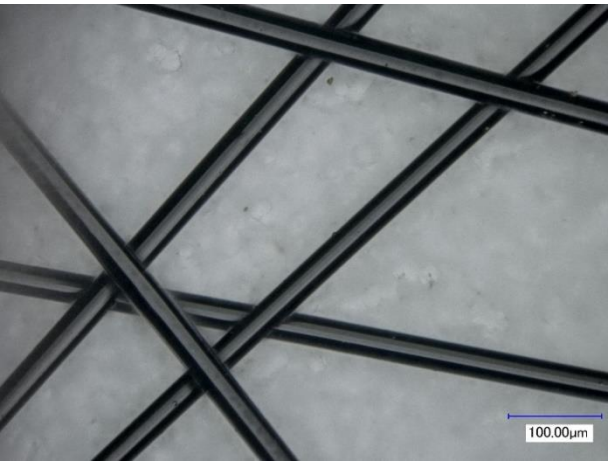
Integrated Computational Materials Engineering (ICME) Predictive Tools for Low-Cost Carbon Fiber



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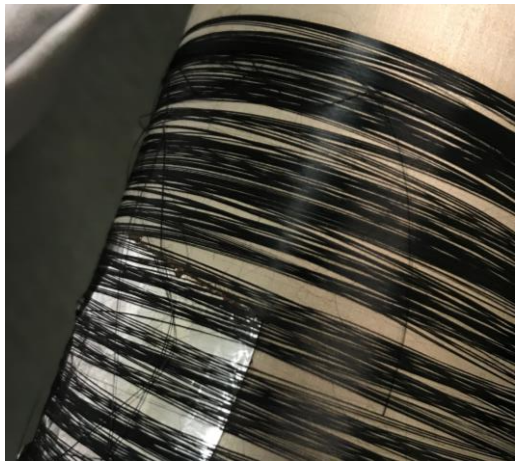
Project ID #: MAT125 **June 19, 2018**



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Overview

Timeline:

Start: October 2017
End: September 2020
Completion: 15%

Budget:

Total: $5,242,820
DOE Share: $3,745,413
Cost Share Total: $1,497,407 (28.6%)
FY 2018 DOE Share: $1,371,684
FY 2018 Cost Share: $792,199

Barriers (US Drive Material Technology Roadmap for CF Composites)

-Low-cost high-volume manufacturing
-Low-cost fibers
-Predictive modeling

Partners

Oakridge National Laboratories (ORNL)
Massachusetts Institute of Technology (MIT), Jeff Grossman Group
Southern Research Institute (SRI)
Advanced Carbon Products, LLC (ACP)
University of Wyoming (UW)
Ramaco Carbon, LLC (RAMACO)
Solvay Composites (Industry advisor)

Relevance & Objectives

Overall Objectives

-**Develop an integrated computational materials engineering (ICME) suite** capable of predicting select mechanical properties of carbon fiber (CF) tow all the way down to the feedstock chemicals

-**Provide a map of common high-volume low-cost major feedstocks** from petroleum, coal and biomass relative to CF production and end CF mechanical properties

Technical Targets

-ICME ≥ 15% of predicted properties

-Mechanical properties of CF resin: strength (250 Ksi), modulus (25 Msi), strain (1%)

