Mg,Fe)SiO₃ (pyroxene) by grinding together suitable pure powders (MgCO₃, SiO₂, Fe₂O₃) and sintering them. The sintered pellet was broken and reground three times and then pressed onto a platinum loop which was held in a vertical tube furnace at temperatures between 1300 and 1400 °C. Experimental changes were first studied by scanning electron microscope to determine phase assemblages and then, after polishing, by electron microprobe analyzer to determine precise atomic compositions of phases. Results of selected experiments will be shown and principles of the kinetics of these systems discussed.

PERIODIC TABLE

The Periodic Table of the Elements

PROCESSES

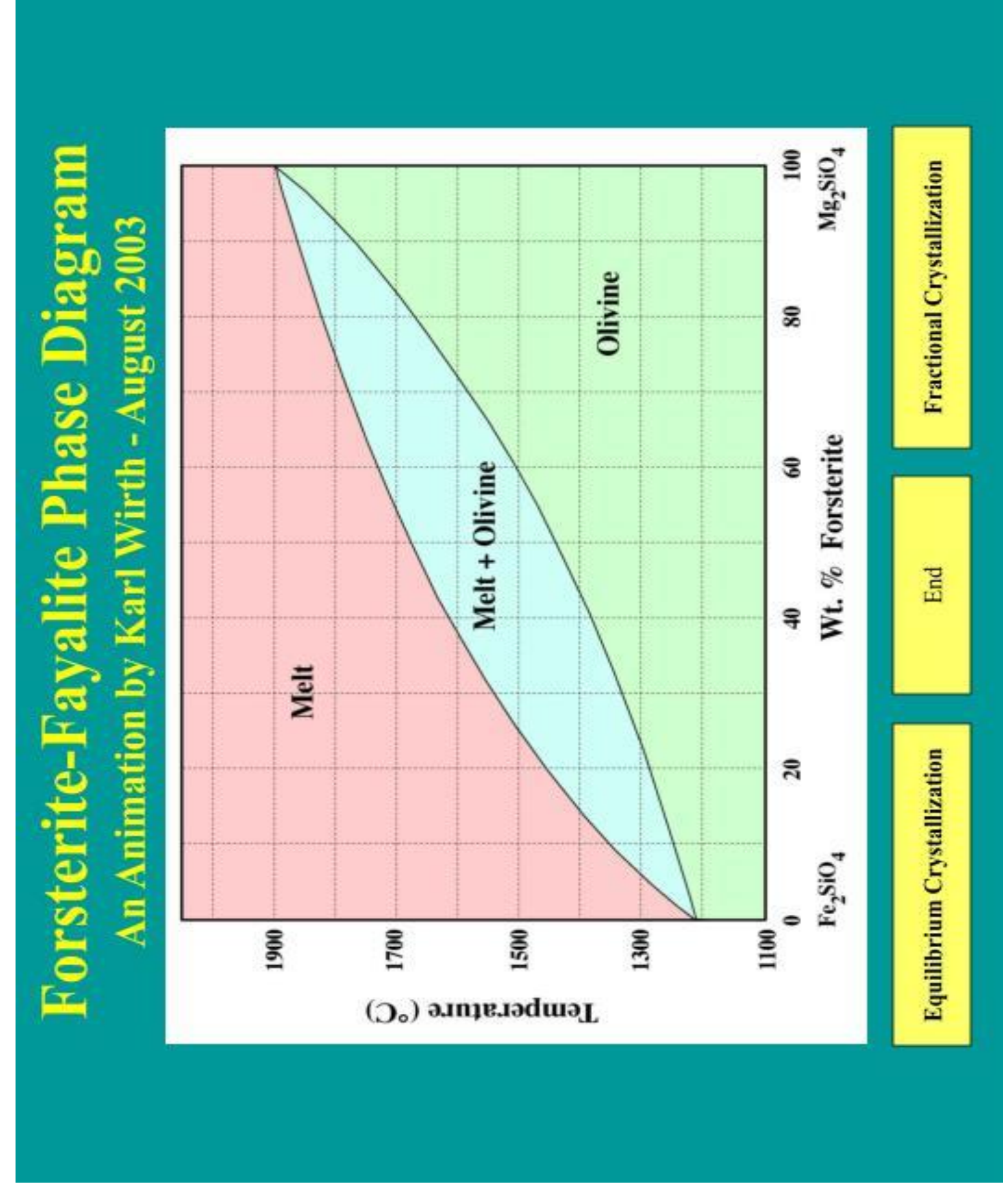
Separating the Components of a Mixture

Mixtures are not unique to chemistry; we encounter them on a daily basis. The food and drinks we consume, the fuel we use in our vehicles, building materials, soil, air, and ordinary water are all mixtures. In fact, very few common materials in the world are pure. Any material made up of two or more substances that are not chemically combined is a mixture. It is not difficult to separate the components of a mixture if you take advantage of differences in physical properties of the components.

- Distillation. This is the process of heating a mixture in order to remove a liquid that evaporates more easily, leaving behind a matter with high vaporization temperatures, whether liquid, solid, or both.
- Sublimation. Some substances change directly from a solid to a gas when they are heated. The reverse process, when the vapor goes back to the solid phase without a liquid state in between, is called deposition. Some solids which sublime are iodine, caffeine, and paradichlorobenzene (mothballs). Dry ice sublimates also.
- Extraction. This uses a solvent to selectively dissolve one component of the solid mixture. With this technique, a soluble substance can be separated from an insoluble substance.
- Decantation. This separates a liquid from insoluble solid sediment by carefully pouring the liquid from the solid without disturbing the solid.
- Filtration. This separates a solid from a liquid through the use of a porous material as a filter. Paper, charcoal, or sand can serve as a filter. These materials trap the solid but let the liquid pass through.

Purpose:

1. To separate the components of a mixture using physical methods.
2. To calculate the percent composition of a mixture.



RESULTS

Homogeneity

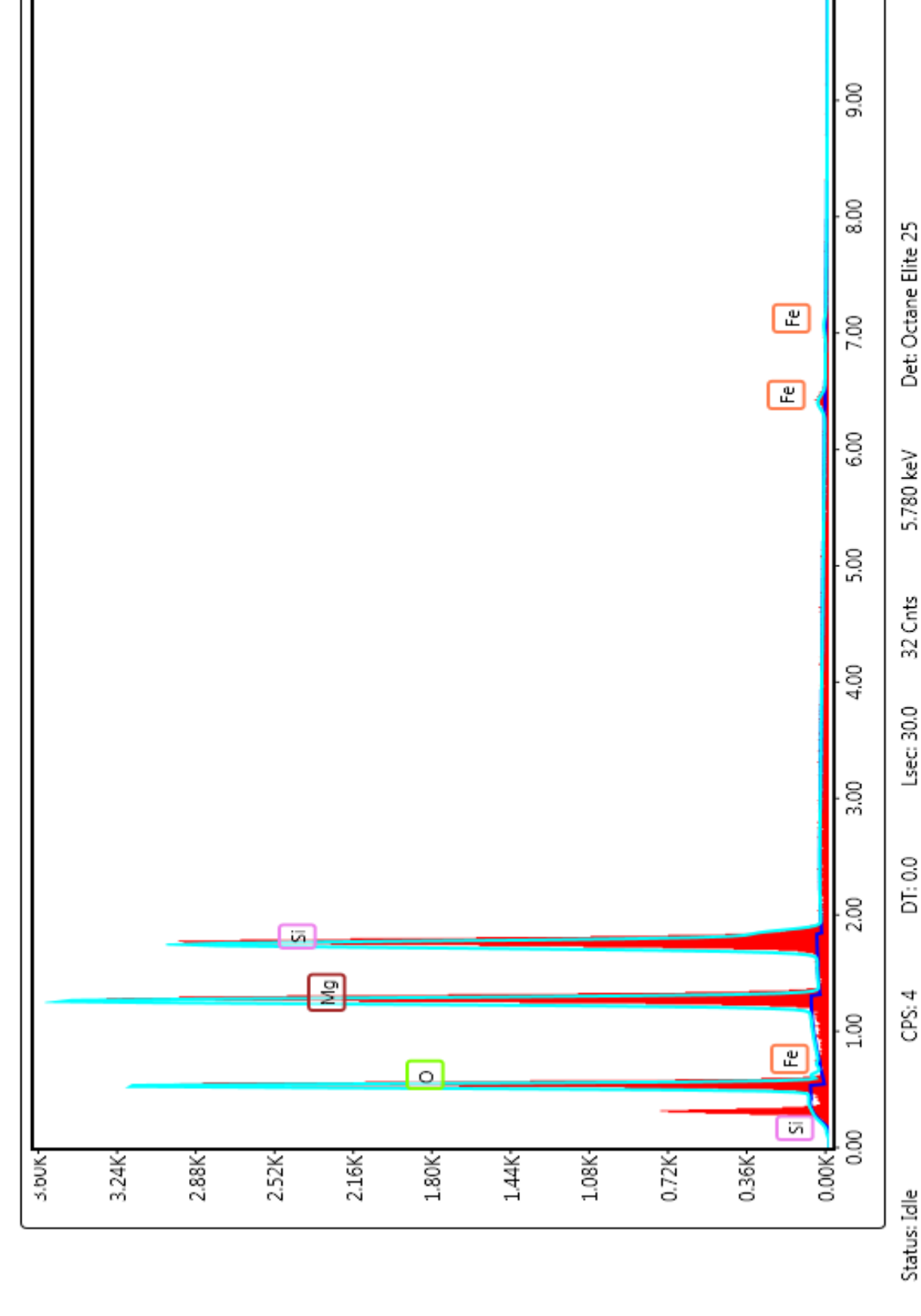
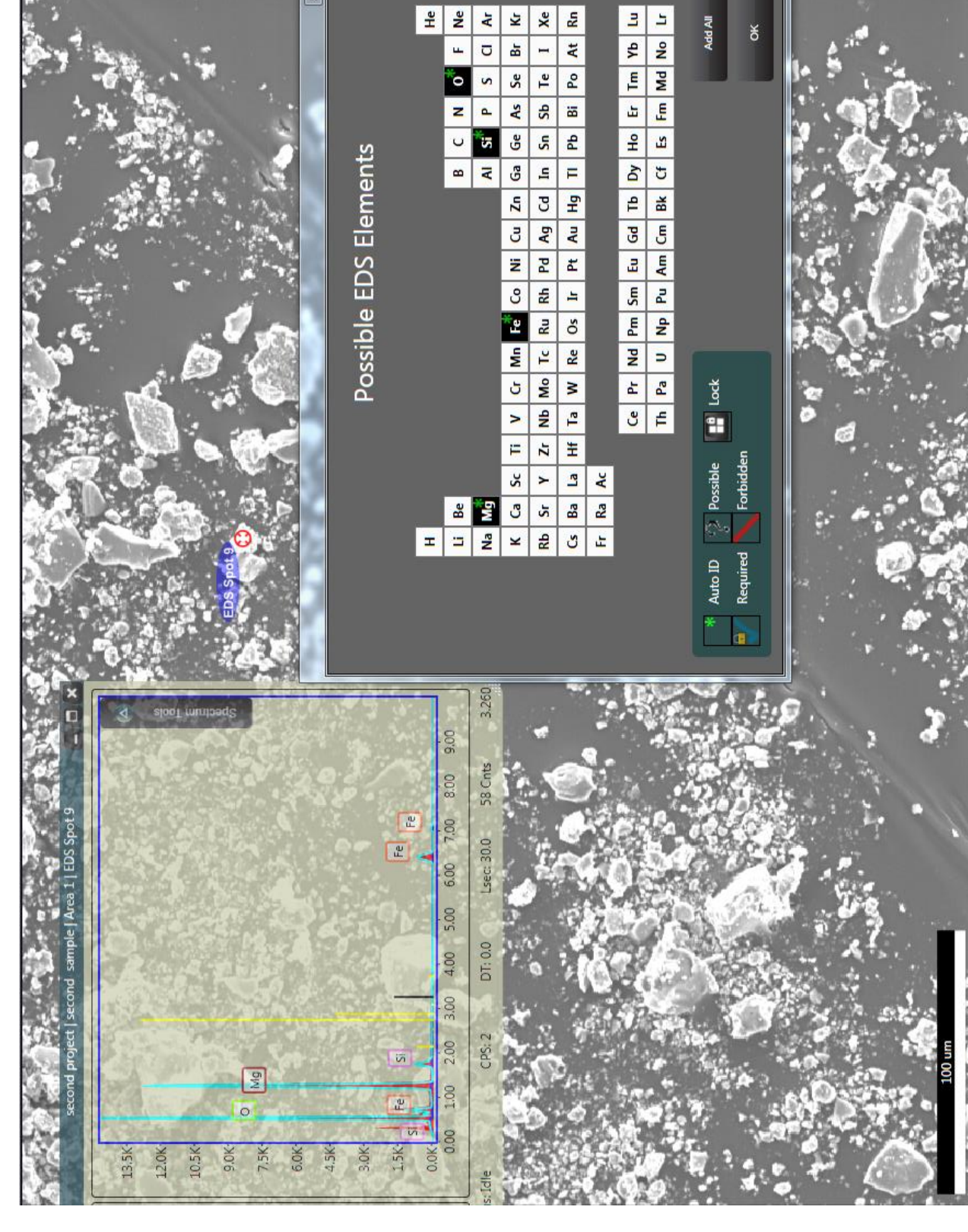
- A homogeneous mixture has the same uniform appearance and composition throughout. Many homogeneous mixtures are commonly referred to as solutions.

Heterogeneity

- A heterogeneous mixture consists of visibly different substances or phases. The three phases or states of matter are gas, liquid, and solid.

• Analysis Using the SEM

(Scanning Electron Microscope)



CONCLUSION

Experiments were performed to synthesize magnesium-iron silicates from their component oxides. Comparison of the electron micrographs of the run products show that initial experiments in air were heterogeneous with iron oxides not being incorporated into the silicates, probably because the iron remained in the trivalent state (Fe³⁺). Synthetic experiments in reducing environments yielded homogeneous material as the iron, reduces to the divalent state (Fe²⁺) substituted for Mg²⁺ in the silicates.

FUTURE WORKS

- Substitution of a rare element on the octahedral site of the silicate can produce a chroma center if the rare earth can occupy excited states as well as a ground state. Energy absorbed in any form to excite the rare earth will be re-released as a fixed quantum and so of constant wavelength reflecting the energy differences between the two states.

FUTURE USES

NASA has an initiative to send a space shuttle to MARS for exploration. Sustainability is a concern for the space mission. This process to make glow sticks to be used as a form of light.

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2. “Separating the Components of a Mixture.” retrieved from <https://www.Quia.com/files/quia/users/>
3. “What Is the Difference Between Heterogeneous and Homogeneous Mixtures?” ThoughtCo., retrieved from <https://www.thoughtco.com/heterogeneous-and-homogeneous-mixtures-606106>

•ACKNOWLEDGEMENT

- This work is supported by REEMS (NSF DMR 1460564)
- And in part by Grants from the State of Texas to JKM through the Texas Center for Superconductivity.

Partition of the Phases in a Ternary System Phosphor and the Effect of the Crystal Structures Created on Luminescence

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When a solid is sourced with a form of energy, it may emit photons in excess of thermal radiation in a process called luminescence. In inorganic solids, luminescence is emitted as the result of electronic transitions between quantum mechanical states with different levels of energy. Transitions through intermediate metastable states determine the duration of the luminescence, if prolonged after the supply of energy is cut off from the solid it is referred to as phosphorescence. Phosphors are used as powders in fluorescent lamps, cathodoluminescent television screens, and are a promising future source for alternative lighting (Yacobi & Holt)^[1]. However, it is unclear how the phases present in a ternary system phosphor affect its luminescence. To tackle this, the ratio of concentrations in the compound of the mixture of immiscible phases were explored in a series of powdered Mg_2SiO_4 samples doped with Mn^{2+} , and co-activated with an Al_2O_3 impurity and rare earths (such as Dy^{3+} and Eu^{3+}), which were prepared and sintered with 95% Ar, 5% H_2 gas at different temperatures in a tube furnace, and treated with different quenching techniques in a thermocouple system, in order to achieve cathodoluminescence, and homogeneity in the system of samples. A Scanning Electron Microscope (SEM) was used to look for both mentioned characteristics above, and Electron Microprobe Analysis (EMPA) was employed to obtain the precise chemical compositions in the crystal structures of the compounds. Samples that were co-activated by Al_2O_3 displayed cathodoluminescence more intensely, as opposed to those that were not. These samples, in particular were observed to have spinel, corundum, and a clear solid state cordierite crystal structure exhibiting the luminescence phenomena. By investigating the effects of the partition coefficient in this specific phosphor it creates the opportunity of formulating a more effective luminescent outcome for future applications.

This work is supported by the National Science Foundation Division of Materials Research REEMS (NSF DMR 1460564) and by grants from the State of Texas to JKM through the Texas Center for Superconductivity.

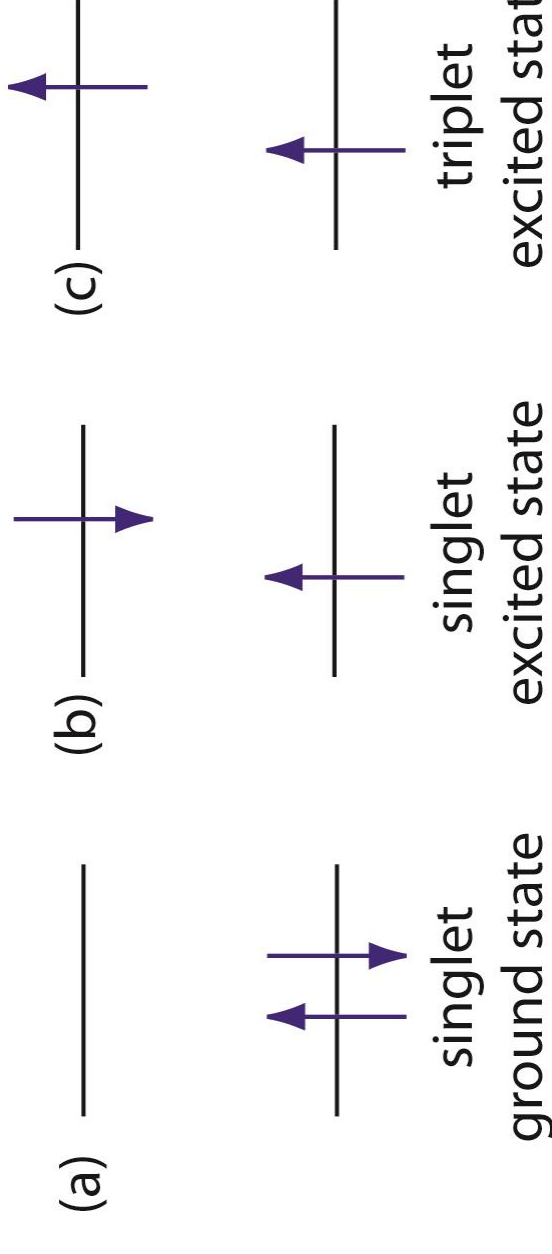
^[1] Yacobi, B. G., and D. B. Holt. *Cathodoluminescence Microscopy of Inorganic Solids*. New York and London: Plenum Press, 2010. Print.

PARTITION OF THE ELEMENTS BETWEEN PHASES IN A TERNARY SYSTEM PHOSPHOR AND THE EFFECTS ON LUMINESCENCE

Martinez, M.^{1,2}; Arceneaux, B.^{1,2}; Vu, B.^{1,2}; Meen, J. K.²; Mueller, K.²
¹REEMS Program, Houston Community College; ²Texas Center for Superconductivity, University of Houston

• What is a Phosphor?

- ✓ Absorption of Energy
- ✓ Continued Emission of Photons
- ✓ Intersystem Crossing from Singlet to Triplet State

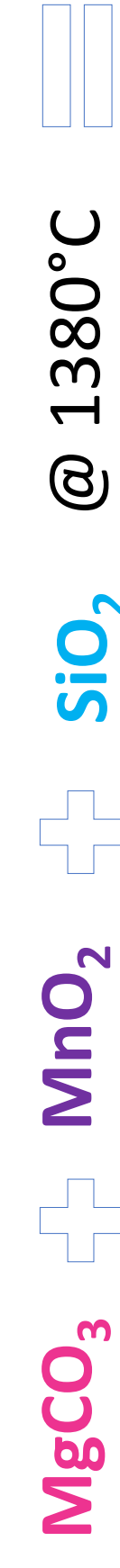


• Importance of a Ternary System Phosphor Exploration

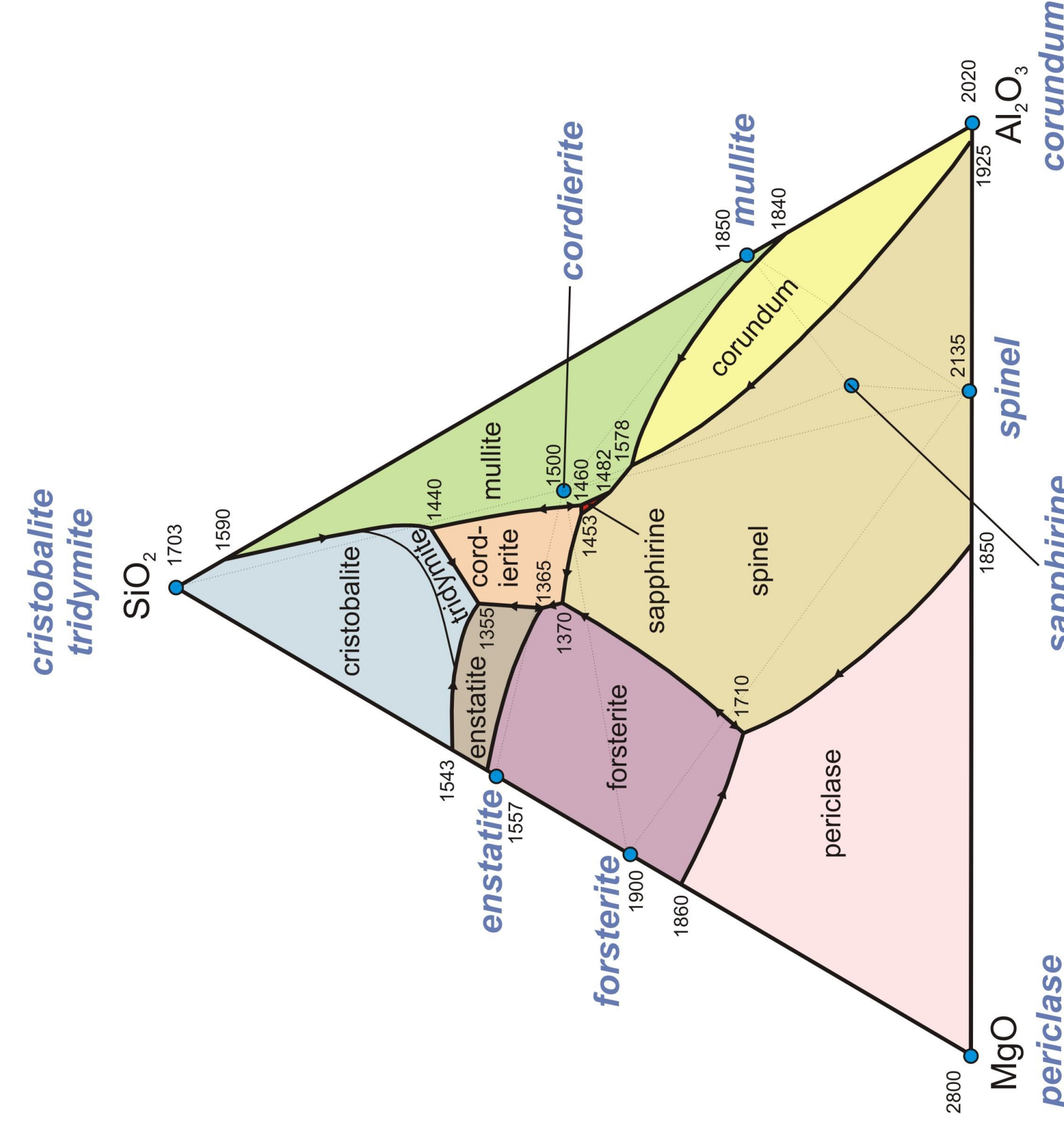
Phosphors are a promising source for alternative lighting but it is unclear how the phases in a ternary system affect their luminescence.

