

Economic Impact of Chemical Metrology Programs

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Senior Policy Makers Dialogue Forum
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NIST
National Institute of
Standards and Technology
U.S. Department of Commerce



Time Flies When You're Having Fun!

First InterAmerican Workshop on Metrology in Chemistry

Rio de Janeiro, Brazil
November 3-4, 1997

*This was the beginning of serious efforts in Brazil
and the Americas to develop strong chemical
metrology programs!*

Time Flies When You're Having Fun!

A Global View of Chemical Metrology: Recent Developments and Basic Concepts

Hratch G. Semerjian

The Importance of Chemical Metrology

“Chemical measurements are of great importance because they relate to almost every aspect of our life: the quality of the air we breathe, the water we drink, or the food we eat. In the manufacturing sector, from the production of chemicals and pharmaceuticals to semiconductors, chemical metrology plays a critical role in the development of products and processes. We have come to expect quality health care and the assurance of public safety and environmental quality based on decisions that depend to a great extent on chemical measurements. By its very nature, chemical metrology is very complex, requiring substantial resources and effort, to ensure reliable results that impact such a broad range of applications.”

Driving Forces for Improved Metrology

... Have evolved over the years

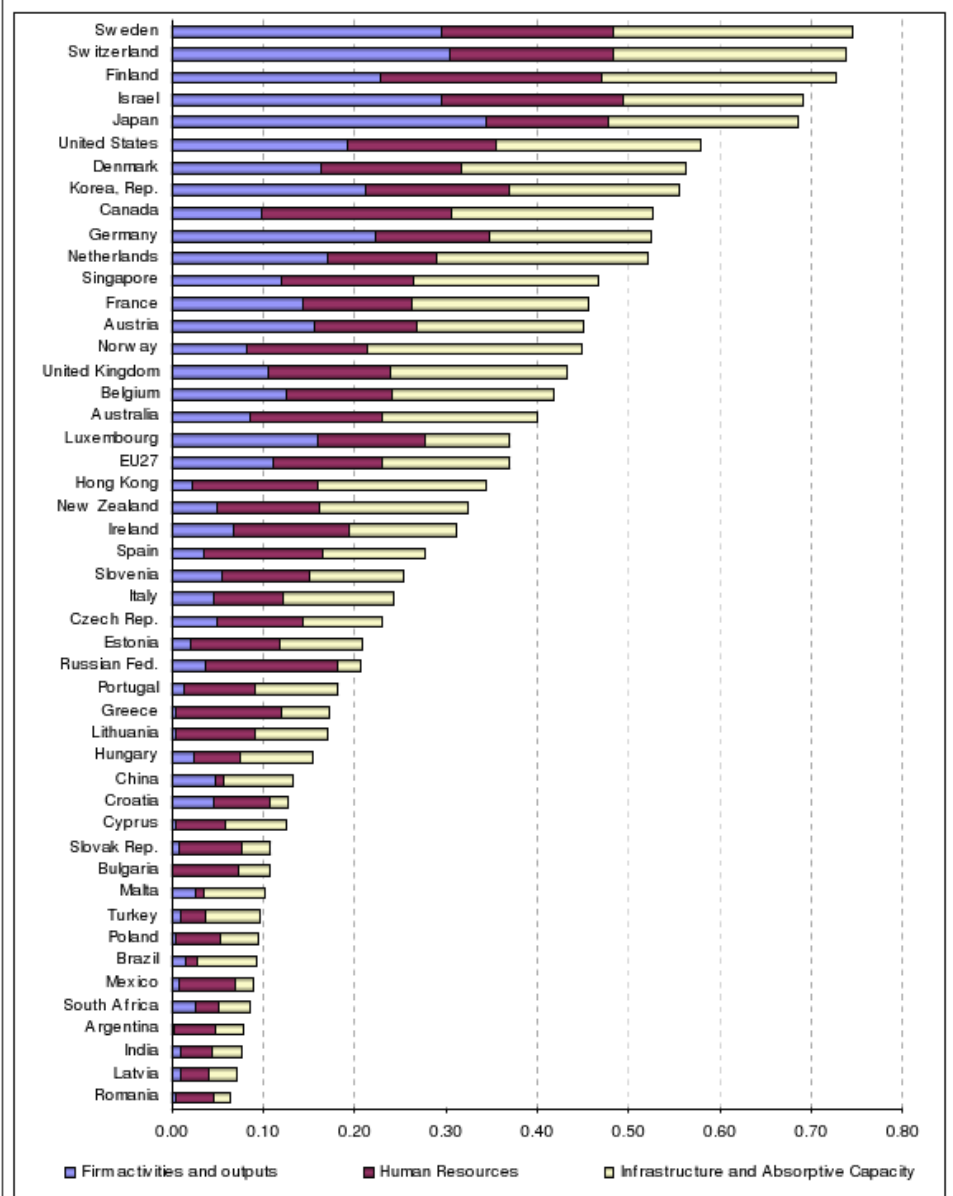
- ***domestic commerce***
- ***international trade***
 - ***innovation***
 - ***global competitiveness***
- ***quality of life***
 - ***personal and global***

all have economic implications!

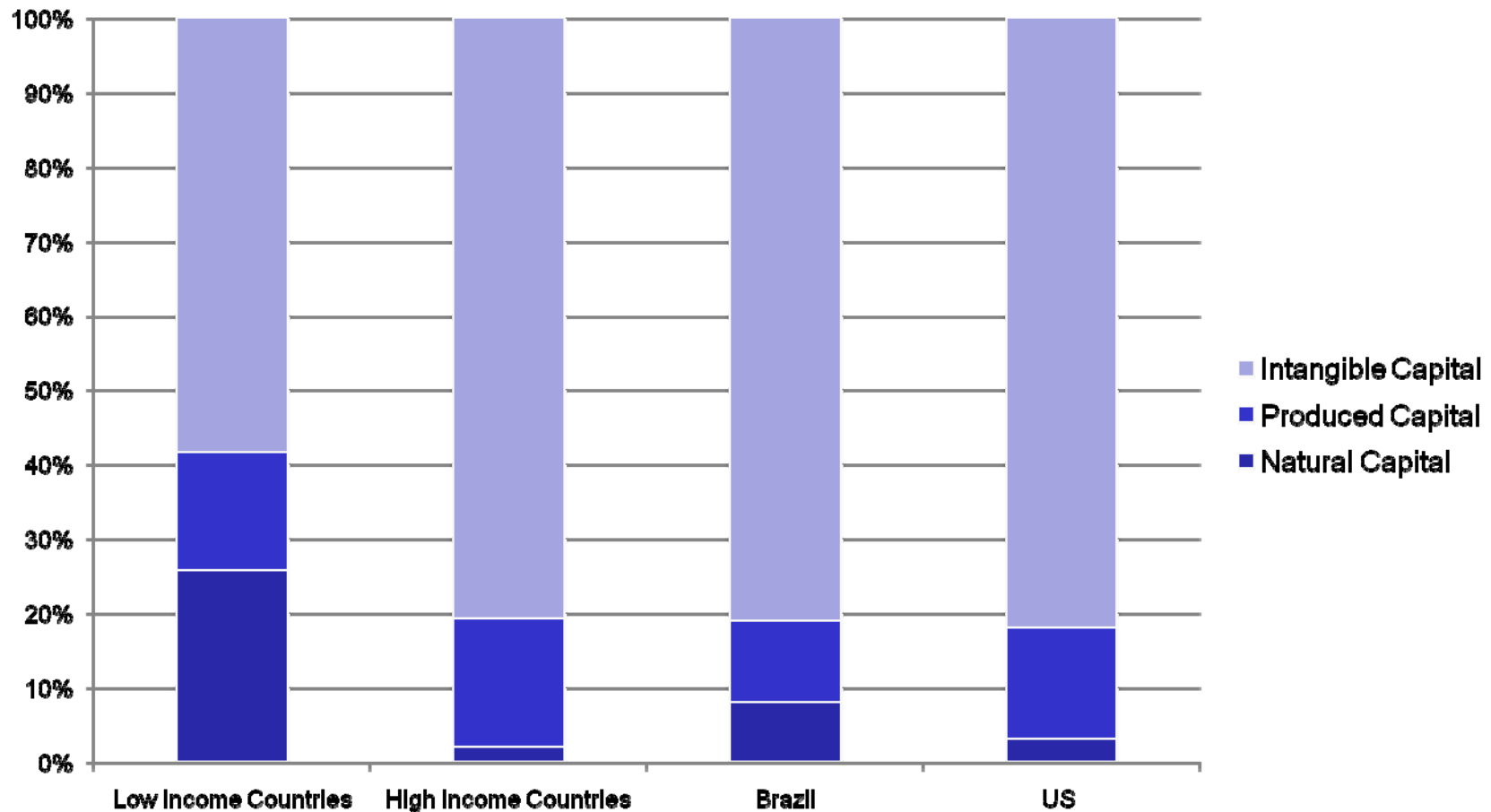
How do we evaluate them on a quantitative basis?

