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Final Report: A Network-Science-Integrated Feedback Loop for Design of Multifunctional Polymeric Rod-Like Nanocomposites

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RPPR Final Report
as of 18-May-2020

Agency Code:

Proposal Number: 69422MS | **Agreement Number: W911NF-16-1-0356**

INVESTIGATOR(S):

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DUNS Number: 608195277 EIN: 566001393
Report Date: 09-Aug-2020 Date Received: 12-May-2020
Final Report for Period Beginning 10-Jun-2016 and Ending 09-May-2020
Title: A Network-Science-Integrated Feedback Loop for Design of Multifunctional Polymeric Rod-Like Nanocomposites
Begin Performance Period: 10-Jun-2016 **End Performance Period:** 09-May-2020
Report Term: 0-Other
Submitted By: Mark Forest Email: forest@unc.edu
Phone: (919) 962-9606
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STEM Degrees: 1 **STEM Participants:** 2

Major Goals: Discoveries and realizations over the last 20 months have disrupted the conventional wisdom that "higher loading of SWCNTs achieves better performance properties". This has been proven demonstrably false in the new class of SWCNT-polyetherimide (PEI) nanocomposites developed by the Dingemans lab. Figure 1a below reveals a striking, non-monotone, strain @ failure relationship, with a strong peak of 12-24% strain at 0.1% volume loading of SWCNTs in the ODPA-P3 neat polymer. This extremely promising peak performance behavior is followed by a sharp decline, already below the neat polymer 4% strain failure by 0.6% loading, that degrades even more for all higher loadings. Furthermore, Figure 1b reveals the average toughness (~ 10 J/g) has a similar peak at 0.1% loading, and Figure 1c reveals the average yield strength (~ 90 MPa) rises to a maximum plateau at 0.1% with no gains at higher loading. Figure 1d reveals that only the elastic modulus rises monotonically with vol% loading, from the already high performance 2.5 GPa of the neat polymer, to 2.6-3.0 GPa at 0.1%, and then 3.0-4.5 GPa with high variability until 4.4% and higher loadings.

These results point to a completely new performance class of SWCNT-PNCs, anchored in the novel conformational flexibility of PEI polymers at SWCNT interfaces to template a crystalline interphase. This new performance class has a unique combination of performance properties: preservation and gains in the high-performance thermoelectric [1] and mechanical property ranges of the ODPA-P3 neat polymer shown in Figure 1, and, unprecedented temperature-usage ranges (above 200 oC for the neat polymer, and higher with SWCNT loadings [2-4]).

Our research effort involves tight collaboration and feedback between experimental, theoretical, and computational expertise, combining the experiences and perspectives of this diverse set of PIs and their trainees. The resulting effort to explore and model these novel composite systems has focused on tools that provide feedback to and from experimental data. Once validated, these tools will provide explanations of PEI-SWCNT multifunctional performance properties, and guide the next iterations of experiments toward identifying bounds on collective properties and the specifications across design space to achieve optimal material performance.

Accomplishments: Three activities comprise the work performed: 1) Experiments on SWCNT-PEI and related polymer nanocomposites by Dingemans, Hegde, and Fox; 2) Analysis and computation of crystallization and the unique properties that arise at extremely low SWCNT loadings by Forest, Mucha, Heroy and Bubnovich; and 3) Theoretical-computational understanding of mechanical percolation and rigidity by Forest, Mucha, Heroy, and Taylor. The results of these activities were published in several leading peer-reviewed journals in materials science.

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Training Opportunities: Ryan Fox was partially supported and received his PhD this May, and has a position in the private sector that will start this summer. Sam Heroy was partially supported and received his PhD two years ago, and took a postdoc position at Oxford University upon graduation. Sam Bubnovich was partially supported and continues to work on materials science related projects between Forest, Mucha, and Dingemans. Postdoc Dane Taylor was partially supported and took a tenure-track job in Mathematics at the University at Buffalo two years ago. Staff scientist Maruti Hegde was partially supported and continues to publish high profile papers with Dingemans and other collaborators.

