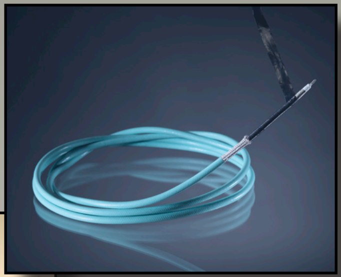
Realizing the Promise of Carbon Nanotubes

Challenges, Opportunities, and the Pathway to Commercialization

Technical Interchange Proceedings
September 15, 2014



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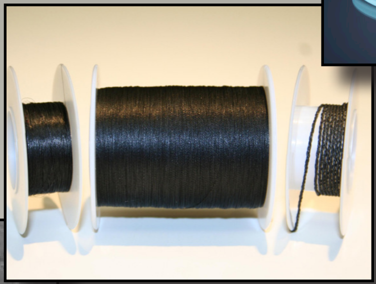

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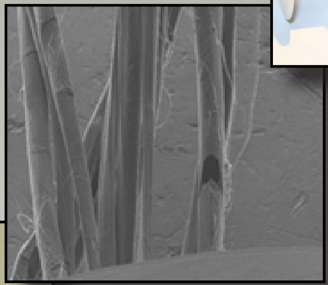

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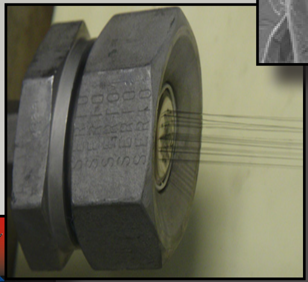

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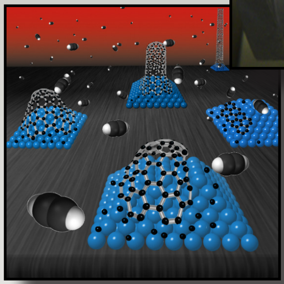

Modeling

About the National Nanotechnology Initiative

The National Nanotechnology Initiative (NNI) is a U.S. Government research and development (R&D) initiative involving 20 Federal departments, independent agencies, and independent commissions working together toward the shared and challenging vision of a future in which the ability to understand and control matter at the nanoscale leads to a revolution in technology and industry that benefits society. The combined, coordinated efforts of these agencies have accelerated discovery, development, and deployment of nanotechnology to benefit agency missions in service of the broader national interest.

About the Nanoscale Science, Engineering, and Technology Subcommittee

The Nanoscale Science, Engineering, and Technology (NSET) Subcommittee is the interagency body responsible for coordinating, planning, implementing, and reviewing the NNI. NSET is a subcommittee of the Committee on Technology (CoT) of the National Science and Technology Council (NSTC), which is one of the principal means by which the President coordinates science and technology policies across the Federal Government. The National Nanotechnology Coordination Office (NNCO) provides technical and administrative support to the NSET Subcommittee and supports the Subcommittee in the preparation of multiagency planning, budget, and assessment documents, including this report. More information about the NSET Subcommittee, the NNI, and the NNCO can be found at www.nano.gov.

About the Nanotechnology Signature Initiatives

The Federal agencies participating in the National Nanotechnology Initiative have identified focused areas of national importance that may be more rapidly advanced through enhanced coordination and collaboration of agency research and development efforts. These Nanotechnology Signature Initiatives (NSIs) provide a spotlight on critical areas and define the shared vision of the participating agencies for accelerating the advancement of nanoscale science and technology to address needs and exploit opportunities from research through commercialization. They are intended to be dynamic, with topical areas rotating and evolving over time. More information about the NSIs can be found at www.nano.gov/signatureinitiatives.

About this Document

This document is the report of the technical interchange meeting on Realizing the Promise of Carbon Nanotubes: Challenges, Opportunities, and the Pathway to Commercialization, held September 15, 2014, in Washington, DC, in support of the *Sustainable Nanomanufacturing: Creating Industries of the Future* NSI. The meeting was sponsored by the NNI and co-sponsored by the National Aeronautics and Space Administration (NASA). The objectives of this meeting were to identify, discuss, and report on technical barriers to the production of carbon nanotube-based bulk materials and composites with optimal electrical and mechanical properties, and to explore ways to overcome these barriers. Any opinions, findings, conclusions, or recommendations expressed in this report are those of the authors and meeting participants and do not necessarily reflect the views of the United States Government or the authors' or other meeting participants' parent institutions. This report is not a consensus document but rather is intended to reflect the diverse views, expertise, and deliberations of the meeting participants.

About the Report Cover and Book Design

Book layout was designed by NNCO staff. Report cover design is by Kristin Roy of the NNCO. The five images on the front cover illustrate five aspects of research on carbon nanotubes that are needed to realize their promise: (1) modeling, (2) synthesis and processing, (3) characterization, (4) commercial products, and (5) applications development. Image credits from left to right: (1) National Institute of Standards and Technology, Center for Nanoscale Science and Technology, (2) Rice University,[1] (3) NASA, and (4–5) Nanocomp Technologies, Inc.