• Synthesis of Samples

- ✓ Sintering of Samples
- ✓ Quenching Techniques
- ✓ Forming Gas (95% Ar & 5% H₂)

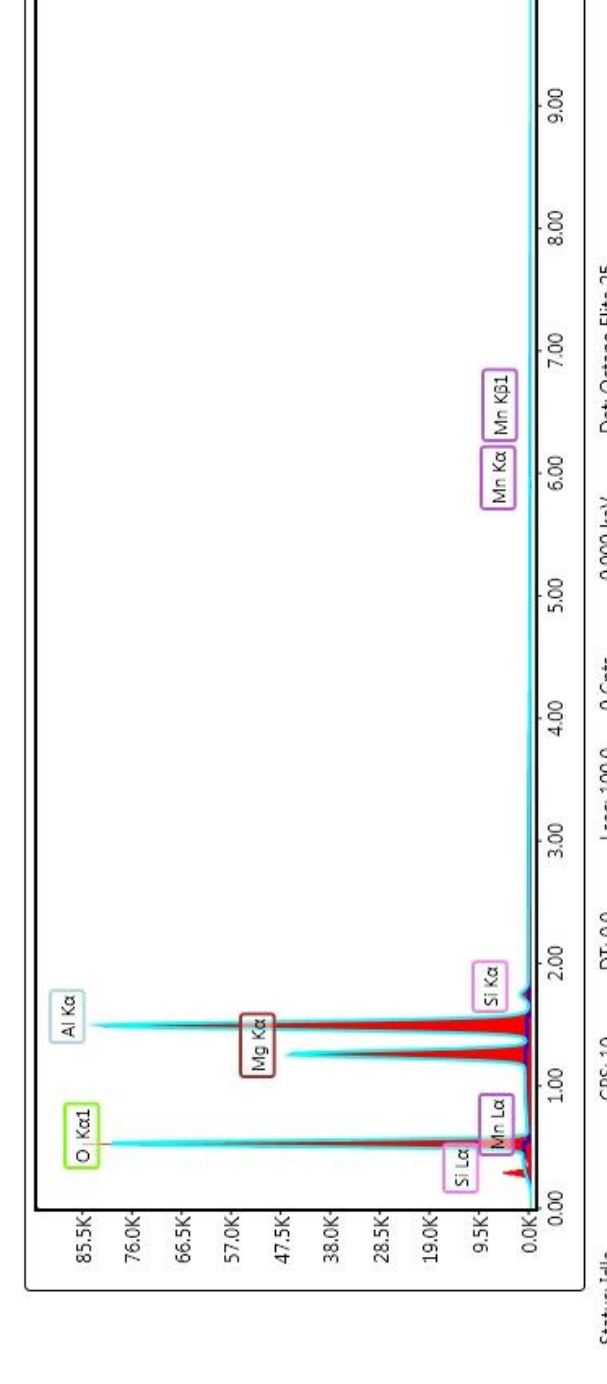
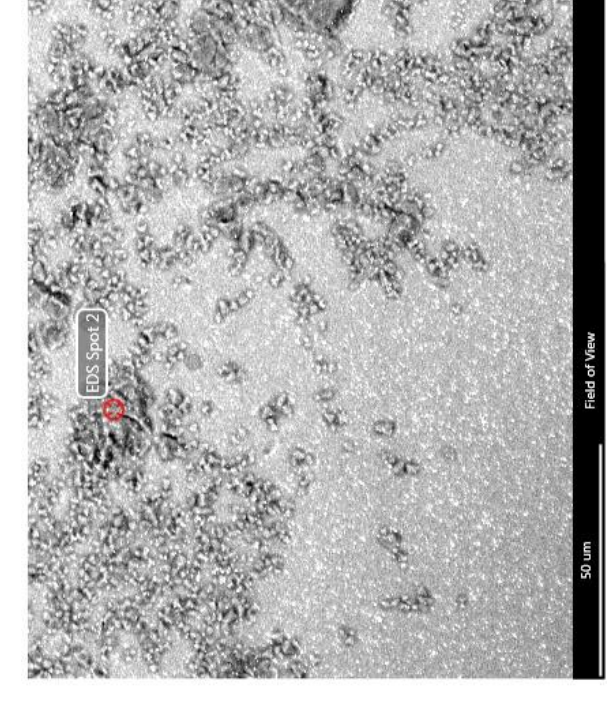
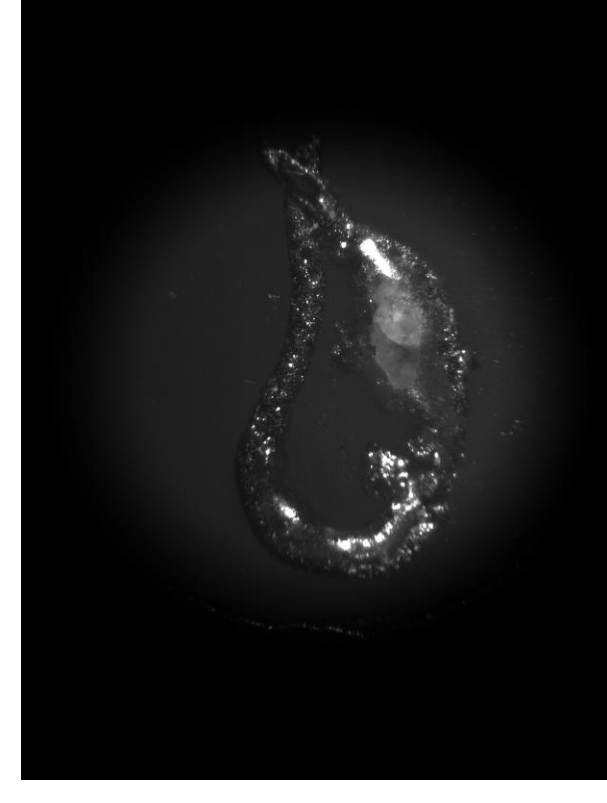


- ✓ Added Al₂O₃, Creating a Ternary System
- ✓ Temperature Dynamic 1300° C and Above



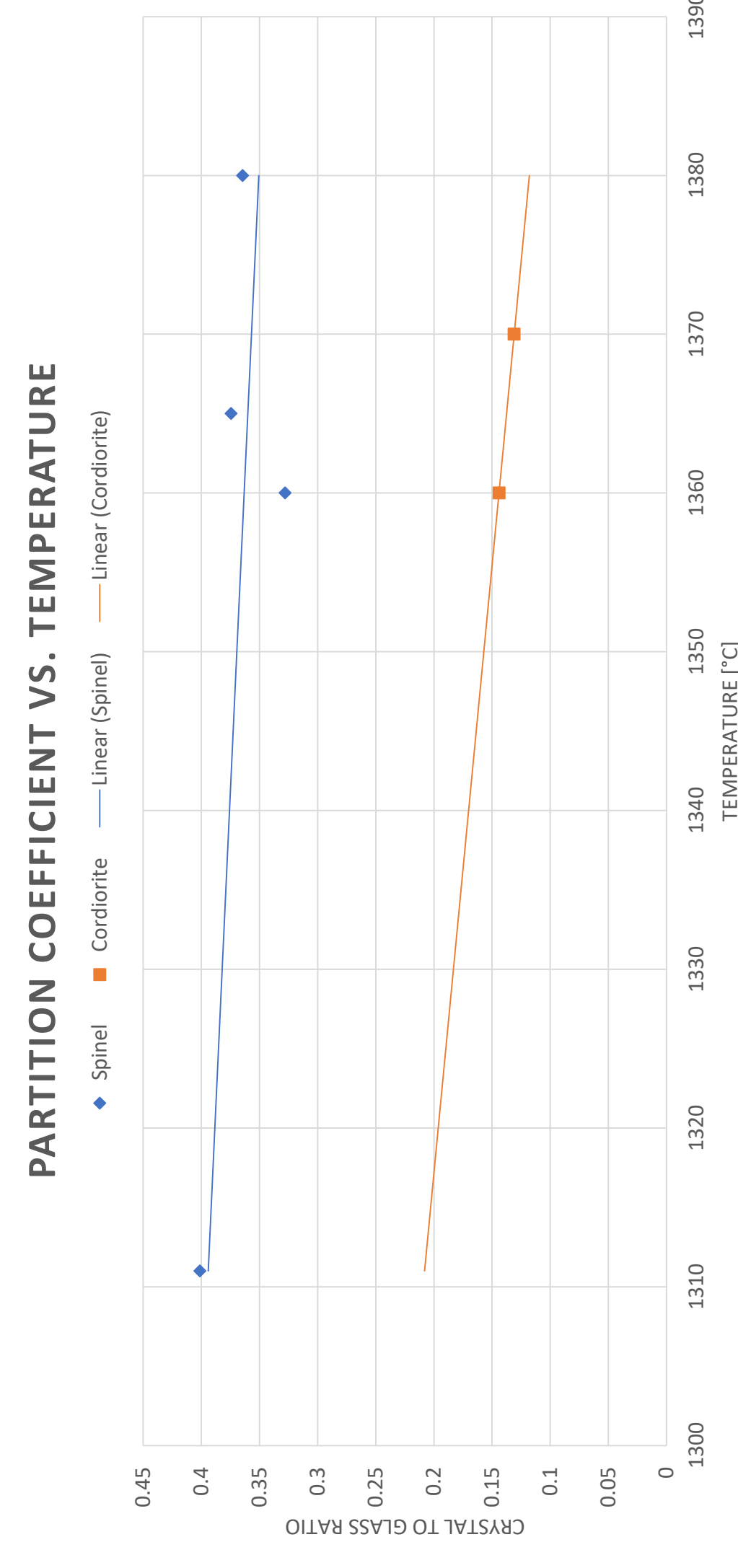
• Composition of Crystal Structures Created

- ✓ Scanning Electron Microscope (SEM) Analysis
 - ❖ Cathodoluminescence & Homogeneity
- ✓ Electron Microprobe Analysis (EMPA)
 - ❖ Composition and Concentration of Compounds

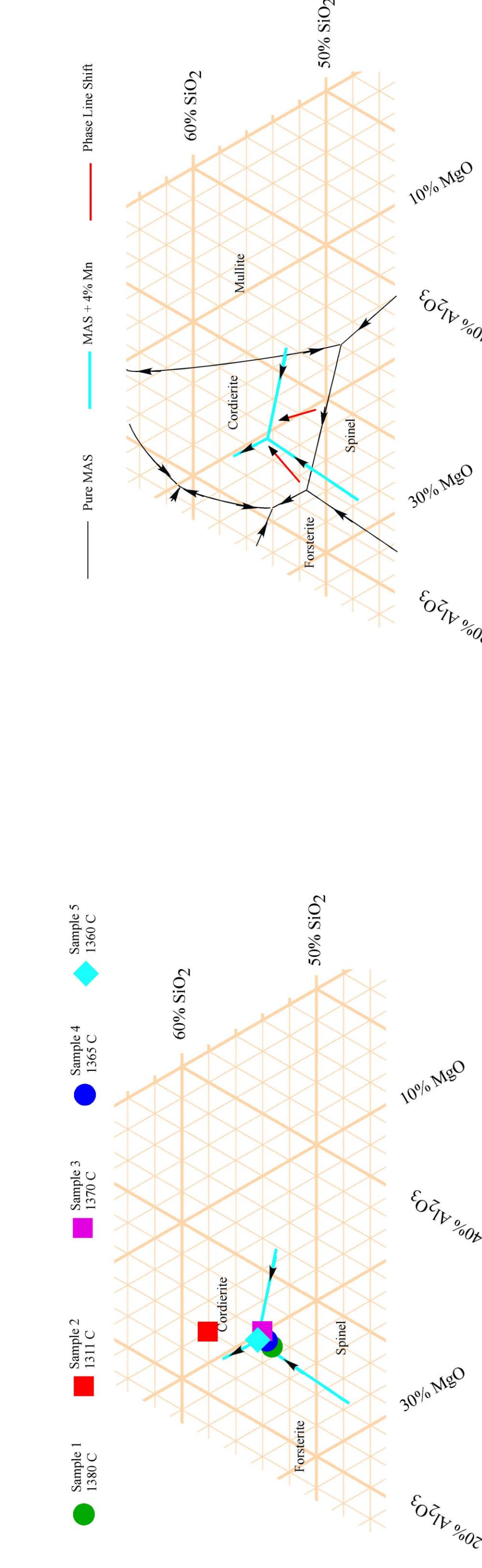


• Ratio of Concentrations of Mn in Crystal Structures

- ✓ Spinel $\frac{\text{Spinel}}{\text{Glass}} = 0.37$
- ✓ Cordierite $\frac{\text{Cordierite}}{\text{Glass}} = 0.14$
- ✓ Coexisting Crystals $\frac{\text{Spinel}}{\text{Cordierite}} = 2.67$



• Shift of Phase Fields



- Data points indicate the compositions of glass coexisting with crystals.
- Black lines illustrate the interrelations of phase fields in pure MgO, SiO₂, Al₂O₃ (MAS) ternary system, and the blue ones determine the shift caused by Mn in the MAS system.

• Discussion

- Phase relations and phase compatibility relations in MnO, MgO, SiO₂, Al₂O₃ were investigated in solid state experiments in a reducing environment.
- ✓ Addition of MnO to the MgO, SiO₂, Al₂O₃ caused a freezing point depression, although the crystallization temperatures of both spinel and cordierite were suppressed.
- ✓ The multiply saturated liquid line (spinel & cordierite) moved away from the spinel composition point.
- ✓ Partitioning of Mn between the phases was consistent with the phase relations.
- ✓ Pure Mg spinels and cordierite are white and do not luminesce, in the spectral range investigated.
- ✓ Mn bearing spinels exhibited significant cathodoluminescence.
- ✓ Coexisting Mn bearing cordierite did not exhibit the cathodoluminescence.

• Future Work

- ✓ Calculation of Gibbs Free Energy
- ✓ Check for Photoluminescence
- ✓ Measure the Wavelength of Luminescence
- ✓ Add Rare Earths

• Acknowledgements

- ✓ This work is supported by the National Science Foundation Division of Materials Research REEMS (NSF DMR 1460564) and by grants from the State of Texas to JKM through the Texas Center for Superconductivity.
- ✓ Special thanks to Dr James K. Meen and Dr Karoline Mueller at the Texas Center for Superconductivity.

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Experimenting With Cobalt Doped Phosphors and Phosphorescence

Brandon Vu^{1,2}, Monica Martinez^{1,2}, Brenda Arceneaux¹, and Dr. James Meen²

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As nations around the globe continue to reduce fossil fuel usage, a renewable resource must take its place. Phosphorescent materials have recently begun to show their potential as a new source for renewable light. Currently, Mn doped phosphors mixed with rare earths have shown emission times of 10 hours. However, red light emission only last four hours. To combat this problem we created a Al-Si-Mg sample doped with Co, another transition metal, which will hopefully provide a basis for a new phosphorescent material when mixed with a rare earth. The sample was created by mixing Al₂O₃, SiO₂, MgCO₃, and Co₂O₄ powder and compressing the sample into a platinum loop. The sample was then heated to 1350 °C for 10 minutes with forming gas (95% Ar-5% H₂) before reducing the heat and leaving it for 30 minutes. The lower equilibration temperature was varied over multiple trials and ranged from 1150-1370 °C to create the crystal phases cordierite, forsterite, and spinel. The finished samples were examined under a scanning electron microscope (SEM) and showed signs that the three phases exist within the samples. Further examination under a microprobe will determine precise chemical compositions that will allow determination of elemental partition coefficients between phases and provide details on the influences of the contents of cobalt and rare earth elements (Dy, Eu, etc.) on the luminescence, if any, of these silicate phases.

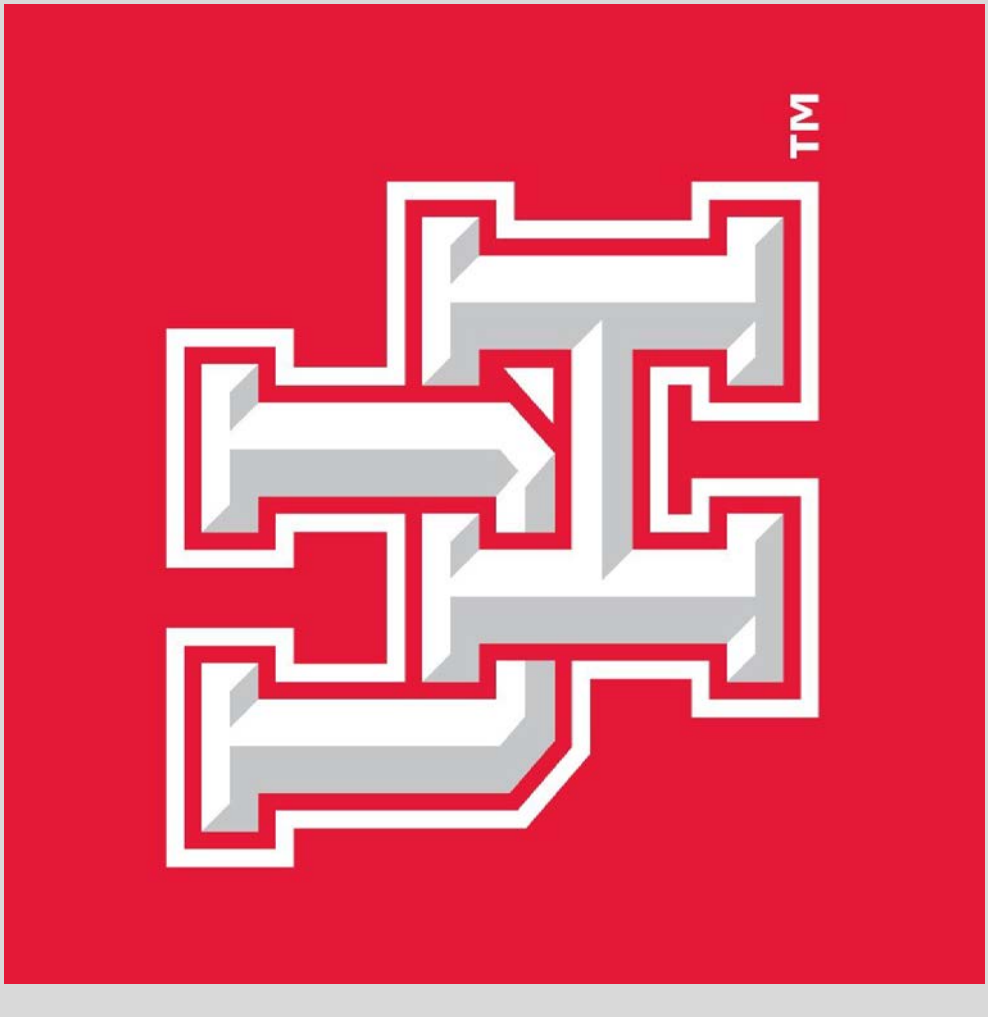
This work is supported in part by the National Science Foundation Division of Materials Research REEMS (NSF DMR 1460564) and in part by grants from the state of Texas to JKM through the Texas Center for Superconductivity.