Results Dissemination: Multiple papers were published and both posters and oral presentations were given at professional meetings. The papers have been uploaded. Ryan Fox gave a series of presentations and posters including multiple prizes / awards, including:
Department of Energy Office of Science Graduate Student Research (SCGSR) Fellowship; July 2019
2nd Place, Oral Presentation – Future of Materials Research III Workshop, NC State; Jan 2019
Outstanding Oral Presentation (top 4) – 13th National Graduate Research Polymer Conference; Jun 2018
1st Place, Oral Presentation – Future of Materials Research II Workshop, NC State; Jan 2018
1st Place, Oral Presentation – Carolina Science Symposium, NC State; Nov 2017

Honors and Awards: Ryan Fox received a Department of Energy Office of Science Graduate Student Research (SCGSR) Fellowship in July 2019. Awards for oral presentations for Ryan Fox were listed in the Dissemination category and repeated here:
2nd Place, Oral Presentation – Future of Materials Research III Workshop, NC State; Jan 2019
Outstanding Oral Presentation (top 4) – 13th National Graduate Research Polymer Conference; Jun 2018
1st Place, Oral Presentation – Future of Materials Research II Workshop, NC State; Jan 2018
1st Place, Oral Presentation – Carolina Science Symposium, NC State; Nov 2017

Protocol Activity Status:

Technology Transfer: Nothing to Report

PARTICIPANTS:

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)
Participant: Maruti Hegde
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

ARTICLES:

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Entropy
Publication Identifier Type: DOI Publication Identifier: 10.3390/e18060202
Volume: 18 Issue: 6 First Page #: 202
Date Submitted: 7/18/16 12:00AM Date Published: 5/1/16 8:00AM
Publication Location: Open Source
Article Title: Hydrodynamic Theories for Flows of Active Liquid Crystals and the Generalized Onsager Principle
Authors: Xiaogang Yang, Jun Li, M. Forest, Qi Wang
Keywords: active liquid crystals; nonequilibrium thermodynamics; hydrodynamics; free surface boundary conditions
Abstract: We articulate and apply the generalized Onsager principle to derive transport equations for active liquid crystals in a fixed domain as well as in a free surface domain adjacent to a passive fluid matrix. The Onsager principle ensures fundamental variational structure of the models as well as dissipative properties of the passive component in the models, irrespective of the choice of scale (kinetic to continuum) and of the physical potentials. Many popular models for passive and active liquid crystals in a fixed domain subject to consistent boundary conditions at solid walls, as well as active liquid crystals in a free surface domain with consistent transport equations along the free boundaries, can be systematically derived from the generalized Onsager principle. The dynamical boundary conditions are shown to reduce to the static boundary conditions for passive liquid crystals used previously.
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Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Nucleic Acids Research
Publication Identifier Type: DOI Publication Identifier: 10.1093/nar/gkw510
Volume: Issue: First Page #:
Date Submitted: 7/18/16 12:00AM Date Published: 6/1/16 12:00PM
Publication Location: Open Source
Article Title: Entropy gives rise to topologically associating domains
Authors: Paula A. Vasquez, Caitlin Hult, David Adalsteinsson, Josh Lawrimore, Mark G. Forest, Kerry Bloom
Keywords: polymer models, chromosomes, entropy, topological domains
Abstract: We investigate chromosome organization within the nucleus using polymer models whose formulation is closely guided by experiments in live yeast cells. We employ bead-spring chromosome models together with loop formation within the chains and the presence of nuclear bodies to quantify the extent to which these mechanisms shape the topological landscape in the interphase nucleus. By investigating the genome as a dynamical system, we show that domains of high chromosomal interactions can arise solely from the polymeric nature of the chromosome arms due to entropic interactions and nuclear confinement. In this view, the role of bio-chemical related processes is to modulate and extend the duration of the interacting domains.
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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Rheology
Publication Identifier Type: DOI Publication Identifier: 10.1122/1.4943988
Volume: 60 Issue: 3 First Page #: 379
Date Submitted: 7/18/16 12:00AM Date Published: 5/1/16 8:00AM
Publication Location: do not know
Article Title: Maximum likelihood estimation for single particle, passive microrheology data with drift
Authors: John W. R. Mellnik, Martin Lysy, Paula A. Vasquez, Natesh S. Pillai, David B. Hill, Jeremy Cribb, Scott A
Keywords: Maximum likelihood; passive microbead rheology; diffusion in the presence of drift
Abstract: Volume limitations and low yield thresholds of biological fluids have led to widespread use of passive microparticle rheology. Themean-squared-displacement (MSD) statistics of bead position time series (bead paths) are either applied directly to determine the creep compliance [Xu et al., Rheol. Acta 37, 387–398 (1998)] or transformed to determine dynamic storage and loss moduli [Masonand Weitz, Phys. Rev. Lett. 74, 1250–1253 (1995)]. A prevalent hurdle arises when there is a nondiffusive experimental drift in the data. Commensurate with the magnitude of drift relative to diffusive mobility, quantified by a Peclet number, the MSD statistics are distorted, and thus the path data must be “corrected” for drift. The standard approach is to estimate and subtract the drift from particle paths, and then calculate MSD statistics. We present an alternative, parametric approach using maximum likelihood estimation that simultaneously fits drift and diffusive model parameters from the path data...
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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Soft Matter
Publication Identifier Type: DOI Publication Identifier: 10.1039/C5SM00852B
Volume: 11 Issue: 32 First Page #: 6393
Date Submitted: 7/18/16 12:00AM Date Published:
Publication Location: Open Source
Article Title: Kinetic attractor phase diagrams of active nematic suspensions: the dilute regime
Authors: M. Gregory Forest, Qi Wang, Ruhai Zhou
Keywords: kinetic phase diagram; active nematic nanorod suspensions
Abstract: Large-scale simulations by the authors of the kinetic-hydrodynamic equations for active polar nematics revealed a variety of spatio-temporal attractors, including steady and unsteady, banded (1d) and cellular (2d) spatial patterns. These particle scale activation-induced attractors arise at dilute nanorod volume fractions where the passive equilibrium phase is isotropic, whereas all previous model simulations have focused on the semi-dilute, nematic equilibrium regime and mostly on low-moment orientation tensor and polarity vector models. Here we extend our previous results to complete attractor phase diagrams for active nematics, with and without an explicit polar potential, to map out novel spatial and dynamic transitions, and to identify some new attractors, over the parameter space of dilute nanorod volume fraction and nanorod activation strength. The particle-scale activation parameter corresponds experimentally to a tunable force dipole strength (so-called pushers with propulsion