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Technical Interchange Proceedings

Realizing the Promise of Carbon Nanotubes: Challenges, Opportunities, and the Pathway to Commercialization

September 15, 2014

Acknowledgements

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Meeting Manager

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We are grateful to all of the participants for interesting and lively discussions during the meeting, and to the note takers who helped capture the meeting output. Thanks are also due to staff members at National Aeronautics and Space Administration headquarters in Washington, DC, for their assistance in hosting the meeting.

Preface

This report on *Realizing the Promise of Carbon Nanotubes: Challenges, Opportunities, and the Pathway to Commercialization* is the result of a joint National Nanotechnology Initiative (NNI)–National Aeronautics and Space Administration (NASA) technical interchange meeting convened September 15, 2014, in Washington, DC. This report was made possible with the help of the Nanoscale Science, Engineering, and Technology (NSET) Subcommittee of the National Science and Technology Council and with staff support from the National Nanotechnology Coordination Office (NNCO). The meeting builds on efforts by Federal agencies participating in the Nanotechnology Signature Initiative *Sustainable Nanomanufacturing: Creating Industries of the Future* (Nanomanufacturing NSI) to accelerate the development of industrial-scale methods for manufacturing functional nanoscale systems. The Nanomanufacturing NSI has focused on production-worthy scaling of two classes of sustainable materials—high-performance carbon-based nanomaterials and cellulosic nanomaterials—that have the potential to affect multiple industry sectors with significant economic impact.

In his landmark speech at the California Institute of Technology on January 21, 2000, in which he announced the establishment of a new national initiative in nanotechnology, President Clinton imagined the possibility of creating “materials with 10 times the strength of steel at a fraction of the weight.” Carbon nanotubes, because of their remarkable mechanical properties, have the potential to make this dream a reality. However, the properties of carbon nanotube bulk materials, e.g., fibers, fabrics, and composites, currently fall short of those of individual nanotubes and of conventional carbon fiber reinforced composites. This one-day meeting brought together some of the Nation’s leading experts in carbon nanotube synthesis, modeling, processing, and applications from industry, academia, and Government to identify technical barriers to achieving bulk materials with electrical and mechanical properties that more closely match those of individual nanotubes, and to propose approaches to overcoming these barriers and promoting more widespread commercialization of this important class of nanoscale materials. In addition to addressing these objectives, meeting participants proposed a pathway for new collaborations to solve the technical challenges they identified, and to facilitate technology transfer and commercialization.

On behalf of the NSET Subcommittee, we thank Lisa Friedersdorf and Alex Liddle for taking the lead in organizing and co-chairing this technical interchange meeting with Mike Meador. We also thank the speakers, discussion leaders, and other participants for their valuable contributions. We would also like to thank NNCO staff and personnel at NASA Headquarters for their logistical support and assistance in planning and executing this meeting. We trust that you will find this report to be a valuable resource for the NNI, the nanomaterials and nanomanufacturing communities, and all other stakeholders as we work together to promote the NNI’s vision of creating “a future in which the ability to understand and control matter at the nanoscale leads to a revolution in technology and industry that benefits society.”

Lori Henderson	Lloyd Whitman	Michael Meador
Co-Chair	Co-Chair	Director
NSET Subcommittee	NSET Subcommittee	NNCO

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Executive Summary

This report is a summary of the discussions that occurred during the National Nanotechnology Initiative (NNI) technical interchange meeting on Realizing the Promise of Carbon Nanotubes: Challenges, Opportunities, and the Pathway to Commercialization, held at the National Aeronautics and Space Administration (NASA) Headquarters on September 15, 2014. The goals of the meeting were to identify, discuss, and report on technical barriers to the production of carbon nanotube (CNT)-based bulk and composite materials with electrical and mechanical properties nearer the ideal, and to explore ways to overcome these barriers.

A number of common themes and areas requiring focused attention were identified:

- **Increased efforts devoted to manufacturing, quality control, and scale-up are needed.**
  The development of a robust supply of CNT bulk materials with well-controlled properties would greatly enhance commercialization and spur use in a broad range of applications.
- **Improvements are needed in the mechanical and electrical properties of CNT-based bulk materials (composites, sheets, and fibers) to approach the properties of individual CNTs.**
  The development of bulk materials with properties nearing ideal CNT values would accelerate widespread adoption of these materials.
- **More effective use of simulation and modeling is needed to provide insight into the fundamentals of the CNT growth process.**
  Theoretical insight into the fundamentals of the growth process will inform the development of processes capable of producing high-quality material in quantity.
- **Work is needed to help develop an understanding of the properties of bulk CNT-containing materials at longer length scales.**
  Longer length scale understanding will enable the development of predictive models of structure–process–properties relationships and structural design technology tailored to take advantage of CNT properties.
- **Standard materials and protocols are needed to guide the testing of CNT-based products for commercial applications.**
  Advances in measurement methods are also required to characterize bulk CNT material properties and to understand the mechanism(s) of failure to help ensure material reliability.
- **Life cycle assessments are needed for gauging commercial readiness.**
  Life cycle assessments should include energy usage, performance lifetime, and degradation or disposal of CNT-based products.
- **Collaboration to leverage resources and expertise is needed to advance commercialization of CNT-based products.**
  Coordinated, focused efforts across academia, government laboratories, and industry to target grand challenges with support from public–private partnerships would accelerate efforts to provide solutions to overcome these technical barriers.

