Nanomaterials by Design – R&D Priorities for Nanotechnology Commercialization

Presented at SME Conference on Nanotechnology and Manufacturing

August 23, 2006

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OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

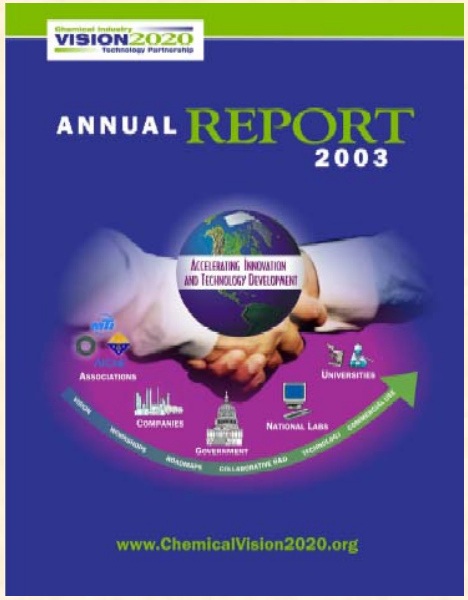
Overview

- **Nanomaterials by Design R&D Roadmap**
- **Roadmap Implementation**
  - **Nanotechnology working groups**
  - **Nanotechnology projects**
  - **Chemical-semiconductor industry joint efforts**
- **Example Project**

Chemical Industry Vision2020

In 1997, the U.S. DOE in concert with the chemical industry - represented by CMA (now ACC), SOCMA, ACS, AIChE, and the CCR - created Vision 2020 *"to outline a path of research, development, and technology demonstration for the chemical industry to continue as the global leader into the next century."*

In 2003, nearly 150 industry, academic and government organizations participated in Vision 2020 activities



Chemical Industry VISION2020 Technology Partnership

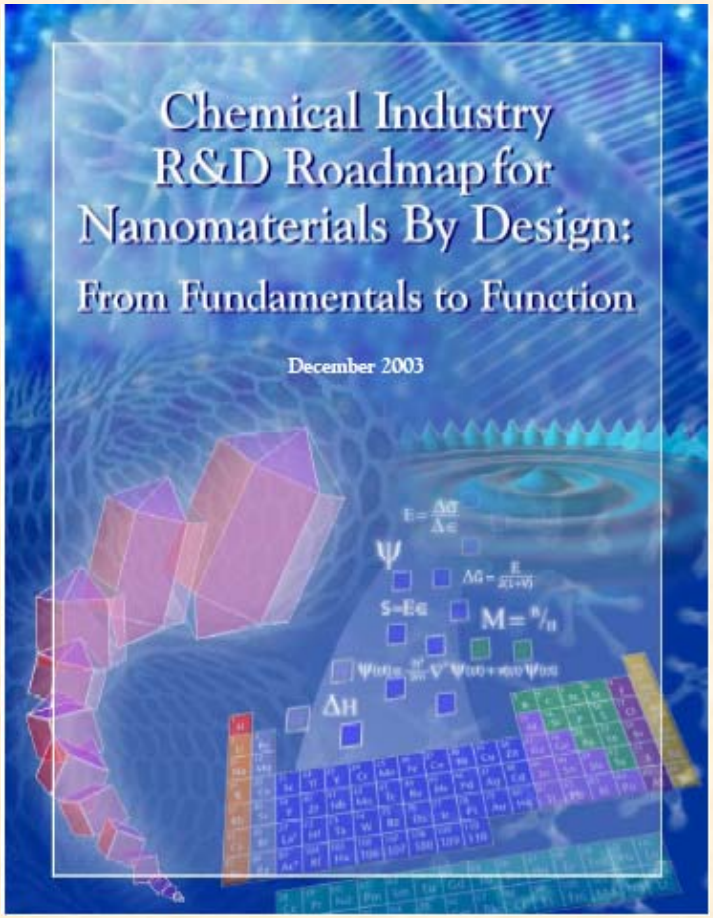
An industry-led program to accelerate technology development and innovation by leveraging technical and financial resources

- Air Products & Chemicals Inc.
- BP
- Cargill
- Ciba Specialty Chemicals
- The Dow Chemical Company
- E.I. du Pont de Nemours and Company
- Eastman Chemical Company
- General Electric Company
- Honeywell
- Praxair, Inc.
- Rohm and Haas Company
- American Chemical Society
- American Institute of Chemical Engineers
- Council for Chemical Research
- Materials Technology Institute

Visit us at www.ChemicalVision2020.org

Chemical Industry R&D Roadmap for Nanomaterials by Design

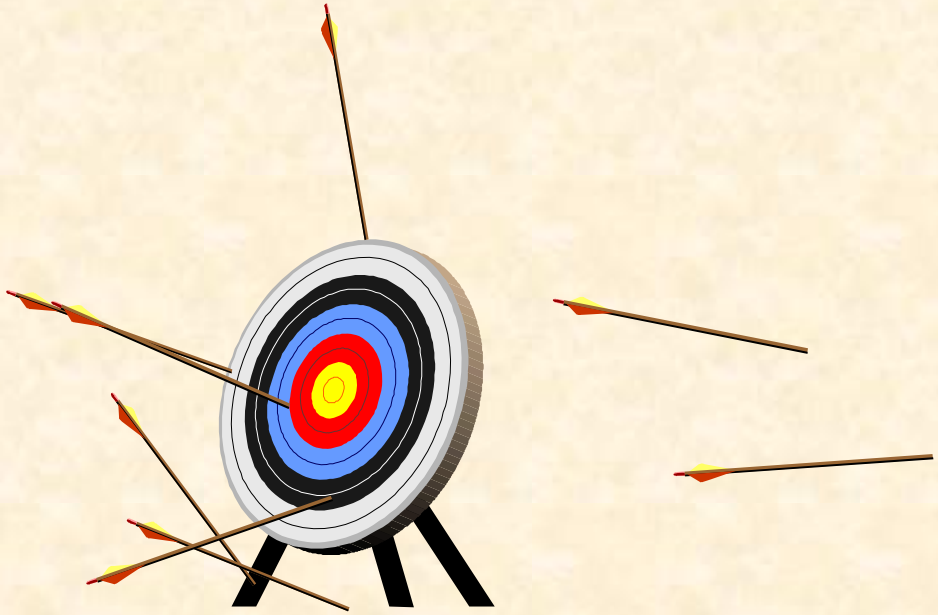
- NNI and DOE partnered with Vision 2020 to develop an R&D roadmap
- Objective to provide industrial perspective on activities to accelerate commercialization
- Over 100 participants in workshop - Oct. 2002
- Roadmap published in Dec. 2003