Experimenting With Cobalt Doped Phosphors and Phosphorescence

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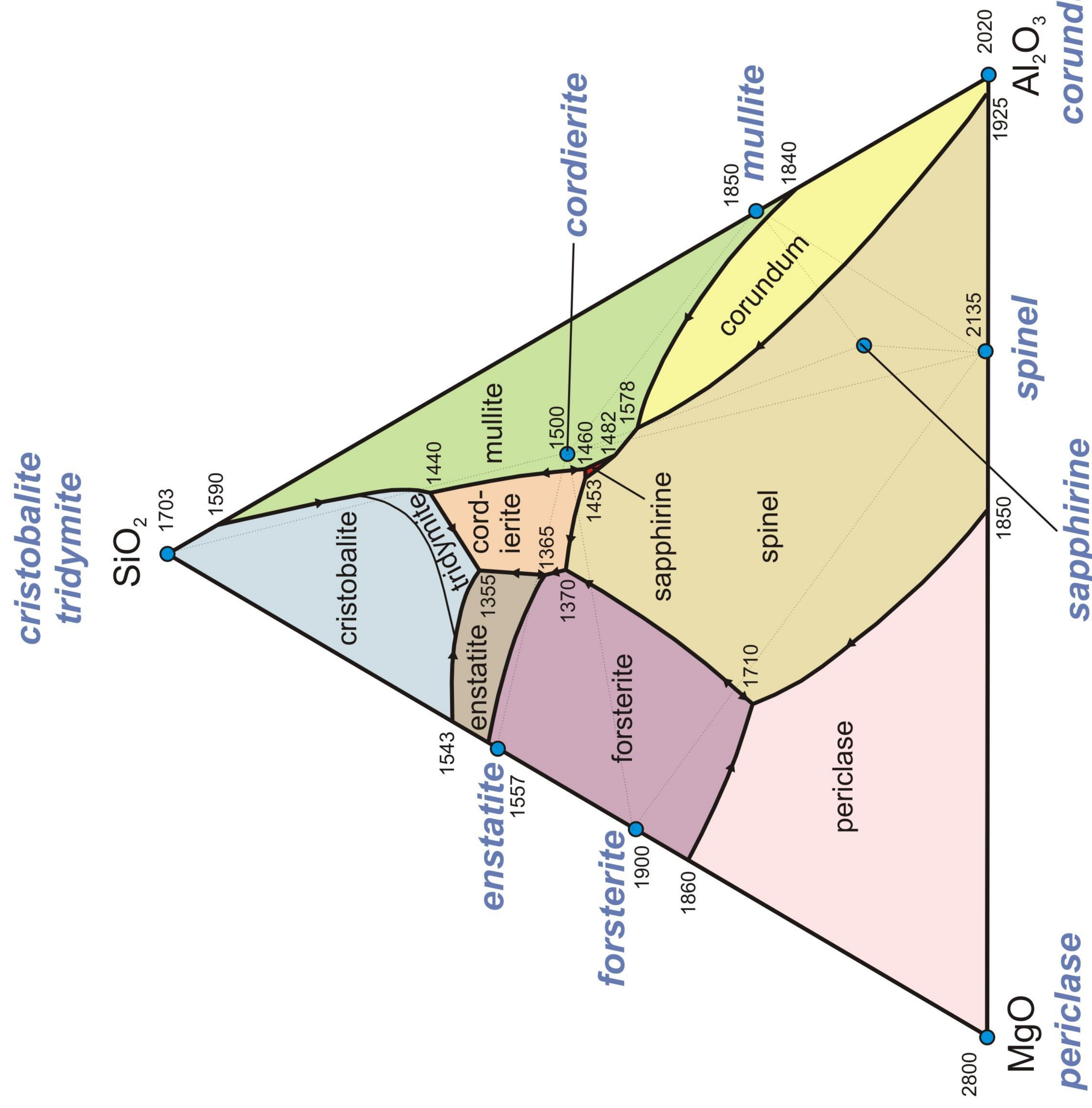


Background

- What is a Phosphor?**
- A substance that exhibits luminescent properties
 - Usually composed of oxides with a transition metal and rare earth
- Applications**
- Potential source of renewable light

Objective

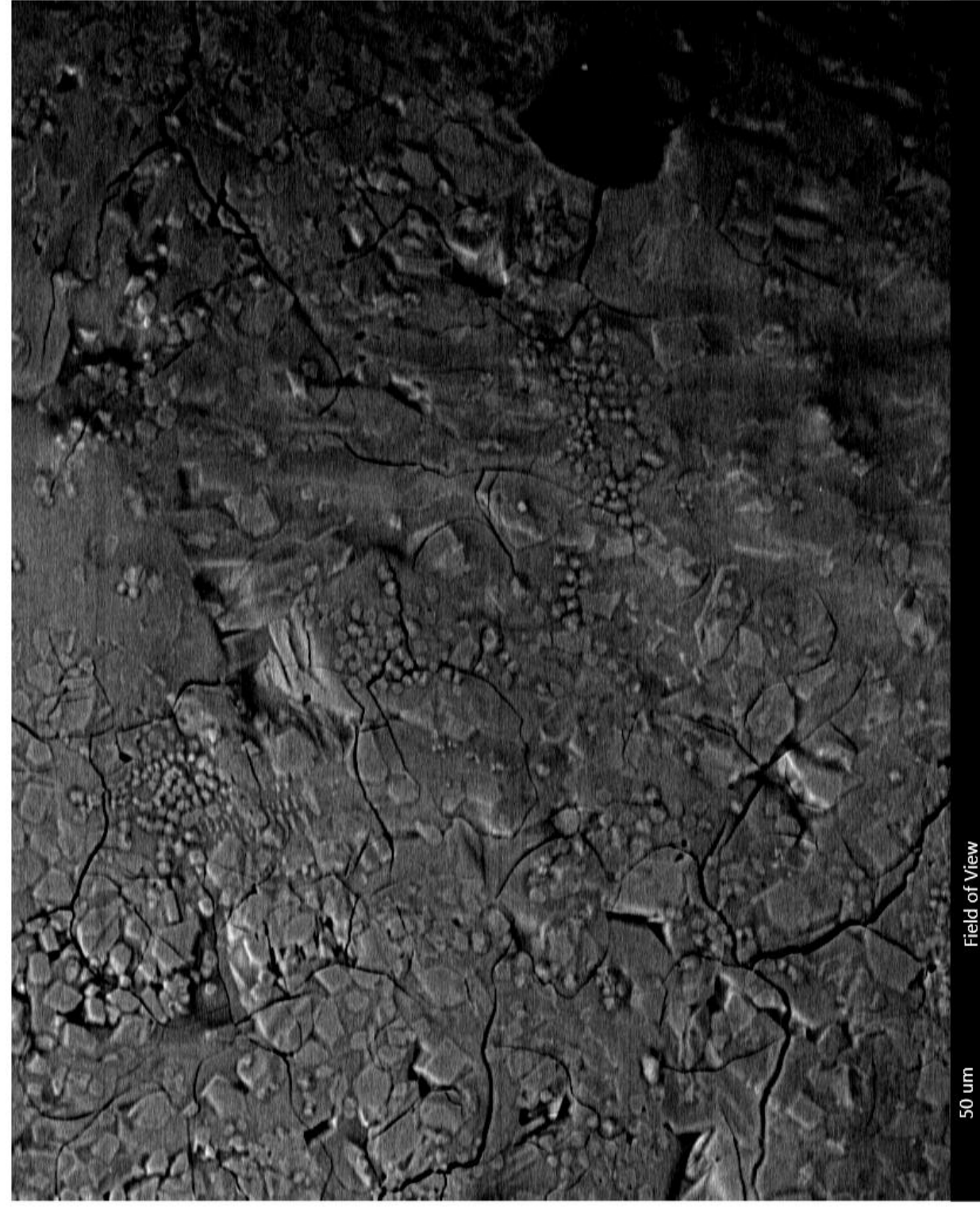
- Observe properties of a Mg-Al-Si phosphor doped with Co
- Form crystal structures to create long lasting phosphorescence



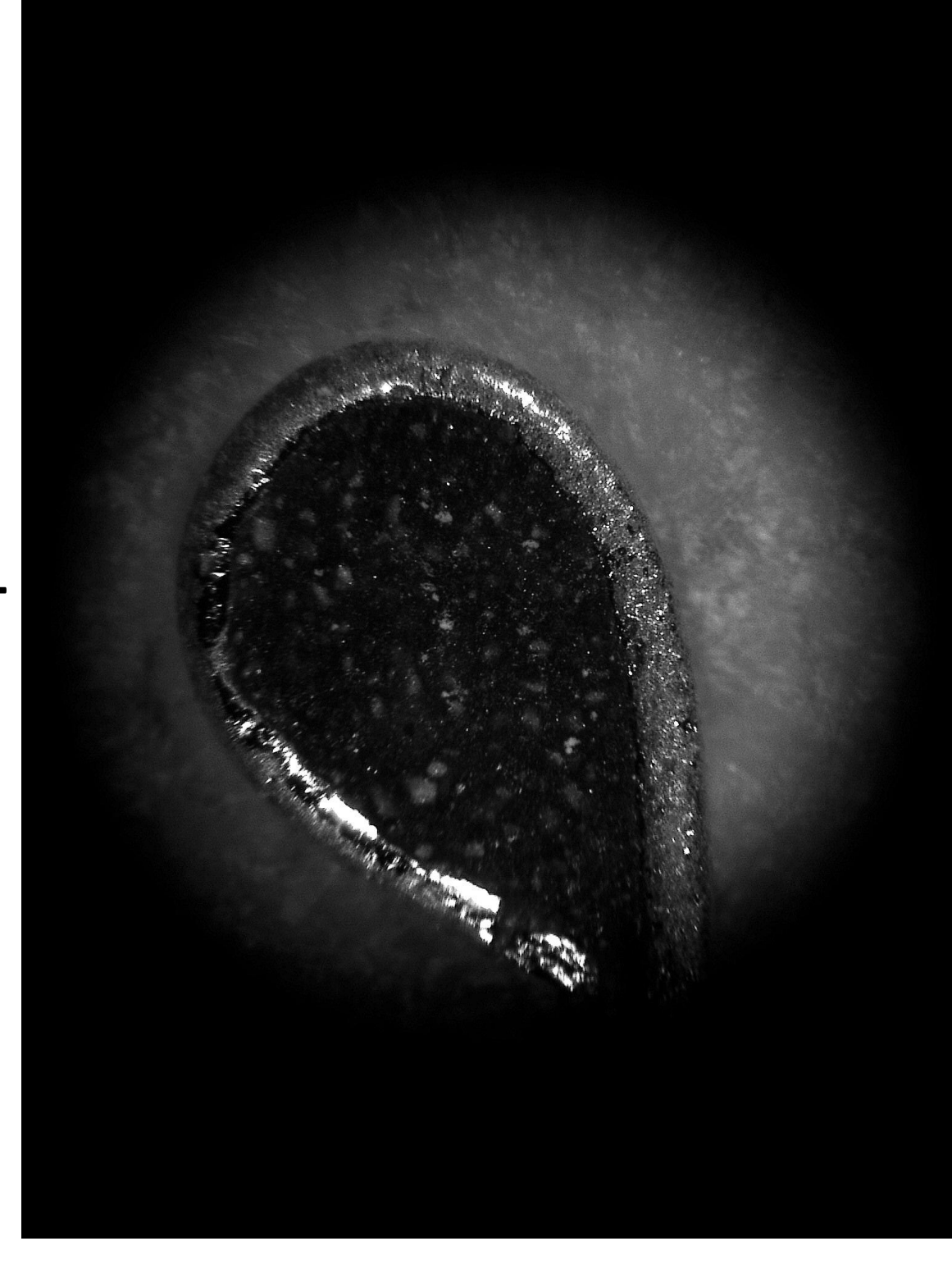
Methods

- Preparation**
- (Sample 1) Combine 0.048g of cobalt oxide, 1.263g magnesium carbonate, and 0.687g of silicon oxide
 - (Sample 2) Use remaining sample and add 20% aluminum oxide
 - (Sample 3) Use remaining sample and add 2.5% europium and 2.5% terbium
- Heating**
- Press into tablet and heat at 1300 °C for 12 hours
 - Press sample into platinum loop and heat to 1380 °C for 10 minutes before lowering temperature for 30 minutes
 - Run 95% Ar-5% H gas into furnace while heating
 - Lowered temperature ranged from 1150-1375 °C

Results



Sample 2



Sample 3

Crystal Phases Observed (Sample 2)

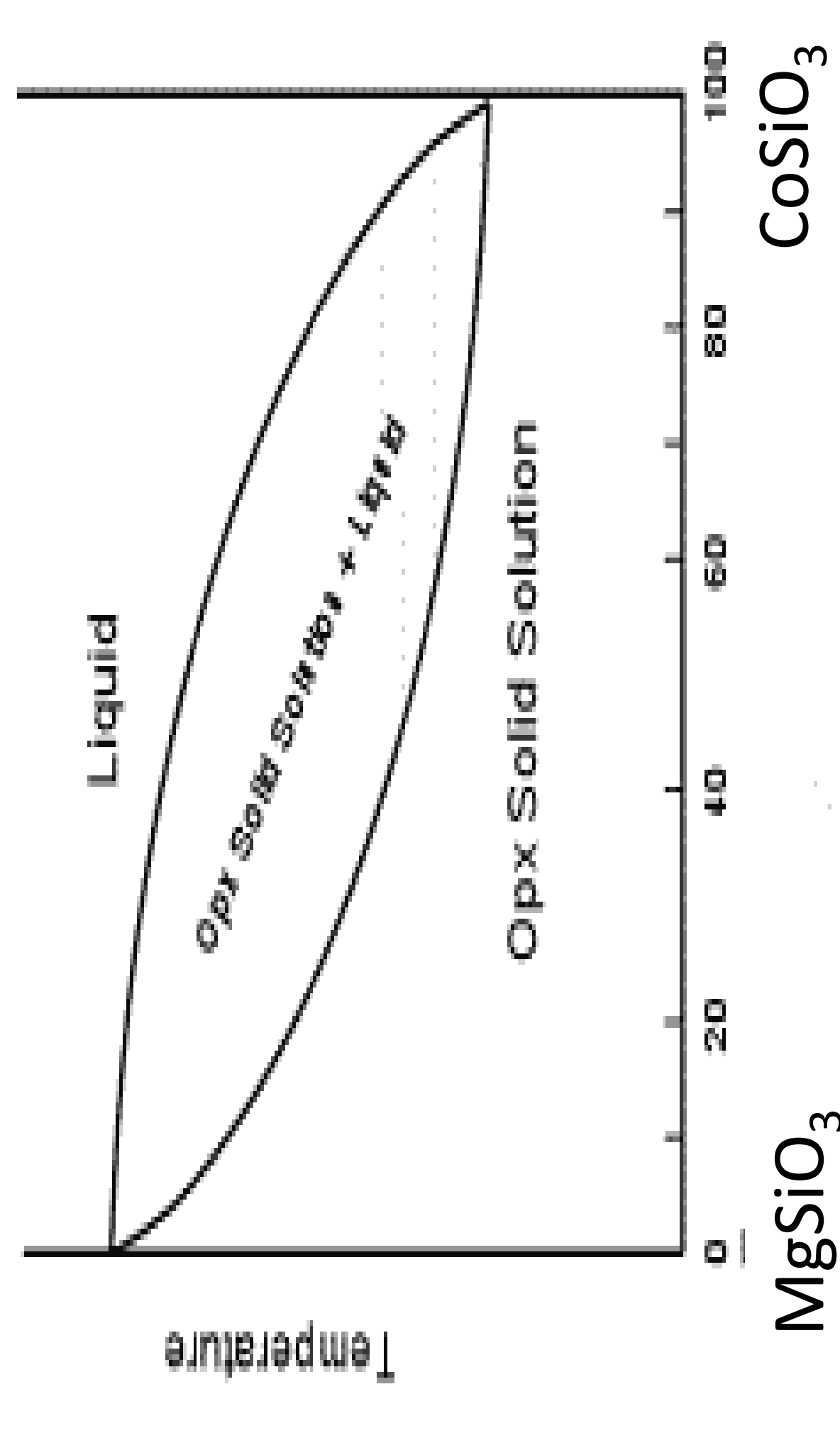
- Spinel
 - Enstatite
 - Olivine
- Observations**
- Cobalt seems to have completely replaced Aluminum in spinel
 - Results in new phase relations

Crystal Phases Observed (Sample 3)

- 2 new phases that haven't been properly characterized
 - Mg₂Al₂Si₂O₉
 - Mg₂Al₂Si₂O₁₅

Conclusion

- No signs of any luminescent properties from any sample
- Data indicates new phase relations with the addition of Co, Eu, and Tb rather than a shift
- Future research could analyze the new phase relations
 - Creation of new phase diagram



Acknowledgements

- Special thanks to Dr. James Meen and Dr. Karoline Mueller at the Texas Center for Superconductivity
- This work is supported by the National Science Foundation (DMR 1460564) and grants from the state of Texas to JKM at the Texas Center for Superconductivity

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**Effect of Side Chain Length on the Physical Properties of Linear Polymers
with a Transient Network**

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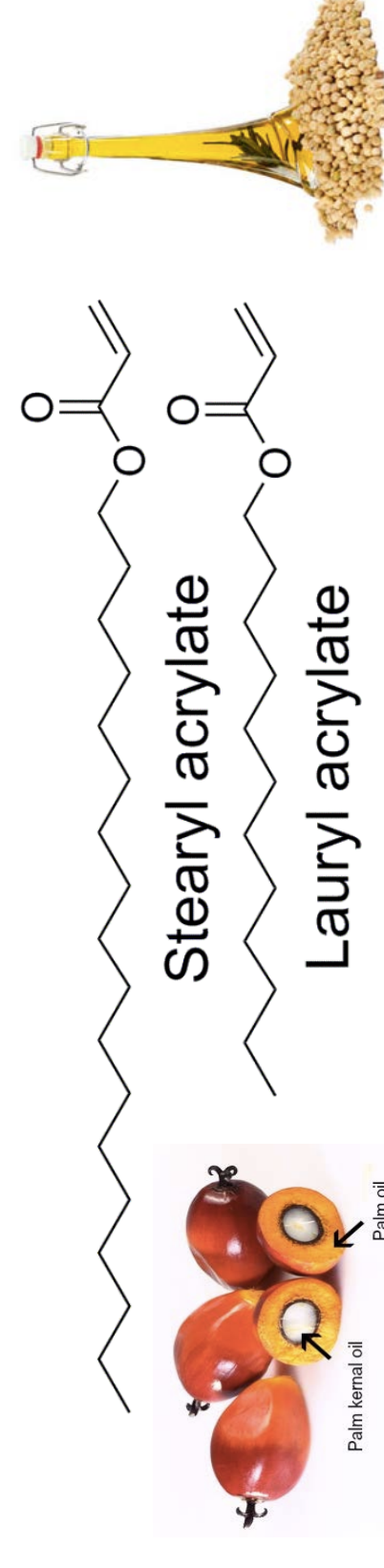
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The increasing demand to create innovative and sustainable materials with improved quality while reducing overall costs is crucial in order to overcome the challenges of scarcity of raw material sources such as petroleum oils. An attractive solution is to create biorenewable polymers with desirable properties that are derived from renewable resources. Vegetable oils and their fatty acids are useful raw material sources for polymers due to their lack of toxicity, worldwide availability, and ease of functionalization. We probed the properties of copolymers derived from fatty acids, poly(stearyl acrylate-co-lauryl acrylate). The two acrylate monomers differ in the length of their side chain, in which stearyl acrylate and lauryl acrylate contain 18 and 12 carbon atoms per side chain, respectively. In order to improve their physical properties, we have incorporated a transient network in the copolymer through copolymerization with acrylamide, which undergoes hydrogen bonding. We examined the effect of the side chain length of the polyacrylate on physical polymer properties, including melting temperature and rheological properties, both with and without copolymerization with acrylamide. The melting point increased with increasing stearyl acrylate content in the copolymer. Copolymerization with acrylamide had negligible effect on the melting temperature. Copolymers containing acrylamide exhibited higher storage and loss moduli. The presence of hydrogen bonding produced deviations from typical terminal region behavior.

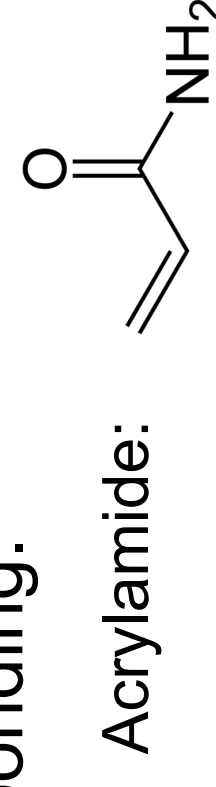
This work is supported by the National Science Foundation (CMMI-1334838 and DMR- 1611376), the HCC REEMS Program (National Science Foundation Division of Materials Research 1460564), and the Norman Hackerman Advanced Research Program of the Texas Higher Education Coordinating Board (003652-0022-2013)

Motivation

The increasing demand to create innovative and sustainable materials with improved quality while reducing overall costs is crucial in order to overcome the challenges of scarcity of raw material sources such as petroleum oils. In this project we explore vegetable oils and their fatty acids as sources for polymers. We are focusing on two long chain acrylate monomers derived from fatty acids, stearyl and lauryl acrylates.



To improve the properties of polymers derived from fatty acids, we are exploring the incorporation of supramolecular interactions, such as hydrogen bonding. Supramolecular polymers exhibit dynamic properties such as self-healing. We will copolymerize the acrylate monomers with acrylamide, which undergoes hydrogen bonding.



