

Materials Design Workshop Report
CHiMaD Headquarters: Northwestern University

Organizing Committee

Professor G. B. Olson (Northwestern University)

Dr. Emine Begum Gulsoy (Northwestern University)

Dr. Ricardo K. Komai (Northwestern University)

Dr. Wei Xiong (Northwestern University)

Significance

Developing Systems Design Charts for each Use-Case Group will facilitate collaboration as this framework can be applied to any material system. These serve as a method to identify and direct research strengths and goals. The workshop also further connected researchers from each Use-Case Group to interact with one another and learn about each other's research progress.

Goals

Short-Term goals:

1. Develop a Material Summary for each Use-Case Group/Project
2. Develop a Systems Design Chart for each Use-Case Group/Project
3. Use these tools to identify strengths and weaknesses of current CHiMaD research
4. Identify attendees' roles in the design and development of their material

Long-Term Goals:

1. Inform and educate attendees on the complete picture of their material systems with tools, models, or experiments
2. Build and refine the Systems Design Chart to assess and evaluate the research direction of each Use-Case Group/Project

Results *(see attached)*

Achievements

Strengthen materials design knowledge with postdocs and students. Systems Design Charts were developed for each Use-Case Group. Some possible future collaborations between Use-Case Groups were identified. Quarterly meetings will serve as opportunities to update the entire CHiMaD community regarding progress in research.

Acknowledgements

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Attendees

Name	Organization	Use-Case Group
Pavan Kolluru	Northwestern University	Polymer Matrix Materials
Xiaolin Li	Northwestern University	Polymer Matrix Materials
Hadallia Bergeron	Northwestern University	Low-dimensional Nanoelectronic Materials
Xiaochen Ren	Northwestern University	Low-dimensional Nanoelectronic Materials
Cameron Gross	Northwestern University	Precipitation-Strengthened Alloys
Orion Kafka	Northwestern University	Precipitation-Strengthened Alloys
Shahab Nahavi	Northwestern University	Precipitation-Strengthened Alloys
Daniel Souza	Northwestern University	Precipitation-Strengthened Alloys
Zequn Wang	Northwestern University	Precipitation-Strengthened Alloys
Cheng Yu	Northwestern University	Precipitation-Strengthened Alloys
Matt Peters	Northwestern University	In-Situ Si-Composite Materials
Jiaxing Ren	University of Chicago	Directed Self-Assembly of Block Co-polymer Films for Lithographic Applications
Samanvaya Srivastava	University of Chicago	Soft Matter Design based on Charge Complexation
Lu Li	University of Chicago	Soft Matter Design based on Charge Complexation
Matthew Goldey	University of Chicago	Organic Bulk Heterojunction Polymer Solar Cells
Alex Schneider	University of Chicago	Organic Bulk Heterojunction Polymer Solar Cells
Qinghe Wu	University of Chicago	Organic Bulk Heterojunction Polymer Solar Cells
Tianyue Zheng	University of Chicago	Organic Bulk Heterojunction Polymer Solar Cells
Alona Furmanchuk	Northwestern University	Data Mining
Vinay Hegde	Northwestern University	Data Mining
Qiao Kang	Northwestern University	Data Mining
Amar Krishna	Northwestern University	Data Mining
Ruoqian (Rosanne) Liu	Northwestern University	Data Mining
Arindam Paul	Northwestern University	Data Mining
Yichi Zhang	Northwestern University	Data Mining
Logan Ward	Northwestern University	Data Mining
Narut Sereewattanawoot	Northwestern University	Phase Field
Dr. Ida Berglund	QuesTek Innovations, LLC	
Dr. Jifeng Zhao	QuesTek Innovations, LLC	
Prof. G.B. Olson	Northwestern University	
Dr. Emine Begum Gulsoy	Northwestern University	
Dr. Ricardo K. Komai	Northwestern University	
Dr. Wei Xiong	Northwestern University	

Agenda



Agenda

CHiMaD Materials Design Workshop

*CHiMaD Headquarters, Hogan Building, Suite 1160
2205 Tech Drive, Evanston, IL, 60208*

September 24, 2015 (Thursday)

- | | |
|-------------------------|--|
| 09:00am | Welcome & Breakfast |
| 09:30am | Materials Genome: The First Half Century
<i>Greg Olson</i> |
| 11:00am | Development of Systems Design Charts for Materials Design
<i>Ricardo Komai</i> |
| 12:00pm | Lunch |
| 12:30pm – 5:00pm | Building Systems Design Charts |

September 25, 2015 (Friday)

- | | |
|-----------------------|--|
| 09:00am | Breakfast |
| 09:15am | Cybermetals Innovation: Application of Systems Design Chart
<i>Wei Xiong</i> |
| 10:00am | Presentation of System Design Charts & Discussion |
| 12:00pm | Lunch |
| 12:30pm 4:00pm | Presentation of System Design Charts & Discussion |

Coffee & snack station at CHiMaD headquarters will be available all day.