www.chemicalvision2020.org/nanotechnology.html

A New Strategic Approach

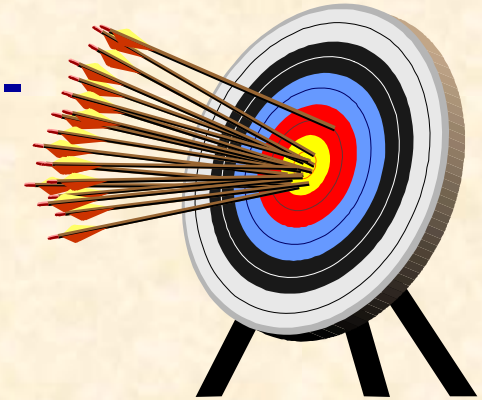
Discovery-based Product Development



Time

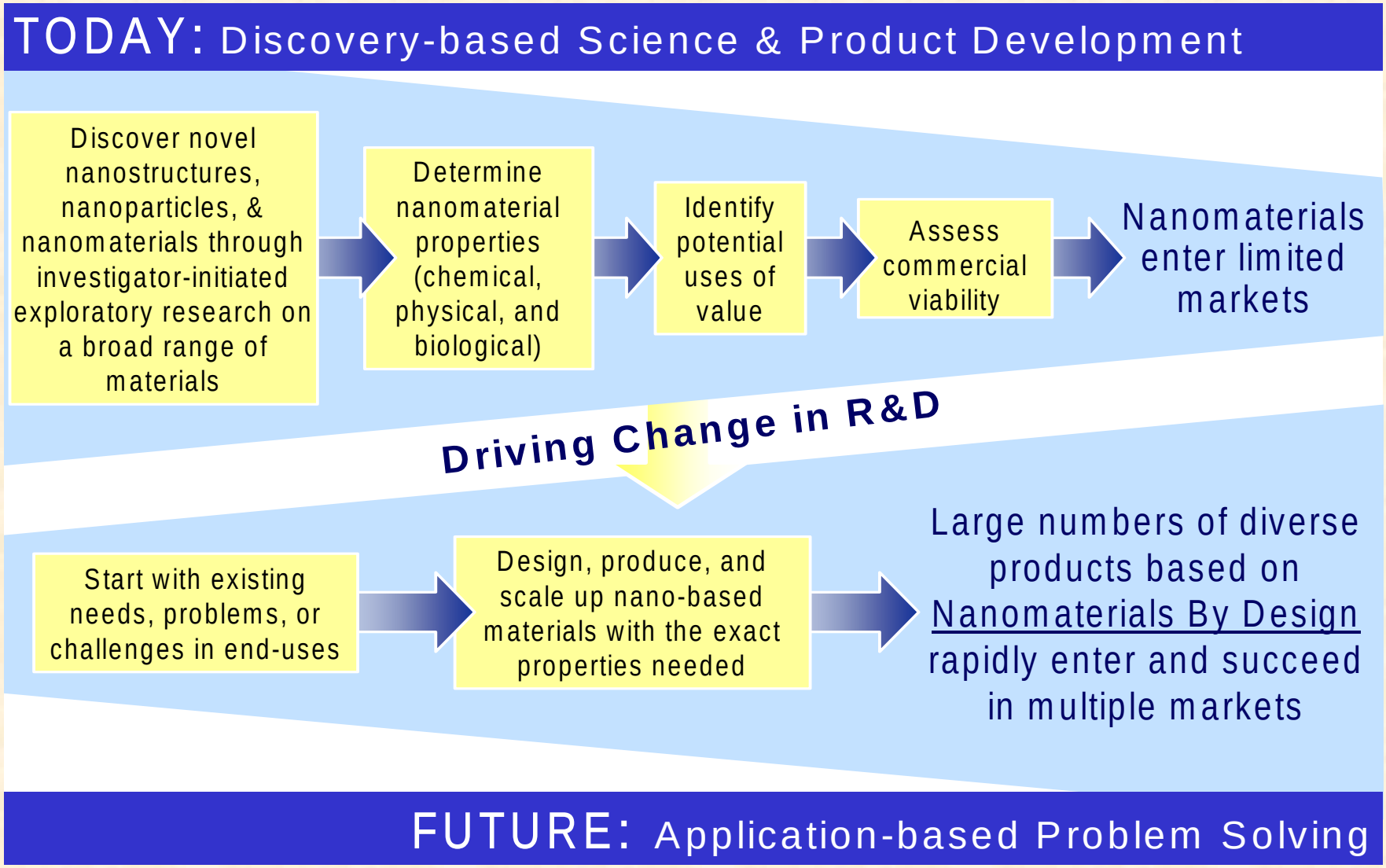
Nanomaterials By Design

Application-based Problem Solving

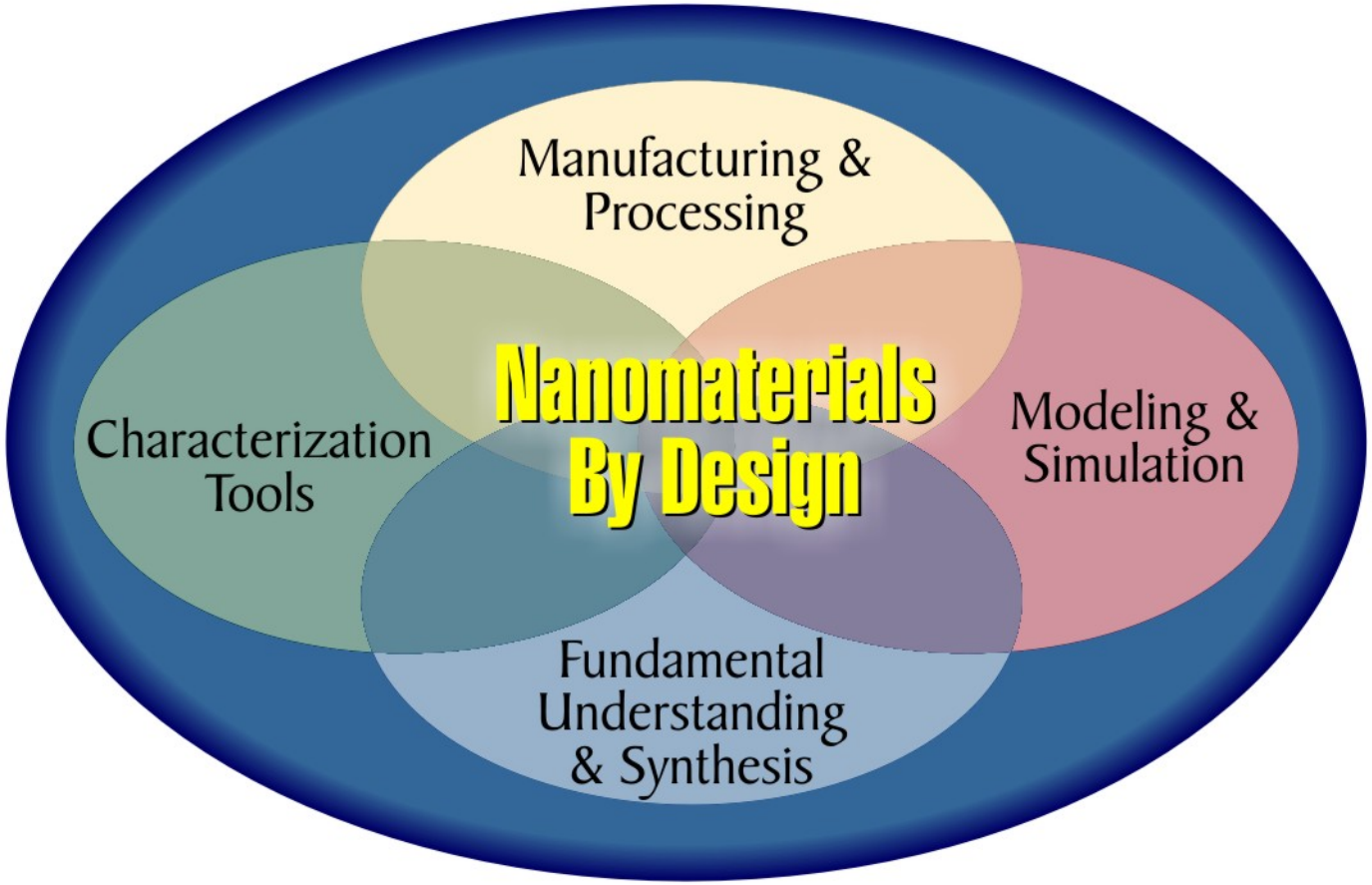


Time

The Roadmap Vision: Nanomaterials by Design



Implementation of Roadmap Strategy: Multidisciplinary, Interdependent, R&D Integrated From Fundamentals to Function



Priority Research Requirements

- Report identified over 30 priorities in 9 categories
- Specific recommendations were offered to bolster the effectiveness of the strategy
- Ultimate goal:

  "accelerated commercialization of innovative technology based on nanomaterials"

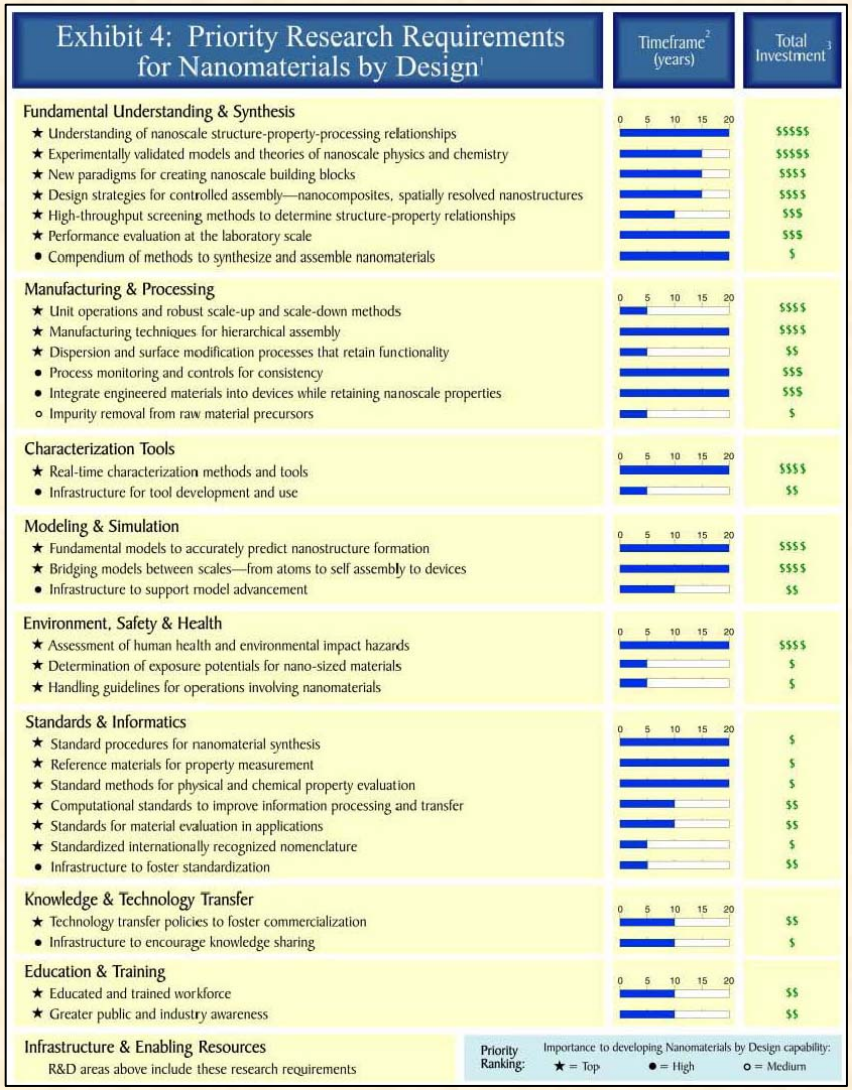


Exhibit 4: Priority Research Requirements for Nanomaterials by Design[1]	Timeframe[2] (years)	Total Investment[3]
Fundamental Understanding & Synthesis		
★ Understanding of nanoscale structure-property-processing relationships		$$$$$
★ Experimentally validated models and theories of nanoscale physics and chemistry		$$$$$
★ New paradigms for creating nanoscale building blocks		$$$$
★ Design strategies for controlled assembly—nanocomposites, spatially resolved nanostructures		$$$$
★ High-throughput screening methods to determine structure-property relationships		$$$
★ Performance evaluation at the laboratory scale		$$$
● Compendium of methods to synthesize and assemble nanomaterials		$
Manufacturing & Processing		
★ Unit operations and robust scale-up and scale-down methods		$$$$
★ Manufacturing techniques for hierarchical assembly		$$$$