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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Nucleic Acids Research
Publication Identifier Type: DOI Publication Identifier: 10.1093/nar/gkx741
Volume: Issue: First Page #:
Date Submitted: 10/18/17 12:00AM Date Published: 8/1/17 4:00AM
Publication Location:
Article Title: Enrichment of dynamic chromosomal crosslinks drive phase separation of the nucleolus
Authors: Caitlin Hult, David Adalsteinsson, Paula A. Vasquez, Josh Lawrimore, Maggie Bennett, Alyssa York, Dia
Keywords: stochastic modeling, biological polymers, DNA, dynamic crosslinks
Abstract: Regions of highly repetitive DNA, such as those found in the nucleolus, show a self-organization that is marked by spatial segregation and frequent selfinteraction. The mechanisms that underlie the sequestration of these sub-domains are largely unknown. Using a stochastic, bead-spring representation of chromatin in budding yeast, we find enrichment of protein-mediated, dynamic chromosomal cross-links recapitulates the segregation, morphology and self-interaction of the nucleolus. Rates and enrichment of dynamic crosslinking have profound consequences on domain morphology. Our model demonstrates the nucleolus is phase separated from other chromatin in the nucleus and predicts thatmultiple rDNA loci will form a single nucleolus independent of their location within the genome. Fluorescent labeling of budding yeast nucleoli with CDC14- GFP revealed that a split rDNA locus indeed forms a single nucleolus. We propose that nuclear subdomains, such as the nucleolus, result from phase ,,,,,
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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Nature Communications
Publication Identifier Type: DOI Publication Identifier: 10.1038/s41467-017-00739-6
Volume: 8 Issue: 1 First Page #:
Date Submitted: 10/18/17 12:00AM Date Published: 10/1/17 4:00AM
Publication Location:
Article Title: A blueprint for robust crosslinking of mobile species in biogels with weakly adhesive molecular anchors
Authors: Jay Newby, Jennifer L. Schiller, Timothy Wessler, Jasmine Edelstein, M. Gregory Forest, Samuel K. Lai
Keywords: nanoparticles, Matrigel®, antibody, IgG
Abstract: Polymeric matrices are ubiquitous in biology and can impede transport of nanoparticulates and pathogens by entropic or direct adhesive interactions. In addition, matrices can harness “third party” molecular anchors to crosslink nanoparticulates to matrix constituents. The trapping potency of such molecular anchors is naturally dictated by their association rates and affinities to both the nanoparticulates and the matrix; the widely held dogma is that long-lived, high-affinity bonds to both species facilitate optimal trapping. Here, we combine experimental evidence using IgG antibodies and Matrigel®, a theoretical explanation based on numerous competing timescales, and rigorous computational modeling to reveal a new paradigm. Among numerous parameters that influences anchor design, we show that anchors that bind and unbind rapidly from the matrix will accumulate on nanoparticulates much more quickly than anchors that form high-affinity, long-lived bonds with the matrix, leading to.....
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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Polymers
Publication Identifier Type: DOI Publication Identifier: 10.3390/polym9100548
Volume: 9 Issue: 12 First Page #: 548
Date Submitted: 8/28/18 12:00AM Date Published: 10/1/17 4:00AM
Publication Location:
Article Title: Atomistic Molecular Dynamics Simulations of the Initial Crystallization Stage in an SWCNT-Polyetherimide Nanocomposite
Authors: Victor Nazarychev, Sergey Larin, Alexey Lyulin, Theo Dingemans, Jose Kenny, Sergey Lyulin
Keywords: polyetherimides; crystallization; molecular dynamics; nanocomposite; ├–├ interactions
Abstract: Crystallization of all-aromatic heterocyclic polymers typically results in an improvement of their thermo-mechanical properties. Nucleation agents may be used to promote crystallization, and it is well known that the incorporation of nanoparticles, and in particular carbon-based nanofillers, may induce or accelerate crystallization through nucleation. The present study addresses the structural properties of polyetherimide-based nanocomposites and the initial stages of polyetherimide crystallization as a result of single-walled carbon nanotube (SWCNT) incorporation. We selected two amorphous thermoplastic polyetherimides ODPA-P3 and aBPDA-P3 based on 3,30,4,40-oxydiphthalic dianhydride (ODPA), 2,30,3,40-biphenyltetracarboxylic dianhydride (aBPDA) and diamine 1,4-bis[4-(4-aminophenoxy)phenoxy]benzene (P3) and simulated the onset of crystallization in the presence of SWCNTs using atomistic molecular dynamics. For ODPA-P3, we found that the planar phthalimide and phenylene moieties show pr
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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Composites Science and Technology
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.compscitech.2017.12.030
Volume: 156 Issue: First Page #: 158
Date Submitted: 2/17/20 12:00AM Date Published: 3/1/18 10:00AM
Publication Location:
Article Title: All-aromatic SWCNT-Polyetherimide nanocomposites for thermal energy harvesting applications
Authors: Lazaros Tzounis, Maruti Hegde, Marco Liebscher, Theo Dingemans, Petra Pötschke, Alkiviadis S. Paipe