This meeting identified a number of the technical barriers that need to be overcome to make the promise of carbon nanotubes a reality. A more concerted effort is needed to focus R&D activities towards addressing these barriers and accelerating commercialization. The outcomes from this meeting will inform the future directions of the NNI Nanomanufacturing Signature Initiative and provide specific areas that warrant broader focus in the CNT research community.

1. Background

Since their reported discovery by Iijima in 1991 [*1*], carbon nanotubes (CNTs) have attracted considerable interest due to their remarkable combination of high electrical and thermal conductivity together with outstanding strength and stiffness [*2–4*]. For example, individual CNTs have extraordinarily high strength-to-weight ratios [*5*] compared to conventional structural materials such as steel, potentially enlarging the design space for structures dramatically and enabling the development of multifunctional materials and components. Investments in CNT research over more than two decades [*6*] have led to significant improvements in the availability of CNTs for research and product development activities and in the production of carbon nanotube-based products such as lightweight data cables and CNT-augmented composites. However, the properties of CNT-based bulk materials (yarns, sheets, and fibers) and composites remain short of those measured for individual carbon nanotubes and conventional carbon fiber composites, respectively, thus limiting their commercial use [*7*, *8*]. The observed limited performance can be attributed to several factors. For example, the presence of defects and other variations in individual nanotube structures, as well as the alignment, dispersion, and interfacial interactions of the CNTs within a matrix, have a dramatic effect on bulk material properties [*8*]. Identifying the properties that depend on raw material quality and those that depend on processing-induced structure is essential to realizing the full potential of these materials.

The NNI's Nanotechnology Signature Initiative *Sustainable Nanomanufacturing: Creating the Industries of the Future* (Nanomanufacturing NSI) was created in 2010 to accelerate the development of industrial-scale methods for manufacturing functional nanoscale systems (www.nano.gov/NSINanomanufacturing). The Nanomanufacturing NSI has focused on production-worthy scaling of two classes of sustainable materials—high-performance carbon-based nanomaterials and cellulosic nanomaterials—that have the potential to affect multiple industry sectors with significant economic impact. The formation of consortia with industry, government, and academic representation is a key aspect of the specific material thrusts. As previously reported [*9*], an essential prerequisite for the development of cost-effective nanomanufacturing is the availability of high-throughput, inline metrology to enable closed-loop process control and quality assurance. Metrology is therefore also a key component of the Nanomanufacturing NSI. Success of this initiative will result in the immediate extension of production methods developed in the laboratory to more complex components and systems as future nanodevices mature, which will help secure and strengthen the U.S. manufacturing base.

The objectives of this technical interchange meeting were to identify, discuss, and report on technical barriers to the production of carbon nanotube-based materials with electrical and mechanical properties nearer the ideal, and to explore ways to overcome these barriers [*10*]. Obstacles to full exploitation of the multifunctional nature of carbon nanotube materials were also discussed. Perspectives on realizing the promise of carbon nanotubes were shared by subject matter experts in the following topical areas:

- Modeling and simulation of bulk CNTs.
- Synthesis and scale-up of bulk CNT materials, such as sheets and nonwoven fabrics, fibers, and yarns.
- Structural materials.
- Electrical materials.

Breakout session talks and discussions focused on the broad technical challenges associated with carbon nanotube materials in these four topical areas (see the list of discussion points in Appendix A). For example, during the modeling and simulation session, participants addressed current limitations in modeling the properties of bulk CNT materials, and the state of progress in correlating theoretical modeling to experiments on those materials. For the synthesis and scale-up session, discussion focused on the challenges to developing scaled-up synthesis of high-quality CNT materials and on the fundamental science needed to understand CNT growth mechanisms and their control. For the other sessions on structural and electrical properties, participants explored which properties of CNTs have the greatest potential to improve materials beyond the current state of the art. Participants were asked to identify the present challenges to making the outstanding structural and electrical properties of individual CNTs available in bulk form, and to determine the research needed to enable the incorporation of bulk CNTs into large structural components, data and power distribution systems, and electrically conductive composites in order to help realize desired applications. The output from the discussions will help inform the future directions of the Nanomanufacturing Signature Initiative, including the development of public-private partnerships.

The full meeting program can be found at www.nano.gov/2014CNTTechInterchange.

2. Summary of Perspectives on Realizing the Promise of Carbon Nanotubes

Since their discovery, CNTs have shown promise for a variety of applications [*11*], which can be divided into four groups: small-scale mechanical applications such as resonators, sensors, and channels; large-scale structural-mechanical applications such as fibers, cables, composites, shock-absorbers, and flywheels; small-scale electronics/devices such as transistors, interconnects, and photo-sensing elements; and large-scale systems such as electrical power transmission or motors. These applications have dramatically different requirements in terms of CNT type (chirality, size, single-wall vs. multi-wall, level of defects) and purity, and in the required product volume. Chirality, for instance, defines the optical and electronic properties of CNTs. Scalable synthesis of CNTs with controlled chirality is essential to fully exploiting their commercial potential [*8*].