★ Dispersion and surface modification processes that retain functionality		$$
● Process monitoring and controls for consistency		$$$
● Integrate engineered materials into devices while retaining nanoscale properties		$$$
○ Impurity removal from raw material precursors		$
Characterization Tools		
★ Real-time characterization methods and tools		$$$$
● Infrastructure for tool development and use		$$
Modeling & Simulation		
★ Fundamental models to accurately predict nanostructure formation		$$$$
★ Bridging models between scales—from atoms to self assembly to devices		$$$$
● Infrastructure to support model advancement		$$
Environment, Safety & Health		
★ Assessment of human health and environmental impact hazards		$$$$
★ Determination of exposure potentials for nano-sized materials		$
★ Handling guidelines for operations involving nanomaterials		$
Standards & Informatics		
★ Standard procedures for nanomaterial synthesis		$
★ Reference materials for property measurement		$
★ Standard methods for physical and chemical property evaluation		$
★ Computational standards to improve information processing and transfer		$$
★ Standards for material evaluation in applications		$$
★ Standardized internationally recognized nomenclature		$
● Infrastructure to foster standardization		$$
Knowledge & Technology Transfer		
★ Technology transfer policies to foster commercialization		$$
● Infrastructure to encourage knowledge sharing		$
Education & Training		
★ Educated and trained workforce		$$
★ Greater public and industry awareness		$$
Infrastructure & Enabling Resources		
R&D areas above include these research requirements		