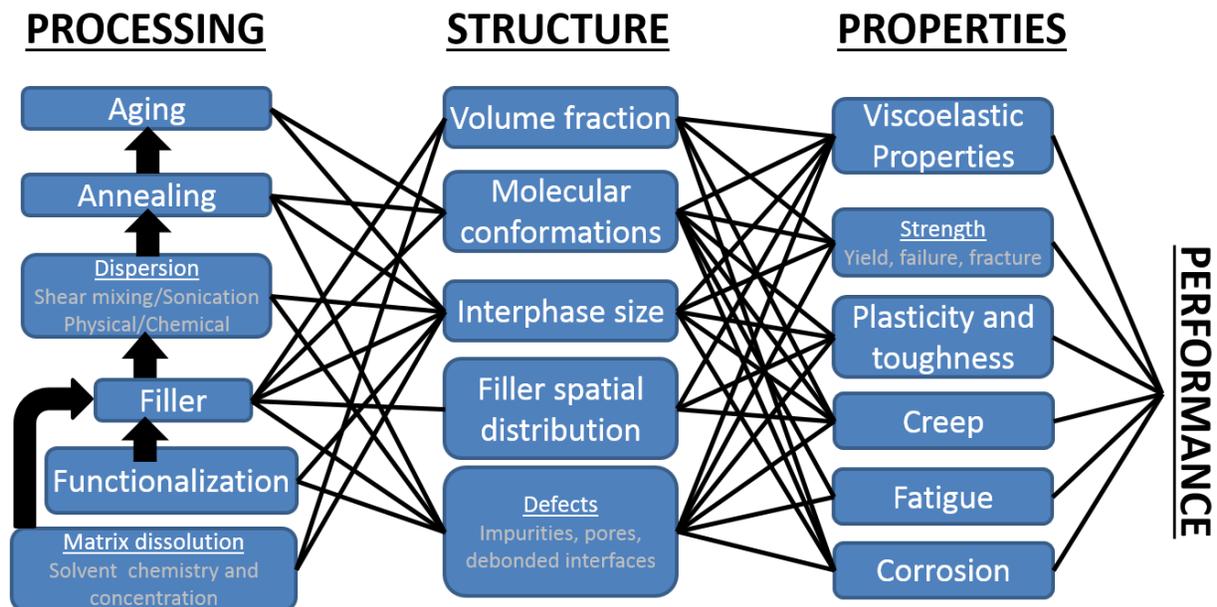
Polymer Matrix Materials

Participants:

Pavan Kolluru (NU, Brinson)

MATERIAL SUMMARY:

In polymer matrix composites, the molecular chains in the vicinity of the filler phase are spatially restricted from taking up their natural/unrestricted conformations and achieving their bulk-like mobility owing to the physical presence of the filler phase. Additionally any chemical interactions arising from the chemical functionalization of the filler surfaces, used to achieve better bonding and/or dispersion, also result in such spatial restrictions). These conditions result in a gradual transition of physical and functional properties between the filler and the matrix phases over a length scale, l , which often referred to as the 'interphase' between the filler and matrix 'phases'. The hypothesis of such an interphase has been further strengthened, in polymer nanocomposites, wherein by the discord between the experimentally observed mechanical properties cannot be explained without invoking models having a tertiary (graded) phase. A multitude of physical and chemical properties at the interface between a polymer and the filler phases can be envisaged to control the interphase structure and behavior. Identifying these fundamental characteristics by using local AFM-based mechanical experiments, and following-up with subsequent data mining analysis is expected to provide a comprehensive data-maps describing the structure-property relationships in a polymer interphase.



Low-Dimensional Nanoelectronic Materials

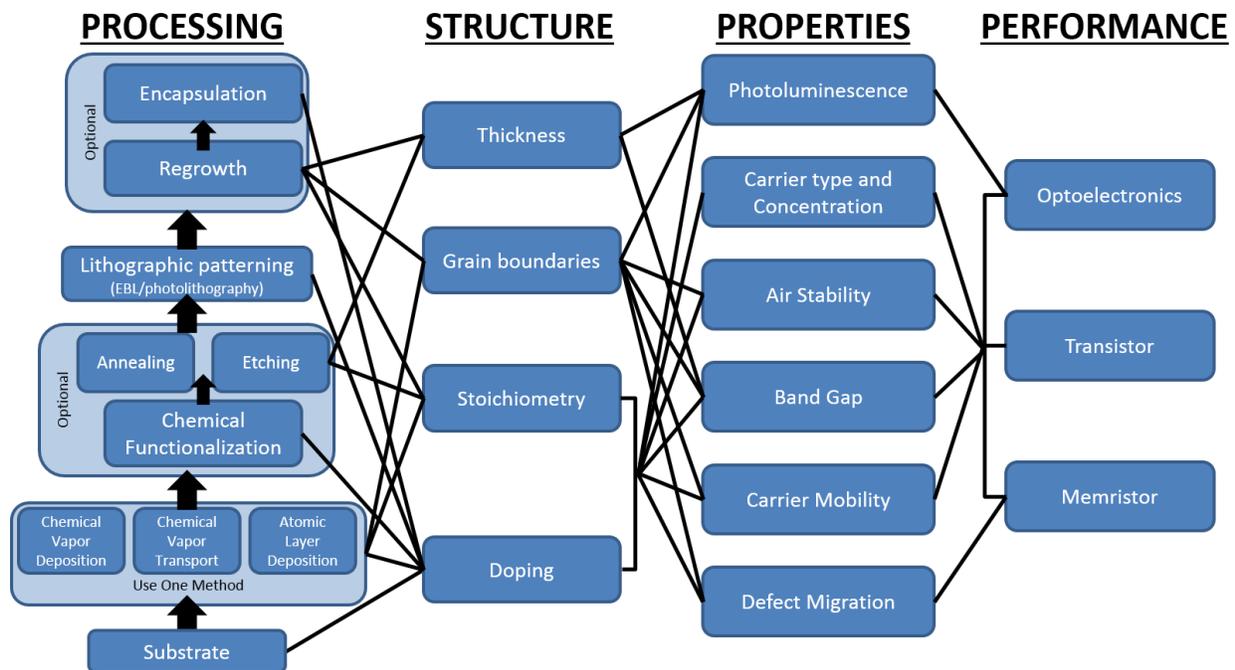
Participants:

Hadallia Bergeron (NU, Hersam)

Xiaochen Ren (NU, Lauhon)

MATERIAL SUMMARY:

Molybdenum disulfide (MoS_2), a transition metal dichalcogenide (TMD) van der Waals solid, can be synthesized in monolayer form via chemical vapor deposition (CVD). An emerging nanoelectronic device and fundamental circuit element, the memristor, was recently realized with gate-tunable properties using monolayer CVD grown MoS_2 . In particular, the memristive behavior of the MoS_2 devices is tied to the stoichiometry of the material and the hysteretic migration of defects such as grain boundaries and sulfur vacancies across the device channel. The performance of the MoS_2 memristor is characterized by the switching state set voltage, switching ratio, conductance of the switching states, and the presence of a pinched resistive loop and negative differential resistance regime. The CVD parameters that affect the stoichiometry of the resulting MoS_2 as well as its crystal domain size and density include the growth pressure, peak temperature, temperature ramping rate, and precursor amount. Post-growth processing methods such as thermal annealing and plasma etching can also be used to induce sulfur vacancies. The role of grain boundary geometry and migration in the MoS_2 memristor can be investigated via the process of re-growth, wherein a second cycle of CVD-grown MoS_2 is nucleated from previously deposited CVD MoS_2 domains. The boundary between the first and second cycle is controlled by tuning the first and second cycle growth parameters. This method can be expanded via photolithographic patterning of the CVD-grown MoS_2 seeds for predictable grain boundary position and geometries upon regrowth, enabling greater control over the memristive mechanism in CVD MoS_2 devices.



Precipitation-Strengthened Alloys

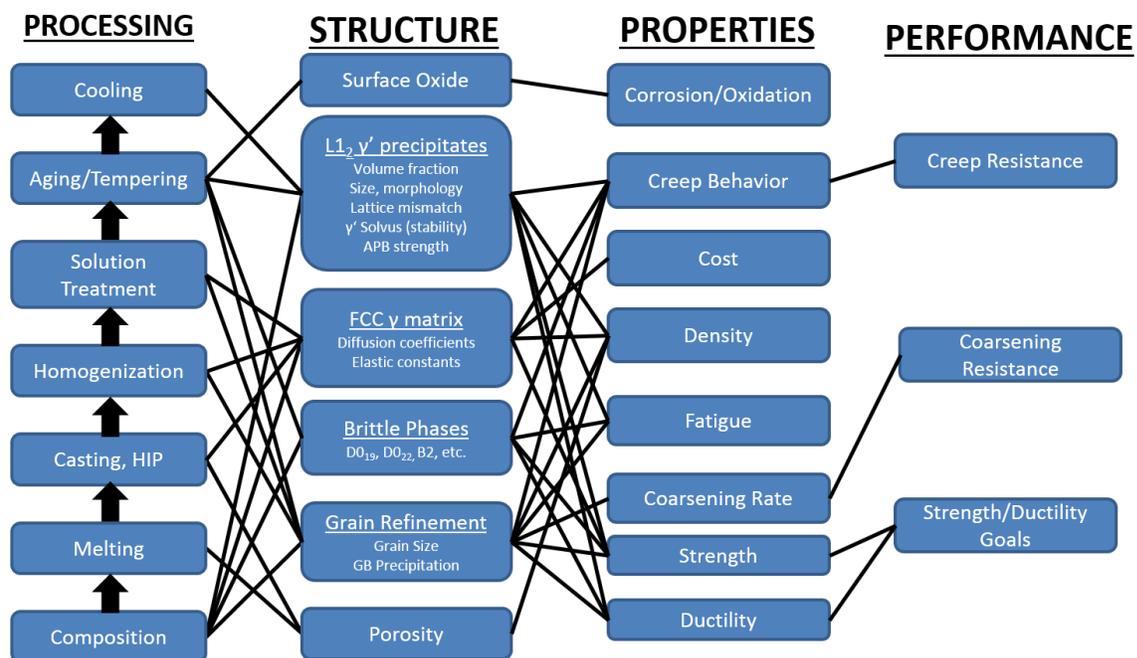
Participants:

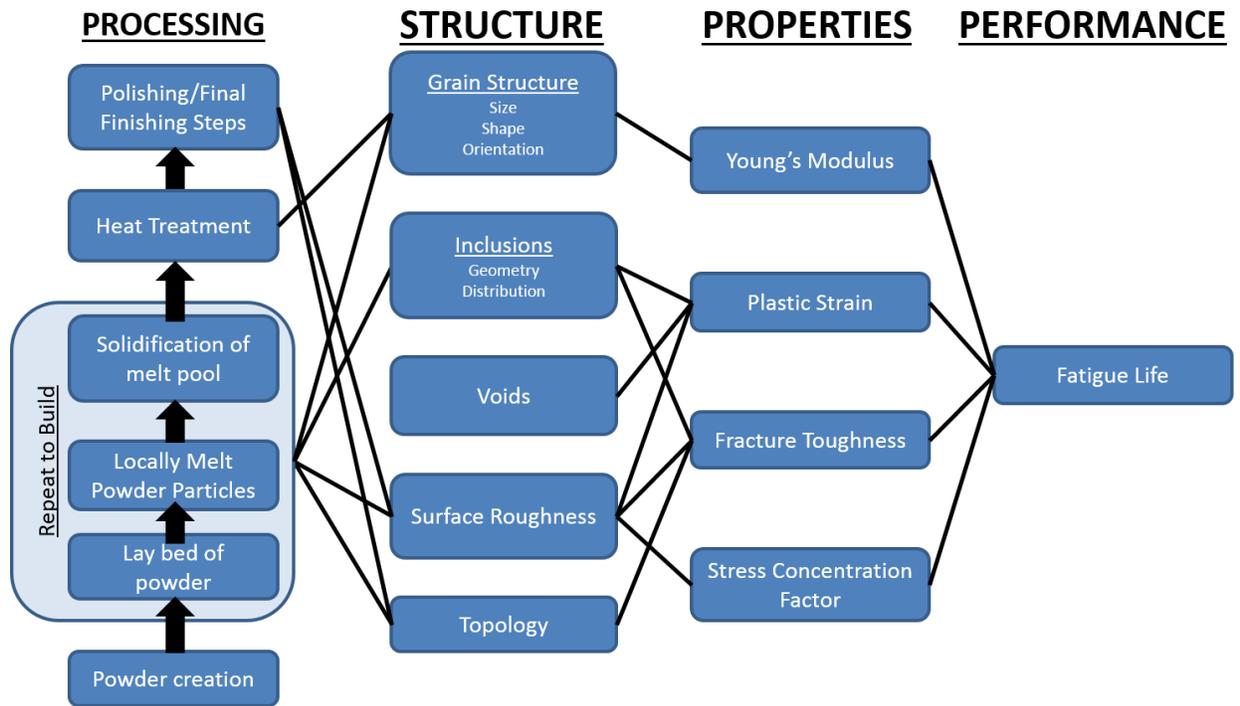
- Cameron Gross (NU, Chung)
- Vinay Hegde (NU, Wolverton)
- Orion Kafka (NU, Liu)
- Shahab Naghavi (NU, Wolverton)
- Daniel Sauza (NU, Dunand/Seidman)

Cobalt Superalloys

MATERIAL SUMMARY:

Cast Co-base superalloys are initially melted using a process such as plasma-arc melting or vacuum induction melting. Melting is typically repeated several times in order to promote homogeneity of the constituent elements before final casting. In the case of single-crystal specimens, directional solidification is employed to ensure the predominance of a single crystallographic orientation throughout the cast component. Hot isostatic pressing (HIP) densifies the casting, removing internal porosity. The alloy is then subjected to a homogenization treatment to mitigate elemental segregation or phases formed as a result of the HIP cycle. Solution treatment at a temperature above the γ' solvus promotes a single-phase f.c.c. γ matrix, in which γ' precipitates begin to nucleate upon cooling. The alloy composition can be chosen to tune the coarsening rate of the γ' precipitates. If the selected alloy composition is prone to quench-cracking, a cooling rate must be selected such that cracking can be avoided. The subsequent temper conditions (aging time and temperature) are directly linked to the resulting size distribution and volume fraction of the strengthening γ' precipitates, which in turn affect the mechanical properties of interest: creep resistance, ductility, and tensile strength at ambient and elevated temperatures. The tempering step also introduces surface oxides that provide corrosion resistance. The size of grains and formation of grain boundary phases such as borides may also be induced during cooling from solution and the subsequent tempering step; if controlled properly, these phases can also be beneficial to mechanical performance. A composition or temper outside of the two-phase $\gamma + \gamma'$ phase field may result in the nucleation and growth of deleterious topologically close packed (TCP) phases, which drastically reduce performance - these phases should be avoided.