-Cost: ≤ $5 lb

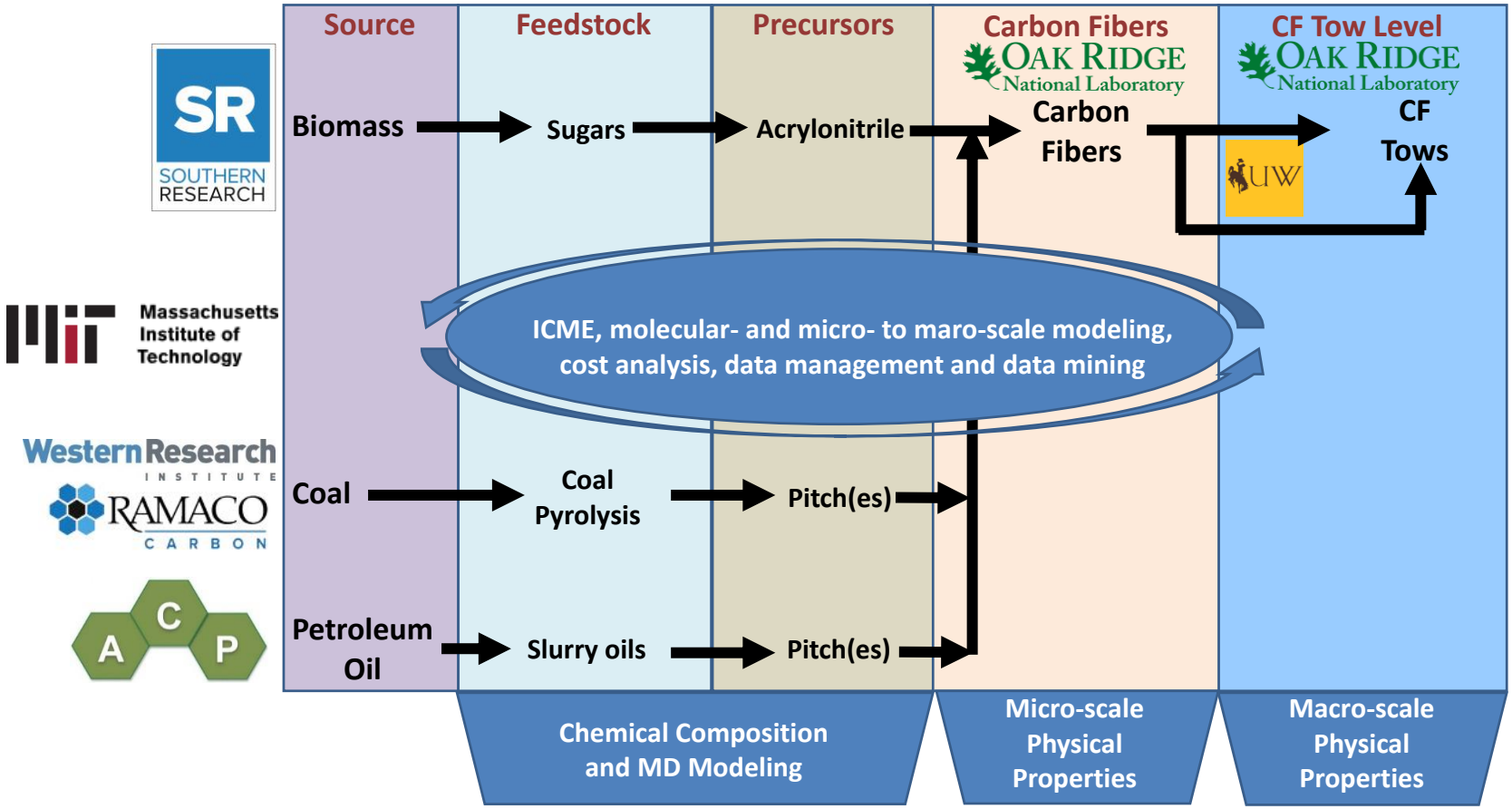
Impact

-Reduction in vehicle mass

-Accelerate sustainable implementation of affordable light weight CF in vehicle use

- Achieving the above mentioned objectives, while also providing long term sustainability by providing a portfolio of different materials capable of achieving the same desired properties that mitigates the risks and market fluctuations associated from becoming exclusively dependent on any one high-volume source of feedstock, while being flexible for the future

Approach & Milestones



FY 2018 Milestones (% Complete): Execute subcontracts (95%), evaluate feedstock materials (50%), make CF (50%)