Established views regarding current understanding of CNT dynamics [*12*] were discussed during the modeling and simulation session for both individual CNTs as well as assemblies. Recent developments in simulations of defect formation and growth mechanisms [*13*], in particular what is needed for growing very long continuous tubes or for growth of specific chiralities, were included. For example, results from recent molecular dynamics simulations of CNT growth indicate that tube chirality controls growth rate, with armchair nanotubes growing the fastest [*14*–*16*]. Ensuing discussions highlighted the opportunity for simulating CNT–CNT interactions and interfaces in bulk materials (Figure 1).

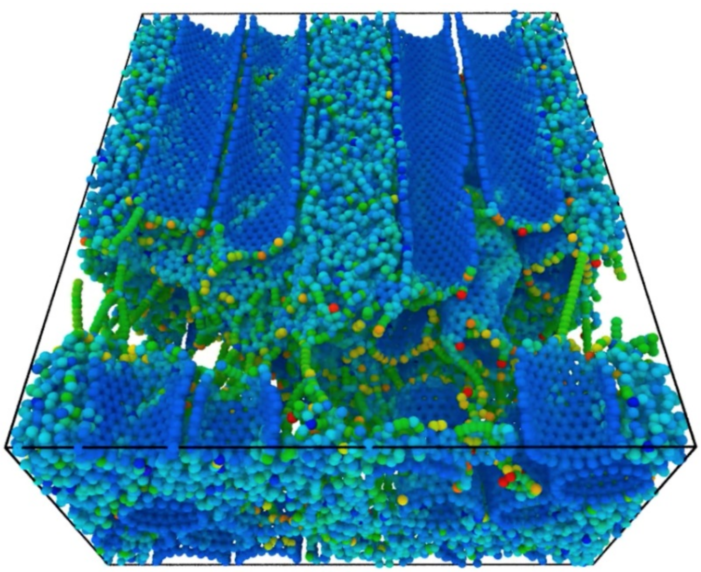

Figure 1. Molecular mechanics modeling of CNT bundle tensile failure (source: NASA).

Global production of CNTs, currently in excess of several thousand tons per year [*8*], has enabled their incorporation into various commercial products ranging from rechargeable batteries to sporting goods. Nevertheless, scalable manufacturing of organized macrostructures of CNTs, with the capacity to deliver the promised exceptional mechanical and electrical properties approaching those of the individual tubes, remains a largely unmet challenge. Moreover, it is imperative to develop process–structure–property relationships that enable design and optimization of CNT synthesis conditions to achieve target material performance for specific applications. Recent progress in the synthesis, characterization, and performance of aligned CNT materials was discussed, specifically pertaining to CNT forests and fibers (such as the CNT yarn in Figure 2). For example, analysis of CNT population dynamics during synthesis [*17*, *18*] yields a measure of diameter and alignment of CNTs as well as the number of CNTs at any position from the forest floor to canopy. Results indicate that CNT–CNT contacts are essential for forest growth, and that mechanical interactions between CNTs degrade properties. Several challenges in optimizing the synthesis of CNTs were highlighted. For example, more research efforts need to be focused on understanding how to ensure that a large fraction of catalyst particles are active for CNT growth and how to prolong their lives, to enable the synthesis of longer CNTs and thus improve the properties of fibers made from them. Automated, fully-instrumented growth systems, currently in short supply, would also be an attractive means to screen the multivariate parameter space involved in CNT synthesis and to identify optimum growth conditions for specific tube types [*19*]. Competitive growth mechanisms for individual CNTs should be investigated due to their effect on bulk-level CNT properties. To accelerate commercial adoption of CNT-related materials, quantitative models and characterization techniques must be used to build structure–process–property relationships. User facilities such as synchrotron x-ray facilities and microscopy centers (see nano.gov/userfacilities), along with finite element methods programmed with nanoscale contact and transport behavior, can be leveraged for these studies.

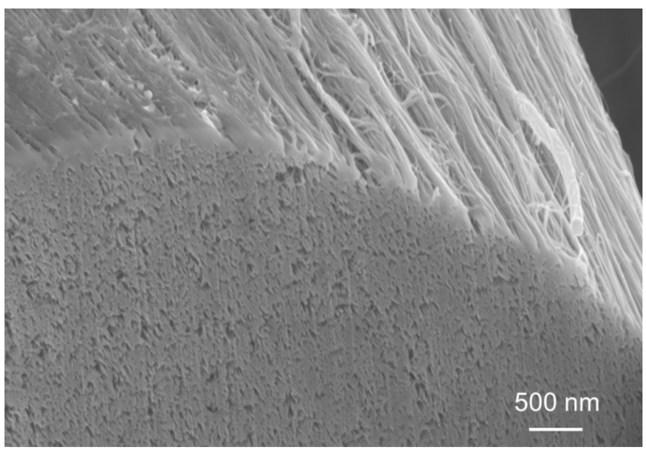

Figure 2. Scanning electron microscopy image of the cross-section of a CNT yarn (source: NASA).