Major Roadmap Recommendations

- **Implement effective protocols to assure health and safety in nanomaterial R&D, production, transport, use, and disposal.**
- **Invest significantly and concurrently in the priority R&D areas—fundamentals, synthesis, manufacturing, characterization, and modeling.**
- **Facilitate intensive coordination and integration among these interdependent and multidisciplinary research areas.**
- **Work with NSET to develop effective means of collaboration between NSET and the U.S. chemical industry to foster effective roadmap implementation.**
- **Encourage NSET to adopt this roadmap as a core strategy for its Grand Challenge in Nanomaterials By Design.**

Roadmap Implementation

Chemical Industry Consultative Board for Advancing Nanotechnology (NNI-ChI CBAN)

- **Partnership established in May 2004**
  - **National Nanotechnology Initiative**
  - **Council for Chemical Research**
  - **Chemical Industry Vision2020**
- **Purpose**
  - **Identify and promote new R&D in key areas**
  - **Expand nanotechnology R&D in industry and academia**
  - **Enhance communication**
- **Working Groups**
  - **Research Focus**
  - **ES&H Focus**
  - **Joint Semiconductor Industry CBAN Teams**

NNI-ChI CBAN working groups have broad participation by industry, government and NGOs

Research Focus Working Group

Don Anthony, CCR
Jim Murday, DOD

Art Ellis, NSF
Rick Barto, Lockheed Martin
John Carberry, DuPont
David DePaoli, ORNL
Rajeev Gorowara, DuPont
Bill Grieco, Rohm & Haas
Geoffrey Holdridge, NNCO
Katie Hunt, Rohm & Haas
John Miller, DOE
Miodrag Oljaca, Cabot
Mike Roco, NSF/NSET
James Rudd, NSF
Douglas Rundell, BP
Cheryl Sabourin, GE
John Sargent, DOC
Glenn Schrader, NSF
Peter Shirmann, Ciba
Robert Shull, NIST
Kevin Snow, Honeywell
Jack Solomon, Praxair
Bryan Tweedy, ACS
Brian Valentine, DOE
Hank Whalen, ACS

NNI-ChI CBAN working groups have broad participation by industry, government and NGOs

ESH Working Group

Emory Ford, MTI

Barbara Karn, EPA

Larry Andrews, Rohm and Haas	Monika Maier, Degussa
John Carberry, DuPont	John Miller, DOE
John DiLoreto, ACC	Vladimir Murashov, NIOSH
David DePaoli, ORNL	Elizabeth Nesbitt, USITC
Bronek Drozdowicz, Air Products	Ravi Prasad, Praxair
Geoff Holdridge, NNCO	Mike Roco, NSF/NSET
Steven Kinsler, Intel	Nora Savage, EPA
Fred Klaessig, Degussa	John Small, NIST
Kristen Kulinowski, Rice Univ.	Jack Solomon, Praxair
Tim Landry, Dow	Clayton Teague, NNCO
Stephen Lingle, EPA	David Warheit, Dupont
Don Marlow, FDA	Al Wiedow, Ciba

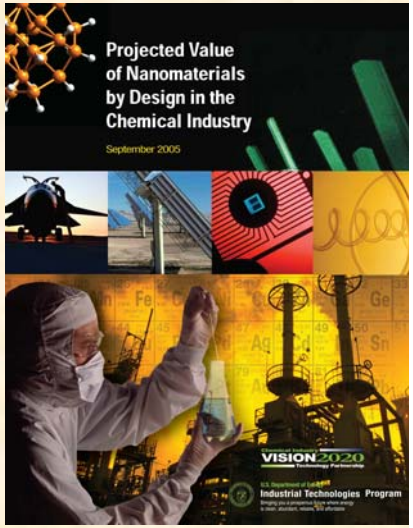
DOE Industrial Technologies Program has supported NNI-ChI CBAN efforts

- **Nanotechnology Benefits Analysis**
- **Responsible Development of Nanotechnology**
  - **EHS Database**
  - **R&D Recommendations for EHS**
- **Nanomaterials by Design Roadmap Implementation**

- **Real-Time Nanoparticle Characterization project**

Vision2020/LANL Benefits Study

- **Study by Los Alamos National Laboratory**
- **Methodology**
  - **Identify nanomaterials impact (e.g., cost savings, yield improvements) for key industrial applications**
  - **Use REMI model to estimate economic effects**
  - **Narrow set of materials**
    - **Catalysts**
    - **Coatings**
    - **Membranes**
  - **Limited set of applications**
    - **Chemicals, petroleum refining and natural gas production, automotive, maritime, manufacturing**



- **Projected Impact:**
  - **Value Creation: $10-20 billion/year**
  - **Energy Savings: 0.5-1.1quadrillion BTU/year**
  - **GNP increase: $30 – 63B**
  - **Employment increase: 455,000 – 975,000 jobs**

http://www.chemicalvision2020.org/pdfs/LANL Nano Rept Final 4-17-06.pdf

Responsible Development of Nanotechnology

Responsible Development R&D Needs

- **Recommendations on R&D directions**
  - **Toxicity of Nanomaterials**
  - **Measurement and Detection of Nanomaterials**
  - **Worker Protection and Industrial Hygiene**

- **Joint Semiconductor Research Corporation CWG5 Research Challenges**
  - **Metrics for nanoscale particle toxicity**
  - **Exposure monitoring methodologies**
  - **Risk assessment methodology**
  - **Testing strategy for toxicity**
  - **Societal communication and education**

Chemical Industry VISION2020 Technology Partnership

SRC

Joint NNI-ChI CBAN and SRC CWG5 Nanotechnology Research Needs Recommendations

http://www.chemicalvision2020.org/pdfs/cban_recommendedtopics.pdf
www.src.org/member/news/snb_12_06_05.asp?bhcp=1

Nanomaterials ESH Literature Database

AUTHOR	TITLE	JOURNAL	PI
	Nano's Troubled Waters: Latest toxic warning shows nanoparticles cause br	Genotype, Thursday, 1 April 2004	
Alberti G, Casciola M, Pica	Preparation of nano-structured polymeric proton conducting membranes for ι	Ann N Y Acad Sci. 2003 Mar;984:208-25. Review.	PMID: 1
Allemann E, Gurny R, Doel	Distribution, kinetics, and elimination of radioactivity after intravenous and int	J. Controlled Release; Vol 28 ISS Feb 1994	
Allemann E, Gurny R, Doel	Distribution, kinetics, and elimination of radioactivity after intravenous and int	J. Controlled Release; Vol 28 ISS Feb 1994	
Allen TM			PMID: 1
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Alyau			PMID: 1
Ande			PMID: 1
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Balint			PMID: 1
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Barro			
Beck			PMID: 8
Benn			PMID: 1
Bhad			PMID: 1
Blago			PMID: 1
Boeh			PMID: 1