Go/No Go: Meets DOE strength and < $5/lb

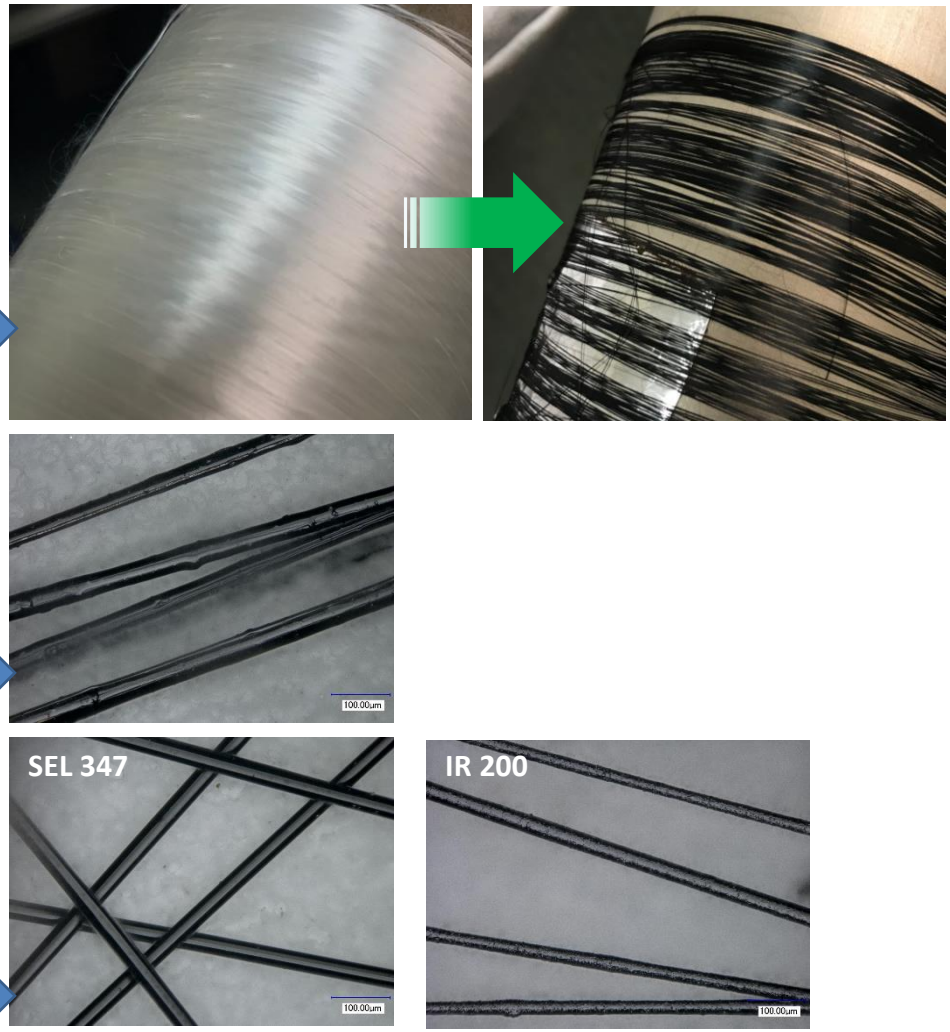
FY 2019 Milestones: macro-scale modeling ± 15%, micro-scale modeling ± 15%, CF tow strength to weight ratio is 30 to 50% steel, use machine learning to identify precursor materials and combinations for CF

Go/No Go: Meets DOE strength and < $5/lb for scaled up batches of precursor material