One example of a structural and multifunctional application of CNTs is their use in improving the properties of conventional fiber materials [*20*, *21*]. Polyacrylonitrile (PAN) fibers exhibit dramatically reduced shrinkage, as well as dramatically reduced polymer molecular mobility, with the incorporation of CNTs. PAN fibers also become thermally and electrically conductive upon the incorporation of CNTs into the polymeric fiber [*22*, *23*]. Gel spinning and continuous carbonization facilities have been recently established in “class 1000” cleanrooms [*24*]. The facilities can produce up to 2000-filament tow carbon fibers. By adding carbon nanotubes in the PAN precursor fibers, carbon fibers can be produced with 100% higher thermal conductivity than current state-of-the-art carbon fibers [*25*]. Similarly, the inclusion of CNTs into polypropylene fibers induces crystallization, demonstrating the potential of converting commodity polymers into high-performance plastics [*26*]. Such polymer fibers exhibit vastly improved solvent and fatigue resistance [*27*]. CNTs also impart a high degree of electromagnetic wave absorption tailoring capability to polymeric fibers [*21*]. A number of technical issues required to make further improvements in the properties of polymeric and carbon fibers were discussed, including the opportunity to investigate the effects of CNTs as nucleation agents, and the need to improve the design of the PAN precursor [*27*]. In addition, much work remains to be done to understand the effect of CNTs on the ability to process polymeric materials. If these challenges are successfully addressed, a new generation of high-performance materials will be developed that can be processed by low-cost, mass-production methods.

CNTs have remarkable electrical, thermal, and mechanical properties, and thus are uniquely suited as building blocks for novel conductors [*28*, *29*]. However, many applications of nanoscale carbon to real-world problems have largely gone unrealized because of difficult and irreproducible material synthesis methods and laborious processing. Treating CNTs as hybrids between polymer molecules and colloidal particles and designing fluid-phase, directed assembly routes for soft conductors [*30*, *31*] can help overcome this hurdle. Even at minute concentrations, CNTs form complex fluid phases with intriguing properties. In crowded environments (e.g., gels), CNTs reptate like stiff polymers [*32*]; surprisingly, the small bending flexibility of CNTs strongly enhances their motion. CNTs can be solution-processed in strong acids, their sole true solvents.

At low CNT concentrations, these solutions can be used to make transparent, conducting, and flexible films and coatings [*33*], as well as highly porous, soft, three-dimensional structures (foams). At high concentrations, CNTs form liquid crystalline solutions [*34*] that can be scalably spun into high-performance multi-functional fibers (see Figure 3). These fibers combine high conductivity, strength, and the emergent property of softness; they are already finding their way into high-value applications such as aerospace electronics, high fidelity audio cables, and field emission devices [*35*]. As soft, exceptionally fatigue-resistant conductors, CNT fibers provide a natural interface to the electrical function of the human body as restorative sutures for electrically damaged heart tissue, electrodes for stimulating and sensing the activity of the brain, and replacements for nerve fibers [*36*, *37*]. Solution processing allows the direct coating of shielding conductors in coaxial cables. In test cases, directly coated CNT shielding meets the military attenuation standard (MIL-C-17) while rendering the shielding layer an essentially negligible fraction of the total mass of the cable. As an added benefit, the resistance of the cable to flex fatigue is also improved [*38*].

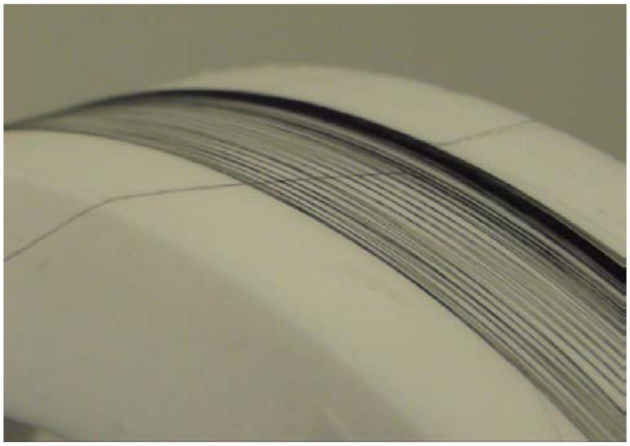

Figure 3. Image of wet-spun carbon nanotube fibers. The fibers on the drum are bundles of several fiber filaments with each filament having a diameter of approximately 25 micrometers (source: Rice University).

3. Summary of Key Challenges and Needs for Carbon Nanotube-Based Applications

The purpose of the breakout sessions at this meeting was to identify key technical challenges and research needs to enable the successful integration of CNTs into bulk materials or composites for commercial applications. Breakout sessions were grouped into four topical areas: modeling and simulation of bulk CNTs; synthesis and scaling; structural materials; and electrical materials. Key inputs from the breakout sessions are summarized in Table 1 below.

Table 1. Technical challenges and research needs identified during the breakout sessions

Topical Area	Key Challenge(s) for CNT-Based Applications	Suggested Research Needs
Modeling and Simulation	Limited modeling capabilities for simulating CNT properties in bulk form	• Better understanding of the interactions of individual tubes. • Improved coarse-grain models of bundled CNT structures. • Simulation techniques for probing and optimizing the alignment process in which entangled mats of CNTs are converted into oriented forms. • Databases for matching catalyst composition and size to the synthesis of specific types of CNTs.
Synthesis and Scaling	Poor yield, slow production rate, variations in material quality, and lack of real-time process control	• Production baseline for the highest volume of CNTs that can be produced for a certain set of quality specifications. • Better understanding of CNT growth mechanisms. • Robust, validated models of large-scale growth reactors. • Closed-loop process control of CNT production for specific material applications, including *in situ* diagnostics.
Structural Materials	Limited structural enhancements achieved using bulk CNTs or CNT-based composites	• Reliable, high-volume manufacturing of consistent, high-quality tubes to enable the necessary evaluation of these materials in applications. • Understanding of the mechanism for load transfer in structures from tube to tube, bundle to bundle, and matrix to tube/bundle. • Materials property databases to enable structural design with these materials. • Competitive life cycle costs from cradle to grave. • Accelerated technology insertion through efficient certification processes. • Understanding of the environmental, health, and safety (EHS) life cycle implications of CNTs early during product development to enable manufacturers to achieve regulatory clearance.