- **Generated by Borges et al., ORNL**
- **Most comprehensive public database**
  - Initially 1,342 records for pertinent articles on ES&H issues related to nanoscale materials
- **Transferred to Rice Univ. CBEN**
  - Web-accessible through ICON **(International Council on Nanotechnology)** site
    - http://icon.rice.edu/research.cfm
  - Living database
    - On-line comment/input capability
- **Current focus of ICON efforts**
  - Generated roadmap for improving and expanding
  - Currently summarizing existing information

Database has been acknowledged broadly

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Nanotechnology Database Focuses on Safety Questions

The International Council on Nanotechnology (ICON) and Ric
19 launched the world's first online database of scientific find

Dennis Kucinich

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Nano coalition unveils environmental

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The International Council on Nanotechnology (ICON) and Ri
Biological and Environmental Nanotechnology (CBEN) today laun
database of scientific findings related to the benefits and ris
database can be accessed at http://icon.rice.edu/research

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outdoor use

This environmental health and safety (EHS) database marks th
and diverse scientific literature on the impacts of nanoparticles,
with dimensions measuring between 1 and 100 nanometers a
thousands of atoms. (One nanometer is one-billionth of a mete
smaller than the width of a human hair.) The database is the
Rice researchers, the chemical industry and the U.S. Departm
be updated and enhanced over the next year.

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p. 33
SCIENCE & TECHNOLOGY

Nano Database Goes Online

Collection of papers on environmental and health impacts of nanomaterials is the first of its kind

Bethany Halford

Sorting through the scientific literature on the environmental and health impacts of nanomaterials can be downright confusing. Because nanoscience cuts across many disciplines, a report on the toxicity of fullerenes, for example, is as likely to be published in a chemistry-heavy journal like *Nano Letters* as it is to be reported in *Environmental Health Perspectives*.

Related Stories

- Nanomaterials: Safe Or Unsafe? C&EN, Apr. 28, 2003
- Nanotechnology Under The Scope C&EN, Dec. 9, 2002
- NanoFocus C&EN Archive

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What the ICON EHS Database Contains:

The ICON Environmental, Health and Safety (EHS) database contains summaries (abstracts) and citations for research papers related to the EHS implications of nanoscale materials. This database was developed initially by Dr. Tim Borges and Ms. LeeAnn Wilson at Oak Ridge National Laboratory - Learn more.

This database includes only abstracts or summaries of the papers. Some entries have links to full papers, although site registration or payment may be required to access the full content of many of these articles. Feedback on the database is welcome and can be provided via the addition/correction link.

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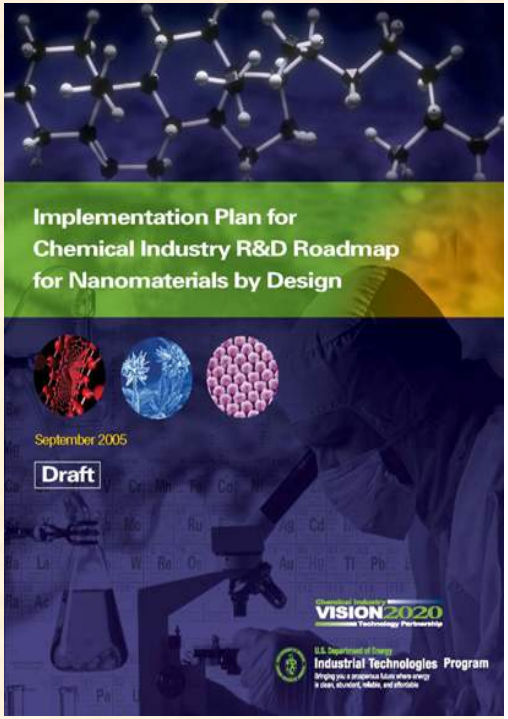
Implementation Plan

Implementation Plan Effort

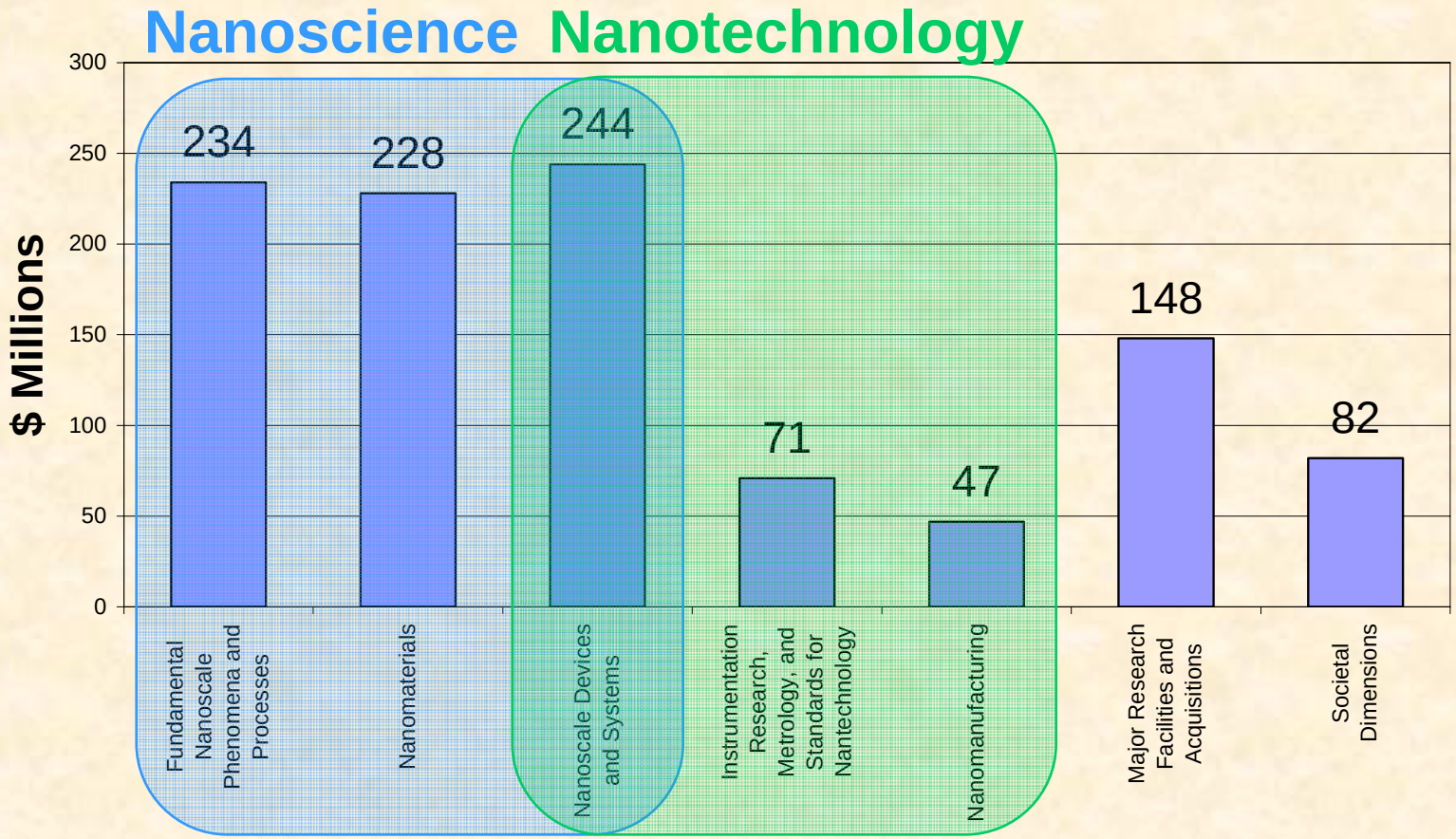
Goal: To provide a detailed implementation plan for the R&D Roadmap