Project objectives:

- Tune the physical properties of polymers derived from fatty acids through incorporation of supramolecular interactions
- Investigate the effect of the side chain length on the polymer properties

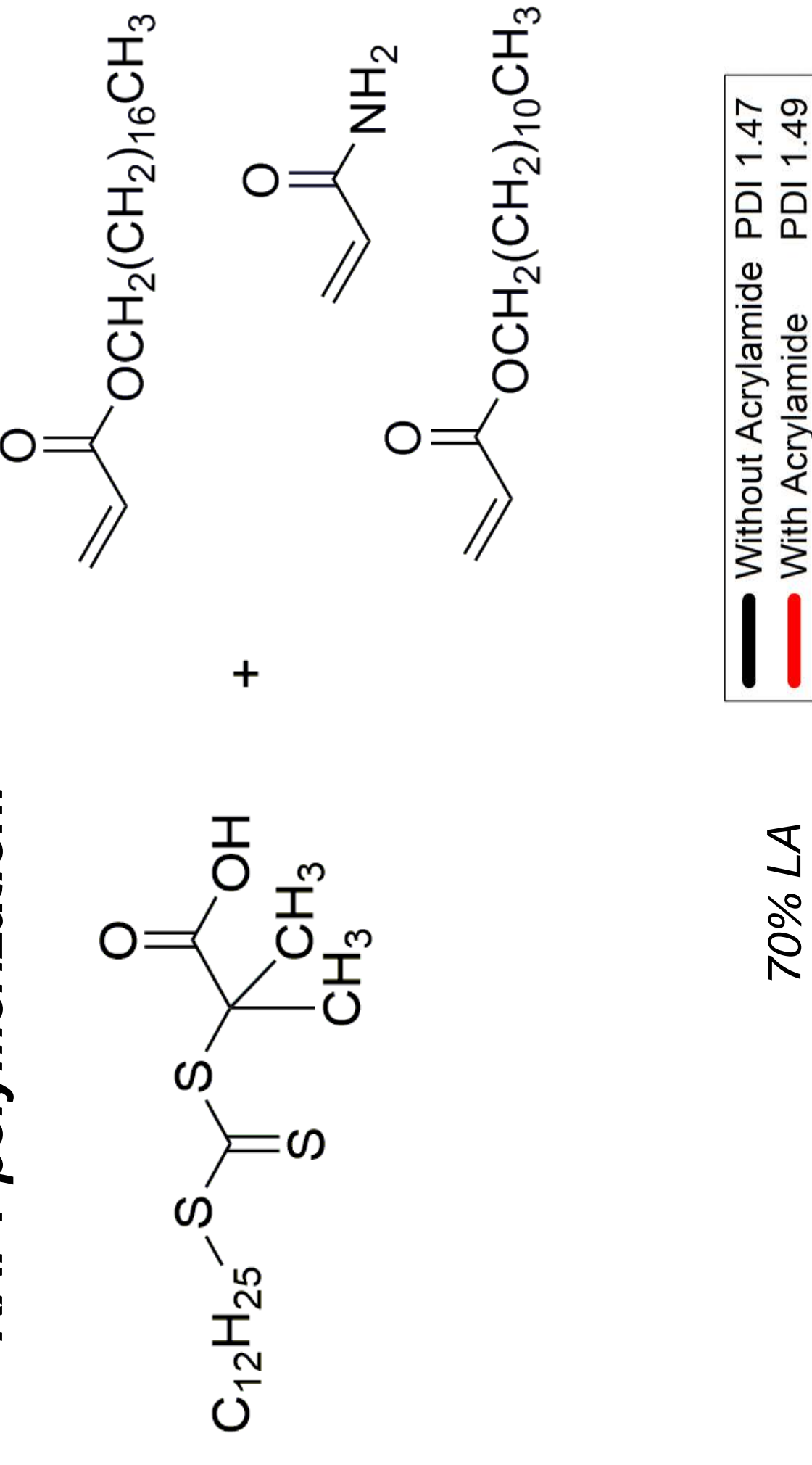
Materials & Methods

- Polymers synthesized with reversible addition-fragmentation chain transfer (RAFT) polymerization
- RAFT: a "controlled" polymerization technique
- Polymer composition and molecular weight distribution characterized with nuclear magnetic resonance and gel permeation chromatography
- Thermal properties explored with differential scanning calorimetry
- Dynamic moduli characterized with rheology
- Polymer compositions explored:
 - % lauryl acrylate (relative to total lauryl and stearyl acrylate content) varied from 10-90 mol%
 - Acrylamide added at a concentration of 4 wt%

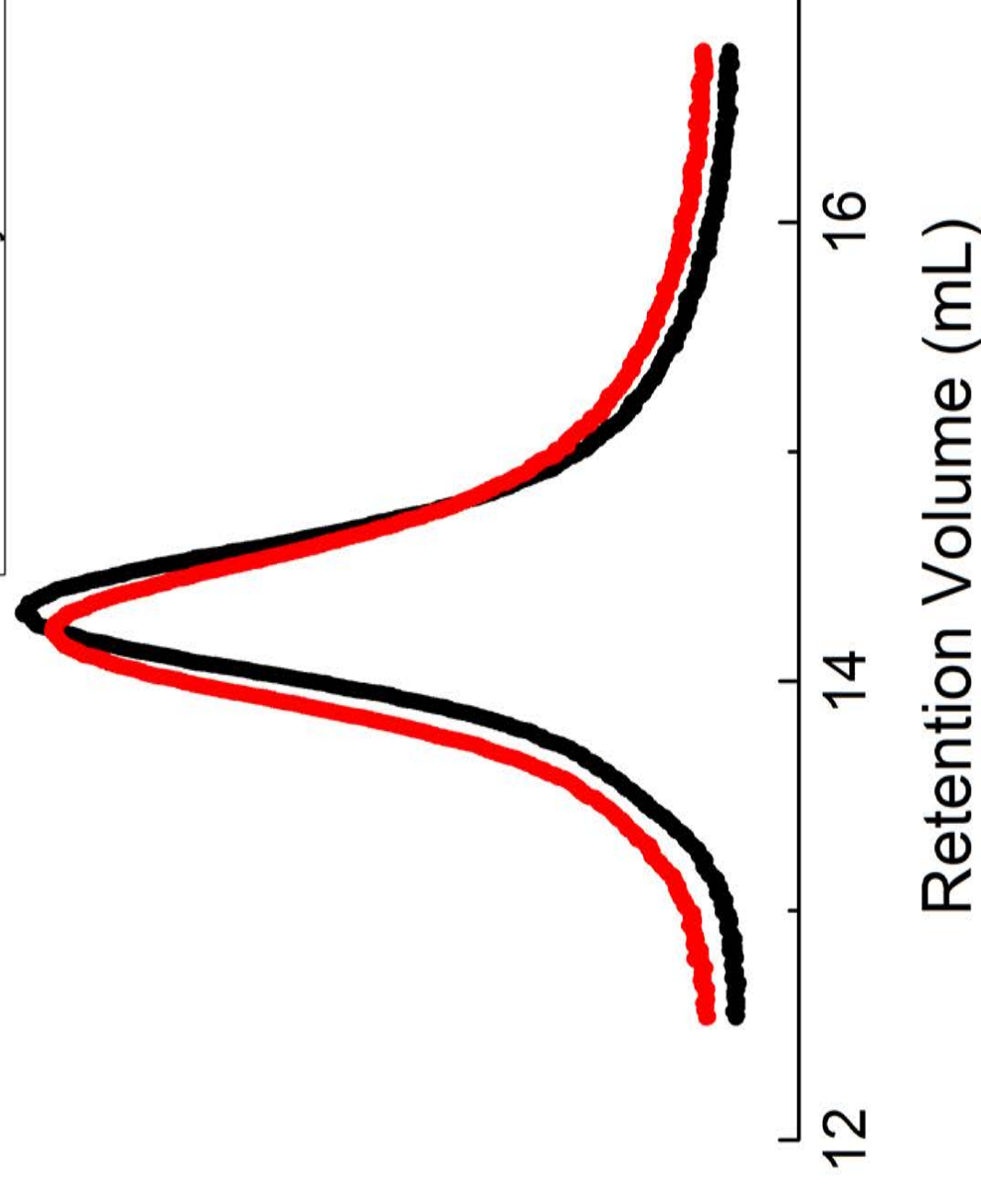
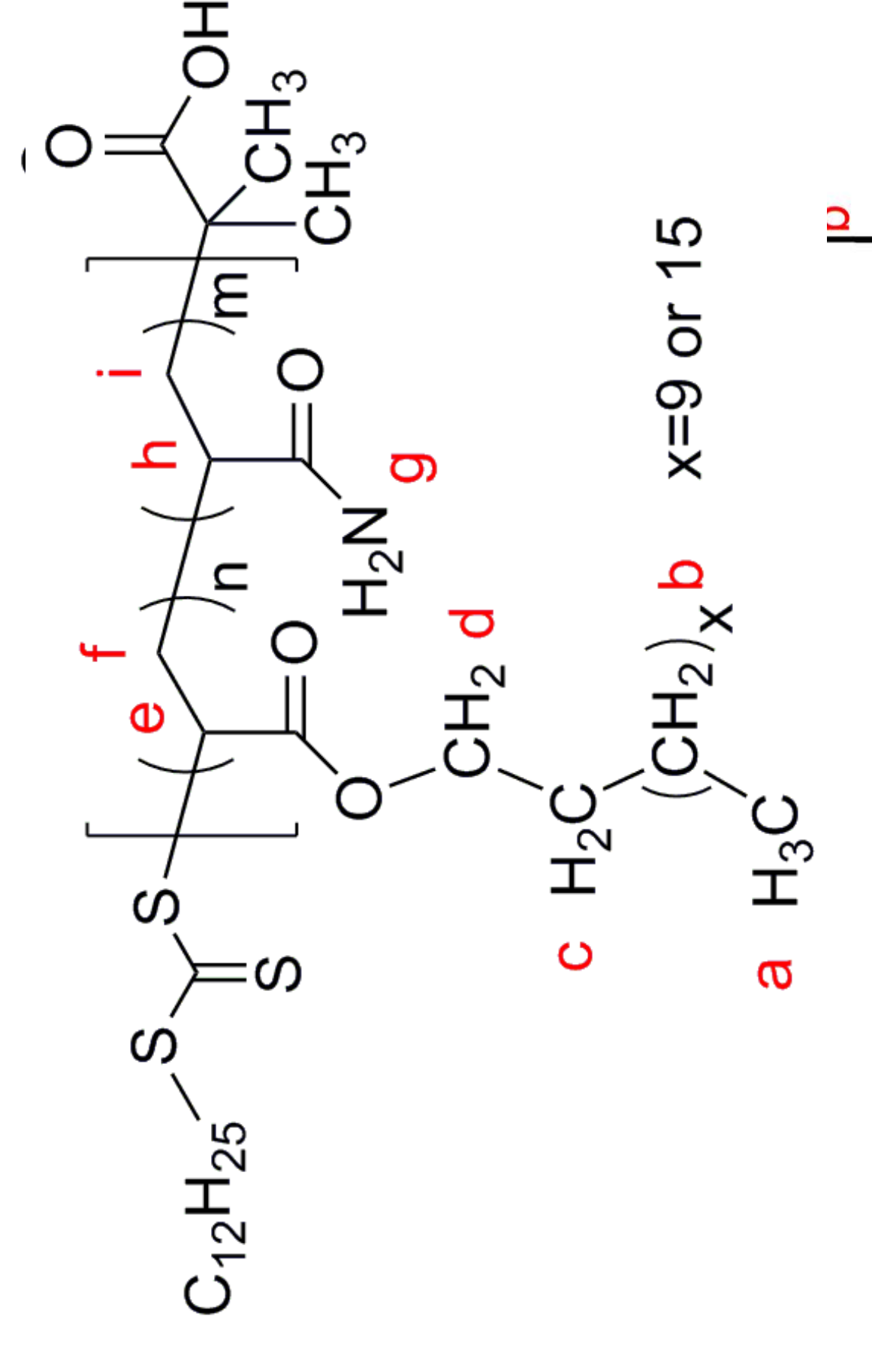
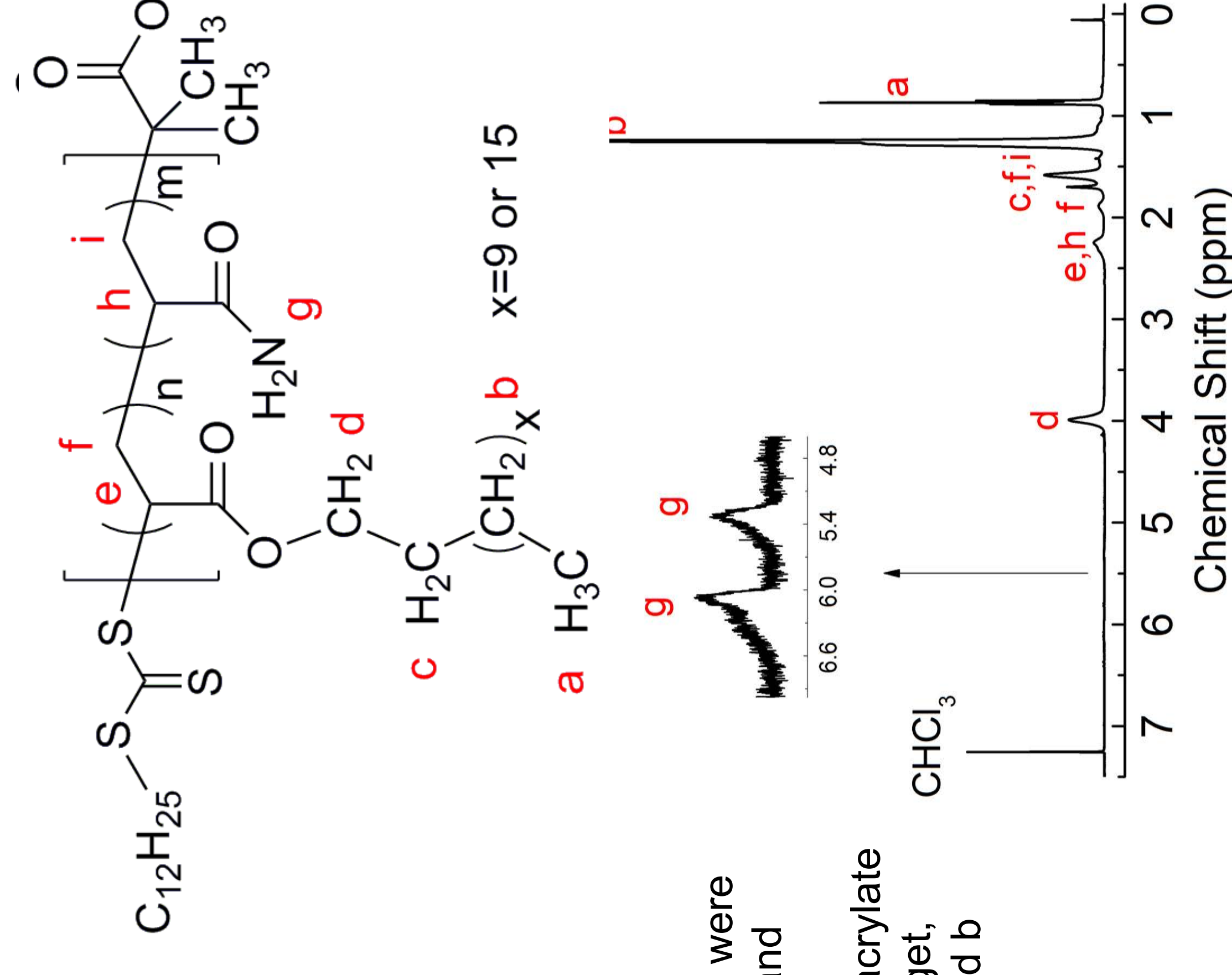


Synthesis of Poly(lauryl acrylate-co-stearyl acrylate-co-acrylamide) Copolymers

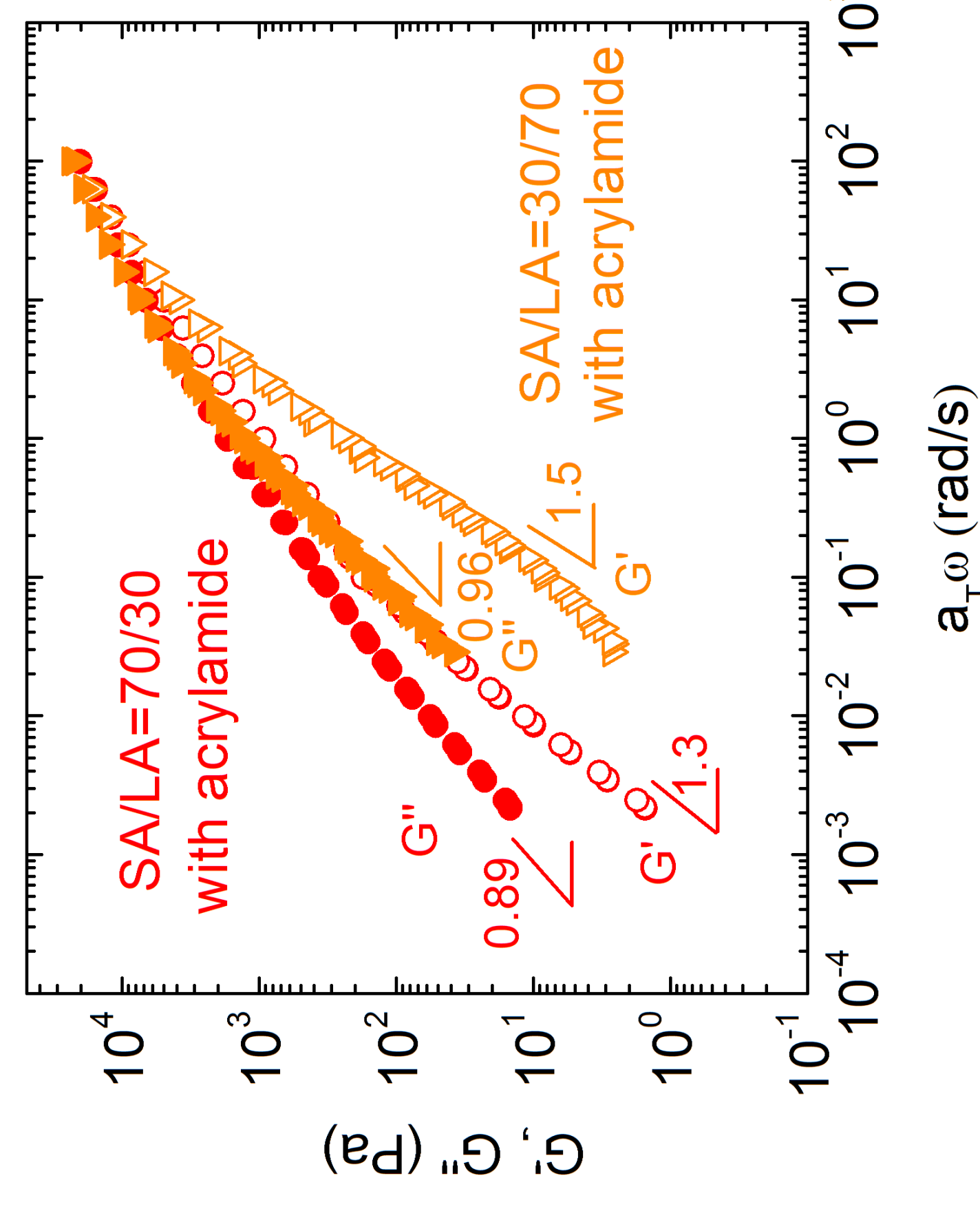
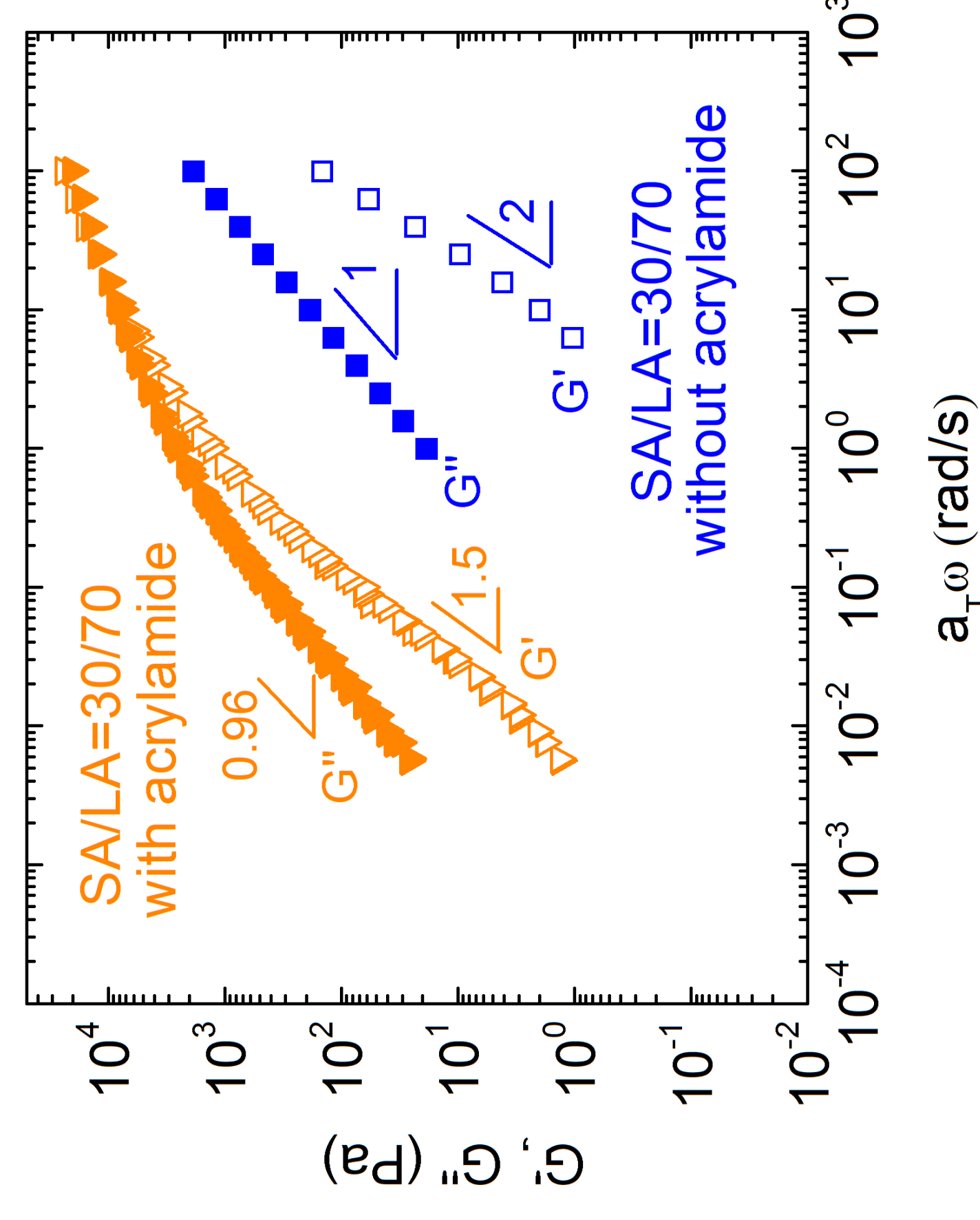
RAFT polymerization:



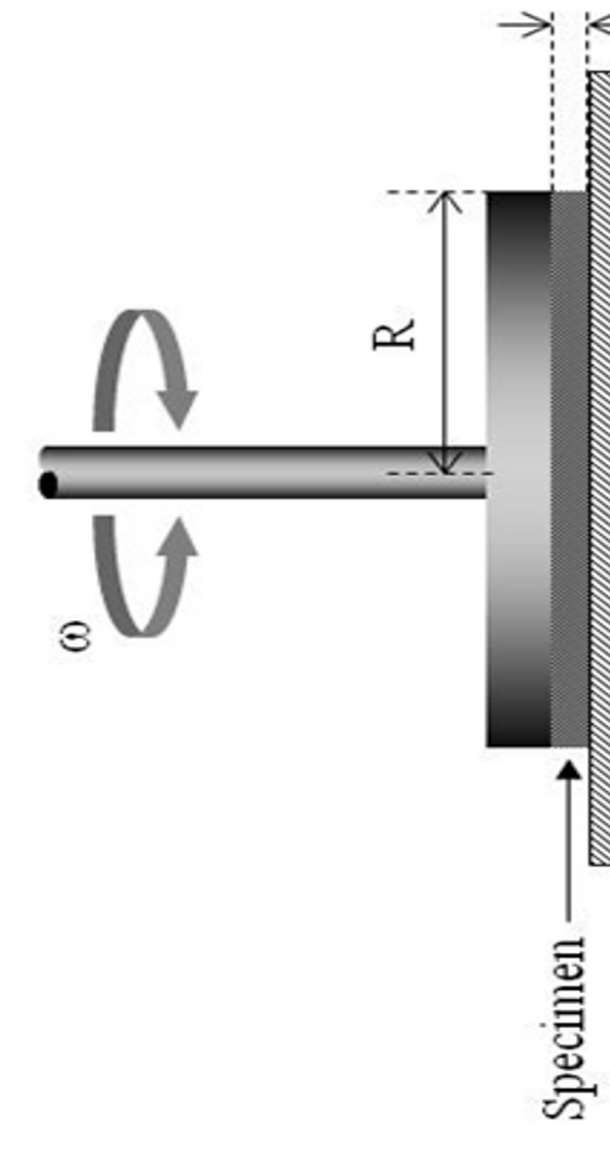
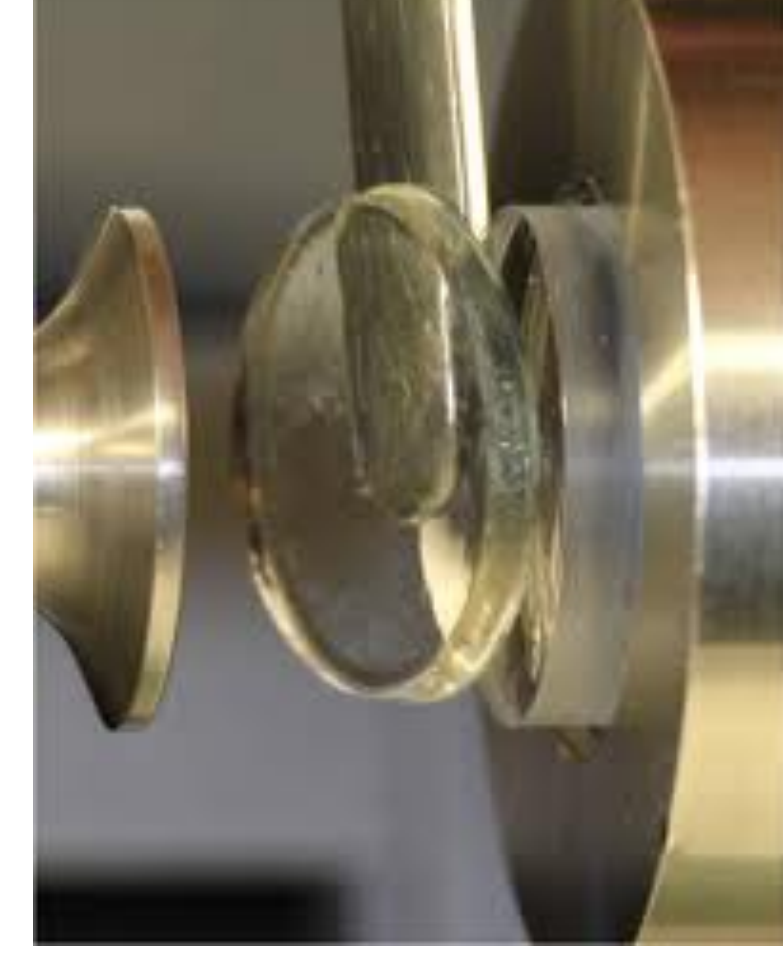
- Molecular weight distributions were similar for the polymers with and without acrylamide
- NMR confirmed the % lauryl acrylate composition was near the target, using the areas of peaks a and b (labeled on spectrum)



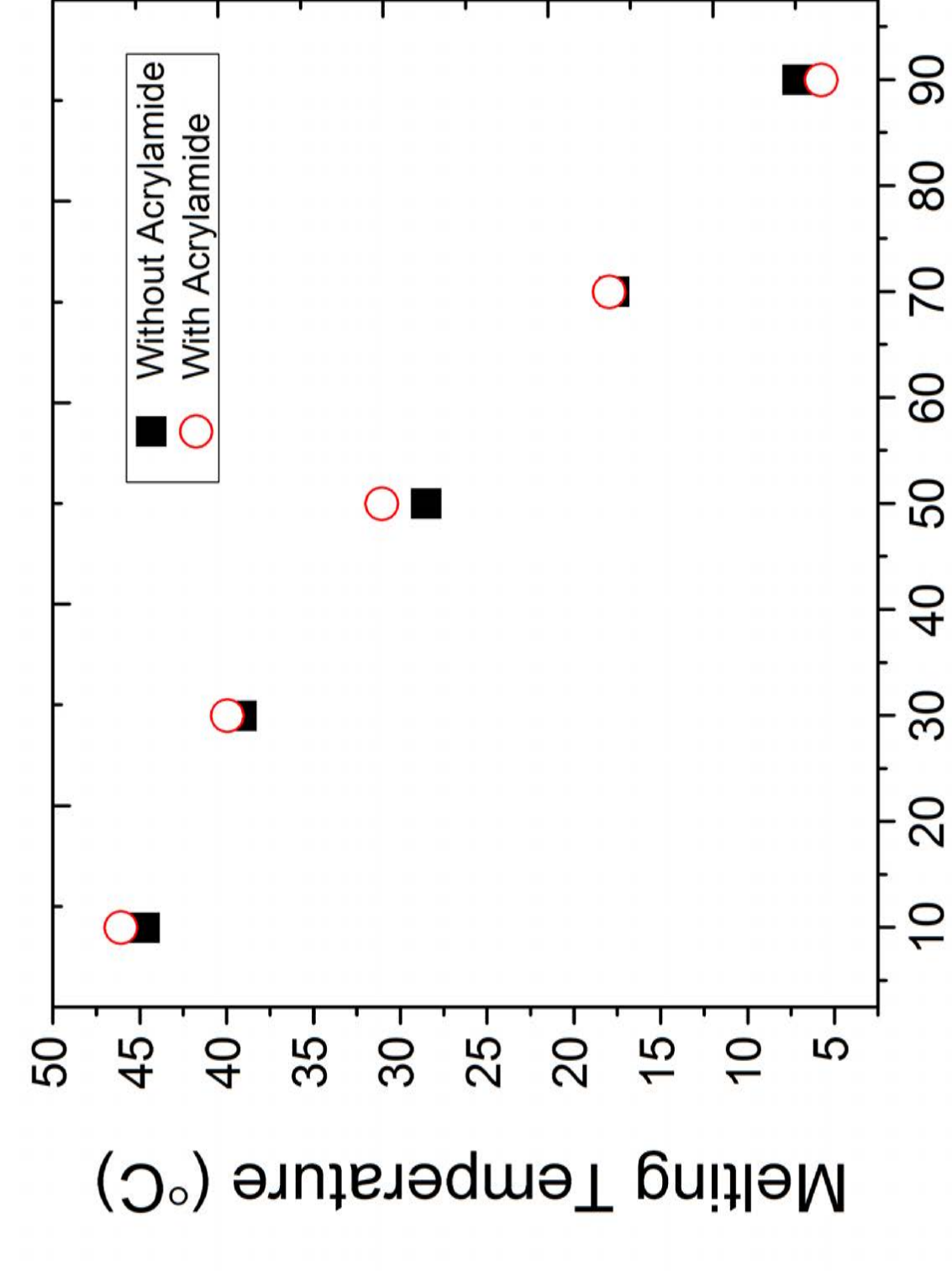
Rheological Properties Impacted by Presence of Hydrogen Bonding



- The storage modulus (G') and loss modulus (G'') reflect the solid-like and liquid-like behavior of the sample, respectively
- By adding acrylamide, both moduli increase significantly indicating the presence of hydrogen bonding interactions
- The sample without acrylamide shows typical terminal region behavior for a linear polymer melt (at low reduced frequency $a_{t,\omega}$):
 - G' proportional to ω^2
 - G'' proportional to ω
- Adding acrylamide results in deviations in the terminal region:
 - G' proportional to $\omega^{1.5}$
 - G'' proportional to $\omega^{0.96}$
- Varying the SA/LA content from 70/30 to 30/70 did not greatly change terminal region behavior



Thermal Properties Independent of Acrylamide Content



- Copolymerization with acrylamide had negligible effect on the melting temperature
- The melting point decreased with increasing lauryl acrylate content in the copolymer

Conclusions

- Copolymers of stearyl acrylate and lauryl acrylate exhibited tunable melting temperatures, based on the acrylate content
- Copolymerization with acrylamide had negligible effect on the melting temperature
- Copolymers without acrylamide exhibited rheological behavior that is typical of polymer melts
- Addition of acrylamide increased the dynamic moduli (G' , G''), and impacted the terminal region, indicating possible presence of hydrogen bonding
- Future experiments will explore the impact of hydrogen bonding in these systems on mechanical behavior, offering a viable route to improve the physical properties of fatty acid-derived polymers

Acknowledgements

This work is supported by the National Science Foundation (DMR-1611376), including the HCC NSF-REEMS Program (DMR-1460564). We are grateful to all the members of the Robertson research group. We also thank NSF-REEMS and all participating members of the REU program.

- Abstract & References QR Code



Enhancing Flexibility of Polymer Conductor through Surfactant and Solvent AdditivesJoshua Jackson¹, Jorge Wu Mok², and Rafael Verduzco²¹REEMS REU Program, West Houston Center for Science & Engineering, Houston Community College 77082²*Department of Biomolecular and Chemical Engineering, Rice University, TX 77005*

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Organic photovoltaic (OPVs) devices have emerged as a promising source for harvesting renewable energy from sunlight. Despite tremendous advances on the OPV technology, mechanical failure still the limiting factor that prevents the marketability of these devices. Here, we improve the mechanical flexibility and stretch-ability of poly(3,4-ethylenedioxythiophene) PEDOT:PSS electrodes by using a combination of ionic additives and solvents. PEDOT: PSS has poor mechanical properties and cracks and fractures occur at minimal tensile strains. Also, when PEDOT: PSS was processed in a thin film we found it has low electrical conductivities. In order to improve both mechanical and electronic properties, we tested the effects of different additives, such as Capstone FS-30 and Zonyl FS-300 for improved flexibility and stretch-ability; and dimethyl sulfoxide (DMSO) for improved conductivities. We prepared blends with various compositions of PEDOT: PSS, DMSO, Zonyl or Capstone. Throughout the research it was shown that with increased concentration of Capstone fs-30, PEDOT: PSS will become more stretchable but less conductive. However, adding DMSO made PEDOT: PSS more conductive but less stretchable. We found that blends with 75 wt.% PEDOT.PSS, 20 wt.% Capstone FS-30 and 5 wt.% DMSO demonstrated significant improvements in mechanical strains and conductivities. In summary, we this work demonstrates that ionic additives can be used to improve the mechanical strains and electronic conductivities of PEDOT: PSS thin films. Future work I want to try to use different additives such as Bis (trifluoroethane) sulfonamide lithium salt and 4-(3-Butyl-1-imidazolio)-1-bultanesulfonic acid triflate to test mechanical and electronic improvements.

Acknowledgments

This work was supported by the National Science Foundation REU-REEMS program (DMR- 1460564) and the NSF CAREER DMR- 1352099.



Enhancing Flexibility of Polymer Conductor through Surfactant and Solvent Additives

Joshua Jackson^{1,2}, Rodrigo Munoz^{1,2}, Jorge Wu Mok^{1,2}, Rafael Verduzco¹

¹ Department of Chemical and Biomolecular Engineering, Rice University, Houston, Texas

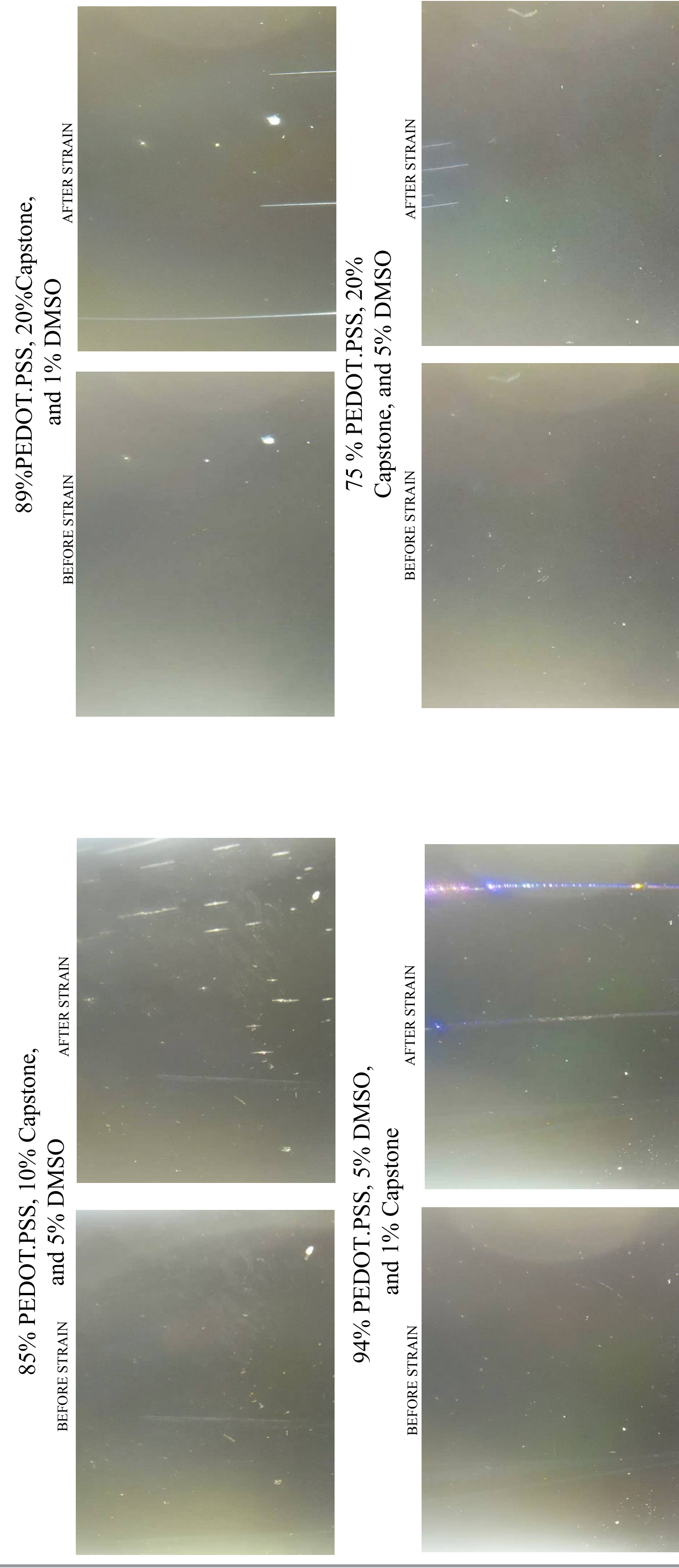
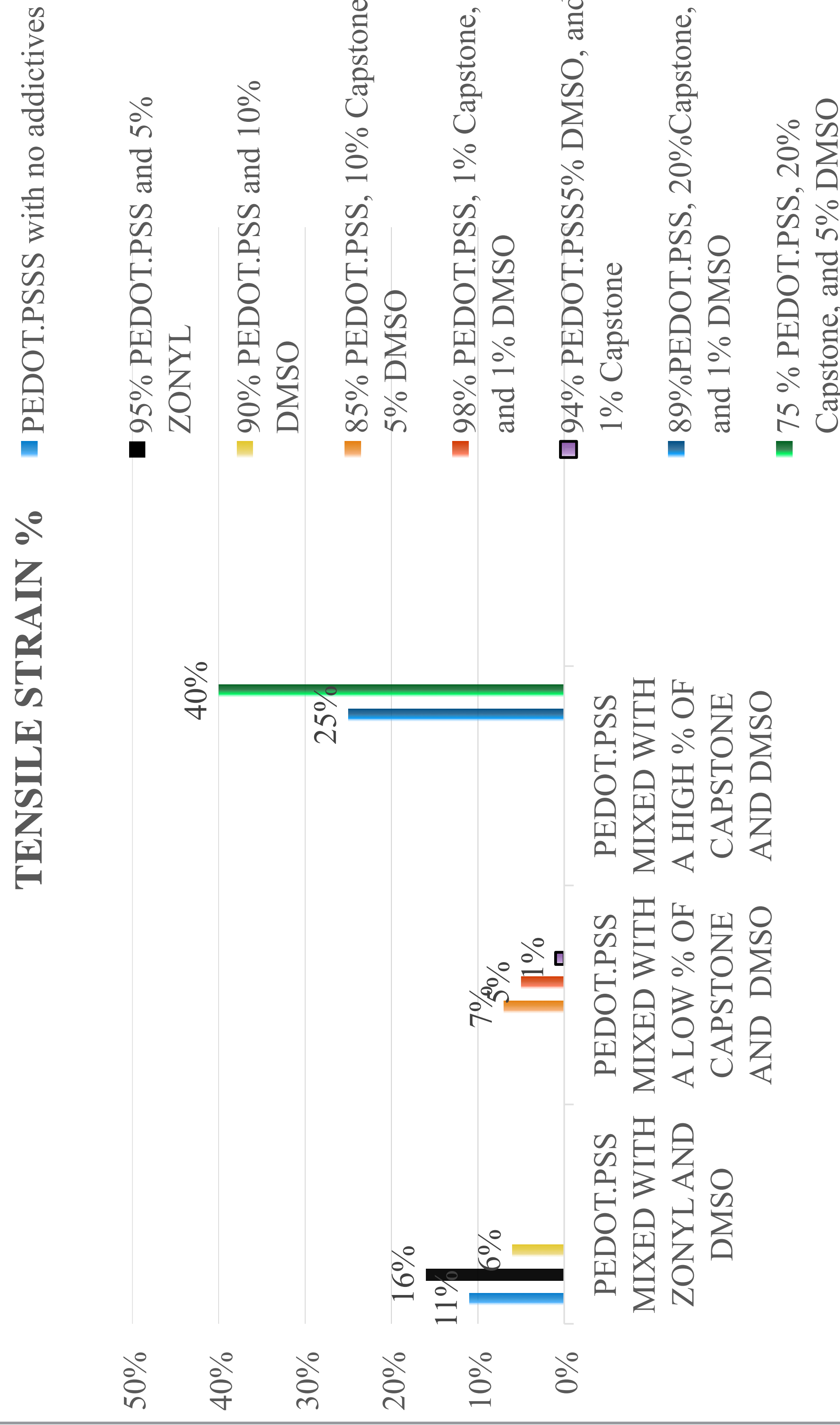
² REEMS program, Houston Community College, Houston, Texas