Topical Area	Key Challenge(s) for CNT-Based Applications	Suggested Research Needs
Electrical Materials	Limited impact of bulk CNTs in data and power distribution systems and in electrically conductive composites	• Demonstration of CNT conductivity that at least matches current standards (copper) while enabling weight reductions of 20% to 70%. • A niche transition product enabled by CNTs to bridge the gap while conductivity improvement takes place. • Understanding of the EHS life cycle implications of CNTs early during product development to enable manufacturers to achieve regulatory clearance.

Modeling and Simulation

As described in the Nanomanufacturing NSI white paper [*9*], a long-term vision for nanomanufacturing is to create flexible, "bottom-up" or "top-down/bottom-up" continuous assembly methods that can be used to construct elaborate systems of complex nanostructures. Advances in the CNT manufacturing enterprise depend on the enabling infrastructure of simulation and models, validated by experiment. A robust informatics infrastructure [*39*] means providing engineers with tools to optimize manufacturing processes and product performance, including capabilities to accelerate the launch of CNT-enabled products from prototypes [*40*]. Participants identified the following research needs to advance the state of progress in CNT-based simulations:

- Better understanding of the interactions of individual tubes, including nanotribology-based phenomena and the role of defects in tube–tube interactions, for modeling CNT properties in bulk form.
- Improved coarse-grain models of bundled CNT structures that take into account their interactions and traction forces, both in their ideal cylindrical form and when they are deformed.
- Simulation techniques for probing and optimizing the alignment process in which entangled mats of CNTs are converted into a highly oriented form with higher density and improved mechanical and electrical properties.
- A database for matching catalyst composition and size to the synthesis of specific types of CNTs.

Synthesis and Scaling

Although several methods have been established for the production of CNTs, efforts pertaining to the scale-up of CNT manufacturing processes still face ongoing challenges such as poor yield (e.g., low carbon utilization and rapid catalyst inactivation), slow production rate (e.g., low nucleation efficiencies), unacceptable variations in material quality, and lack of real-time process control. Unless overcome, these challenges will continue to significantly inhibit the maturation of CNT-based manufacturing, specifically related to batch-to-batch variability, high cost of production, and minimal market footprint. So far, research funding has focused primarily on the applications of CNTs. More research on the mechanisms of CNT growth and manufacturing scale-up would facilitate better control of material properties such as aspect ratio, chirality, and purity [*15*, *19*]. As for current production processes, standardized measurement methods could guide the quality assessment of CNTs. Participants identified the following needs to achieve scalable, controlled production of CNTs:

- A "production baseline" for the highest volume of CNTs that can be produced for a certain set of quality specifications.
- Better understanding of CNT growth mechanisms, specifically:
  - The kinetics of each synthesis step.
  - Nucleation efficiency.
  - Chiral selection.
  - Effect of catalyst system on CNT growth (catalyst, support, promoters, etc.).
  - Nucleation mechanisms for supported vs. floating catalysts.
  - Influence of experimental conditions (humidity, etc.) on CNT production processes.
  - Automated and autonomous experimentation as critical to discovering the fundamental growth mechanisms and exploiting them for commercial production.
- Robust, validated models of large-scale growth reactors.
- Closed-loop process control of CNT production for specific materials applications, including *in situ* diagnostics.
- Market studies on the potential applications of CNTs to identify market size, material quality requirements, required manufacturing volumes for various applications, and current state of technology and manufacturing readiness; and to assess the global competitive landscape (i.e., can CNTs be disruptive to specific market segments with regard to incumbent technologies?).
- Assessment of the technology gaps for application maturity versus supply chain maturity for nanotubes.
- Public-private consortia to advance the development of CNT-based products.

Structural Materials

Among the most notable properties of CNTs are their exceptional mechanical properties. The tensile specific strength and specific modulus of CNTs at the nanoscale are far higher than state-of-the-art light-weight structural materials such as carbon fiber. These properties, together with superior electrical and thermal conductivities, have led to speculation that carbon nanotubes will be a disruptive technology that can enable revolutionary structural concepts [*41*]. However, in the more than two decades since the novelty of CNTs was recognized, demonstrating these incredible nanoscale mechanical properties at the macroscale has been elusive. Much of the work in the area of structural nanocomposites has been confined to low-concentration CNT doping of polymeric matrices, with mechanical property enhancements being measured against polymer resin properties. While the resulting improvements relative to polymer properties are significant, they are still far below the properties required to realize the revolutionary concepts initially envisioned for this material. Participants identified the following needs to fully achieve the promise of CNT structural materials:

- Better understanding of the mechanism for load transfer in structures from tube to tube, bundle to bundle, and matrix to tube/bundle.
- Consistent tube quality.
- Reliable, high-volume manufacturing of high-quality tubes to permit the necessary evaluation of these materials in applications.
- Low-cost materials competitive with state-of-the-art materials.
- Materials property databases to enable structural design with these materials.
- Efficient certification processes to accelerate technology insertion.
- Competitive life cycle costs from cradle to grave.
- Better understanding of potential health and safety concerns associated with nanomaterials.