- **Workshop held Feb 15, 2005 in Baltimore**
- **Identified key industry needs over next five years and provided next level of detail to the roadmap**
- **Project team commissioned to identify appropriate agencies for each aspect and develop interactions**
  - **National Laboratories**
  - **NSF Nanomanufacturing Center**
  - **Industrial Steering Team**
    - **20 companies**
- **Chemical-semiconductor joint teams**

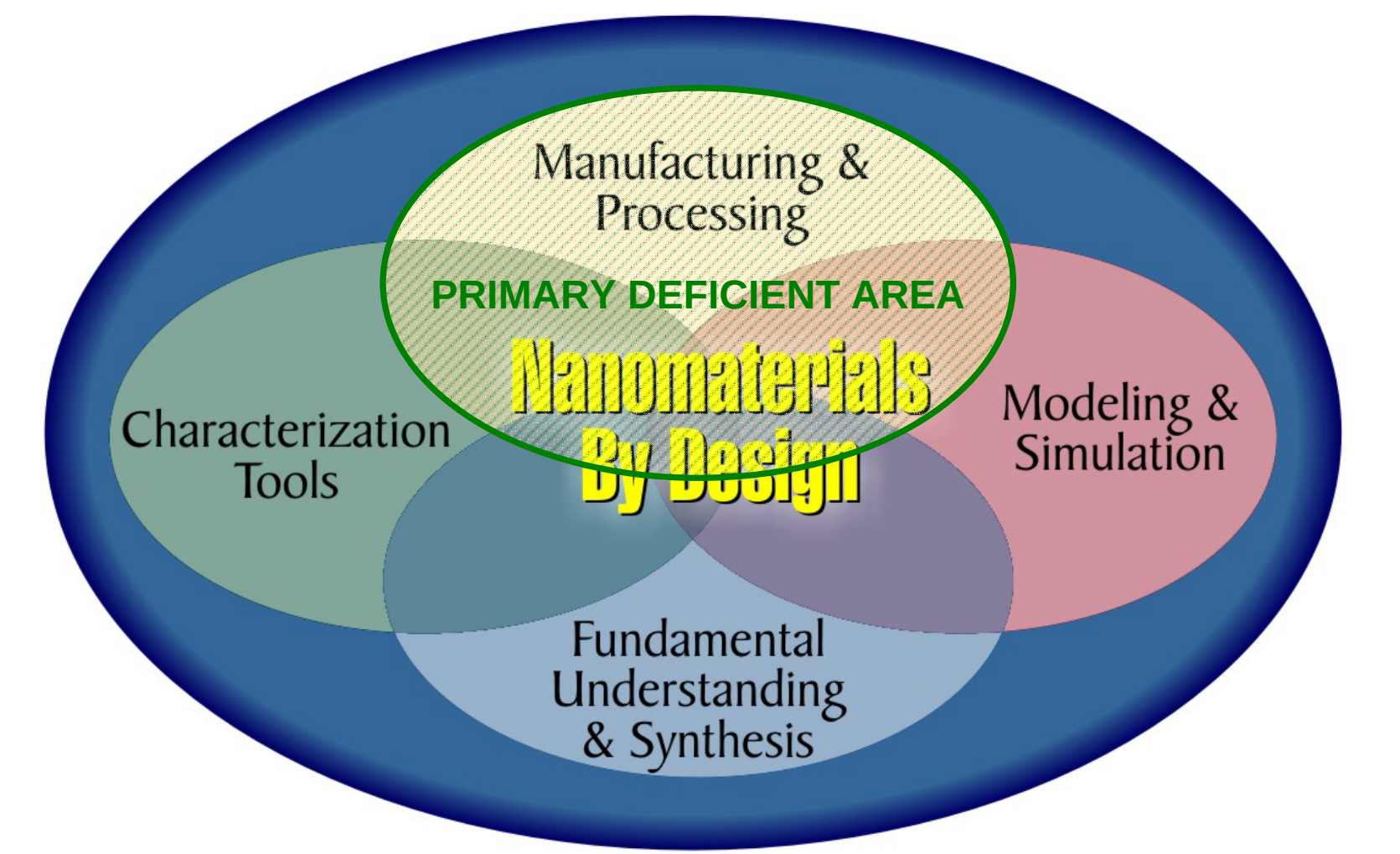


NNI Investment Favors Nanoscale Science

FY 2006 Requested Funding by Program Component Area



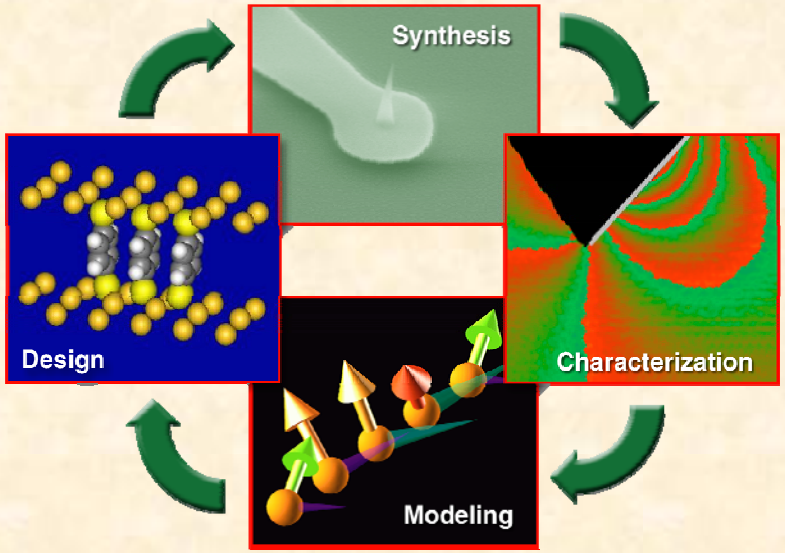
Issues for Commercialization: The Chemical Industry View



Strong intersection of needs in manufacturing & processing!