Global Innovation Performance

Figure 14: Global Innovation Performance – 2005



Total Wealth of Nations



*Where is the Wealth of Nations?
The World Bank 2006*

Fostering Innovation

- **Understanding Innovation**

 - Local improvements ...adopting available technologies

 - Competitive industries ..using technologies from other countries

 - New innovations of global significance

- **Tapping into Global Knowledge and Technology**

- **Stimulating and Supporting Innovation**

- **Providing Research and Technology Infrastructure**

 - “metrology, standards and quality control, extension services, information and training programs....”

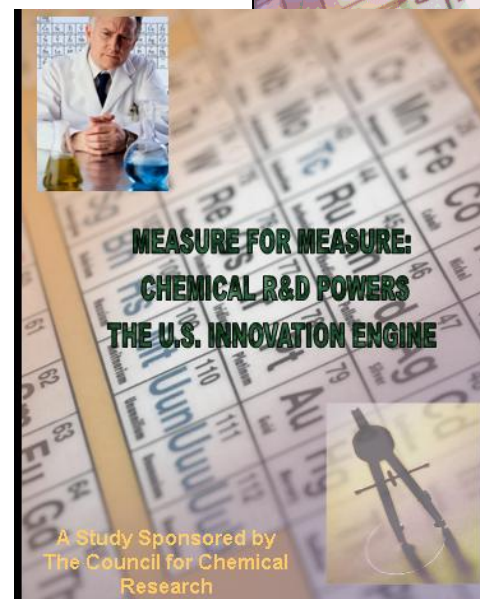
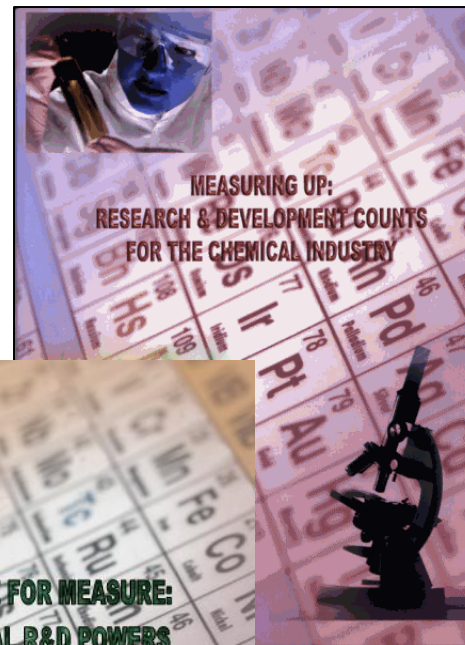
- **Export Sector Policies**

- **Intellectual Property Rights**

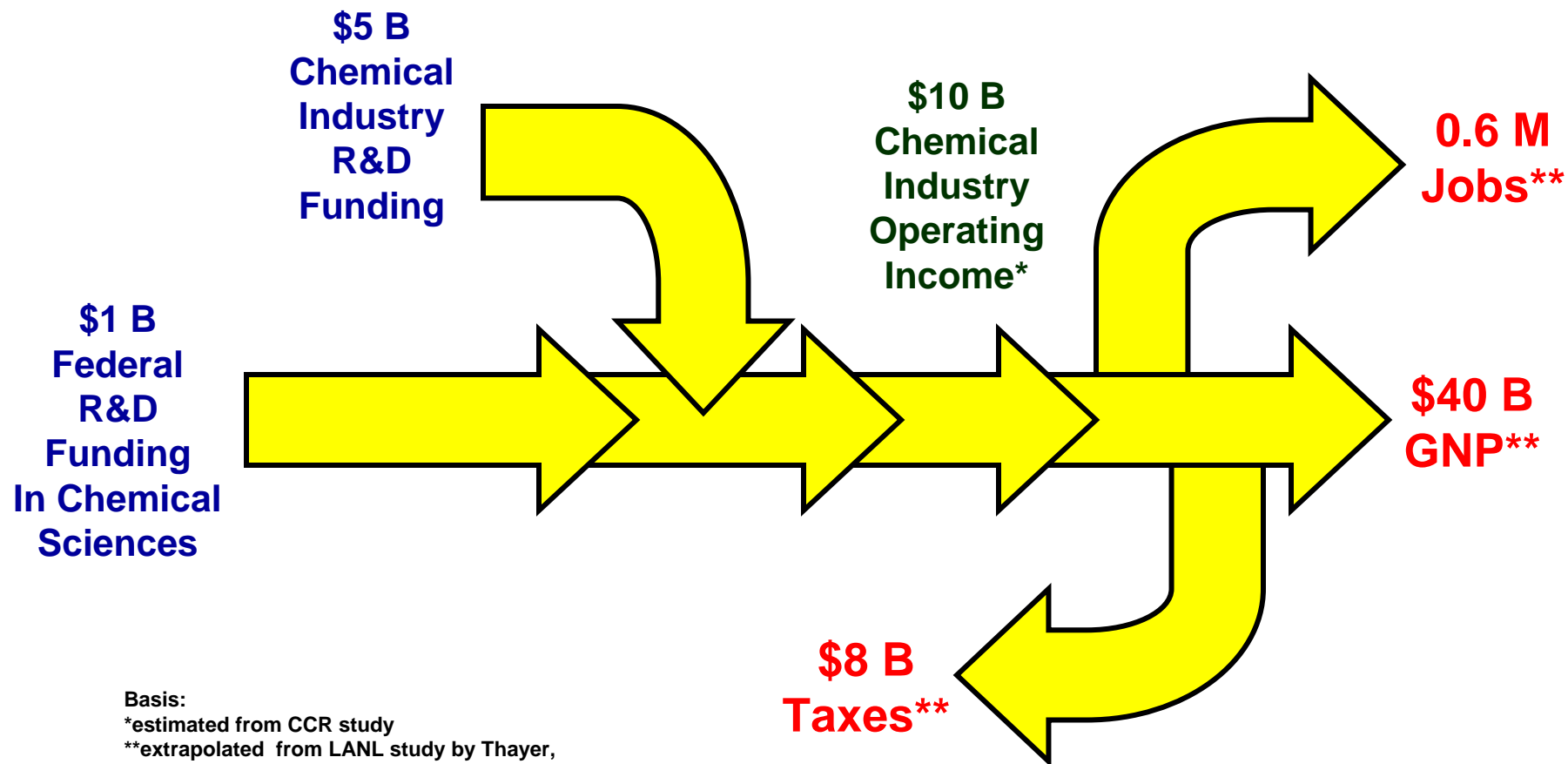
*Building Knowledge Economies
World Bank Institute 2007*

CCR Study on R&D Investments

- 10 Results of the 5 year (2 phase) study were published in two reports:
- ***“Measuring Up: R&D Counts for the Chemical Industry” – 2001***
 - ***“Measure for Measure: Chemical R&D Powers the U.S. Innovation Engine” - 2005***



Macroeconomic Implications



Basis:

*estimated from CCR study

**extrapolated from LANL study by Thayer, et al., April 2005 using REMI economic model

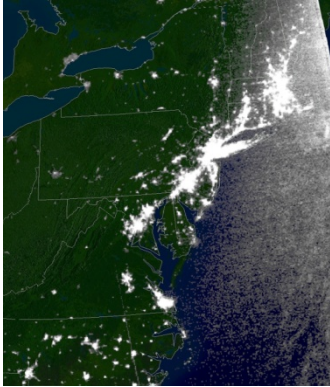
The Council for Chemical Research

CCR Studies - Overall Conclusions

- **Chemical companies get \$2 of operating income for every \$1 of R&D invested; that's a 17% after tax return**
- **Chemical technology is highly dependent on publicly funded chemical science research**
- **U.S. economy gains roughly \$40 dollars in GDP growth and \$8 in increased tax revenues for every dollar of federal investment in chemical sciences research**
- **Technology quality, innovation speed and strong scientific links deliver greater shareholder value**
- **All industries are significantly impacted by the chemical sciences. It is the most enabling science and technology**
- **The big opportunity is to reduce the 20-year innovation time lag from initial public research funding to commercialization**

Nation's Infrastructure

When things go well...



(Before 2003 blackout)



When things go wrong...