Electrical Materials

An important application area for bulk CNTs that has attracted considerable attention in recent years is electrical wiring. For example, several new commercial products have integrated CNTs into cable platforms for lightweight power applications [*38*]. Although a large parameter space exists for the electrical characterization of CNTs, specific applications should drive the set of required measurements. Key tests include voltage drop measurements, conductivity (direct current [DC] and alternating current [AC]), contact resistance, uniformity, and ampacity (current carrying capacity). Characterization requirements should span the development life cycle for a specific application area, to include measurement needs for early product development, reliability and uniformity measurements for integration, and standardized specifications to meet customer needs. Ongoing challenges remain in incorporating bulk CNTs into data and power distribution systems and into electrically conductive composites. Participants identified the following needs to achieve electrical applications of bulk CNTs:

- Demonstration of performance: at similar price points, conductivity of CNTs should at least match current standards (copper) while enabling weight reductions of 20% to 70%.
- Niche transition products to bridge the gap while efforts to improve conductivity take place, for example, by building a consortium around the development of CNT–copper hybrids.
- Understanding of the EHS risk perceptions of CNTs and the life cycle implications of CNTs early during product development to enable manufacturers to achieve regulatory clearance.

4. Realizing the Promise of Carbon Nanotubes

Improving the electrical and mechanical properties of bulk carbon nanotube materials (yarns, fibers, wires, sheets, and composites) to more closely match those of individual carbon nanotubes will enable a revolution in materials that will have a broad impact on U.S. industries, global competitiveness, and the environment. Use of composites reinforced with high-strength carbon nanotube fibers in terrestrial and air transportation vehicles could enable a 25% reduction in their overall weight, reduce U.S. oil consumption by nearly 6 million barrels per day by 2035 [*42*], and reduce worldwide consumption of petroleum and other liquid fuels by 25%. This would result in the reduction of CO_2 emissions by as much as 3.75 billion metric tons per year. Use of carbon nanotube-based data and power cables would lead to further reductions in vehicle weight, fuel consumption, and CO_2 emissions. For example, replacement of the copper wiring in a Boeing 777 with CNT data and power cables that are 50% lighter would enable a 2,000-pound reduction in airplane weight. Use of carbon nanotube wiring in power distribution lines would reduce transmission losses by approximately 41 billion kilowatt hours annually [*42*], leading to significant savings in coal and gas consumption and reductions in the electric power industry's carbon footprint.

The impact of developing these materials on U.S. global competitiveness is also significant. For example, global demand for carbon fibers is expected to grow from 46,000 metric tons per year in 2011 to more than 153,000 metric tons in 2020 due to the exponential growth in the use of composites in commercial aircraft, automobiles, aerospace, and wind energy [*43*]. Ultrahigh-strength CNT fibers would be highly attractive in each of these applications because they offer the advantage of reduced weight and improved performance over conventional carbon fibers.

This meeting identified a number of the technical barriers that need to be overcome to make the promise of carbon nanotubes a reality. A more concerted effort is needed to focus R&D activities towards addressing these barriers and accelerating commercialization. The development of application-specific, public–private partnerships is one way of providing that focus. This focus could be achieved by one or more institutes for manufacturing innovation such as those that are being established under the U.S. National Network for Manufacturing Innovation [*44*]. Such an approach would provide a vehicle to foster collaborations between the NNI, the Advanced Manufacturing National Program Office [*45*], and the Materials Genome Initiative [*46*]. Alternatively, successful models such as the Nanoelectronics Research Initiative [*47*] could be adapted to leverage resources and capabilities within the Federal Government, industry, and universities to tackle these challenges.

The outcomes from this meeting will inform the future directions of the NNI Nanomanufacturing Signature Initiative and provide specific areas that warrant broader focus in the CNT research community.

Appendix A. Meeting Materials

Meeting Agenda[2]

8:00 Registration and Networking

8:30 Welcome Remarks and Overview: Dr. David W. Miller, National Aeronautics and Space Administration

8:45 Plenary Presentations
- Modeling and Simulation: Dr. Boris Yakobson, Rice University
- Synthesis and Scaling: Dr. John Hart, Massachusetts Institute of Technology

10:15 *Coffee Break*

10:45 Plenary Presentations (Cont.)
- Structural Materials: Dr. Satish Kumar, Georgia Institute of Technology
- Electrical Materials: Dr. Matteo Pasquali, Rice University

12:15 Charge to Breakout Participants

12:30 *Lunch*

13:30 Parallel Breakout Sessions
- Modeling and Simulation session (Concourse level, room CU21)
  - Session Chair: Dr. Kristopher Wise, National Aeronautics and Space Administration
- Synthesis and Scaling session (Main level, Glennan Conference room 1O35)
  - Session Chair: Dr. Benji Maruyama, Air Force Research Laboratory
- Structural Materials session (Concourse level, room CU24)
  - Session Chair: Dr. Emilie Siochi, National Aeronautics and Space Administration
- Electrical Materials session (Main level, STMD small conference room 6W50)
  - Session Chair: Dr. Stefanie Harvey, TE Connectivity Ltd.