Keywords: polyetherimide
Abstract: The thermoelectric properties of amorphous and semi-crystalline high-performance polyetherimideeSWCNT nanocomposites are reported for thefirst time. Nanocomposites based on a non-linear poly-etherimide (PEI) model system, labeled aBPDA-P3, with 0.6, 4.4 and 10 vol% SWCNTs remained amor-phous after the addition of SWCNTs. In contrast, SWCNTs induced crystallization in a linear PEI modelsystem labeled as ODPA-P3. The (thermo)mechanical properties were fully characterized using ther-mogravimetric analysis (TGA), differential scanning calorimetry (DSC) and dynamic mechanical analysis(DMTA). The electrical conductivity was studied by four-probe measurements and showed higher valuesfor the ODPA-P3films reaching 20 S/m at 10 vol% of SWCNTs. The thermoelectric performance revealedby Seebeck coefficient (S) measurements showed values of 40 and 55mV/K for the 0.6 and 4.4 vol% ODPA-P3 SWCNT nanocomposites, while 16 and 47mV/K for aBPDA-P3 amorphousfilms. This enhancement hasbeen attributed to SWC
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Volume: 11 Issue: 43 First Page #: 40551
Date Submitted: 2/17/20 12:00AM Date Published: 9/1/19 4:00AM
Publication Location:
Article Title: Nanofibrillar Ionic Polymer Composites Enable High-Modulus Ion-Conducting Membranes
Authors: Ryan J. Fox, Deyang Yu, Maruti Hegde, Amar S. Kumbhar, Louis A. Madsen, Theo J. Dingemans
Keywords: ionic polymer
Abstract: Polymer electrolyte membranes (PEMs) with high volume fractions of ionic liquids (IL) and high modulus show promise for enabling next-generation gas separations, and electrochemical energy storage and conversion applications. Herein, we present a conductive polymer-IL composite based on a sulfonated all-aromatic polyamide (sulfo-aramid, PBDT) and a model IL, which we term a PBDT-IL composite. The polymer forms glassy and high-aspect-ratio hierarchical nanofibrils, which enable fabrication of PEMs with both high volume fractions of IL and high elastic modulus. We report direct evidence for nanofibrillar networks that serve as matrices for dispersed ILs using atomic force microscopy and small- and wide-angle X-ray scattering. These supramolecular nanofibrils form through myriad noncovalent interactions to produce a physically cross-linked glassy network, which boasts the best combination of room-temperature modulus (0.1–2 GPa) and ionic conductivity (8–4 mS cm–1) of any polymer-IL electr
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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Multiscale Modeling & Simulation
Publication Identifier Type: DOI Publication Identifier: 10.1137/17M1157271
Volume: 16 Issue: 3 First Page #: 1283
Date Submitted: 2/17/20 12:00AM Date Published: 1/1/18 5:00AM
Publication Location:
Article Title: Rigid Graph Compression: Motif-Based Rigidity Analysis for Disordered Fiber Networks
Authors: Samuel Heroy, Dane Taylor, F. Bill Shi, M. Gregory Forest, Peter J. Mucha
Keywords: rigid graph compression
Abstract: Using particle-scale models to accurately describe property enhancements and phase transitions in macroscopic behavior is a major engineering challenge in composite materials science. To address some of these challenges, we use the graph theoretic property of rigidity to model mechanical reinforcement in composites with stiff rod-like particles. We develop an efficient algorithmic approach called rigid graph compression (RGC) to describe the transition from floppy to rigid in disordered fiber networks (``rod-hinge systems''), which form the reinforcing phase in many composite systems. To establish RGC on a firm theoretical foundation, we adapt rigidity matroid theory to identify primitive topological network motifs that serve as rules for composing interacting rigid particles into larger rigid components. This approach is computationally efficient and stable, because RGC requires only topological information about rod interactions (encoded by a sparse unweighted network) rather than ge
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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Soft Matter
Publication Identifier Type: DOI Publication Identifier: 10.1039/D0SM00275E
Volume: 16 Issue: 16 First Page #: 3891
Date Submitted: 5/12/20 12:00AM Date Published: 3/23/20 4:00AM
Publication Location: United Kingdom
Article Title: Observation of transition cascades in sheared liquid crystalline polymers
Authors: Ryan J. Fox, M. Gregory Forest, Stephen J. Picken, Theo J. Dingemans
Keywords: liquid crystalline polymers, steady shear
Abstract: We report on the shear rheology of liquid crystalline solutions composed of charged, rodlike polymers that form supramolecular assemblies dispersed in water. Under steady shear, we observe shear thickening behavior, followed by a hesitation in the viscosity accompanied by an extremely narrow range of negative first normal stress difference. The Peclet number (Pe, shear rate normalized by rod rotational diffusivity) for the onset of shear thickening is in agreement with previous, high-resolution numerical simulations of the Doi–Edwards–Hess kinetic theory. We interrogate these dynamic responses through shear step-down experiments, revealing a complex evolution of transient responses. Detailed analysis of the stress transients provides compelling evidence that the principal axis of the rod orientational distribution, the nematic director, undergoes a cascade of transitions and coexistence of periodic states known as kayaking, tumbling, and wagging, before transitioning to steady flow.
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Acknowledged Federal Support: **Y**