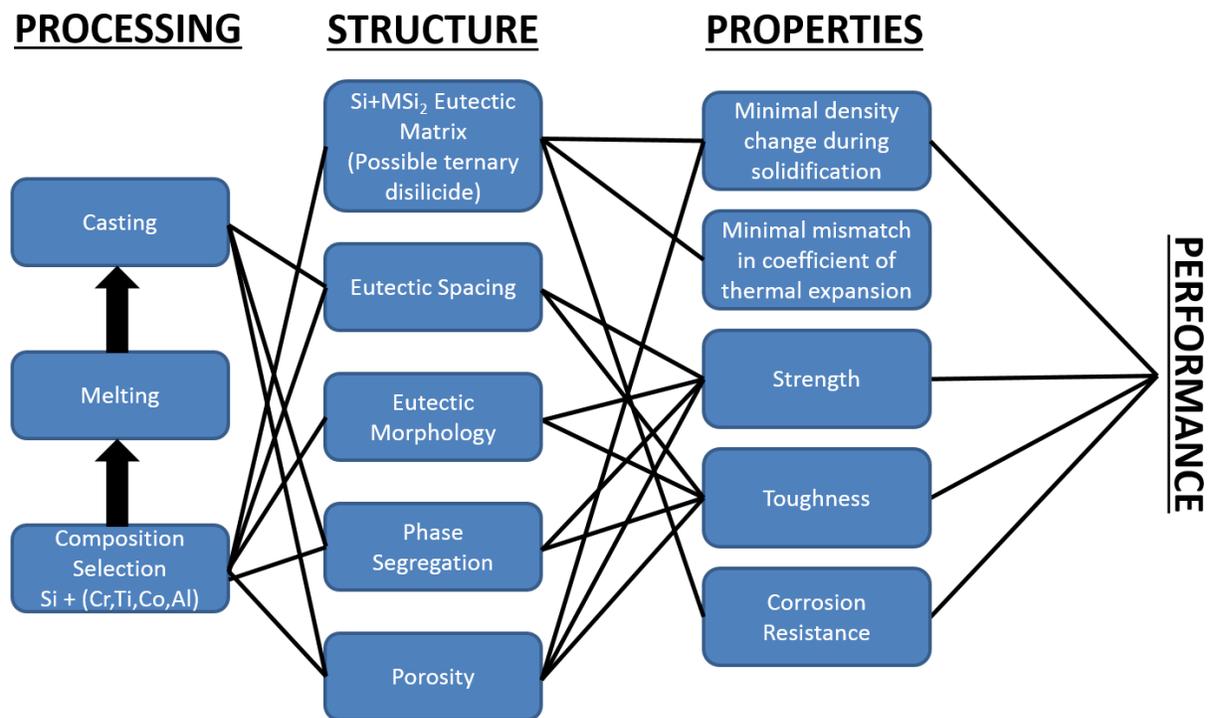


In-Situ Si-Composite Materials

Participants:
Matt Peters (NU, Voorhees)

MATERIAL SUMMARY:

Our team's goal is to design a castable silicon based *in situ* composite of eutectic Si and CrSi₂ that is both strong and has a toughness in the range of 4-6 MPa m^{1/2}. This material has enhanced toughness from pure Si due to crack deflection and bridging mechanisms that occur at the two-phase interface. The toughness can be further increased by decreasing the eutectic spacing of the silicon matrix and reinforcing disilicide. The casting process involves both thermodynamic and kinetic effects of the system, therefore, a complete description of the thermodynamics of the system is a necessity. This is best done through the CALPHAD method, which uses experimental and first principle calculations to create semi-empirical thermodynamic models for the phases involved. In addition, a kinetic model for the eutectic growth must also be created that is based on a modified Jackson-Hunt theory. By having a complete understanding of the kinetic and thermodynamic factors of the system, material selection and processing parameters can be fine tuned to create a fully optimized material. Several issues keep this from being an easy problem and include the drastic change in density as silicon freezes, the faceted microstructure and the morphology being highly sensitive to impurities in the melt.



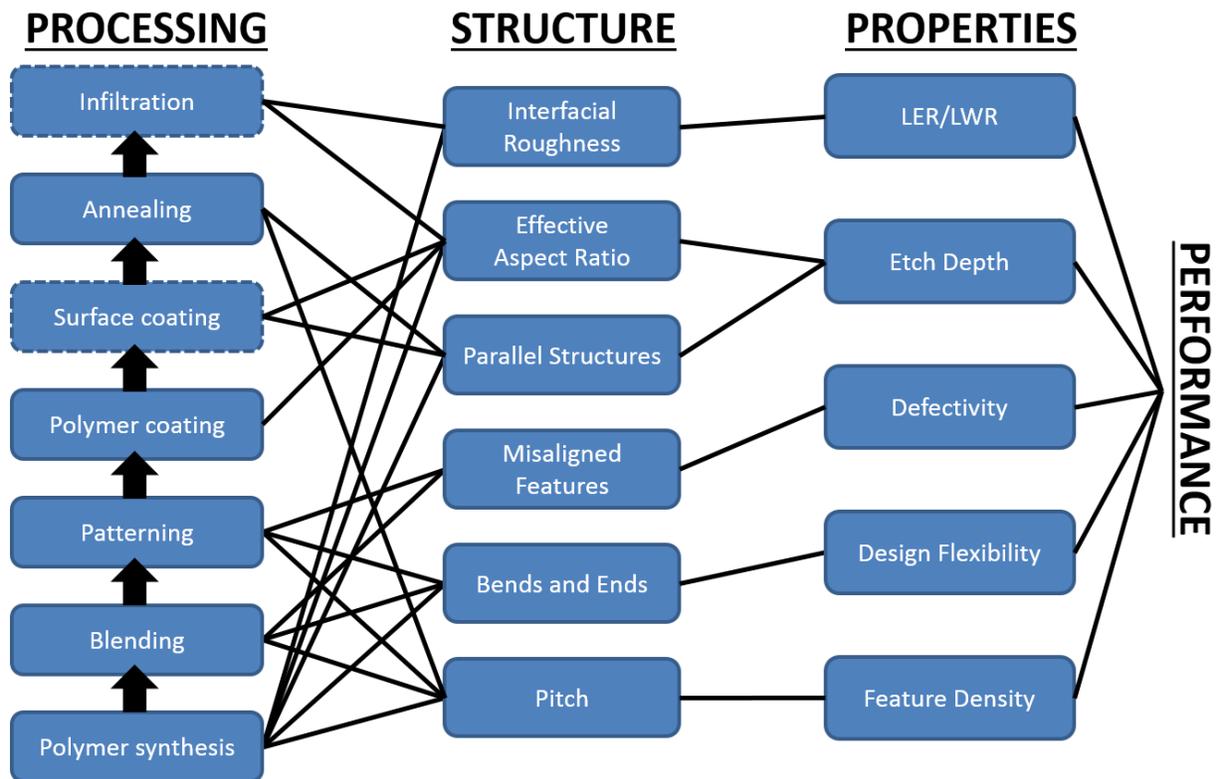
Directed Self-Assembly of Block Co-polymer Films for Lithographic Applications