15:30 *Coffee Break*

16:00 Report Out

17:00 Summary and Next Steps: Dr. J. Alex Liddle, National Institute of Standards and Technology, and Dr. Michael Meador, National Aeronautics and Space Administration

17:30 *Adjourn*

Discussion Points Considered in Breakout Sessions

a. Modeling and Simulation of Bulk CNT Materials:
- What are the limitations to modeling properties of bulk CNT materials?
- How good are the correlations between modeling and experiment?
- What needs to be done to close the gap in accuracy?

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[2] Links to speakers' biographies are available at www.nano.gov/2014CNTTechInterchange.

- What specific material properties are needed and to what level of detail?
- How should we simulate scaled synthesis of CNTs?
- Given the extremely complex, inhomogeneous, multiscale structure of bulk CNT materials, what is the minimum volume of material that must be simulated in order to predict converged bulk properties?
- What advances in theory and simulation will be required to model a bulk CNT system of this size?
- Can we identify which types of models (MD, FEM, etc.) have worked better than others and why?
- Is there any prospect of getting more comprehensive experimental structural information than what is provided by current microscopy and scattering techniques?
- What set of static and dynamic material properties should be used for verification and validation of predicted properties?
- How can we use tools and resources coming from the Materials Genome Initiative to further modeling of nanotube-based materials?

b. Synthesis and Scale-Up

- What are the remaining challenges to developing scaled-up synthesis that can deliver CNTs with controlled aspect ratio, selective chirality, and high purity? What level of control is required for specific applications?
- What fundamental science is left to understand CNT growth mechanisms and their control? Why do most catalyst particles not grow nanotubes? How can we investigate this using simulations?
- What measurements are the basic measurements necessary to specify quality?
- What drives batch-to-batch variability? What should be done to reduce it?
- What metrologies are required?
- What is the “Killer App” to realize large-scale production? Is there a government role?
- What is the current state of U.S. manufacturing capability associated with this technology within the TRL/MRL metrics?
- What is the likelihood that this technology could generate significant cost share to match a government investment?

c. Structural Materials

- Based on the current state of science, which mechanical properties do CNTs have the most potential for improving over the state of the art in load-bearing applications? What are the barriers to achieving these mechanical properties? What CNT characteristics are required to enable these properties?
- How could CNT synthesis and composite manufacturing methods be modified to enable the retention of properties mentioned above on the large scale?
- What unique challenges are there in incorporating bulk CNTs (e.g., sheets, yarns) into composite materials in order to help realize the desired applications? How can these challenges be addressed?
- What are the prospects for developing multifunctional materials from CNT composites? What CNT properties can be exploited to realize this? What are the technical barriers to optimizing these properties in bulk materials?
- What metrologies are required for initial and long-term properties? Are they different for CNT composites? Can we model initial and long-term structural properties?

d. Electrical Materials

- What measurements are required for electrical characterization?
- Why haven't we achieved the anticipated electrical properties of individual CNTs in bulk form (e.g., yarns, sheets, and cables)? What can we do to enable this to happen?
- How could CNT synthesis methods be modified to improve the situation?
- What unique challenges are there in incorporating bulk CNTs (sheets, yarns) into data and power distribution systems and electrically conductive composites in order to help realize the desired applications?
- How do we get to IBM 5-9's semiconducting purity?
- Can conductivity improvements be made across physical scale (nano, micro, meso, macro)?
- Can mixing aspect ratios (CNT + graphene) reduce loading % and increase conductivity?
- Could a CNT/metal hybrid bridge the gap while conductivity improvement takes place? At what scale does the hybridization occur (nano, micro, meso, macro)?

Appendix B. Meeting Participants[3]

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[3] NOTE: Participants' affiliations are as of the date of the workshop.

Appendix C. List of Acronyms

AFRL	Air Force Research Laboratory
AMNPO	Advanced Manufacturing National Program Office
CNT	carbon nanotube
EHS	environment(al), health, and safety
EPA	Environmental Protection Agency
FEM	finite element methods (models/simulations)
MD	molecular dynamics (models/simulations)
MRL	Manufacturing Readiness Level
NASA	National Aeronautics and Space Administration
NIST	National Institute of Standards and Technology
NMSP	Nanoscale Materials Stewardship Program (EPA)
NNCO	National Nanotechnology Coordination Office
NNI	National Nanotechnology Initiative
NRL	Naval Research Laboratory
NRO	National Reconnaissance Office
NSET	Nanoscale Science, Engineering, and Technology Subcommittee of the National Science and Technology Council' s Committee on Technology
NSF	National Science Foundation
NSI	Nanotechnology Signature Initiative
NSTC	National Science and Technology Council
PAN	polyacrylonitrile
R&D	research and development
RXMS	Propulsion, Structures and Manufacturing Enterprise Branch (AFRL Materials and Manufacturing Directorate, Manufacturing and Industrial Technologies Division)
TRL	Technology Readiness Level

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