(After blackout)



Consumers Count on Standards for Equity in Trade



Measurements and Standards Impact Everyday Life

Fossil Fuels

- gasoline
- jet A
- coal
- natural gas



Drinking Water

- flow metering
- quality



Altimeter Calibration



Food and Nutrition

- labeling
- measures



Refrigerants

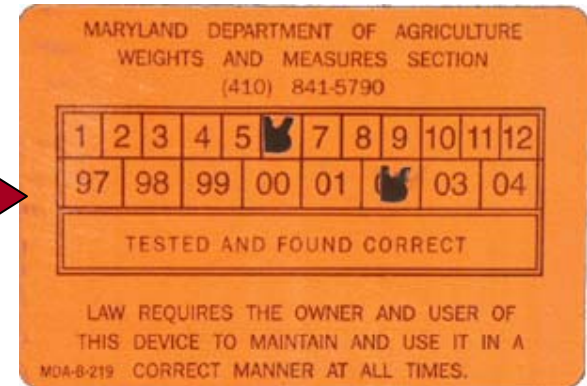
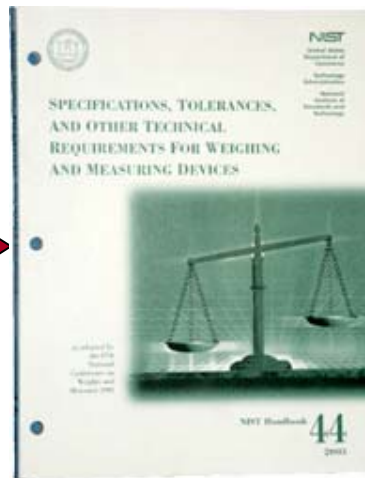
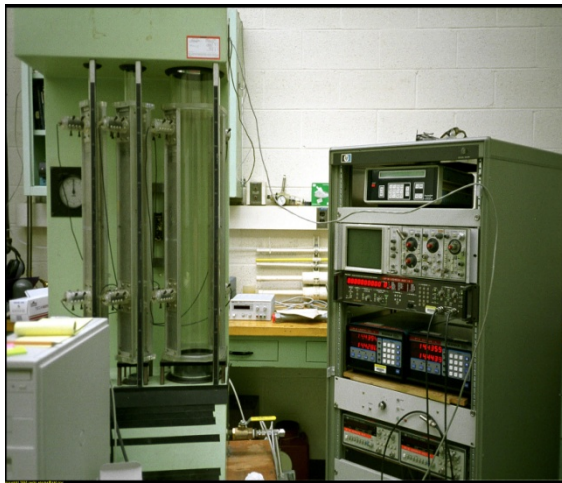


Thermometry

- healthcare
- process metrology



Weights and Measures: *Bringing Equity to the Marketplace*

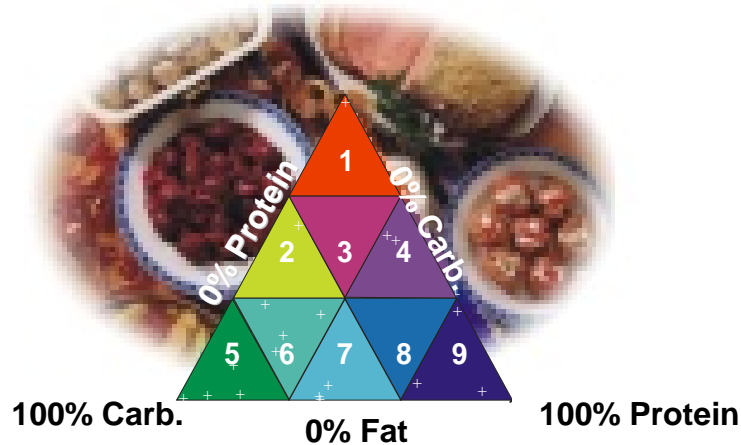


From laboratory, primary fluid-flow and volume standards

To assisting the States in their Weights and Measures regulation

- Responsible for coordination with Standards Development Organizations, such as the American Petroleum Institute (API) and the American Society of Mechanical Engineers (ASME), and the National Conference on Weights and Measures (NCWM)
- US imports 5 B barrels of oil each year; measurement uncertainty of 0.1% would translate to about \$350 M per year.

Food and Nutrition



“Nutrition Labeling is Mostly Accurate on Packaged Food”

“However, 46 percent of foods contained less Vitamin A . . . than their labels claimed, and the labels were accurate for iron just 69 percent of the time.”

US FDA

Washington Post 1/1/97

Quality Assurance: Interlaboratory comparisons involve 20 laboratories from NFPA, plus other collaborating labs

AOAC food triangle populated with appropriate standards to meet current needs – shifting emphasis to new issues such as efficacy and purity of Nutraceuticals

Populating the AOAC Food Triangle

- Sector 1** Cholesterol and Fat-Soluble Vitamins in Coconut Oil, SRM 1563
- Sector 2** Baking Chocolate
- Sector 3** Peanut Butter, proposed
- Sector 4** Meat Homogenate, SRM 1546
- Sector 5** Baby Food Composite, SRM 2383
- Sector 6** Frozen Diet, SRM 1544, Infant Formula, SRM 1846, Typical Diet, SRM 1548a
- Sector 7** Frozen Spinach, SRM 2385
Juncture, Fish Tissue, SRM 1946
- Sectors 4,8,9**

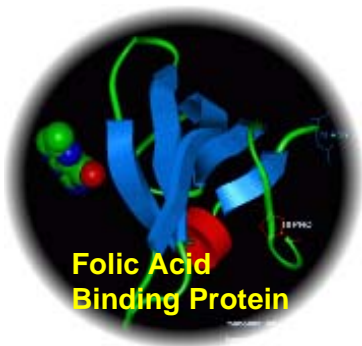
Food SRMs facilitate:

- compliance with nutritional labeling laws
- traceability for food exports needed for international trade
- the provision of accurate labeling information

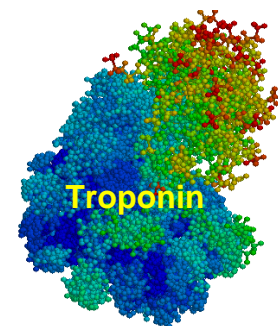
Measurements and Standards Help Reduce Healthcare Costs

Healthcare costs amount to ~ 16% of the GDP, an estimated \$1.8 trillion

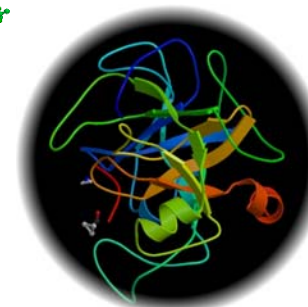
Prevention



Diagnosis



CARDIAC MARKERS



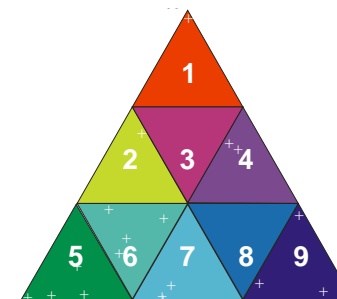
Treatment/Therapy



CSTL Maintains and Refines Definitive Methods for 12 Health Status Markers

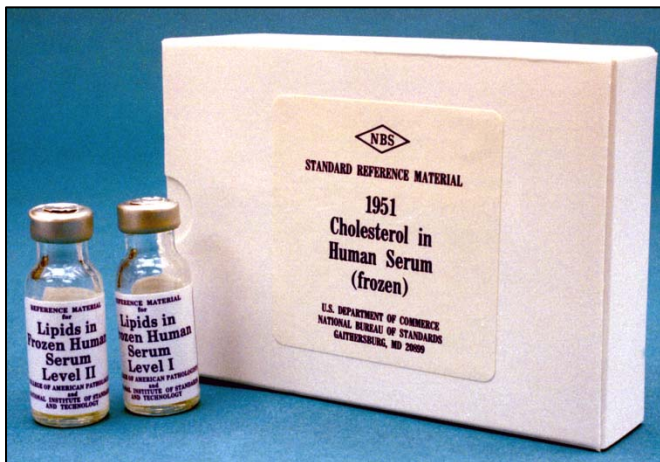
Calcium	<i>Cancer, Blood Clotting</i>
Chloride	<i>Kidney Function</i>
Cholesterol	<i>Heart Disease</i>
Creatinine	<i>Kidney Function</i>
Glucose	<i>Diabetes</i>
Lithium	<i>Antipsychotic Treatment</i>
Magnesium	<i>Heart Disease</i>
Potassium	<i>Electrolyte Balance</i>
Sodium	<i>Electrolyte Balance</i>
Triglycerides	<i>Heart Disease</i>
Urea	<i>Kidney Function</i>
Uric Acid	<i>Gout</i>