Participants

Jiaying Ren (UC, Nealey)

MATERIAL SUMMARY:

Block copolymers self-assemble into periodic structures at the nanometer length scale. The assembly can be directed by lithographically defined patterns with chemical contrast to achieve levels of perfection and pattern complexity that enable the next generation nanomanufacturing. The pattern consists of guide stripes that preferentially wet one block of the polymer and background regions that can wet both blocks. The pitch of the guide stripes is an integer multiple of the natural periodicity of the block copolymer so during thermal annealing the polymer spontaneously assembles following the guide stripes and multiplies the density of features. The quality of registration and the morphology of the polymer is determined by the geometric parameters, i.e. pitch and width of the guide stripes, as well as the chemical parameters of the underlying pattern, i.e. composition of the guide stripe and background regions. When pattern parameters differ from the optimal conditions, misaligned defects and complex three dimensional morphologies could form throughout the film thickness and are often not visible from top down SEM imaging. Three dimensional characterization methods such as TEM tomography and X-ray scattering are developed to reveal and understand these structures.

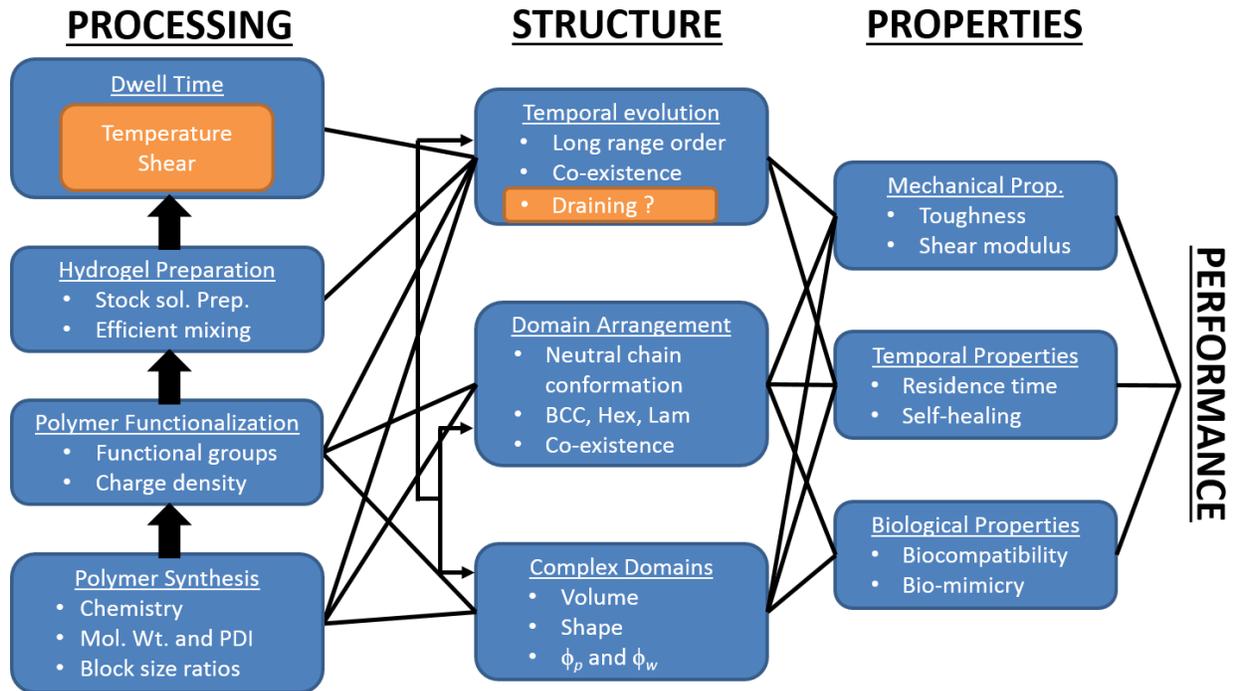


Soft Matter Design based on Charge Complexation

Participants

S. Srivastava (UC, Tirrell)

Lu Li (UC, Tirrell)



Organic Bulk Heterojunction Polymer Solar Cells

Participants:

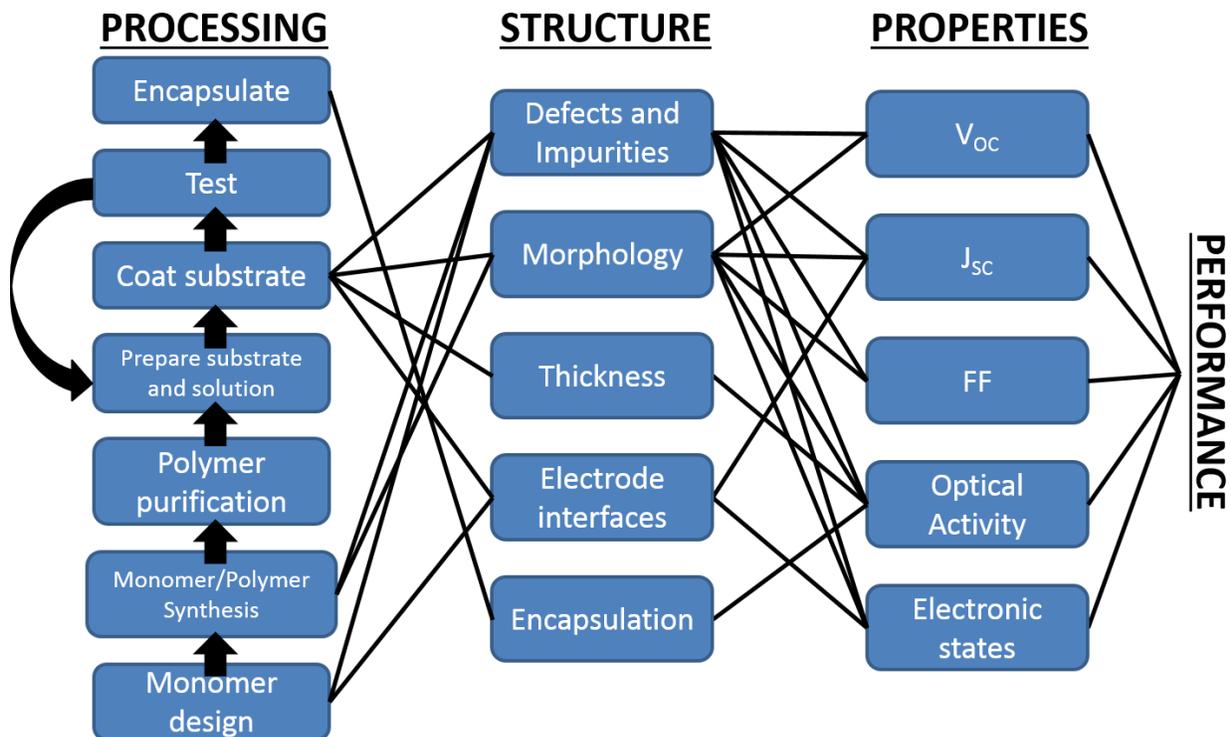
Matthew Goldey (UC, Galli)

Alex Scheider (UC, Yu)

Tianyue Xu (UC, Yu)

MATERIAL SUMMARY:

Organic electronic donor-acceptor polymers are prepared via chemical synthesis. The process begins with monomer synthesis, polymer synthesis, and then purification. A solution of polymer, fullerene-derived acceptors, and additives is prepared. On a clean ITO substrate, PEDOTS:PSS and the active layer material are spin coated in layers. The spin-casting process generates an amorphous bulk heterojunction with intrinsic structural disorder, maximizing interfacial surface area. Finally, a layer of metal (Ca/Al) electrode is vapor deposited onto the surface of the active layer. The spin-casting process produces different active layers upon temperature, time, concentration, ratio of polymer to fullerene, additive nature/concentration, nature of the solvent, and spin-cast rate (speed and time). Relevant structures include defects and impurities, active layer morphologies and thickness, active layer-electrode interfaces, and encapsulation. Important properties governing device performance are the open-circuit voltage, the short-circuit current, the fill factor, optical absorbance, and the electronic states involved in the photoconversion process. Photoconversion efficiency and long-term stability (physical and oxidative) are the figures of merit for our materials.



Data Mining

Participants:

Amar Krishna (NU, Agrawal)

Alona Furmanchuk (NU, Agrawal)

Roseanne Liu (NU, Agrawal)

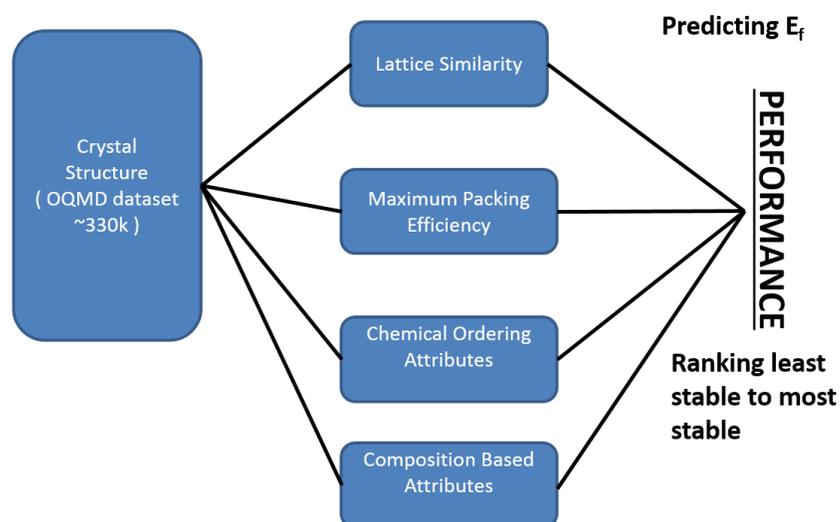
Logan Ward (NU, Wolverton)