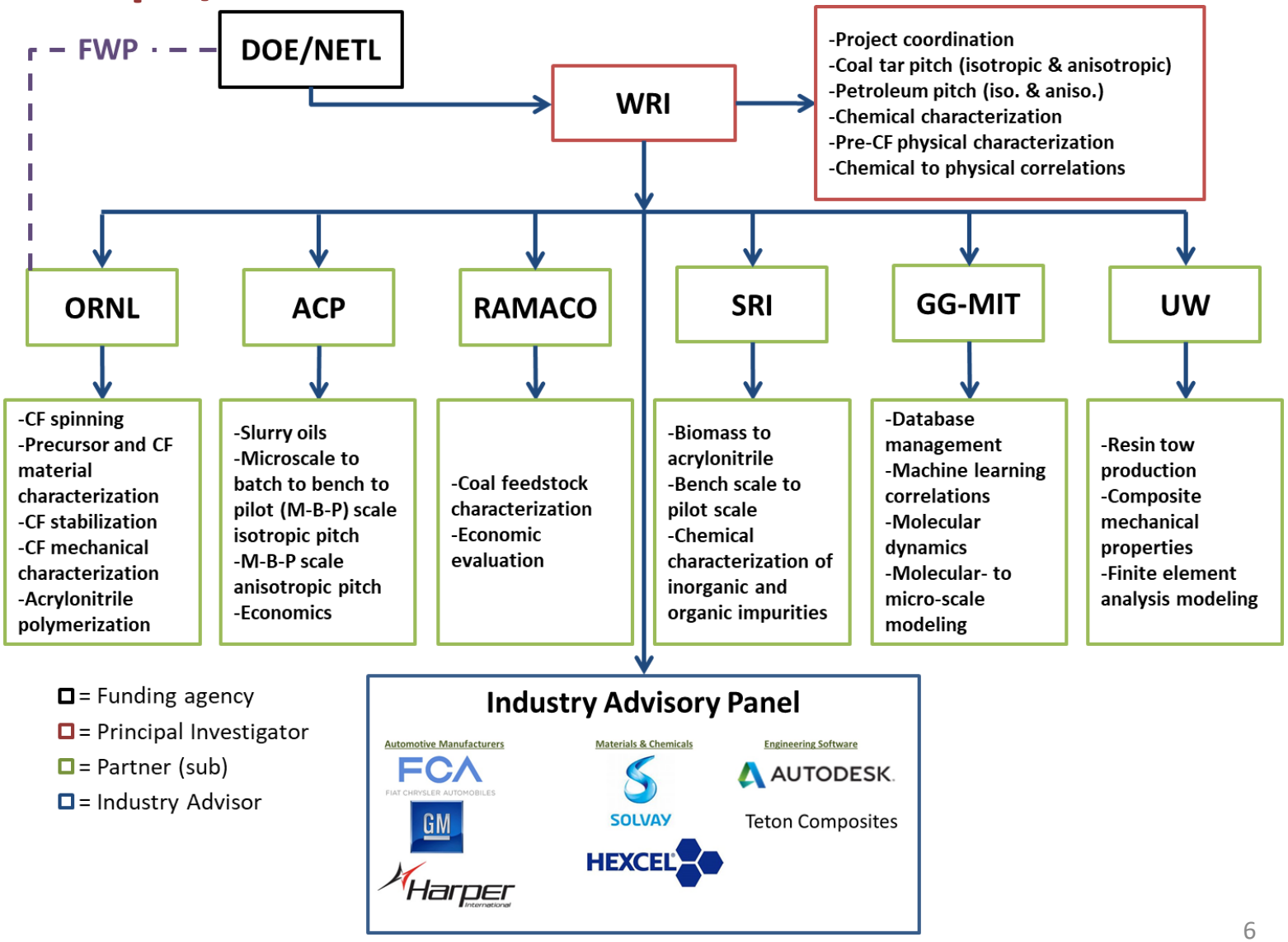
Accomplishments for FY 2018

Feedstock/Intermediate and CF

Source	Feedstock	Precursors
Biomass -Corn Stover -Sugarcane Bagasse -Switchgrass -Wheat Straw -Miscanthus -Sorghum -Hybrid Poplar -Grass Clippings -Lodge Pole Pine	Acrylonitrile	Polyacrylonitrile
		Polyacrylonitrile *Textile Grade
Coal	Pitch/pyrolysis* -High Temp. -Low Temp.	Isotropic* Anisotropic
Petroleum	Pitch* -Slurry Oil -Hydroconverted Bottoms -Gilsonite*	Isotropic* Anisotropic



Partnerships / Collaborations



Proposed Future Research*

Feedstock/Intermediate FY18-19

Coal Tar Pitch, Gilsonite, Hydroconverted Bottoms

-Continue removal of impurities from raw materials; chemical characterization of raw materials, impurities and purified materials
-Continue physical characterization of raw materials and purified material
-Conversion of isotropic pitch to anisotropic (mesophase) pitch to achieve strength requirements

Slurry Oil Pitch

-Reconfiguration of pilot scale equipment to handle bench scale quantities
-Conversion of slurry oil to isotropic pitch and preliminary characterization
-Conversion of isotropic pitch to anisotropic pitch and preliminary characterization
-Microscopic conversion kinetics and morphology evolution of anisotropic pitch

Acrylonitrile

-Continue evaluation of feedstock specific inorganic and organic impurities in bench scale equipment to determine the breakthrough curves and catalyst performance during acrylonitrile production
-Pilot scale production of acrylonitrile
-Polymerization of acrylonitrile into polyacrylonitrile

*Any proposed future work is subject to change base on funding levels

Proposed Future Research*

CF, Modeling and Database, Resins, Economics FY18-19

CF Production and Characterization

-Ongoing production and morphological characterization of CF fibers from various precursor materials
-Stabilization and graphitization of spun CF
-Mechanical testing of CF fibers
-Ongoing evaluation of precursor physical properties

Modeling and Database

-Model kinetics of formation of mesogen molecules from starting material molecules
-Model thermal reactions leading to crosslinking and oxidative stabilization
-Verify model simulation properties to actual material properties
-Define database structure, begin applying machine learning to mine and correlate data

Resin CF Tow Fabrication and Marco-scale Modeling

-Ongoing work in producing model resin systems
-Mechanical testing of the tow and model resin systems
-Application of finite element modeling

Economic Evaluation

-Economic evaluation of feedstock/intermediate/precursor materials

*Any proposed future work is subject to change base on funding levels

Summary

Relevance

-Develop ICME tools to predict CF physical properties from the molecular level up through micro-scale CF and macro-scale CF tow

-Develop a catalogue of materials that can achieve light-weight high-volume CF at < $5/lb with the following requirements: strength (250 Ksi), modulus (25 Msi) and strain (1%)

Approach

-Assemble a consortium to look at various different materials appropriate for CF production from biomass, petroleum and coal

-Characterize the chemical and physical properties of these materials at different stages

-Correlate properties with the resulting CF properties

Accomplishments

-Production of CF from gilsonite, coal tar pitch and textile grade PAN

Future Research

-Further purification and chemical and physical characterization of materials at different stages of production

-Additional CF production from biomass based polyacrylonitrile, coal tar pitch, gilsonite and other petroleum based materials

-Stabilization and graphitization of CF and mechanical testing of the CF and tows

-Implementation of the database along with modeling and machine learning

Response to Previous Year Review Comments

This project was not reviewed at the previous 2017 VTO Annual Merit Review.