Introduction and Background

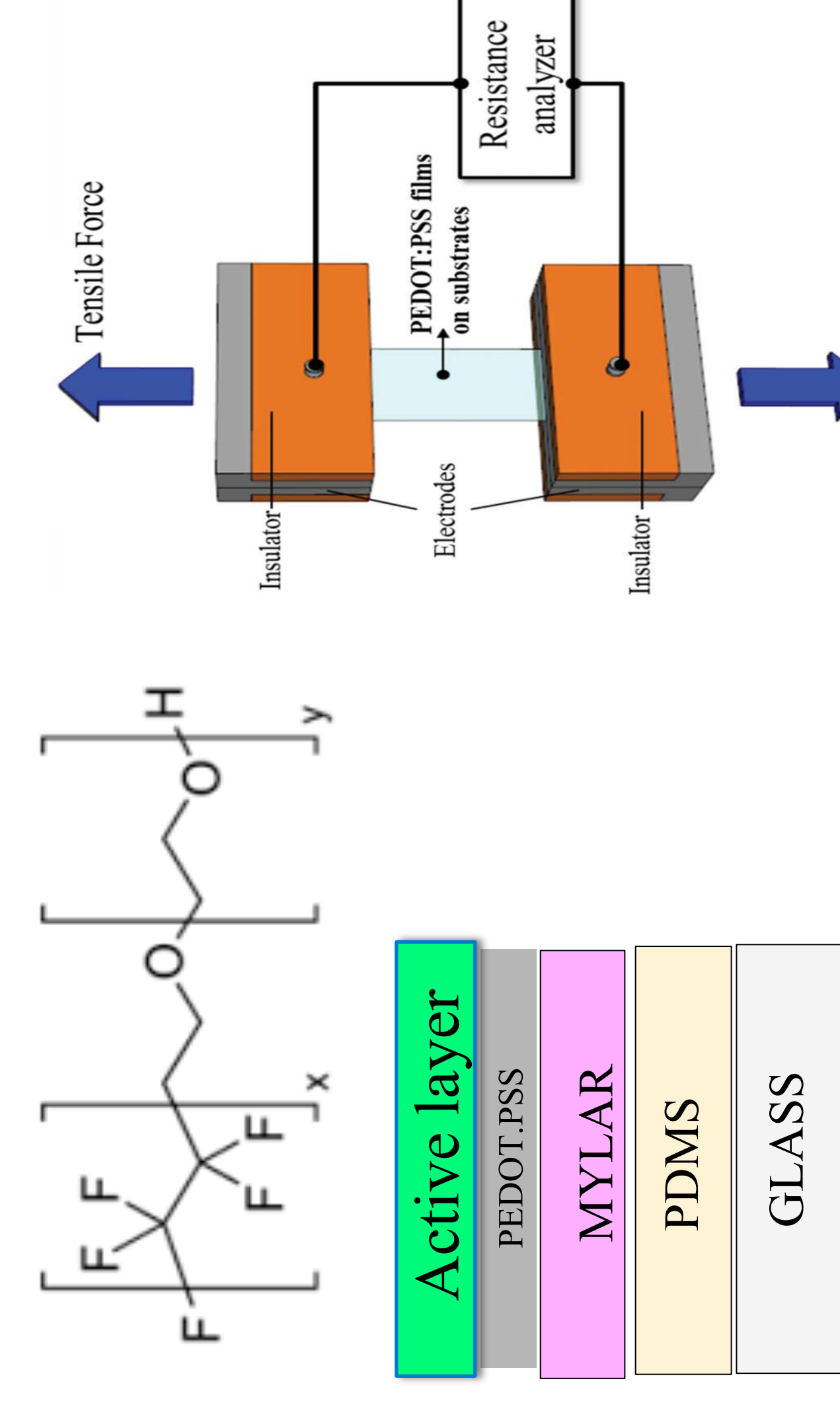
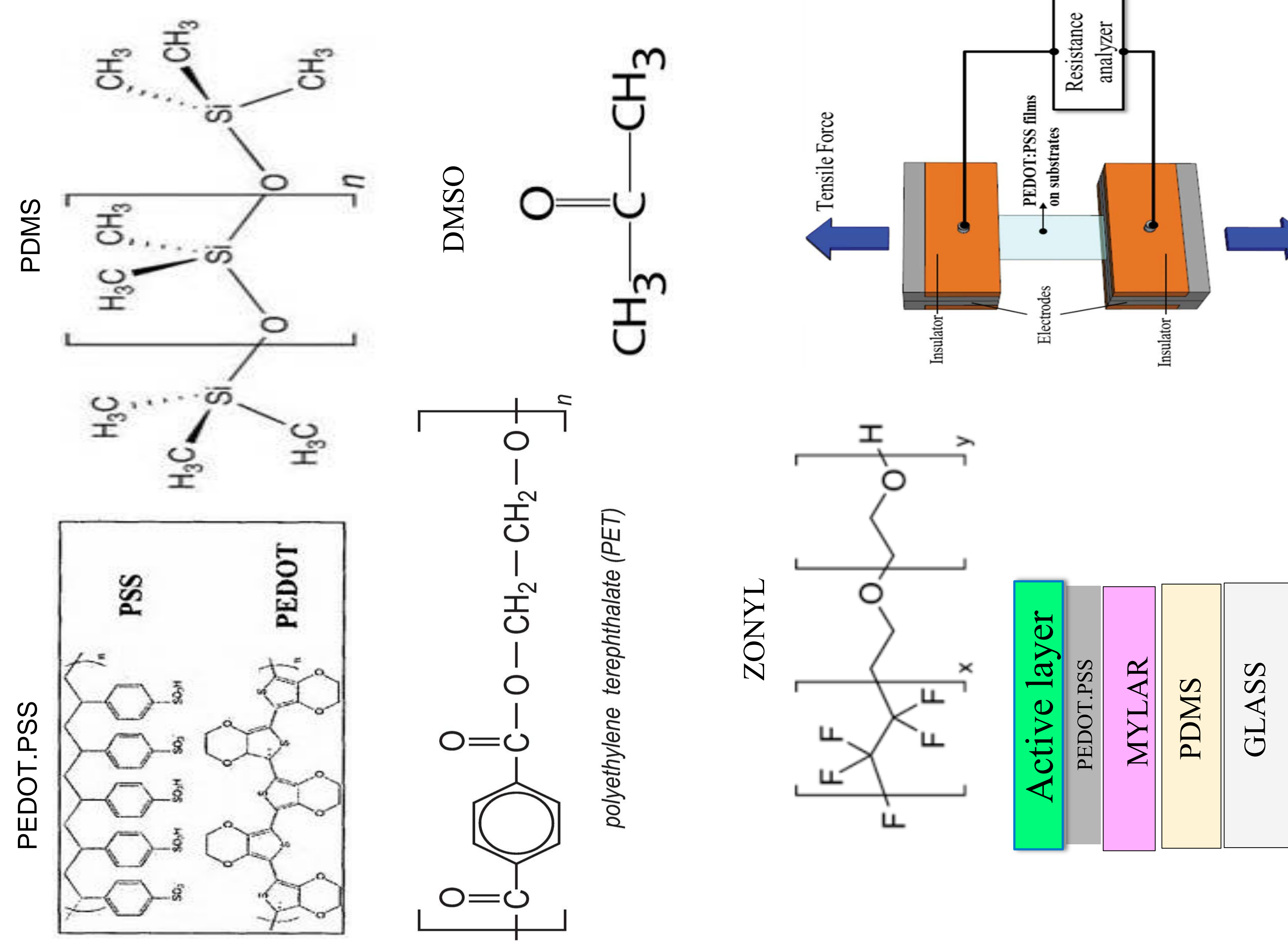
Organic photovoltaic (OPVs) devices have emerged as a promising source for harvesting renewable energy from sunlight. Despite tremendous advances on the OPV technology, mechanical failure is still the limiting factor that prevents the marketability of these devices. Conducting polymers are good candidates because of their flexibility in tuning the molecular structures and electrical and mechanical properties. Their solution process-ability offers additional advantages for large-scale production of flexible electronics. Unfortunately, high conductivity and high stretchability have not been achieved simultaneously for conducting polymers. The polymer that I have been working with is poly(3,4-ethylenedioxythiophene) (PEDOT: PSS). PEDOT:PSS has poor mechanical properties and cracks and fractures occur at minimal tensile strains.

RESULTS



EXPERIMENTAL

In this study, we focused on enhancing both mechanical and electronic properties, we tested the effects of different additives, such as Capstone FS-30 and Zonyl FS-300 for improved flexibility and stretch-ability; and dimethyl sulfoxide (DMSO) a common polar additive for enhancing PEDOT:PSS conductivity. This was placed on top of glass, Polydimethylsiloxane (PDMS), and Mylar (polyethylene terephthalate (pet)). Stretched under a microscope to check for cracks and strains.



1. Clean glass with Hellmanex, DI water, acetone, and Isopropyl Alcohol (IPA)
2. Make PDMS by mixing 10:1 ratio of Silicon curing agent and Silicon base
3. Make PEDOT:PSS solution(s)
4. Spin-coat 300 μ L of PEDOT:PSS at 500 rpm for 120 seconds and 2000 rpm for 30 secs
5. Anneal on a hot plate at 100 C for 10 minutes.
6. Stretch PEDOT:PSS on substrates under a microscope

Conclusion

PEDOT:PSS on Mylar being stretch at 70%



Our results so far have shown that the more capstone that was added to the blend of PEDOT:PSS improves the tensile strain up to 40% compared to PEDOT:PSS 11% tensile strain on top of PDMS. We found that blends with 75 wt.% PEDOT:PSS, 20 wt.% Capstone FS-30 and 5 wt.% DMSO demonstrated significant improvements in mechanical strains and conductivities. We added an active layer on top of the 75 wt.% PEDOT:PSS, 20 wt.% Capstone FS-30 and 5 wt.% DMSO and placed it on Mylar and we noticed up to a 70% strain.

Future Work

- Try to use different additives such as Bis (trifluoroethane) sulfonamide lithium salt and 4-(3-Butyl-1-imidazolyl)-1-bultanesulfonic acid triflate to test mechanical and electronic improvements.
- Finding an efficient way to test conductivity in the polymers.

Acknowledgements

We would like to thank the National Science Foundation for the funding, Dr. Rafael Verduzco, our supervisor, and Jorge Wu Mok, our mentor, in the Chemical and Biomolecular Department at Rice University.

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2. Suchol Savagatrup , Esther Chan , Sandro M. Renteria-Garcia , Adam D. Printz , Aliaksandr V. Zaretski , Timothy F. O'Connor , Daniel Rodriguez , Eduardo Valle , and Darren J. Lipomi. "Plasticization of PEDOT:PSS by Common Additives for Mechanically Robust Organic Solar Cells and Wearable Sensors.
3. A. Elschner , S. Kirchmeyer , W. Lovenich , U. Merker , K. Reuter , PEDOT: Principles and Applications of an Intrinsically Conductive Polymer , CRC Press , New York 2011

Optimization of thiol-ene coupling for substrates for flexible photovoltaic devicesRodrigo Munoz-Zarruk^{1,2}, Joshua Jackson¹, Jorge Wu Mok², and Rafael Verduzco^{2,*}¹REEMS REU Program, West Houston Center for Science & Engineering, Houston Community College, Houston, TX 77082²Department of Biomolecular and Chemical Engineering, Rice University, TX 77005

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Organic Photovoltaic (OPV) devices have the ability to harness energy from solar radiation and produce electricity that can be used in a wide variety of applications. As opposed to clunky and relatively hard-to-process silicon-based solar cells, OPVs can be easily and relatively inexpensively processed into thin films that exhibit good electrical properties. However, producing OPVs that are flexible is still a challenge when trying to maintain acceptable efficiencies because current polymers used in the (electricity producing) layer of cells do not exhibit high enough (tensile strength modulus) before failing and rendering the cell obsolete. Further, devices are tested on hard substrates with electrodes and interlayers that are brittle and prone to cracking. To address the issue, we propose the use of light-activated chemistries for the fabrication of flexible substrates. Specifically, we focused on the polymerization of a tetra functional thiol, pentaerythritol tetrakis(3-mercaptopropionate) (PETMP), and an allyl vinyl ether, pentaerythritol allyl ether (PAE), using two different catalyzation processes: (UV irradiation) and (thermal annealing). 2-Hydroxy-2-methylpropiophenone (HMPP) is used as a photo-initiator during the UV irradiation polymerization, in which we vary UV exposure times, solution concentration and wavelength type in attempts to optimize processing. After using (ChR Profilometry) to measure thickness in polymer thin films, it was found that five minutes of 300 nanometer UV exposure produces acceptable films with thicknesses ranging from (70-90 nanometer). Azobisisobutyronitrile (AIBN) is used as thermal-initiator during heat-catalyzed polymerization process. The following variables were observed during optimization: thermal annealing time, thermal annealing temperature, exposure to air, polymer solution concentration, and percentage of thermal-initiator used. Films attained acceptable thicknesses, per profilometry results, after thermally annealing 30mg/mL solution of polymer network for 5 minutes at 65C. Results indicate ease of processing of successfully cross-linked

thiol-ene network polymers. These materials provide a simple approach to flexible and solution processible photovoltaic devices.



Optimization of thiol-ene coupling for substrates for flexible photovoltaic devices

Rodrigo Munoz-Zarruk^{1,2}, Jorge Wu Mok¹, Rafael Verduzco¹

¹ Department of Chemical and Biomolecular Engineering, Rice University, Houston, Texas

² REEMS program, Houston Community College, Houston, Texas



Introduction and Polymerization

Organic Photovoltaic Devices

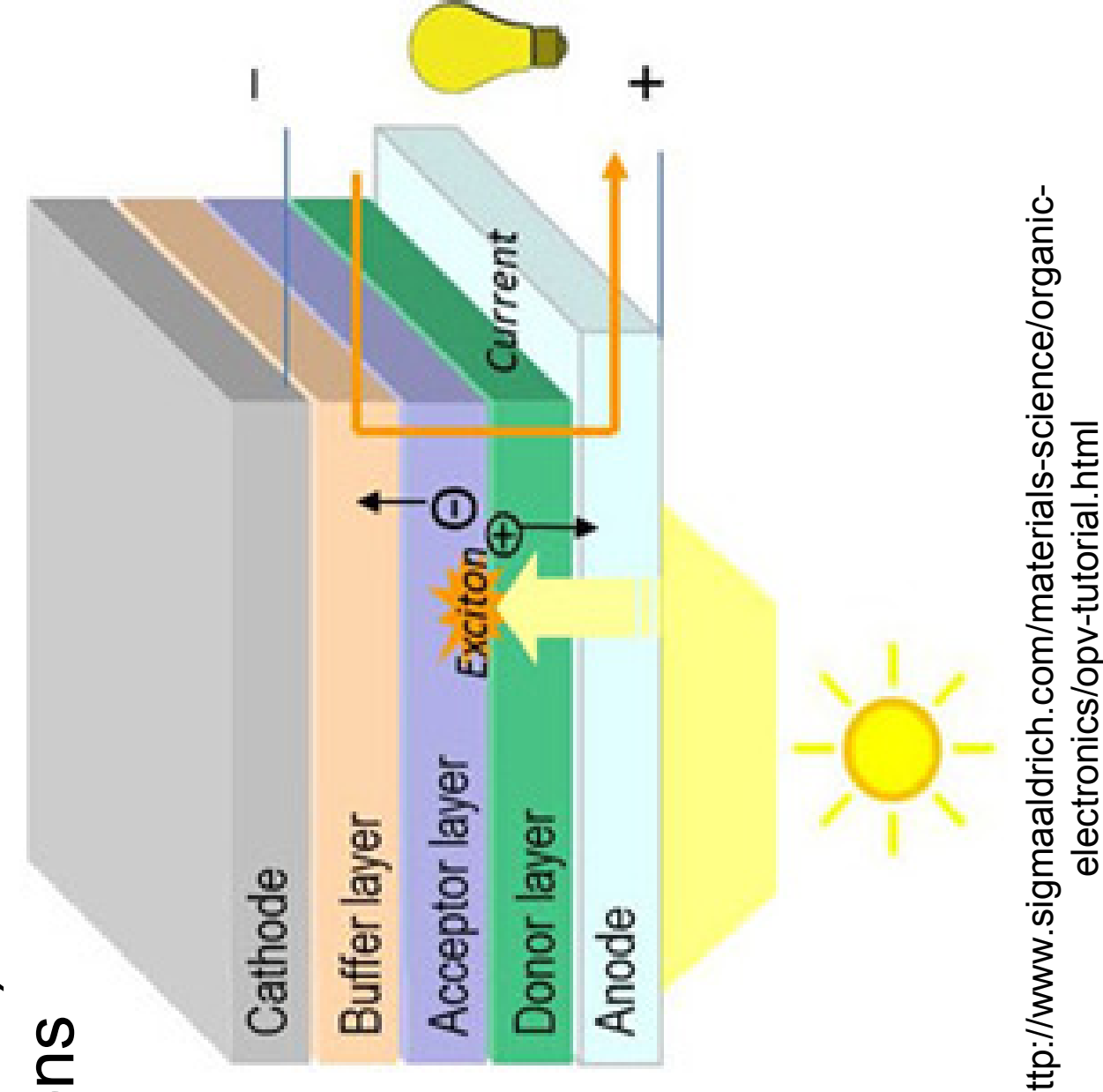
- Harvest energy from the Sun and convert it into electricity
- Low manufacturing costs (R2R production)
- Thin films allow for countless applications

Challenge

- Flexible solar cells exhibit lower efficiencies

Solution

- Optimizing polymerization of thiol-ene network polymers for use in flexible substrates

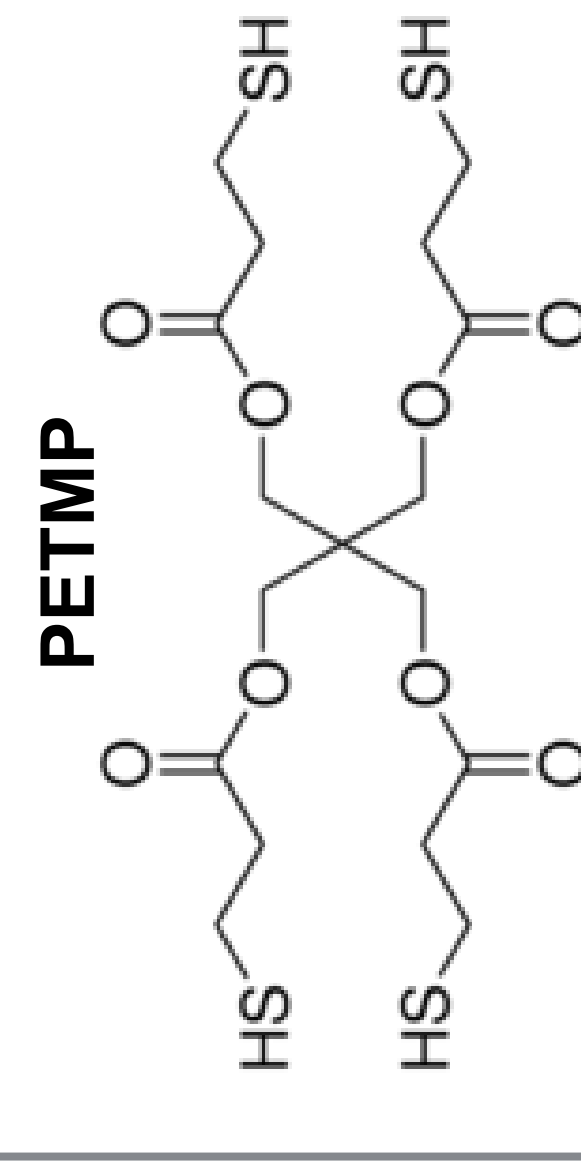


Thiol-Ene Network Polymer

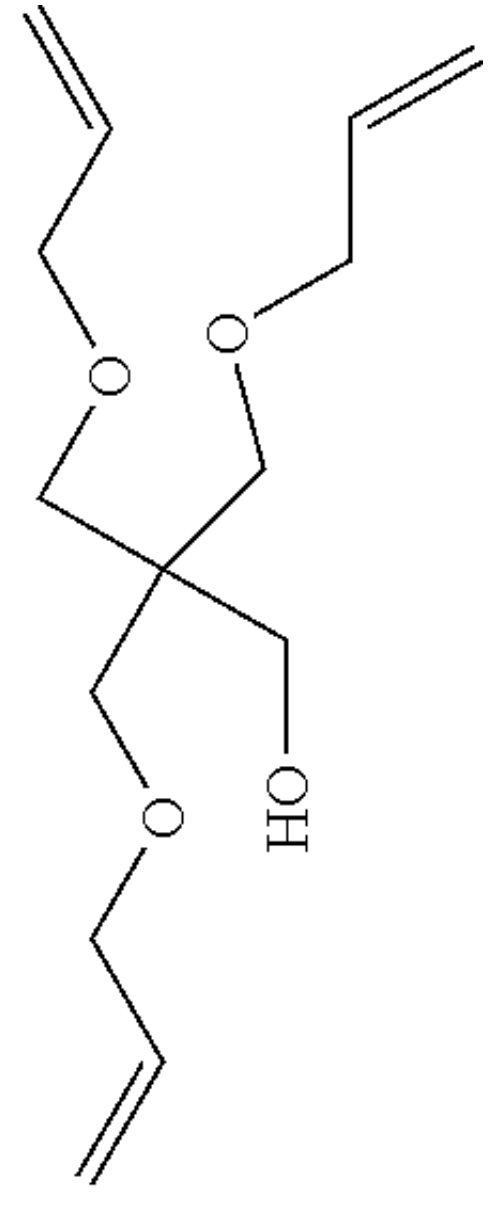
Monomer 1: Pentaerythritol tetrakis(3-mercaptopropionate) (PETMP)

Monomer 2: Pentaerythritol allyl ether (PAE)

Solution: PETMP:PAE (1:1) + Catalyst



PAE



UV Irradiation

Catalyst: 2-Hydroxy-2-methylpropiophenone (HMPP)
Instrument: UV Light (series-model)

Thermal Annealing

Catalyst: Azobisisobutyronitrile (AIBN)
Instrument: Hot Plate (? – model/series)

Optimization Results

Thiol-ene coupling through light-activated and thermal annealing chemistries can both be optimized to keep fabrication/manufacturing processes fairly simple and cost effective.