Nutrition



Cholesterol SRMs

An Economic Impact Study



Title: SRMs for Cholesterol Measurements

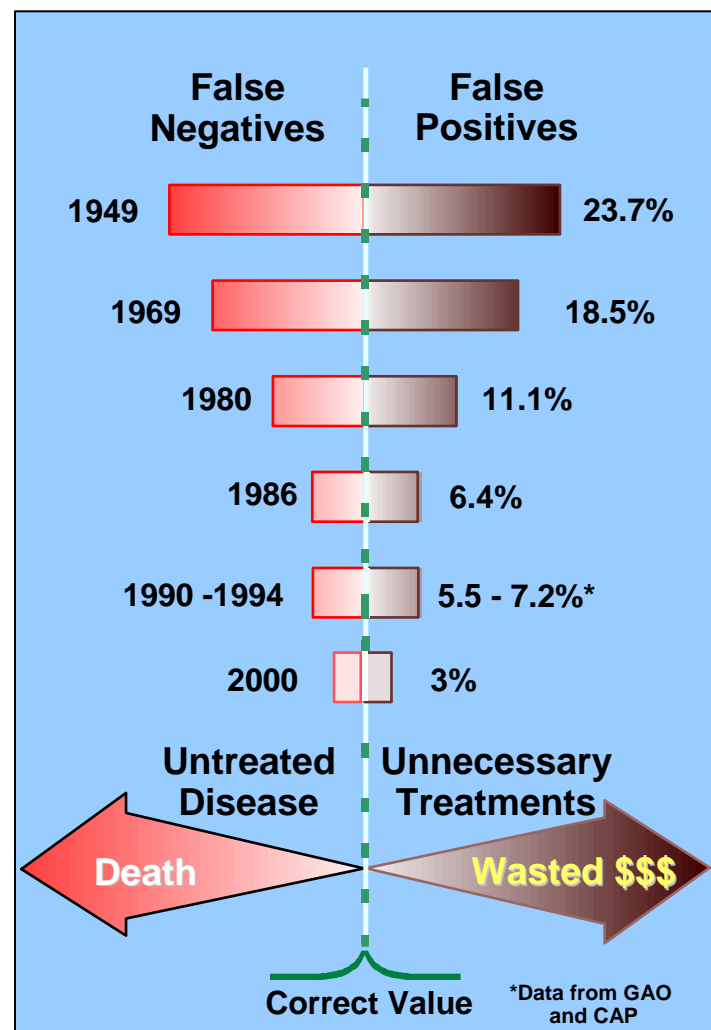
Products: NIST SRMs 911, 909, 1951, 1952

Users Impacted:

- Instrument and reagent manufacturers
- Network laboratories
- Clinical labs and hospitals

Results:

- **Social Rate of Return** 154%
- **Benefit to Cost Ratio** 4.5:1
- **Net Present Value** \$3.5M



Health Care Measurements and EU IVD Directive

Assuring Market Access

Directive went into effect in December 2003

Worldwide *in vitro* diagnostic device market is ~\$20B;
>60% of European market is supplied by U.S.



IVD Calibrators and/or control materials must: be traceable to “*standards of a higher order*”; have traceability and uncertainty statements



US IVD Manufacturers sought NIST help to meet the traceability requirements



NIST response: led industry driven workshops (2000, 2002, 2003), and leadership in the JCTLM

...and in the International Community

- Leading the effort to establish higher order reference methods and standards under JCTLM, recognized by BIPM, WHO, ILAC and IFCC
 - List I: approximately 100 Reference Methods for 58 markers (30 from NIST), and approximately 150 entries for 96 measurands (72 from NIST)
- Webbased information widely accessible through NIST and BIPM

JOINT COMMITTEE on TRACEABILITY in LABORATORY MEDICINE



That global body, consisting of two task oriented Working Groups was established in Paris on 12 June 2002

- **WG1 - Reference Materials and Reference Methods**
- **WG2 - Reference Measurement Services**

A Declaration of Cooperation was established between the International Committee of Weights and Measures (CIPM), the International Federation for Clinical Chemistry and Laboratory Medicine (IFCC), and the International Laboratory Accreditation Cooperation (ILAC)

Greenhouse Gas Emissions Measurements

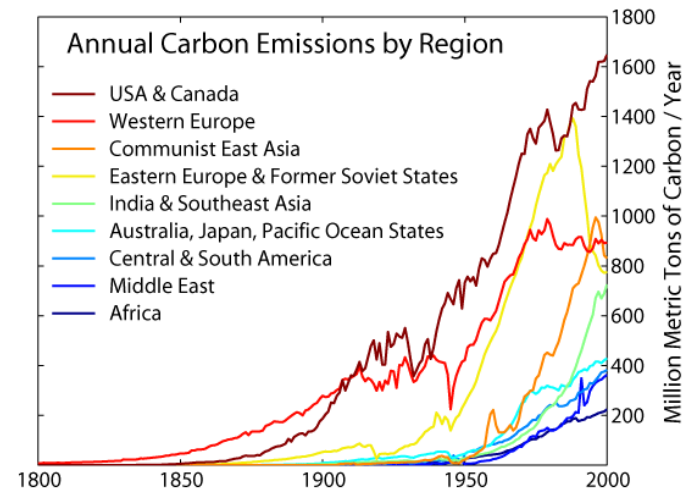
Effective mitigation of greenhouse gas-induced global warming will require precise and comparable measurements to:

- Determine accurate emissions levels and baselines
- Monitor GHG levels over sources and sinks
- Assess impact of mitigation strategies

This will require:

- Point emission source monitoring and standards
- Remote monitoring and standards
- Accreditation of private and state laboratory networks
- International comparability of GHG emission measurements

Huge Economic Implications!



Credit: R. Rohde



Gas Mixture NIST Traceable Reference Material (NTRM) Program

Potential Model for underpinning a cap-and-trade program

History and Drivers

- 1990 Amendment to Clean Air Act required significant increase in pollution monitoring
- Market for standards for compliance with EPA air quality regulations too large for demand to be met directly with the NIST Gas SRM program
- Acid Rain Emissions Trading program required robust traceability to provide comparability

NIST Response

- Established NTRM program in 1992
 - Commercially produced
 - Market driven
 - Well-defined traceability linkage to NIST primary standards
 - NIST works directly with commercial Specialty Gas Companies (SGCs) for dissemination

“... the NTRM program has served as an excellent vehicle for production of the high quality standards - of known pedigree - required by both industry and the regulatory community in the ***implementation of Title IV (SO₂ emissions trading) of the 1990 Clean Air Act.***”

*Stephen Miller, Technical Director
Scott Specialty Gases*

Gas-Mixture NTRM Program

An Economic Impact Study

Title: The Economic Impact of the Gas-Mixture NTRM Program

Products: Gas-Mixture NTRMs

Users Impacted:

- Specialty Gas Companies
- End Users: Electric Utilities, Transportation Equipment Firms, Petrochemical Firms, Commercial Labs, Government Agencies

CSTL works directly with commercial Specialty Gas Companies (SGCs)

AGA

Air Liquide

Air Products

Airgas

BOC Gases

MG Industries

Praxair

Matheson TriGas

Scott Specialty Gas

Spectra Gases



NTRM

Results:

Social Rate of Return	225%
Benefit to Cost Ratio	24:1
Net Present Value	\$56M

Since 1992, **8624** NTRM cylinders have been produced by **15 SGCs**, resulting in the production of **500,000** EPA Protocol Gas Standards, valued at **\$140,000,000**

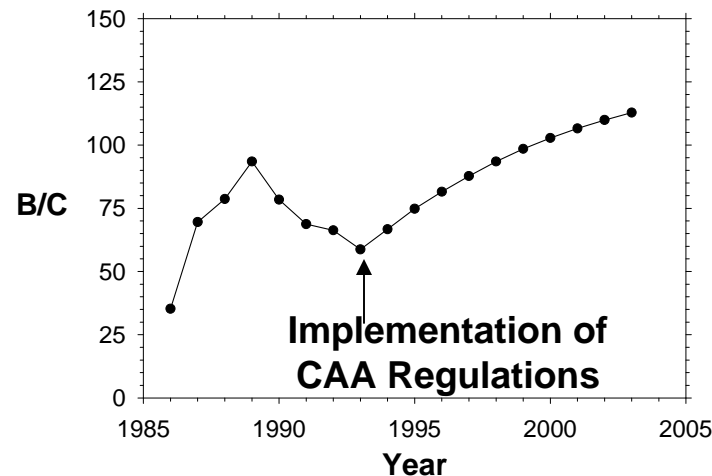
Sulfur in Fossil Fuel SRMs

An Economic Impact Study

improved production efficiency... improved environment... improved health

Industries Impacted:

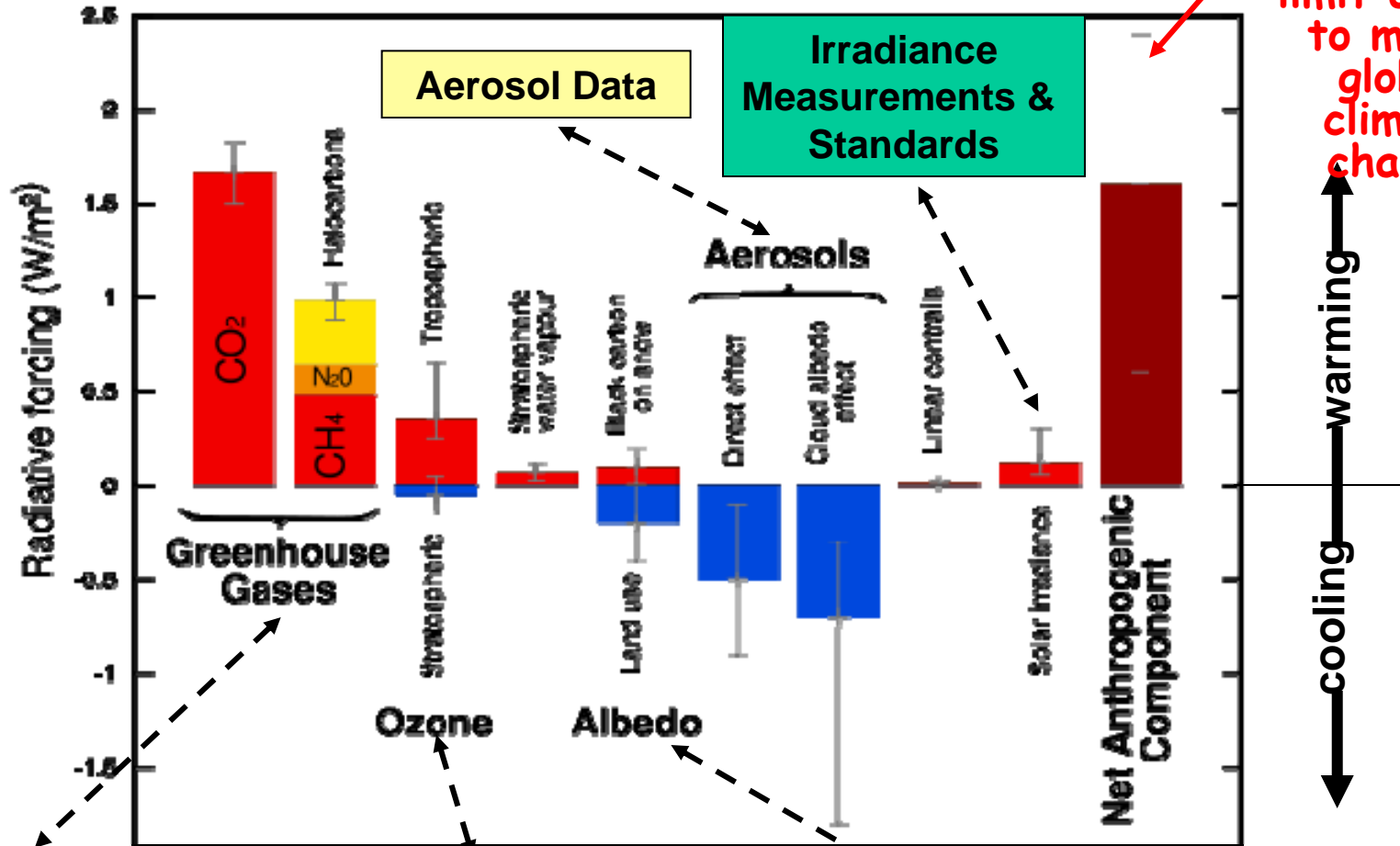
Transportation	Diesel, Gasoline
Energy	Coal
Steel	Coke



Benefit-Cost Ratio	113
Social Rate of Return	1,056%
Net Present Value	\$409M

Certification of NIST SRMs for sulfur in fossil fuels uses a definitive method, developed at NIST, that virtually eliminates bias and significantly reduces the measurement uncertainty ... which translates to improved production efficiency

Measurements and Standards Needed for Climate Change Assessment



Critical measurement uncertainties limit ability to model global climate change

warming
cooling

Greenhouse Gas Measurements & Standards For Cap-and-Trade

Ozone Concentration Standards

Reflectance Standards

chemical
physical

Alternative Refrigerants Research Program

An Economic Impact Study

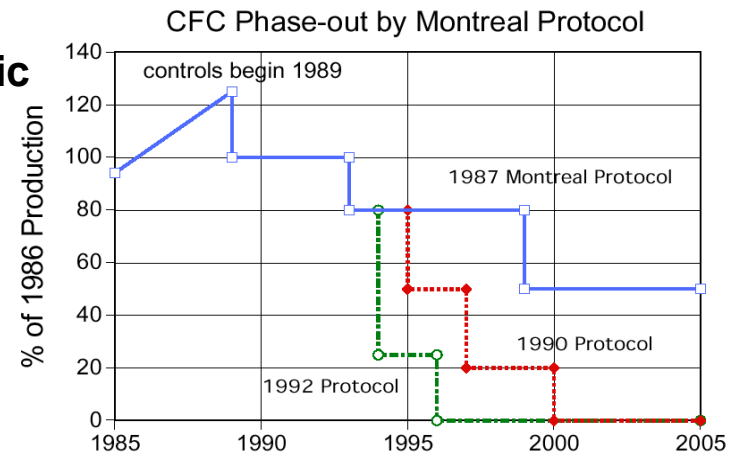
Problem

- CFC and HCFC refrigerants deplete stratospheric ozone and contribute to global warming

NIST was in a unique position to aid transition to CFC replacements

NIST SRD 23 REFPROP database

- Constructed with expt'l data as foundation
 - Models the behavior of refrigerant mixture
 - Effective form of information dissemination
 - Key to developing CFC replacements
 - Facilitated the development of new products that are energy efficient, environmentally safe, timely, and economical
- Internationally Adopted*
- IEA Annex 18 – Int'l Standard Equations of State
 - ISO Standard 86
 - Distributed through ARI, IIR, ASHRAE, etc.



NISTDATA

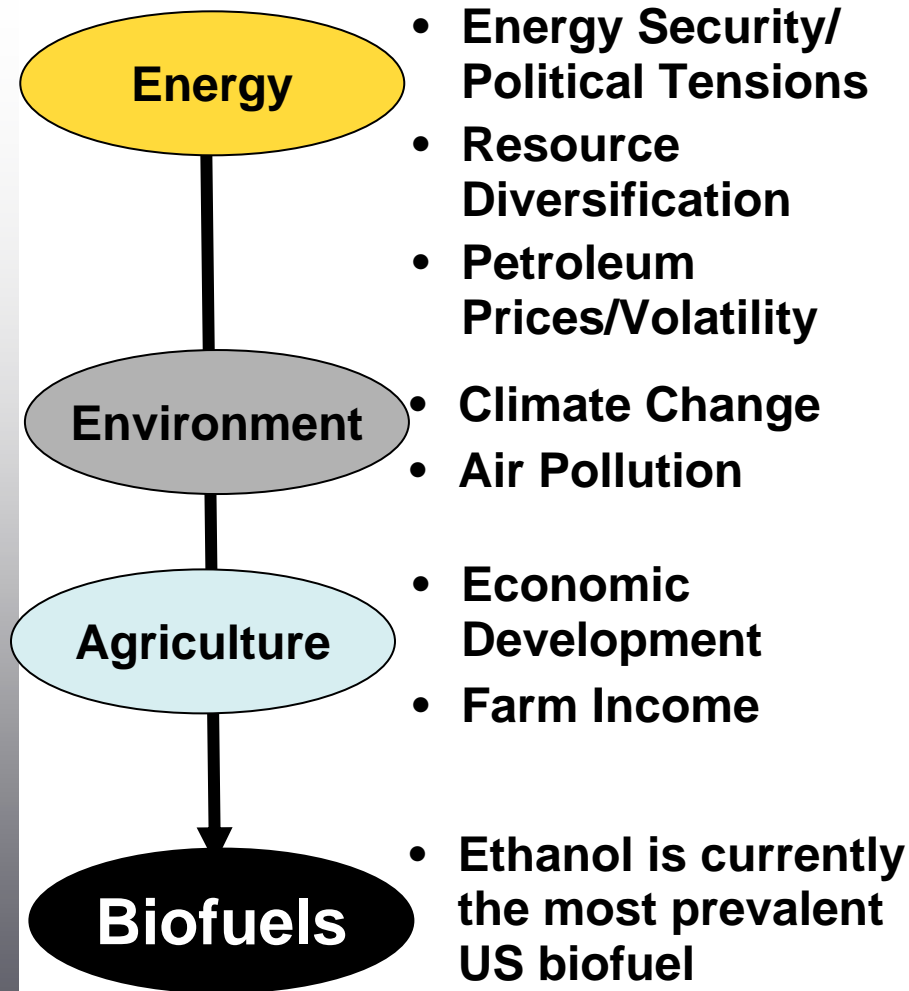
CFCs and HCFCs

Used as refrigerants, solvents, foam-blowing agents (\$28B/year)
Used in manufacturing processes (\$350B worth of installed equipment)

Economic Impact Study: Published January 1998
Comments: Scope of study included manufacturers and users
Internal Rate of Return: 433%



Policy Drivers & Incentives Supporting Biofuels



Examples of Policies

United States

- Energy Policy Act of 2005 (federal policy)
- State tax credits, blend requirements...