Nanomanufacturing R&D: a Major Need

Nanoscale Science R&D
$777M
NSF, DOD, DOE BES, NIH, NIST, NASA…



Nanomanufacturing R&D
$47M
NSF, NIST, DOD

Manufacturing & Processing

Develop unit operations & robust scale-up methodologies for manufacturing
- Synthesis
- Separation
- Purification
- Stabilization
- Assembly

Characterization

Develop real-time tools for process monitoring & control

Commercialization

Priority R&D Needs for Nanotechnology Commercialization

Nanoscale science

Synthesis and Assembly

Develop new paradigms to create nanoscale building blocks

Develop approaches for controlled assembly of nanocomposites and nanostructures

Characterization tools

Develop analytical tools for measuring and characterizing nanomaterials

Modeling and Simulation

Develop models of nanomaterials processing and predict bulk properties of materials that contain nanomaterials

Bridge models between scales, from atoms to self-assembly to devices

Nanotechnology

Manufacturing & Processing

Develop unit operations and robust scale-up and scale-down methodologies for manufacturing

- Synthesis
- Separation
- Purification
- Stabilization
- Assembly

Characterization tools

Develop real-time tools for measuring and characterizing nanomaterials, particularly online and in-process

Chemical Industry Application Areas

Catalysts, coatings, ceramics, sorbents, membranes

Manufacturing & Processing Research Needs

- **Integrated manufacturing and separations processes for consistent, large scale manufacture of <u>carbon nanomaterials</u>**
  - **High purity and low cost processes**
  - **Better catalysts for improved yield**
  - **Better control of tube chirality, diameter, length**
  - **Improved separations to ensure product purity**

- **Integrated manufacturing processes to deliver lower cost <u>metal and metal-oxide nanoparticles</u> at high purity**
  - **Improved control of particle morphology (size/shape)**
  - **Powder collection techniques that prevent particle agglomeration**

Manufacturing & Processing Research Needs

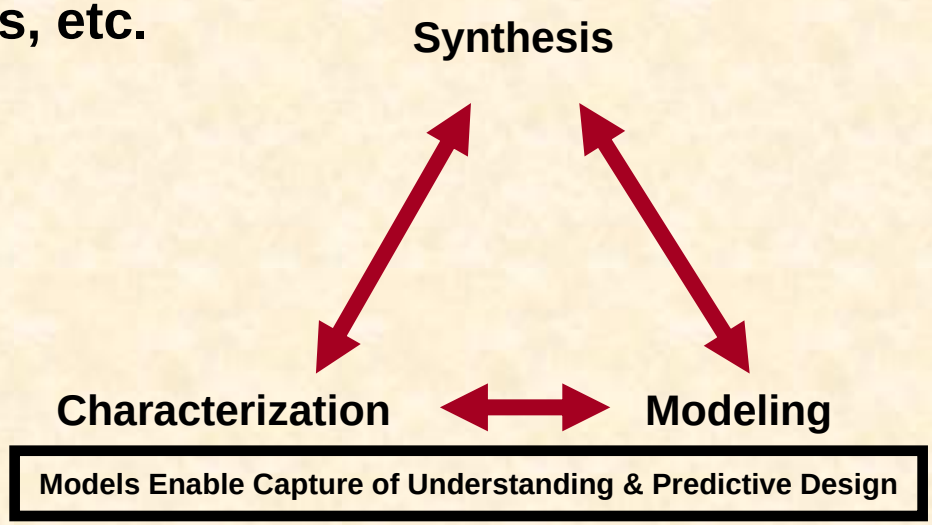
- **Integration of real-time characterization techniques for on-line process monitoring and process control**
  - **Optical and spectroscopic analyses for particle size distribution**
- **Scale-up of self-assembly processes for practical use commercial scale unit operations**
  - **Apply current lab/pilot scale techniques of molecular or biological self-assembly to larger scale processes**
  - **Develop appropriate *in situ* diagnostics and process control schemes to ensure consistent, low cost manufacture of nanostructures using these processes**

Metrology & Characterization:
Key Needs for Manufacturing

- **Characterization of nanotube electronic properties (bulk CNT samples)**
  - **Bandgap distribution**
  - **Could be useful for characterizing other nanoparticles**
  - **On wafers or as-grown**
- **On-line particle characterization (1-50 nm)**
  - **Particle size distribution**
  - **Particle surface morphology distribution**

Modeling Research Needs

- **Effect of synthesis and self assembly conditions on nanostructure and composition**
- **Correlation of nanostructure and composition**
- **Quantitative nanomaterial structure – property correlations**
  - **e.g. CNTs, interfaces, contacts, etc.**
- **New metrology capabilities**



Modeling Needs – Infrastructure

- **Innovative algorithms to model over multiple length and timescales for realistic system sizes**
  - **More foundational long-term algorithm development is needed**
- **Models experimentally validated**
- **Systematic experiments that develop fundamental understanding**
  - **Metrology to characterize structure and properties**
- **Increased access to high-speed computing capabilities**
- **Improved portability of models on existing computing platforms**

Modeling Needs – Technical

- **Designed Synthesis of Nanostructured Materials**
- **Nanomaterial Surface Chemical Reactivity**
- **Nanomechanical & Interface Properties**
- **Electronic Properties & Transport**
- **Self-Assembled Material Properties**
  - **Mechanical, electronic, chemical reactivity, and magnetic**

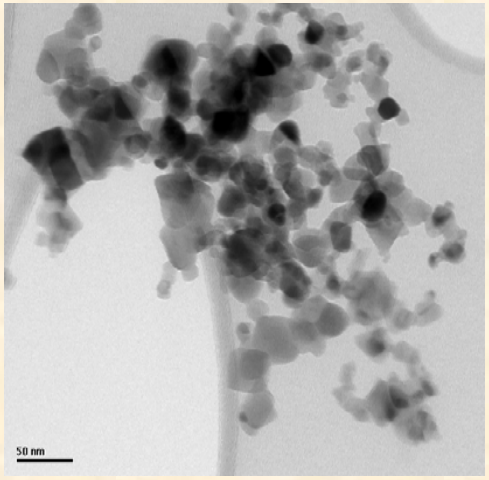
Example Project – Advancing Nanomanufacturing