UV Irradiation Optimized Process:

- UVO cleanse substrates (12 minutes)
- Deposit 180 microliters of PETMP:PAE (1:1) solution at 30 mg/mL concentration
- Spincoat at 1000 rpm for 1 minute and 30 seconds
- Short wave (300 nanometer) Ultraviolet irradiation for 1 minutes

Thermal Annealing Optimized Process:

- UVO cleanse substrates (12 mins)
- Deposit 180 microliters of PETMP:PAE (1:1) solution at 20 mg/mL concentration
- Spincoat at 1000 rpm for 1 minute and 30 seconds
- Thermal anneal on hot plate at 65C for 5 minutes

UV Irradiation

Fabrication Process

- UVO cleanse – 12 mins
- Deposit 180 microliters of solution
- Spincoat 1000 rpm for 1:30 mins
- UV irradiation (Short wave/Long wave)
- Chloroform (CHCl₃) rinse

Solution Formula

PETMP:PAE (1:1)* with HMPP 5% wt

*1:1 by functional groups

Polymer Concentration: 100mg/mL

PETMP: 176.47 mg

PAE: 123.35 mg

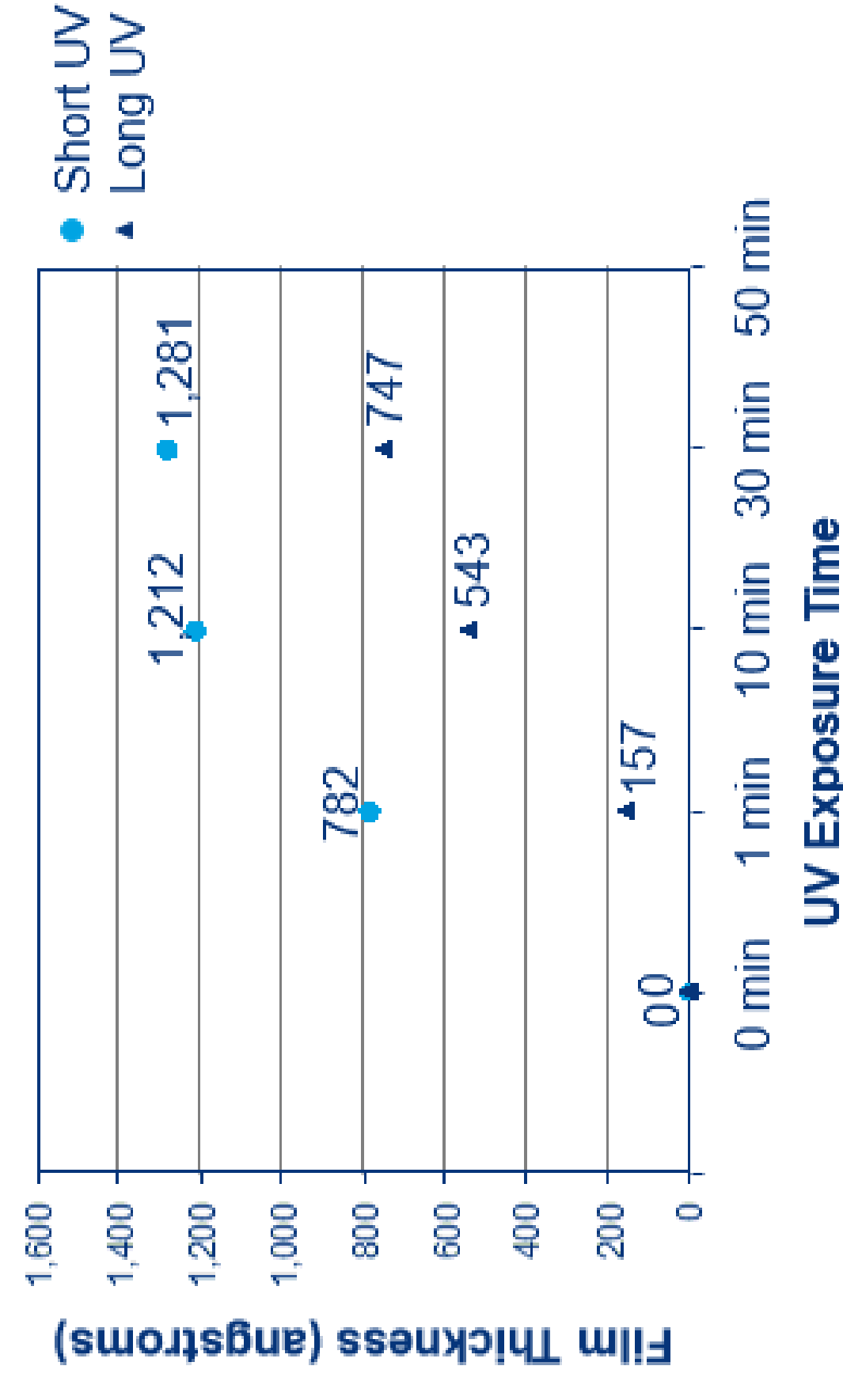
HMPP: 15 mg

Chlorobenzene: 3mL

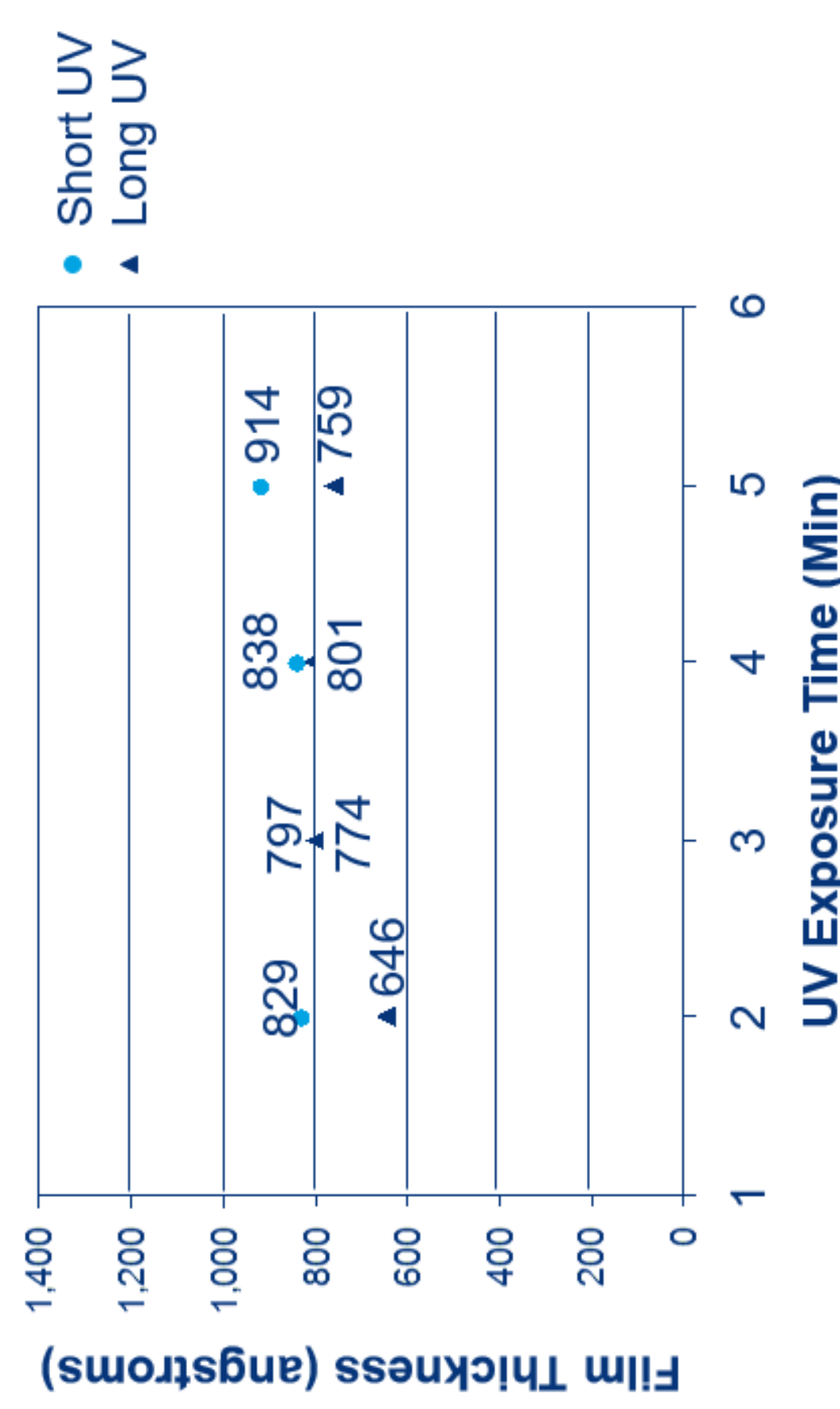
Profilometry

ChR NanoFab Profilometer used to measure Polymer network film thickness

PETMP:PAE (1:1) 30 mg/ml



PETMP:PAE (1:1) 30 mg/ml



Thermal Annealing

Fabrication Process

- UVO cleanse – 12 mins
- Deposit 180 microliters of solution
- Spincoat 1000 rpm for 1:30 mins
- Thermal anneal on hot plate at:
 - 65C
 - 85C
 - 150C
- Chloroform (CHCl₃) rinse

Solution Formula

PETMP:PAE (1:1)* with AIBN 1% wt

*1:1 by functional groups

Polymer Concentration: 100mg/mL

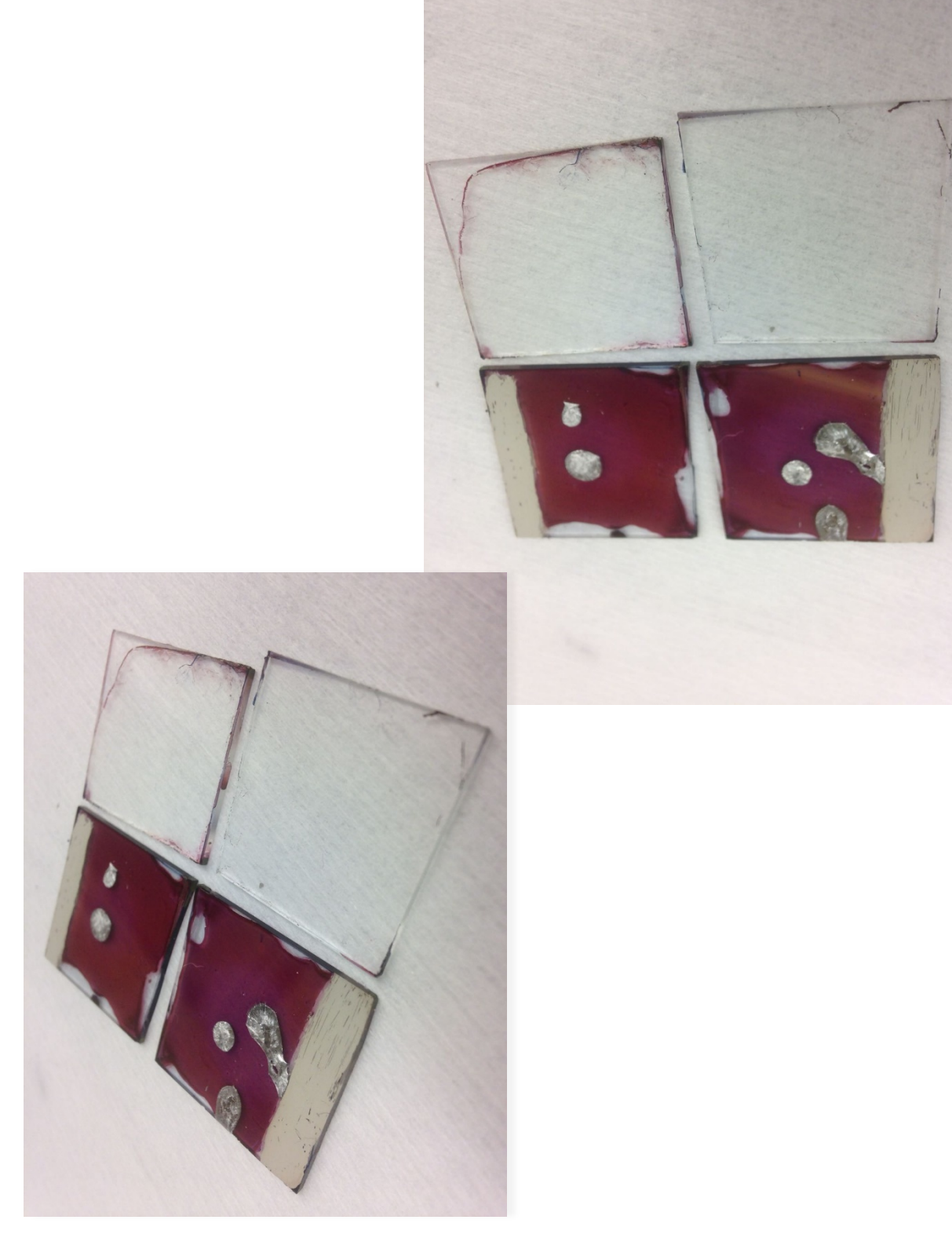
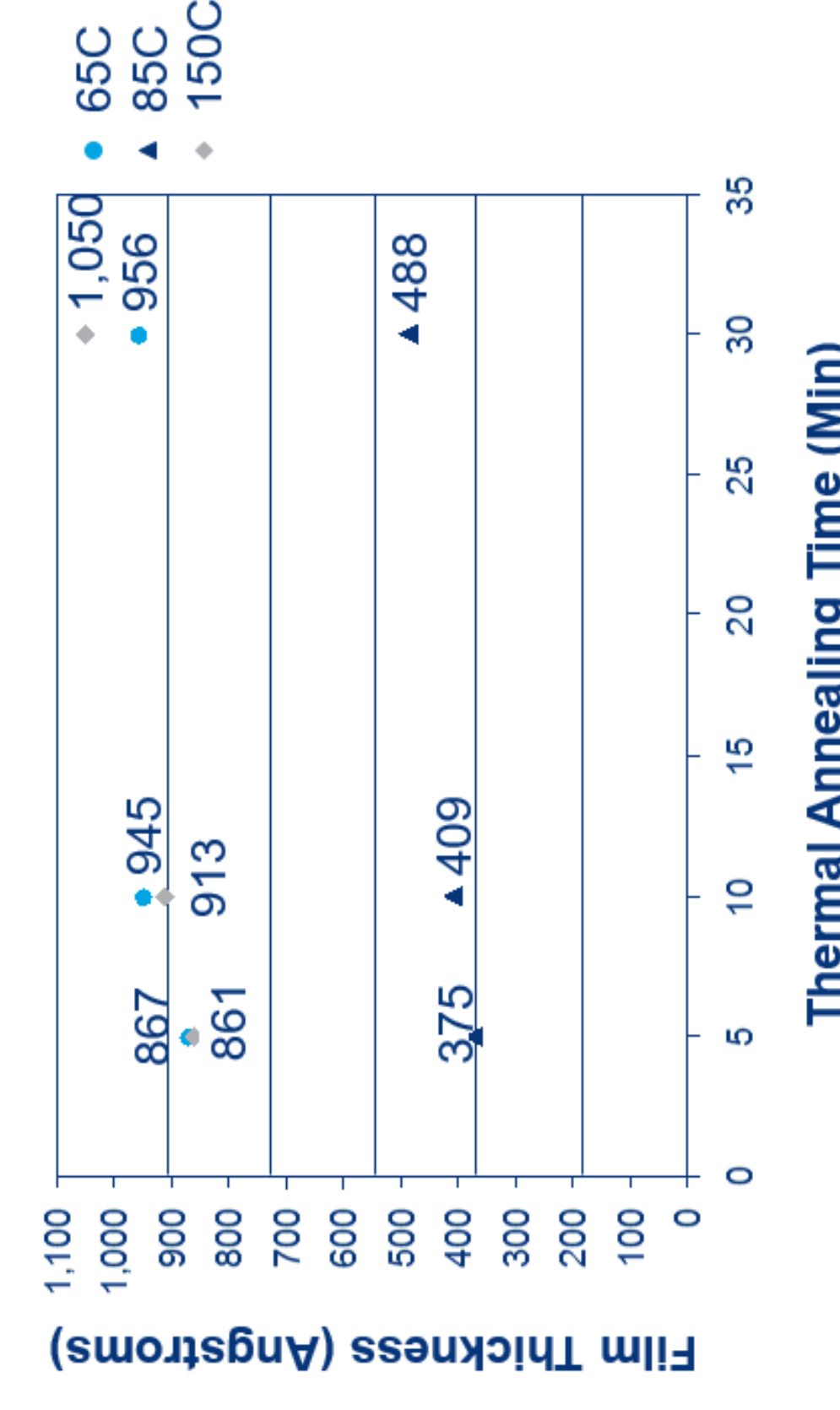
PETMP: 176.47 mg

PAE: 123.35 mg

AIBN: 3 mg

Chlorobenzene: 3mL

PETMP:PAE (1:1) 30 mg/ml



Future Work

- Test mechanical properties of thiol-ene network polymers to determine flexibility.
- Incorporating thiol-ene coupled polymers to OPV devices and testing efficiencies.

Acknowledgements

I would like to thank the National Science Foundation Division of Materials Research (DMR 1460564) and Mr. Bartlett Sheinberg for selecting me to be a part of the Research Experiences and Exploration in Materials Sciences group. I would also like to thank my mentor, Jorge Wu Mok, and Dr. Rafael Verduzco for providing direction and guidance throughout the research experience.

References

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- Hoyle, Charles E. and Bowman, Christopher N. (2010), Thiol-Ene Click Chemistry. *Angewandte Chemie International Edition*, 49: 1540–1573. doi:10.1002/anie.200903924

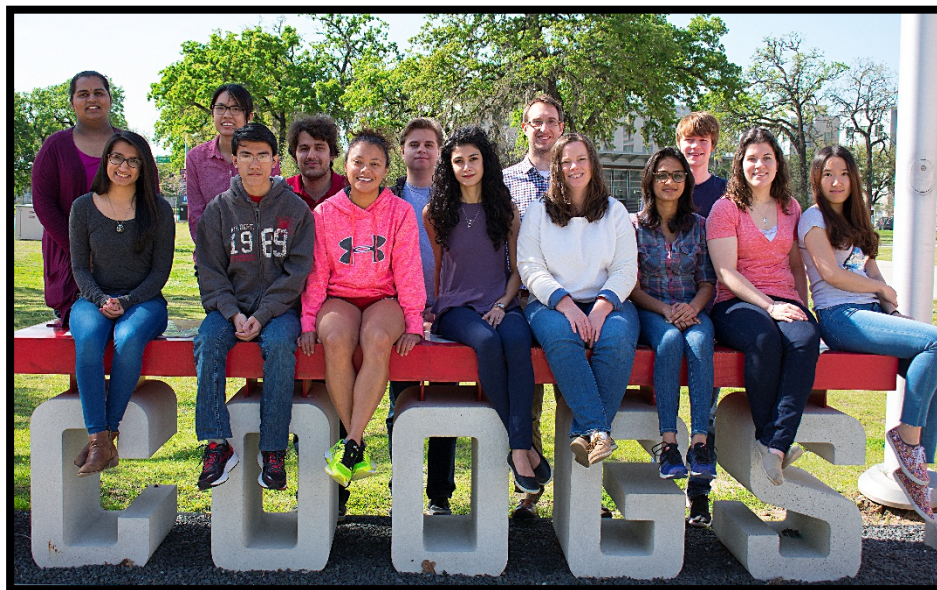
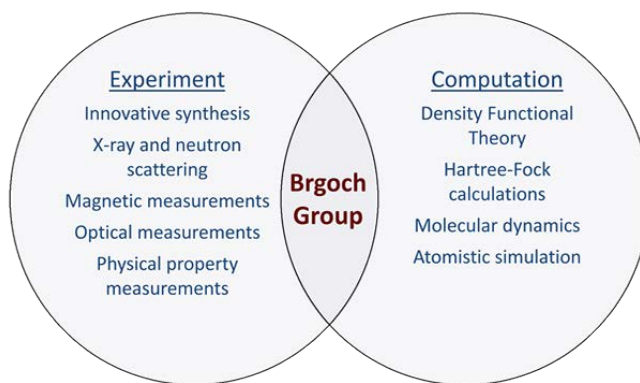
2017 REEMS Research Faculty

Dr. Jakoah Brgoch, Department of Chemistry, University of Houston

<http://jbrgoch.chem.uh.edu/>

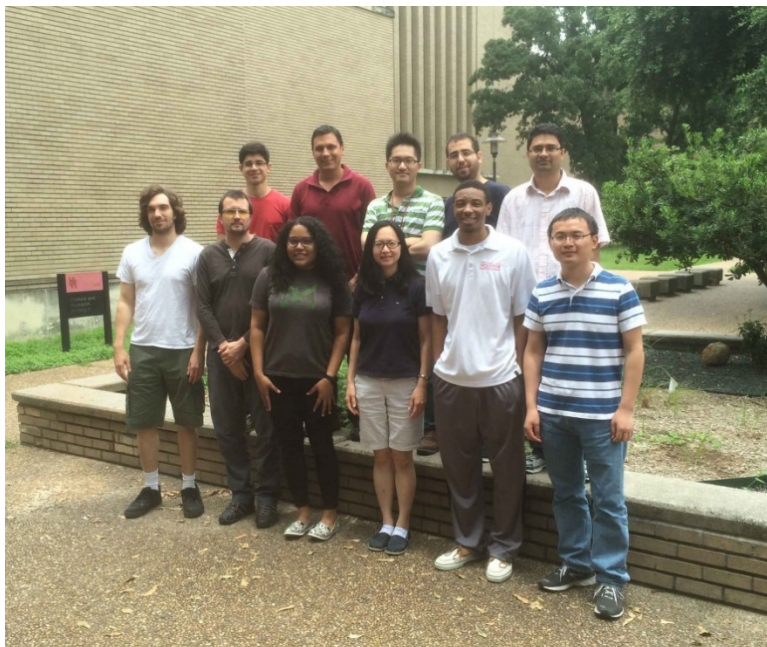
REEMS REU Students: Gelareh Nobakht and Zeshan Rizvi

Students in the Brgoch group are experts in inorganic synthetic chemistry, numerous characterization techniques, and computational chemistry methods. Connecting these research approaches allows the group to solve current problems in a multitude of complex functional inorganic materials.



Front (L-R): Shruti Hariyani, Phu-Cuong Phan, Angelica Cobb, Sogol Lotfi, Erin Finley, Adhessha Danthararayana, Anna Duke, Ya Zhuo *Back (L-R):* Gayatri Viswanathan, Amber Lim, Aria Mansouri, Anton Oliynyk, Jakoah Brgoch, Sean Bailey

Dr. Margaret S. Cheung-Wyker, Department of Physics, University of Houston and Center for Theoretical Biological Physics, Rice University
REEMS REU Student: Frank Kornet



(Left to right). Front row: Jake, Oleg, Lenaya, Dr. Cheung, Rodney, Pengzhi.
Back row: Andrei, Fabio, Victor, Ezzat, Swarnendu.

Theoretical Biological Physics, Soft Condensed Matter, and Clean Energy

<https://mynsm.uh.edu/wiki/projects/cheunggroup>

One of the goals of the Cheung group is to discover interesting macromolecular dynamics under cell-like conditions by applying molecular simulation methods. Cellular milieu is a crowded and concentrated environment that impacts the behavior of macromolecules. It can affect the rate of protein folding, protein association, and even the overall conformational changes that cannot be probed in dilute solutions. Examples of the simulation tools used in our investigations include coarse-grained molecular simulation, all-atomistic molecular simulation, and bioinformatic data-mining to investigate the structural behavior and statistical properties of large biomolecules in cellular milieu. To tackle macromolecular dynamics across multiple orders of magnitude in both space and time, we develop a state-of-the-art multi-scale molecular simulation and the utilization of high-performance computing resources to simulate very large systems efficiently.

Dr. Zachary Cordero, Department of Materials Science and NanoEngineering, Rice University

<https://msne.rice.edu/Content.aspx?id=2147484079>

REEMS REU Students: Andrew Catalanotto and Nathaniel Ocanas



Zachary Cordero

Assistant Professor

Dr. Cordero leads the Additive Lab in the Department of Materials Science and NanoEngineering at Rice University. The Additive Lab has two complementary research thrusts. The first thrust is to develop metal additive manufacturing techniques for printing parts with complex shapes and precisely-controlled microstructures. The second leverages these techniques to probe structure-property relationships in metals.

Dr. Cordero is an assistant professor of Materials Science and NanoEngineering. He earned both his B.S. in Physics and his Ph.D. in Materials Science and Engineering from the Massachusetts Institute of Technology. In between his undergraduate and graduate programs, Dr. Cordero worked at the Lawrence Berkeley National Laboratory, where he was first exposed to powder metallurgy and metals processing. After receiving his PhD, Dr. Cordero spent one year as a post-doctoral fellow at the Manufacturing Demonstration Facility of the Oak Ridge National Laboratory. There, he developed improved process monitoring, quality control, and microstructure design tools for powder-bed, metal additive manufacturing technologies. Dr. Cordero launched the Additive Lab in the Department of Materials Science and NanoEngineering in July 2016.