Europe

- Tax credits: most common incentive
- EU set target for biofuels consumption (similar to RFS, but not a mandate)

Asia

- China, India, and Malaysia introducing policies to support biofuels
- Japan has tax credits in place

South America

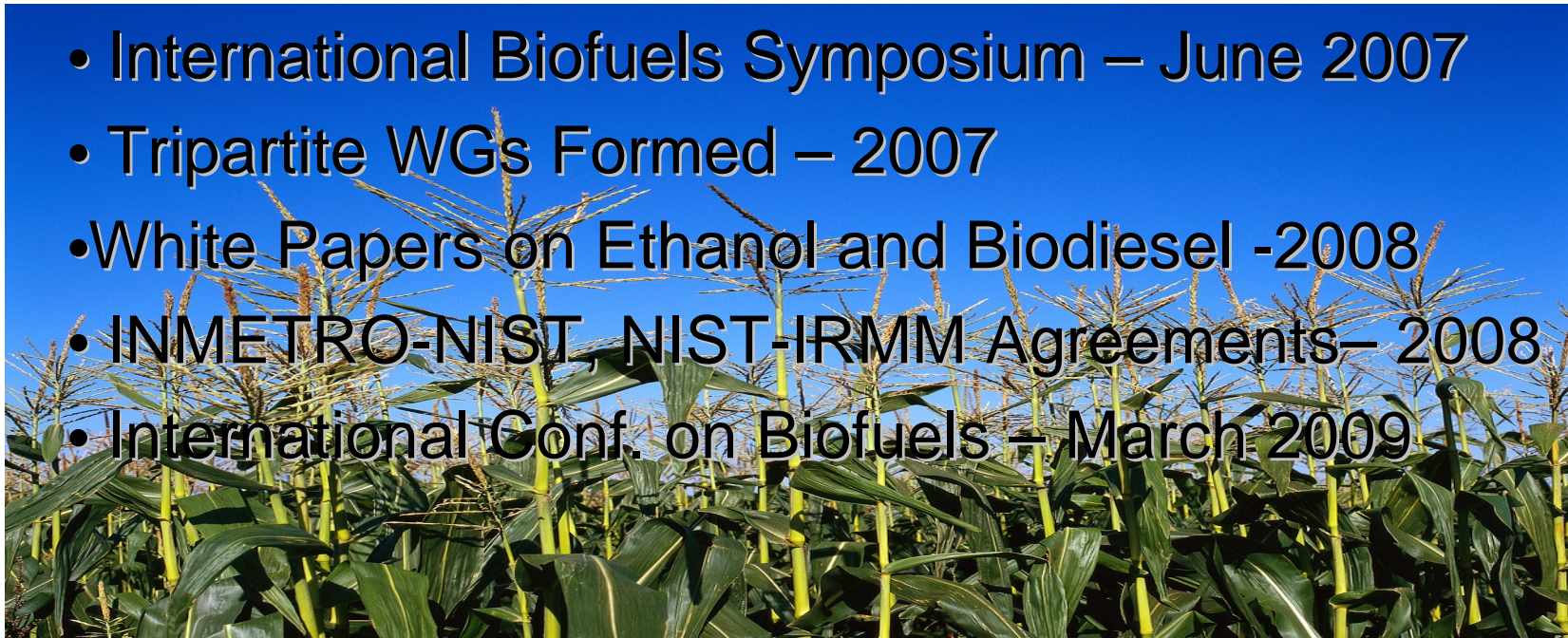
- Brazil: Ethanol blending requirements in place and a requirement for biodiesel starting in 2008

Source: Navigant

Biofuels require a comprehensive & effective policy framework

Measurements and Standards for Biofuels

- Brazil-US Ministerial Meeting – June 2006
- INMETRO-NIST Workshop – Sept. 2006
- EU Conference on Biofuels – Feb. 2007
- IBF Established – 2007
- International Biofuels Symposium – June 2007
- Tripartite WGs Formed – 2007
- White Papers on Ethanol and Biodiesel -2008
- INMETRO-NIST, NIST-IRMM Agreements– 2008
- International Conf. on Biofuels – March 2009



Planned Supportive Activities of the Governments through their National Metrology Institutes

NIST (U.S.), and **INMETRO** (Brazil) have established plans for cooperative development of

Certified Reference Materials:

- **Anhydrous and Hydrated bioethanol**
- **Soy and Animal-based biodiesel**
- for **calibrating** measurement instruments to a known and internationally accepted reference
- for **validating** the accuracy of measurement results and measurement platforms, space and time.

Reference Measurement Methods:

- Chemical pattern recognition to identify feedstock source of biodiesel (e.g. soy, rapeseed, animal fat)
- Isotope metrology to distinguish between renewable/nonrenewable fuels

Advanced Isotope Ratio Measurements to Establish Source-type of Ethanol

- Petroleum-derived ethanol is chemically identical to bio-ethanol
- Measurement strategy needed to distinguish non-renewable sources from renewable sources for:
 - Establishment of appropriate tax credits
 - Metrics to support assessment of achieving national/international fuel composition targets
 - Verification of meeting customer criteria as to source of ethanol,
 - Etc.
- *Carbon-14 and carbon-13 measurements provide a means to authenticate ethanol source*

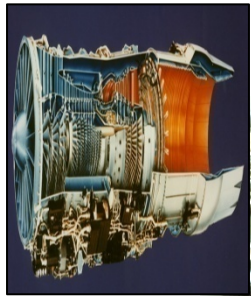
non-renewable

C 14/12 = 10^{-12}
C 13/12 = 0.0111

renewable

C 14/12 ~ 10^{-15}
C 13/12 = 0.0109

Metrology Supports Industrial Competitiveness



Aerospace & Transportation

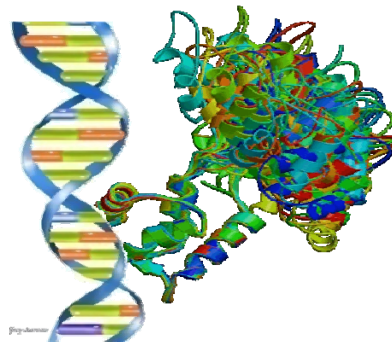


Chemical Processing

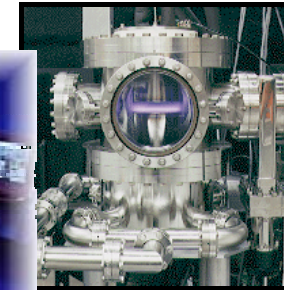
Biotechnology

BDB

Research Collaboratory for Structural Bioinformatics



Energy



Semiconductors



Health and Food

The NIST/EPA/NIH Mass Spectral Library

Reference Standard Mass Spectra for Chemical Identification

Fragments of charged molecules provide reproducible, discriminating fingerprints for small molecules in complex mixtures in:

- Environmental Analysis
- Health Research
- Homeland Security
- Drug Testing
- Chemical Processing
- Food Analysis

Content

- NIST Evaluated spectra for 163,198 compounds
 - QA/QC by documented computer-assisted evaluation
 - Verified, implemented spectrum matching methods
 - Other relevant data: structure, retention, ...