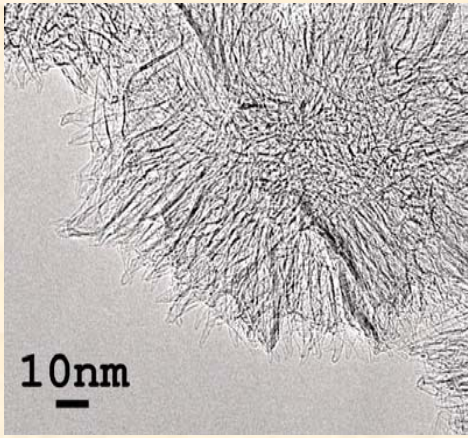
Addressing Real-Time Characterization Need: DOE MPLUS project

- **Project initiated by Materials Subprogram of DOE Industrial Technologies Program**
- **PI – Emory Ford, Materials Technology Institute**
- **Involves ORNL team of R&D experts**
  - **Chemical engineers, physicists, materials scientists, aerosol scientists, and microscopists**
- **Focus: Address priority need identified by chem-semi teams in characterization for nanomanufacturing:**
  - **Real-time, on-process monitoring of nanoscale materials in gas-phase synthesis processes**

Demonstrate Capability of Differential Mobility Analyzer for On-Line Nanoparticle Sizing

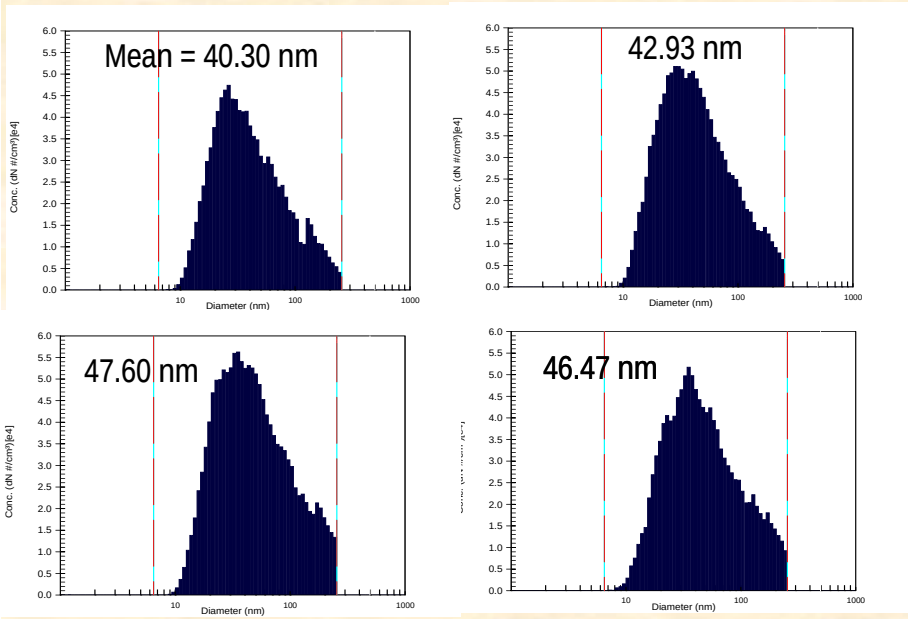
- Test Systems
  - **TiO_2 by chemical vapor deposition**
  - **Carbon nanoparticles by laser ablation**
- Comparison Metrics
  - **Real-time size distribution < 100 nm**
  - **Ability to detect changes in process**
  - **Verification using EM**



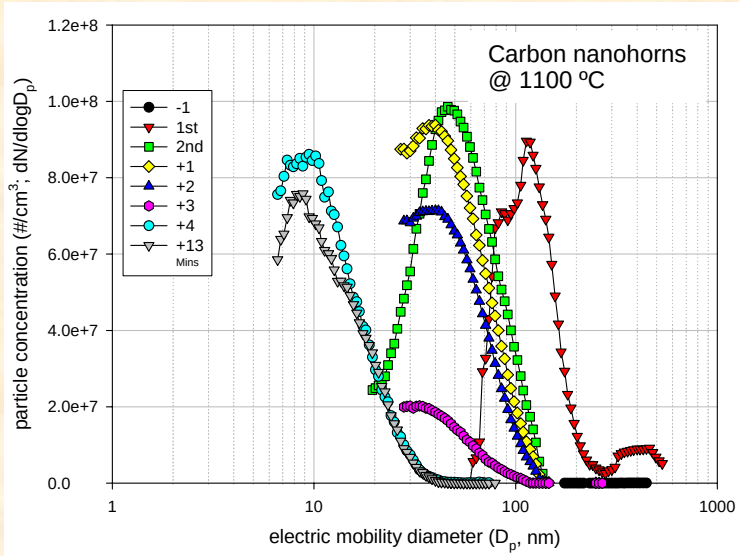


Results indicate that scientific aerosol instrument may be translated to industrial process monitoring

Size distribution shift with variation of $TiCl_4$ flow rate



Shift in carbon nanohorn size with operating parameters



Equipment is portable and suitable for in-plant use

Summary

Industrial teams are working with NNI funding agencies to implement R&D recommendations

- **Meetings and workshops are being held with**
  - **NIH**
  - **NIST**
  - **NSF**
  - **DOE**

For more information:

Chemical Vision2020: Current Activities: Nanotechnology - Microsoft Internet Explorer

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Current Activities

Vision2020 Thrust Area: **Nanotechnology and Nanomaterials By Design**

Project Leader: Jack Solomon

Partners: ACC, ACS, Air Products, BP, Ciba, CCR, General Electric, Dow, DuPont, Honeywell, Intel, MTI, Praxair, Rohm and Haas

Goal: Define nanomaterials/nanotechnology R&D priorities for the chemical and material processing industry to help guide government funding

Nanotechnology is an important new research area. The chemical industry may be the only industry with R&D capabilities and expertise to commercialize nanotechnology advances. Consequently, the chemical industry should have a voice in the selection of R&D topics pursued by the Federal government. The chemical industry, along with the electronics industry, are the two industries that have the most to benefit from guiding the nanotechnology R&D funding.

Roadmap Available

Chemical Industry R&D Roadmap for Nanomaterials By Design: From Fundamentals to Function

Vision2020 is currently working to improve communication with nanotechnology funding agencies to make sure they are focusing on areas relevant to the industry. The systematic research in nanotechnology is just beginning. The infrastructure is forming. The integration of new phenomena into macroscopic systems is not yet being emphasized.

Technical and Scientific Accomplishments

NEW

- Analyzed nanotechnology's potential impacts in report, *Estimated Energy Savings and Financial Impacts of Nanomaterials by Design on Selected Applications in the Chemical Industry*.(PDF 838 KB) The study provides a preliminary analysis of nanotechnology's potential impacts on energy efficiency, economic competitiveness, waste reduction, and productivity in the chemical and related industries. This report supplements the December 2003 roadmap, *Chemical Industry R&D Roadmap for Nanomaterials By Design: From Fundamentals to Function*.

Internet

http://www.chemicalvision2020.org/nanotechnology.html