Dr. James K. Meen, Department of Chemistry and The Texas Center for Superconductivity, University of Houston

<http://www.uh.edu/research/mcf/>

REEMS REU Students: Brenda Arceneaux, Monica Martinez and Brandon Vu.

Materials Characterization Facility of the University of Houston



The Materials Characterization Facility (MCF) is housed in the Houston's Science Center (HSC) building of the University of Houston's Main Campus. We are part of the [Texas Center for Superconductivity of the University of Houston \(TcSUH\)](#). We specialize in **micro-chemical/structural characterization of solid state materials by x-ray and electron beam techniques.**

Areas of active research include:

- Conduct Phase Equilibria Studies on Systems Related to High Temperature Superconductors (HTS) Materials.
- Development of High Temperature and High Pressure Experiments for Synthesizing Materials.
- Development of the Analytical Capabilities of Electron Beam Instruments.
- Conduct Studies in Petrology and Geochemistry (mainly igneous systems)

Dr. Megan Robertson, Department of Chemical and Biomolecular Engineering, University of Houston <http://robertsongroup.chee.uh.edu/>
REEMS REU Student: Kevin Scholtes



**Polymeric Materials
Tailored Structure, Properties, and Function**

The objective of our research group is to develop polymeric materials with enhanced physical properties and function. We specialize in polymer synthetic techniques, structural characterization (small-angle neutron, x-ray and light scattering), thermodynamics and self-assembly, and development of structure-property relationships.

Research projects are focused on the following areas:

Sustainable and biodegradable polymers derived from renewable resources

Advanced materials for wind energy

Structure and dynamics of block copolymer micelles

pH-responsive, antifouling polymer brushes

Multicomponent and multiphase polymer blends

Dr. Laura Smith Callahan, PH.D., Neurosurgery & Center for Stem Cell and Regenerative Medicine

<https://med.uth.edu/neurosurgery/smith-callahan-lab/>

REEMS REU Students: Yasaman Adel and Tasmia Nadeem



The Smith Callahan Laboratory focuses on the developing tissue engineering approaches toward clinical treatments for spinal cord injury, traumatic brain injury and cartilage defects using an interdisciplinary approach involving techniques from cell, molecular, and stem cell biology, chemistry, and material science. Utilizing engineering approaches, the laboratory seeks to optimize scaffold design and the expansion of clinically relevant cell sources.

An Assistant Professor in the Department of Neurosurgery, [Dr. Smith Callahan](#) earned her doctorate in Biomedical Engineering from the University of Michigan, where her work under focused on the effects of nanofibrous scaffolding on the osteogenic differentiation of embryonic stem cells. Upon completion of her thesis, she was awarded a post-doctoral fellowship on the Regenerative Science T90 training grant which allowed her to further study the effects of nanofibrous scaffolding on the neural differentiation of embryonic stem cells. To obtain additional training in peptide and polymer chemistry and soft material characterization, Dr. Smith Callahan transitioned to a post-doctoral position at the Institute of Polymer Science at the University of Akron with Matthew L. Becker. At the University of Akron, her work focused on the effects of bioactive peptides and gradient hydrogels on stem cell differentiation to mesenchymal and neuronal lineages

CURRENT PROJECTS

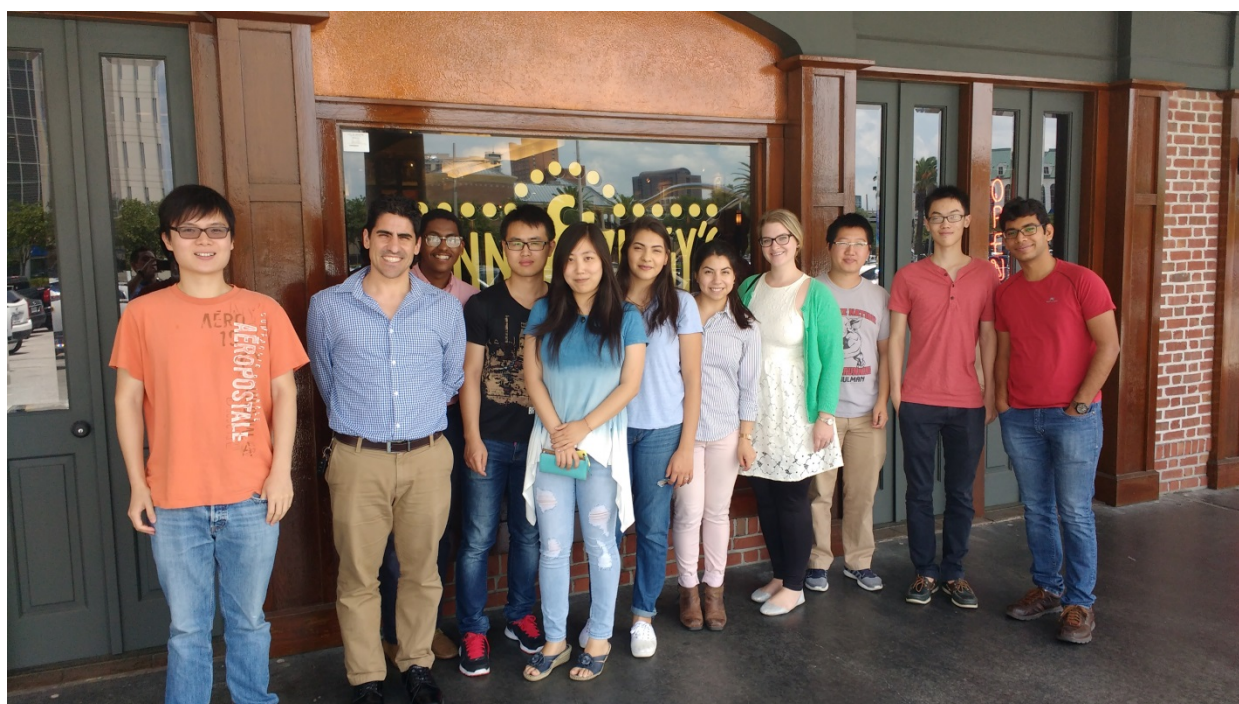
- 1) Development of multi-component scaffolds to facilitate tissue regeneration through better replication of the native extracellular matrix.
- 2) Optimization of culture surfaces for the differentiation of human induced pluripotent stem cells to neural stem cells and oligodendrocyte progenitor cells.
- 3) Identification of optimal artificial matrix properties such as bioactive signaling moiety concentration or mechanical properties using combinatorial approaches.
- 4) Synthesis of novel biomaterials for spinal cord, brain, and vertebral disk repair.

Dr. Rafael Verduzco, Department of Chemical and Biomolecular Engineering, Rice University

<http://verduzcolab.blogs.rice.edu/>

REEMS REU Students: Rodrigo Munoz-Zarruk and Joshua Jackson.

The Verduzco laboratory focuses on the development of complex polymeric materials. We take advantage of advanced polymer synthesis techniques and nanoscale characterization tools to design and characterize polymers at multiple length scales. Current areas of interest include all-conjugated block copolymers for photovoltaics, bottlebrush polymers as responsive surface coatings, liquid crystal elastomers for biomedical applications, and polymers for enhanced oil recovery. The unifying theme of this work is engineering materials at the molecular level to achieve a stronger fundamental understanding of material properties.



2017 REEMS REU JUDGING PANEL

Dr. Forrest J. "Jack" Agee



Dr. Forrest J. "Jack" Agee, a member of the Senior Executive Service, is Director of Physics and Electronics, Air Force Office of Scientific Research, Arlington, Va. He is responsible for the \$80 million Air Force basic research program in physics and electronics, assuring the excellence and relevance of a broad research portfolio. His program encompasses hundreds of university grants and supports work of undergraduates and more than 300 graduate students. This work also supports basic research within the Air Force Research Laboratory, industry and overseas. The research includes novel space-craft engineering, semiconductor device research, nanotechnology, electronic sensors,

polarimetry research, gravitometry, lasers, plasmas, high-power radio frequency sources, high-temperature superconductivity engineering, atomic and nuclear physics, space optics, and imaging and opto-electronics. Agee plans, coordinates and executes a research program conducted by scientists in academia, industry and Air Force laboratories. He was appointed to the SES in 1998.

Prior to beginning his career with the Air Force, Dr. Agee worked as a U.S. Navy physicist in acoustics related to silencing submarines. He also worked in low-temperature physics for the U.S. Army at Fort Belvoir, Va. In the 1970s, he joined the Harry Diamond Laboratory in Adelphi, Md. He handled many assignments of increasing scope and responsibility, initially in nuclear electromagnetic pulse hardening and testing for the Safeguard Anti-Ballistic Missile System and for Army tactical systems. As the Technical Director, he led a major, strategic, Defense Nuclear Agency Electromagnetic Pulse Test for the Commander in Chief of Pacific Forces. For three years he managed strategic command, control and communications programs at The BDM Corp., including the Airborne Command Post. In 1982 Dr. Agee became Director of the Aurora Radiation Test Facility that tested the Peacekeeper missile and other systems at the Harry Diamond Laboratory. In the Army's high-power microwaves program, Dr. Agee led research and

development efforts in sources, and in 1990, became Director of the Army program. His efforts led to developing the AN/VLQ-9 and AN/VLQ-10 Shortstop electronic warfare systems during operations Desert Shield and Desert Storm. The Shortstop System protected U.S. forces in Bosnia and now has seven versions, including two that are deployed in Iraq in a counter-IED role. Dr. Agee formed the Joint Directors of Laboratories Panel on Directed-Energy Weapons in 1990, and chaired the panel until 1993. That same year, he began his Air Force career in the Directed-Energy Program at Phillips Laboratory at Kirtland Air Force Base, N.M., where he led the research program in high-power microwave sources.

Dr. Agee's principal fields of interest are in electrical engineering, pulsed power, microwave generation, electromagnetics and superconductivity. In physics, his interests include nuclear physics, plasma physics, semiconductor physics and lasers. He has written or co-written more than 200 publications and inventions in these areas.

EDUCATION

1963 Bachelor of Science in physics, high honors, Clemson University, Clemson, S.C.

1965 Master of Science degree in physics, University of Virginia, Charlottesville

1967 Doctor of Philosophy degree in physics, University of Virginia, Charlottesville

Dr. Andrew Bean



Dr. Bean is Professor in the Department of Neurobiology and Anatomy at UTHealth McGovern Medical School and Associate Dean in the MD Anderson-UT Health Graduate School of Biomedical Sciences (GSBS). His laboratory has been studying the molecular mechanisms of membrane protein sorting and endosomal trafficking for 20 years. The Bean Laboratory has used molecular, biochemical, genetic, and cell biological approaches to make novel discoveries concerning the mechanisms of membrane trafficking events that have contributed to understanding the role of mutations that alter trafficking events in cancer and neurological disease. In the GSBS, Dr. Bean manages student recruiting, orientation, admissions, and career development.

Mr. Zane Marek



Zane Marek graduated from Texas State Technical College in 1992 with a degree in Electronic Engineering Technology. He began working with JEOL USA as a Field Service Engineer in 1992, assigned to semiconductor equipment (SE) solutions. Zane went back to school while working in the Field Application's Group of JEOL's SE division and received a Bachelor of Science in Business/Marketing from the University of Phoenix. He currently has dual responsibilities as JEOL USA's SE Product Manager and Senior Sales Manager for JEOL's Electron Microscopes.

JAMES K. NELSON, JR., PH.D., P.E., C.ENG., F.ASCE



Dr. James K. Nelson received a Bachelor of Civil Engineering degree from the University of Dayton in 1974. He received the Master of Science and Doctor of Philosophy degrees in civil engineering from the University of Houston. During his graduate study, Dr. Nelson specialized in structural engineering. He is a registered professional engineer in three states, a Chartered Engineer in the United Kingdom, and a fellow of the American Society of Civil Engineers. He is also a member of the American Society for Engineering Education and the SAFE Association.

Prior to receiving his Ph.D. in 1983, Dr. Nelson worked as a design engineer in industry and taught as a lecturer at the University of Houston and Texas A&M University at Galveston. In industry he was primarily involved in design of floating and fixed structures for the offshore petroleum industry. After receiving his Ph.D., Dr. Nelson joined the civil engineering faculty at Texas A&M University. He joined the civil engineering faculty at Clemson University in 1989 as Program Director and founder of the Clemson University Graduate Engineering Programs at The Citadel and became Chair of Civil Engineering in 1998. While at Clemson he received the Award for Faculty Excellence.

In July 2002, Dr. Nelson joined the faculty at Western Michigan University as Chair of Civil and Construction Engineering. At Western Michigan he started the civil engineering undergraduate and graduate degree programs and also chaired the Departments of Materials Science and Engineering and Industrial Design. In May 2005 he joined the faculty at The University of Texas at Tyler. At UT Tyler he was the founding chair of the Department of Civil Engineering and instituted the bachelor's and master's degree programs. In 2006 he became the Dean of Engineering. While serving as Dean, enrollments in the college grew over 250 percent. He returned to Texas A&M in January 2016 and currently serves as the Director of Special Academic Initiatives for the Texas A&M University System.

Dr. Nelson's primary technical research interest is the behavior of structural systems. For over 25 years he has been actively involved in evaluating the behavior of free-fall lifeboats and the development of analytical tools to predict that behavior. His research has formed the basis for many of the regulations of the International Maritime Organization for free-fall lifeboat performance. Since 1988, Dr. Nelson has served as a technical advisor to the United States Delegation to the International Maritime

Organization, which is a United Nations Treaty Organization. In that capacity, he is a primary author of the international recommendation for testing free-fall lifeboats and many of the international regulations regarding the launch of free-fall lifeboats. In 1996 Dr. Nelson received the United States Marine Safety Award for accomplishments furthering the cause of safety in the marine field.

He has authored many technical papers that have been presented in national and international forums and co-authored three textbooks. Dr. Nelson chaired a national committee of the American Society of Civil Engineers for curriculum redesign supporting the civil engineering body of knowledge. He is actively engaged in developing strategies for enhancing the STEM education pipeline in Texas and nationally, and has testified before the Texas Senate and House Higher Education Committees in that regard. He chaired the councils for the Texas Higher Education Coordinating Board developing statewide articulation compacts for several engineering and science programs. He chaired the Engineering Field of Study Committee for the Coordinating Board. Dr. Nelson was the primary architect of the UT Tyler Houston Engineering Center through which UT Tyler's engineering programs are available to students in Houston. He also served on the Texas State Board of Education committee preparing the standards for career and technical education. In addition, Dr. Nelson served as the chair of the academic advisory committee for the Texas Board of Registration for Professional Engineers, and chaired the task committee to enhance faculty licensure. He also served as the representative of ASEE on the NCEES Engineering Education Task Force.

George M. Stancel, Ph. D.

Senior Vice President, Academic and Research Affairs, UTHealth



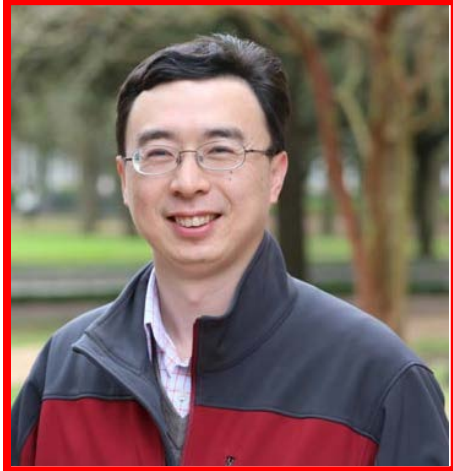
Dr. George M. Stancel currently serves as the Senior Vice President for Academic and Research Affairs at The University of Texas Health Science Center (UTHealth), a position he has held since 2011.

Stancel came to The University of Texas Health Science Center at Houston in 1972 as an assistant professor of Pharmacology at the Medical School. He has assumed many leadership roles before becoming Executive Vice President for Academic and Research Affairs, including president of the Medical School Faculty Senate, president of the Graduate School Faculty, Chairman of the Pharmacology Department at the Medical School, Associate Dean for Education and Research at the Medical School, Executive Vice President for Research of the Health Science Center, Dean of the Graduate School of Biomedical Sciences, and has served on innumerable committees of the Medical School, Graduate School, and Health Science Center. Stancel notes that he has taught every student who has gone through the Medical School here in Houston and has taught at all six UTHealth Schools and MD Anderson during his tenure. He is especially proud of teaching awards he has received. He has also been active in national professional organizations dedicated to biomedical science and medical education. In addition to being the SVP of Academic and Research Affairs, he is currently Professor of Integrative Biology and Pharmacology at the UT Medical School and Professor of Gynecologic Oncology at MD Anderson (adjunct) and continues to teach pharmacology each year to the medical class.

Stancel's training and research programs have received over \$15 million in grants from the National Institutes of Health (NIH) and other sources. His past research has been on the effects of estrogens and related hormones and drugs on the female reproductive system and their role in hormone related cancers although he no longer has his own active research lab since he focuses now on administrative leadership. He has served on a number of research advisory panels and review groups for The National Institutes of Health (NIH) and other professional organizations. He remains actively involved in teaching and research training of graduate students and postdoctoral fellows in UTHealth training programs and those of the Gulf Coast Consortium. He has published over 200 research articles, scientific abstracts, book chapters, and other works.

Stancel was raised in Chicago, and earned a B.S in chemistry from the College of St. Thomas in St. Paul, MN in 1966. He went on to receive a doctorate in biochemistry from Michigan State University in 1970 and did postdoctoral work in physiology at the University of Illinois at Champaign-Urbana for two years. He is married to Mary Lee (Wiepking) Stancel, and they have three children. Mary taught Spanish and English as a Second Language at the high school level for almost 10 years and then taught pre-school at Bellaire United Methodist's School for Little Children for over 30 years where she was selected as the Outstanding Pre-School Teacher of the Year in Houston by the Martel Foundation in 2004. Stancel has been active in scouting and youth sports and his current hobbies include fishing and biking.

Dr. Ming Tang



Dr. Tang is an assistant professor of Materials Science and NanoEngineering at Rice University. He obtained his Ph.D. in Materials Science and Engineering at MIT. Before joining Rice, he worked at the Lawrence Livermore National Laboratory and also Shell Technology Center, Houston. His group is interested in materials phenomena at mesoscale, which bridge between atomistic building blocks and macroscopic properties. Current research topics include microstructure evolution phenomena in energy storage materials, rational design of microstructure in battery electrodes, morphological evolution and control during 2D materials growth and selfassembly process in emulsion systems. Dr. Tang is planning to join the REEMS REU program in the spring of 2018.

Mr. John Vasselli



John J. Vasselli is the Dean of the Houston Community College Engineering Center of Excellence. He possesses over forty years of engineering experience ranging from the Federal research environment, through large corporations, to starting and owning his own engineering businesses. John's career as a scientist, researcher, product developer, and serial entrepreneur gives him a full-spectrum understanding of how to turn a new idea into a global corporation. Three of the companies that John led grew to over \$100M/year in annual sales. He holds several patents, and degrees in electrical, biomedical and systems engineering.

PROFESSIONAL SUMMARY

- Houston Community College System – Dean, Engineering Center of Excellence
- University of Texas – Director, Houston Engineering Center and Executive Director of TxAIRE Research Institute
- Carrier Corp. – Chief of Technology for Indoor Air Quality & Global Technology Fellow
- Syracuse Center of Excellence for Environmental and Energy Systems – Exec. VP
- Green Star Technologies – Founder & President
- Houston Advanced Research Center - President & CEO
- Syracuse Research Corporation, Director of Corporate Development
- Science Applications International Corporation – Corp. Vice President
- Farmers Mills Technologies – Founder & President
- Air Force Research Laboratory & DARPA Program Manager – Sr. Research Engineer
- United States Air Force – Captain

Dr. Marendra A. Wilson- Pham, Ph. D.



Assistant Dean, Diversity and Alumni Affairs
The University of Texas MD Anderson Cancer Center
UTHealth Graduate School of Biomedical Sciences

Dr. Wilson-Pham received her BS in Biology at Dillard University in 2002 and her PhD in Microbiology and Molecular Genetics at The MD Anderson UTHealth Graduate School of Biomedical Sciences (GSBS) in 2007 in the laboratory of Dr. Ambro vanHoof. Her research addressed the understanding the molecular mechanisms of nonstop mRNA metabolism. Following her doctoral research, she accepted her first postdoctoral fellowship in the Biochemistry and Molecular Biology Department at The

UT MD Anderson Cancer Center in the laboratory of Dr. Sharon Y.R. Dent. Her research was focused on understanding how histone modifying complexes regulate gene expression. Her second postdoctoral fellowship, in the Molecular and Human Genetics Department at Baylor College of Medicine in the laboratory of Dr. Grzegorz Ira, was focused on the role of DNA double-strand breaks and repair in the maintenance of genome stability.

She joined the GSBS Deans' Office in 2013 to assist in improving the recruitment and retention rates of underrepresented minority students. She is involved in yearly recruitment activities through attendance of conferences and institutions that serve large populations of minority students. Her retention efforts are focused on providing educational and community support to currently enrolled minority students at the GSBS through monthly lunch-and-learn seminars, workshops and mentorship support. She oversees support to all student organizations and alumni networking initiatives of the graduate school.

REEMS & West Houston Center for Science & Engineering Staff

Mr. Bartlett (Bart) Sheinberg



REEMS Principal Investigator & Center Director,
West Houston Center for Science & Engineering

Mrs. Mary Beth Hurd



REEMS Administrator

REEMS & West Houston Center for Science & Engineering Staff

Dr. Yibrán Perera Mercado



REEMS Program Manager

Dr. Gizelle Davis



HCC Biology Faculty
REEMS Student Mentor

Dr. Amanda Hackler



REEMS External Evaluator

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Faculty Fellow in Chemistry,
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Dr. Alan J. Jacobson, Ph.D.



Director, Texas Center for Superconductivity
University of Houston

Mr. Robert K. (Bob) Ehrmann



Managing Director
Pennsylvania State Center for
Nanotechnology Education &
Utilization