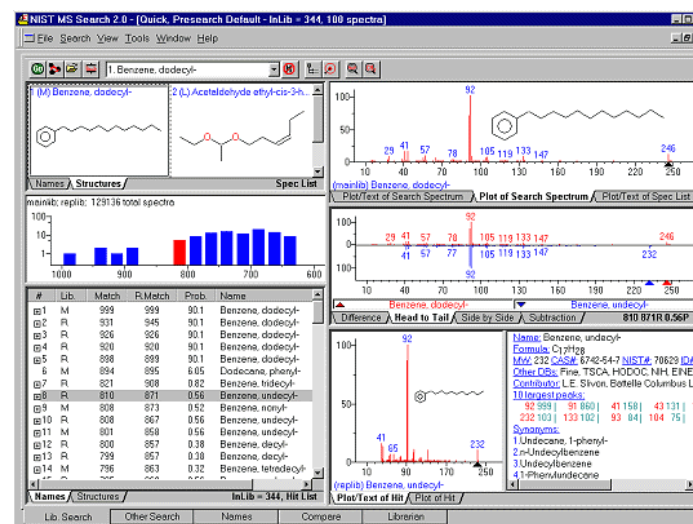


Usage

- Installed on >4000 instruments per year
 - World's most widely used MS library
- Integrated into instruments by distributors
- Common element in GC/MS 'gold standard' identifications

Extensions

- Large molecule 'MS/MS'
 - proteomics, metabolomics, glycomics, ...



Primary Method for Sulfur Determination Finds Wide Range of Applications

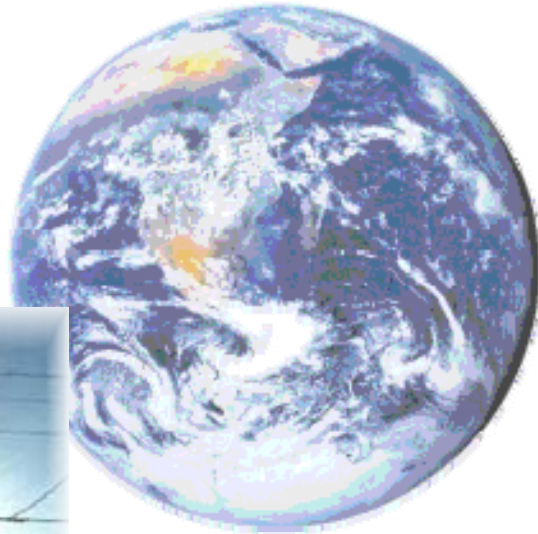
Sulfur in Fossil Fuels



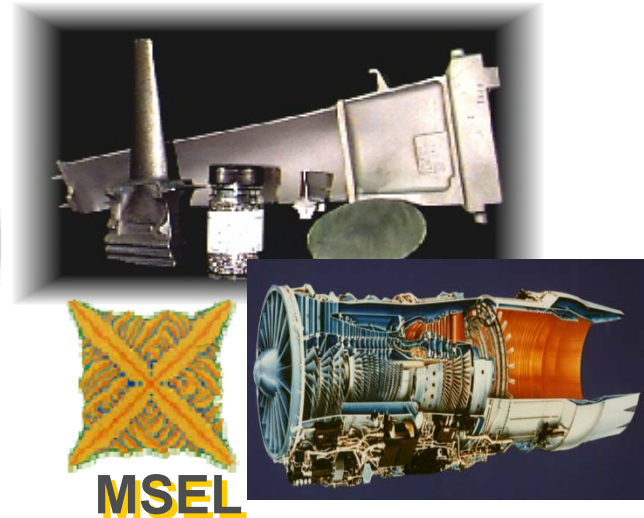
Fossil Fuels SRMs

Kerosenes
Fuel Oil
Coal
Lubricating Base Oil
Fly Ash
Gasoline
Coke

**Acid Rain
Emissions Trading
Catalyst Poisoning**



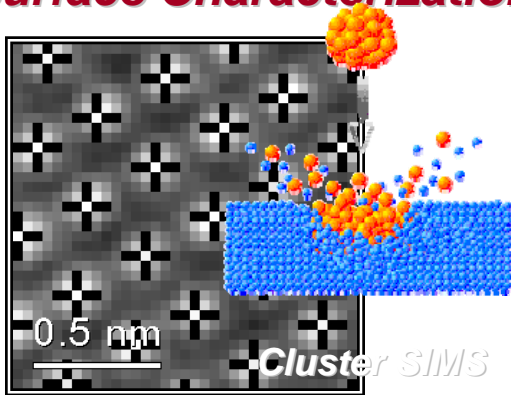
Sulfur in Aerospace Superalloys



- High temperature turbine is the most critical component of jet turbine
- Industry requires sulfur measurements at 1 $\mu\text{g/g}$ and below in Ni-based alloys
- Adherence of protective oxide coating is enhanced by reducing sulfur below 0.5 $\mu\text{g/g}$

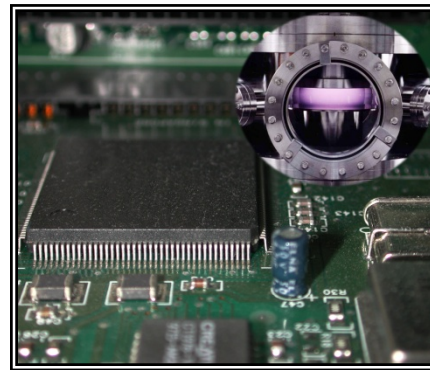
Microelectronics

Surface Characterization



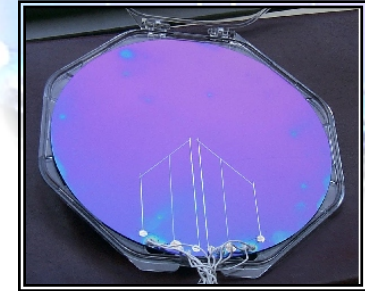
Electron
Micrograph

Value of Semiconductor
Shipments Nearly \$200B

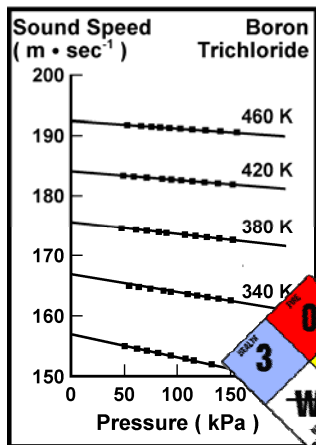


Standards for
Process Control

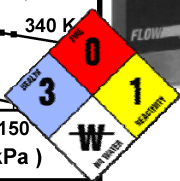
Temperature



Data for Process
Modeling

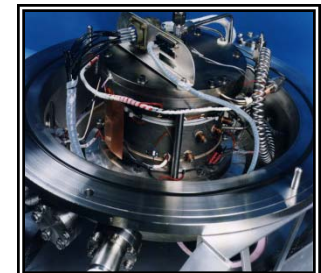
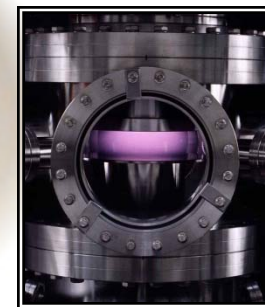


Thermophysical
Properties



SRM 2134, Arsenic in Silicon

Plasmas



Humidity

Ion-Implanted Dopants in Silicon

New SRMs Improve Quality Control in Silicon Wafer Production

- SIMS is the primary tool used in process control in the semiconductor industry
- Ion-implanted reference materials are used routinely for SIMS calibration

SRM 2137 B-10 implant in Si (released 8/93)
SRM 2134 As implant in Si (released 8/00)
SRM 2133 P implant in Si (scheduled release 9/02)

ITRS specifies in-line dopant profile concentration precision requirements ... to 2% in 2008, ... with "low systematic error".



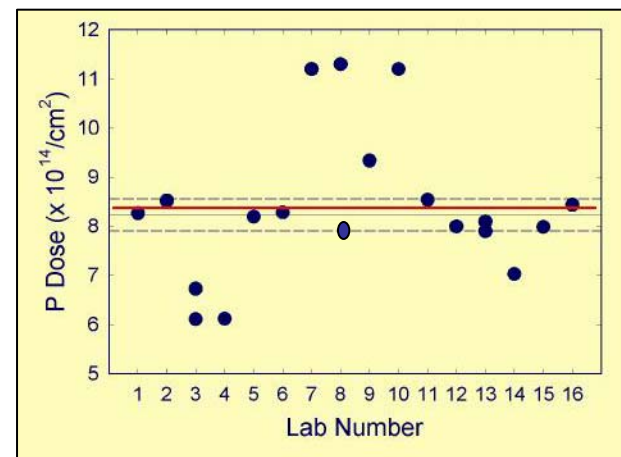
SEMATECH ... identified P, As, and B were identified as having highest priority.