Compound Stability

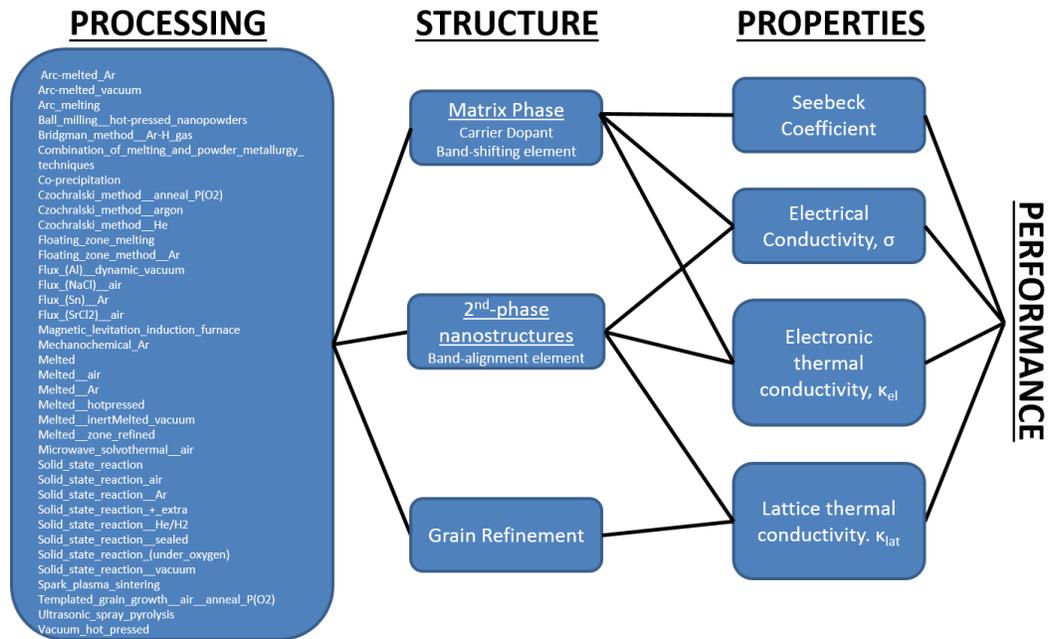
PROCESSING

STRUCTURE

PROPERTIES



Thermoelectrics



Summary

- 33 attendees (including organizers)
- 10 Systems Design Charts (SDC) were developed
- 6 Materials Summaries were developed
- 2 days of lectures, working on charts, results/research presentations, and discussion (Agenda attached)

Comments

- While Systems Design Charts (SDCs) were developed for all Use-Case Groups, not all groups produced a corresponding Materials Summary. Summaries should be developed by the next Quarterly meeting.
- SDCs produced had varying details. In the future all SDCs should have the same level of detail.
- Ideal SDC will describe a material prepared for industrial development, including all major processing and post-processing steps. This will aid with identification of future opportunities and possible collaborations with industry.
- Use-Case Groups had good communication between researchers. Attendees would have benefited from more collaborators participating to provide full picture.
- Some attendees did not know the Use-Case Group/Project to which they belonged.
- Students and Postdocs will benefit greatly from more opportunities to meet and communicate, within their own Use-Case group as well as across Use-Case Groups

Future Outlook

- Polymer Matrix Materials—The SDC developed would benefit from more work and discussion within Use-Case Group. The goals of the final material should be more defined to provide clarity within the SDC. This team lacked input from collaborators, so it is expected that this SDC can be improved.
- Low-Dimensional Nanoelectronic Materials—Excellent adaptation to the SDC framework. This team excelled at demonstrating the many opportunities for this system to become different types of electronic devices. Great potential for further development.
- Precipitation-Strengthened Alloys—The project is very mature and benefits from many research perspectives. The SDC is well-developed and the next step will be to use this to optimize the alloy for the application of turbines. With many groups working on the same problem, communication will be key to aid each individual effort with the resources of the group.
- In-Situ Si-Composite Materials—Excellent progress in identifying research opportunities within the material class. SDC is well-developed. Project would benefit from more collaboration.
- Directed Self-Assembly of Block Co-polymer Films for Lithographic Applications—Excellent job developing SDC and Material Summary. This project combines experimentation with computation and theory well and is on track to material being developed for industry.

- Soft Matter Design based on Charge Complexation—Good first attempt at defining system within the SDC framework. This needs more attention and work to form a more refined picture of the material. Examination of “post-synthesis” techniques to form bulk hydrogels is an area of interest to bridge the fundamental science with material development.
- Organic Bulk Heterojunction Polymer Solar Cells—Good job defining the SDC and relevant research goals. This project would benefit with communication with the Data Mining group in regards to the development of a monomer library.
- Data Mining—This group would benefit from more materials science knowledge. Attendees lacked clarity when explaining the purpose/goal of their work. The CHiMaD community could benefit by using these techniques so more communication is needed between this and other groups.