Army Research Office Proposal Number: 69422-MS
Agreement Number: W911NF-16-1-0356
Final Report May 12, 2020
PI: Forest, Co-PIs: Dingemans, Mucha

Three activities comprise the work performed in the 1-year award plus no cost extension year. 1) Experiments on SWCNT-PEI and related polymer nanocomposites by Dingemans, Hegde, and Fox; 2) Analysis and computation of crystallization and the unique properties that arise at extremely low SWCNT loadings by Forest, Mucha, Heroy and Bubnovich; and 3) Theoretical-computational understanding of mechanical percolation and rigidity by Forest, Mucha, Heroy, and Taylor. A summary of progress for each activity follows.

1) Experimental results on polymer nanocomposites in the Dingemans lab.

The following papers have been or will soon be published:

1- R.J. Fox, S.J. Picken and T.J. Dingemans, "Irreversible shear-activated gelation of a liquid crystalline polyelectrolyte," *ACS Macro Letters*, **2020** in press (DOI 10.1021/acsmacrolett.0c00168) **Note:** Work is featured on the journal cover.

2- R.J. Fox, M.G. Forest, S.J. Picken and T.J. Dingemans, "Observation of transition cascades in sheared liquid crystalline polymers," *Soft Matter*, **2020**, *16*, 3891-3901. **Note:** Work is featured on the journal cover.

3- R.J. Fox, D. Yu, M. Hegde, A.S. Kumbhar, L.A. Madsen and T.J. Dingemans, "Nanofibrilar ionic polymer composites enable High-modulus ion-conducting membranes," *ACS Applied Materials&Interfaces*, **2019**, *11(43)*, 40551-40563. **Note:** Work is featured on the journal cover.

Three additional papers are in various stages of preparation for submission to peer-reviewed journals.

2) Analysis and computation of crystallization and the properties that arise at extremely low SWCNT loadings

Forest, Mucha, Heroy and Bubnovich developed a mesoscale model and code that:

- creates realizations of SWCNT-PEI dispersions under prescribed conditions on SWCNT vol% loading, dispersion quality (i.e., homogeneity vs. different models for heterogeneity), and orientational distribution (isotropic vs. degree of order);
- initiates growth and tracks evolution of the crystalline interphase from each SWCNT-PEI interface, out to a maximum radius for an isolated SWCNT;
- arrests growth of the interphase due to close proximity and relative orientation of neighboring SWCNTs;
- predicts final crystallinity for direct comparison with experimental data, providing the first validation of, and feedback with, experiments at the sparse sampling of vol%.

This work is in rough form that needs polishing prior to submission.

3) Theoretical-computational understanding of mechanical percolation and rigidity

The first results were published in:

“Rigid graph compression: Motif-based rigidity analysis for disordered fiber networks,” S. Heroy, D. Taylor, F. Shi, M. G. Forest & P. J. Mucha, Multiscale Modeling and Simulation **16**, 1283–1304 (2018).

The extension of this work to 3D rod systems is in progress with a paper to be submitted sometime in the next few months: “Rigidity percolation in disordered 3D rod systems”, Samuel Heroy, Dane Taylor, Feng Shi, M. Gregory Forest, and Peter J. Mucha.

Personnel outcomes supported by the award:

Sam Heroy, applied math RA partially supported, received his PhD in May 2018, dissertation is titled “Network analyses of nano-rod composites”; postdoc position at Oxford University and now University College, London.

Dane Taylor, applied math postdoc partially supported, left UNC in 2017 for a tenure-track position at U. Buffalo.

Ryan Fox, applied sciences RA partially supported, received a PhD in May 2020.

Sam Bubnovich, applied math RA partially supported, is progressing toward his PhD at the intersection of applied and computational mathematics and materials science.

Maruti Hegde, research scientist in applied sciences partially supported, performs significant experimental work in the Dingemans lab for the project and is co-author on all research coming out of the Dingemans lab.