- Newly released **SRM 2134**, As in Si, has a rigorously evaluated expanded uncertainty of **0.38%**

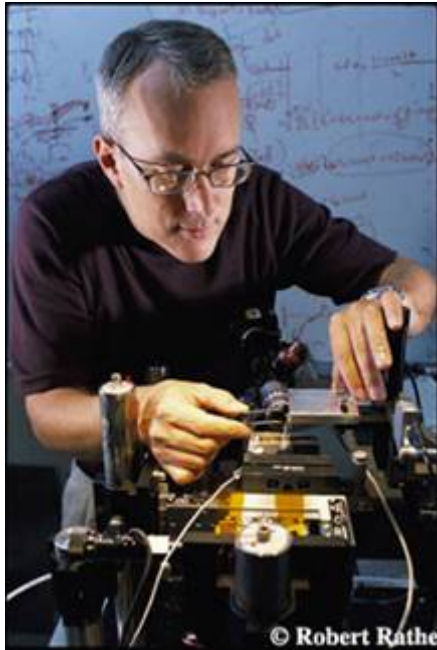
- Certified Reference Materials with low systematic error are required for ISO compliance, international and inter-site comparability, and comparing experimental results with simulation models.
- The use of **SRM 2137**, B in Si, is incorporated into ISO documents 14237 and 17561



Calibration of Phosphorus Implantation Dose in Silicon by RNAA



Nanomanufacturing

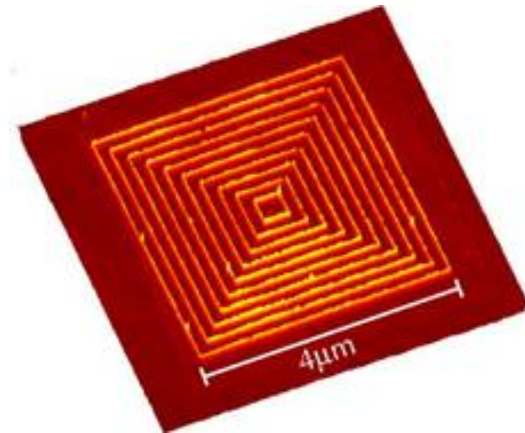


Force Metrology for Nanoscale Measurements and Standards

Nanonewton range -- Force 1 billion times smaller than the force required to hold an apple against Earth's gravity.

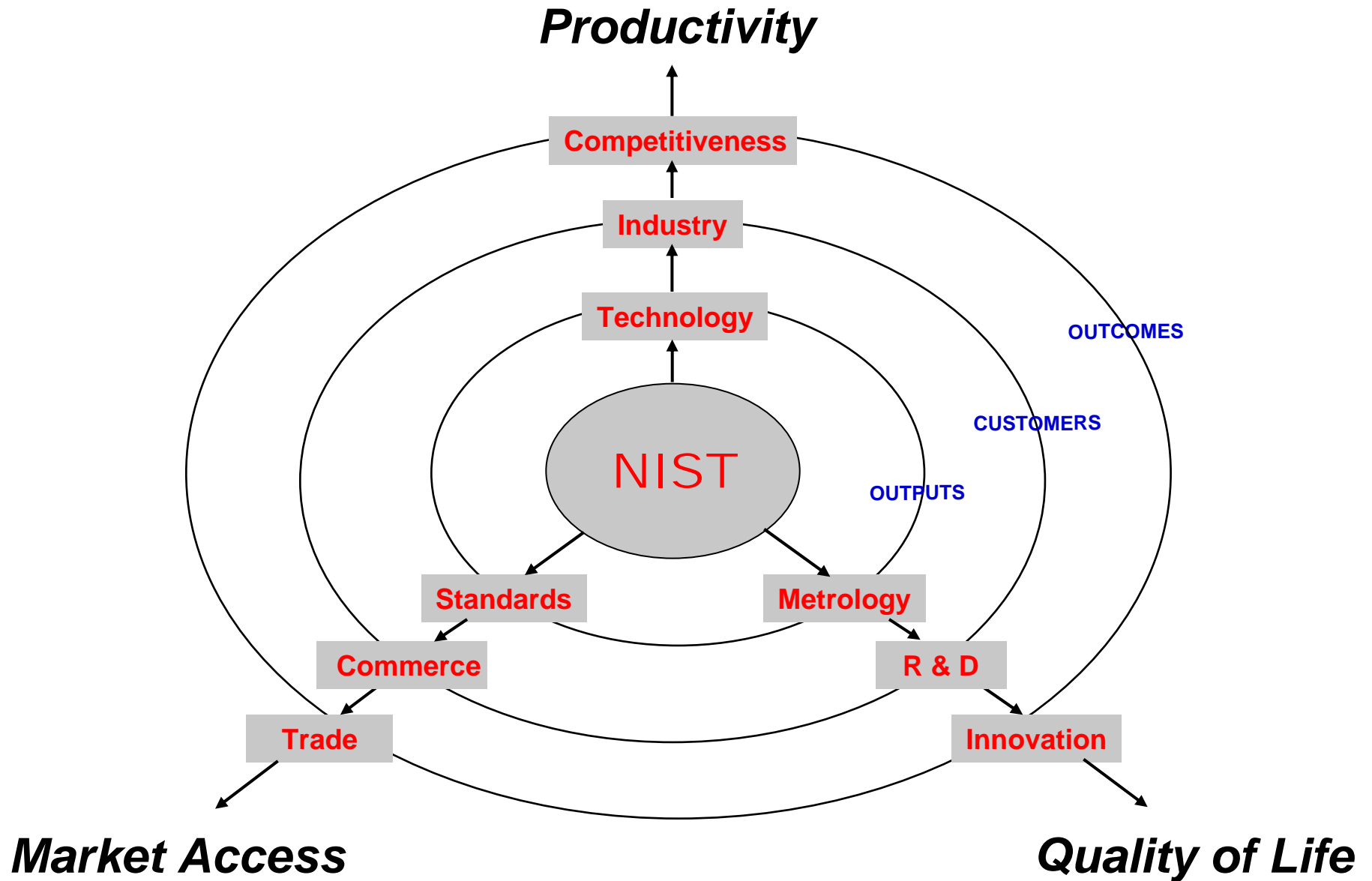
Nano Gauge Blocks

Using the interferometer-guided probe of the Molecular Measuring Machine, accurate calibration patterns can be produced.



Nano-Manipulation of nanowires with "optical tweezers." A highly focused laser beam attracts microscopic objects and can be used to pick up and precisely position nano-components for building semiconductor circuits or biosensors smaller than a red blood cell.

NIST's Pivotal Role in U.S. Economy



NIST Formal Impact Studies

Industry:	Project	SRR	BCR
Semiconductors:	Resistivity	181%	37
	Thermal conductivity	63%	5
	Wire Bonding	140%	12
	Electromigration	117%	12
	Software for design automation	76%	23
Communications:	Electromagnetic interference	266%	
	ISDN	156%	
	Data encryption standards	267-272%	58-145
	Role-based access control, security	44%	109
Automation:	Real-time control systems	149%	
	Machine tool software error compensation	99%	118
Manufacturing:	Standards for product data exchange	32%	21
Photonics:	Optical fiber	423%	
	Spectral irradiance	145%	13
	Optical detection calibration	72%	3
	Laser & fiberoptic power calibrations	43-136%	3-11

***lower transaction costs - lower compliance costs - energy conservation
increase R&D efficiency - increase product quality - enable new markets***

NIST Formal Impact Studies (Cont'd)

<i>Industry:</i>	<i>Project</i>	<i>SRR</i>	<i>BCR</i>
<i>Energy:</i>	Electric meter calibration	117%	12
<i>Computers:</i>	Software conformance	41%	
<i>Electronics:</i>	Josephson voltage standard	87%	5
<i>Materials:</i>	Thermocouple calibration	32%	3
	Phase equilibria for advanced ceramics	33%	10
<i>Pharmaceuticals:</i>	Radiopharmaceuticals	138%	97
	Cholesterol	154%	4.5
<i>Chemicals:</i>	Alternative refrigerants	433%	4
	Sulfur in fossil fuel	1,056%	113
	Gas Mixture NTRMs	225%	24
<i>Construction:</i>	Building codes	57%	
	Roofing shingles	90%	
	Fire safety evaluation systems	35%	

http://www.nist.gov/director/planning/impact_assessment.htm

Summary

- **Historically, metrology has provided the foundation for domestic trade**
- **Globalization of trade has put increasing emphasis on measurements and their mutual recognition**
- **Economic impact of metrology is demonstrated and will continue to be demonstrated**
- **Improved measurement capabilities will be needed to enable *innovation* in the 21st century and meet global challenges**