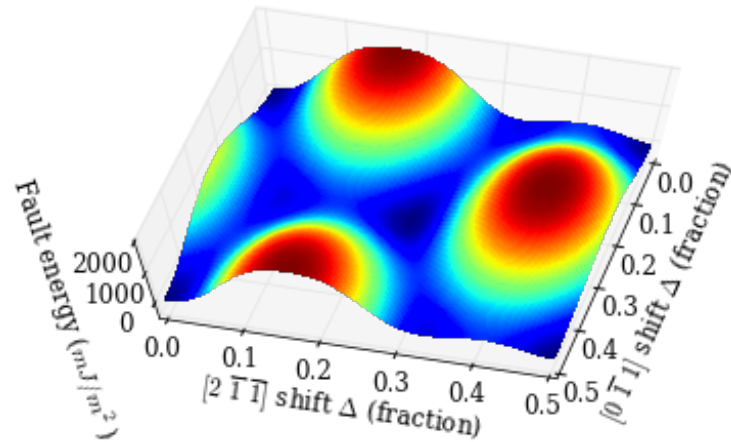
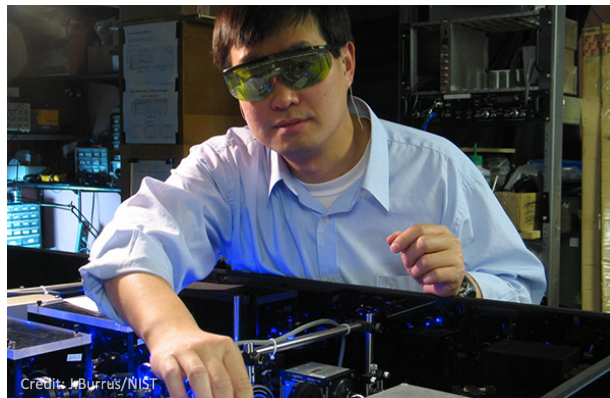


Atomistic Simulations for Industrial Needs

August 5-7, 2020



To promote U.S. innovation and industrial competitiveness by advancing **measurement science, standards, and technology** in ways that enhance economic security and improve our quality of life



MEASUREMENTS ESSENTIAL TO COMMERCE, TRADE, AND INNOVATION

Federal role
established in the
U.S. Constitution

We the People
insure domestic Tranquility, provide for
and our Posterity, do ordain and establish

Article 1

Section 1 All legislative Power herein granted shall be vested in a Congress of the United States, which shall consist of a Senate and House of Representatives.

Section 2 The House of Representatives shall be composed of Members chosen every second Year in each State - but how many Representatives in each State shall have no more than one Representative. No Person shall be a Representative who shall not have attained to the Age of twenty five Years and who shall not, when elected, be seven Years a Citizen of the United States, and who shall not, when elected, be an Inhabitant of that State in which he shall be chosen.

Representatives and direct Taxes shall be apportioned among the several States which may be included within this Union, according to their respective Numbers, which shall be determined by adding to the whole Number of free Persons, including three fourths of all other Persons bound to Service, the actual Number of free Persons in each State, and in such Manner as they shall by Law direct. The Number of Representatives shall not exceed one for every thirty thousand, but each State shall have at least one Representative, and until such Enumeration, there shall be one Representative for every ten thousand. The actual Enumeration shall be made within three Years after the first Meeting of the Congress, and within every subsequent Term of ten Years, in such Manner as they shall by Law direct. The Electors in each State shall have the Qualifications requisite for Electors of the most numerous Branch of the State Legislature. Immediately after they shall be qualified in Congress of the first Election, they shall be divided into three Classes. In the first Class, all the Representatives in the first Term shall be chosen; in the second Class, one third of the Representatives shall be chosen; in the third Class, one third of the Representatives shall be chosen. The Electors in each State shall have the Qualifications requisite for Electors of the most numerous Branch of the State Legislature.

Section 3 The Senate of the United States shall be composed of two Senators from each State, chosen for six Years; and each Senator shall have one Vote.

Immediately after they shall be qualified in Congress of the first Election, they shall be divided into three Classes. In the first Class, all the Senators in the first Term shall be chosen; in the second Class, one third of the Senators shall be chosen; in the third Class, one third of the Senators shall be chosen. The Electors in each State shall have the Qualifications requisite for Electors of the most numerous Branch of the State Legislature. The Senate shall be the more noble Body, in which the Senators shall be chosen for six Years; and each Senator shall have one Vote. The Electors in each State shall have the Qualifications requisite for Electors of the most numerous Branch of the State Legislature.



The patent system ... added the fuel of interest to the fire of genius in the discovery and production of new and useful things.

Abraham Lincoln – April 6, 1858



U.S. Patent No. 6469



...Giving effectual encouragement as well to the introduction of **new and useful inventions** from abroad as to the exertions of skill and genius in producing them at home, and of facilitating the intercourse between the distant parts of our country...

George Washington, State of the Union Address, January 8, 1790

EARLY DRIVERS FOR STANDARDS AND MEASUREMENTS



1904

Out-of-town fire companies arriving at a Baltimore fire cannot couple their hoses to the hydrants. 1526 buildings razed.

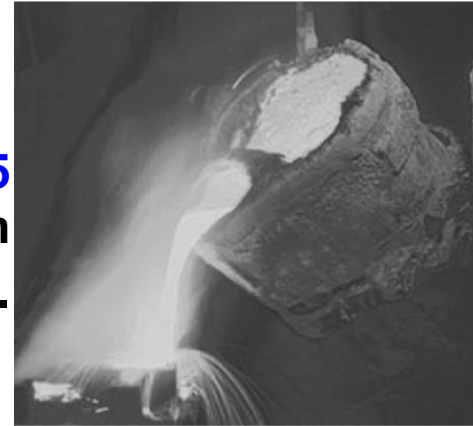


1912

41,578 train derailments in the previous decade lead to NBS measurement and test program.

1905

Standard samples program begins with standardized irons.



NIST AT A GLANCE

Industry's National Laboratory



3,400+

FEDERAL
EMPLOYEES



5

NOBEL PRIZES



2 CAMPUSES

GAITHERSBURG, MD [HQ]
BOULDER, CO



3,500

+



10

COLLABORATIV
E



400+

BUSINESSES USING
NIST FACILITIES



ManufacturingUSA®

14

NATL OFFICE FOR
MANUFACTURING
INSTITUTES



51

MANUFACTURING
EXTENSION
PARTNERSHIP CENTERS



U.S. BALDRIGE
PERFORMANCE
EXCELLENCE PROGRAM

REDEFINING THE WORLD'S MEASUREMENT SYSTEM: SI UNITS



On November 16, 2018, at Versailles, France, the world's scientific and technical community redefined four of the seven base units for the International System of Units (SI). The affirmative vote means the kilogram (mass), kelvin (temperature), ampere (electric current) and mole (amount of substance) are now determined by fundamental constants of nature instead of by physical objects. This historic change is the largest single shift in international measurement since the Treaty of the Meter was signed in 1875. Scientists expect this change will spur technological innovation and lower the cost of many high-tech manufacturing processes.

NIST Priority Research Areas



Fotocrisis/shutterstock

Advanced
manufacturing



IT and cybersecurity



Bioeconomy



@Matt DeLaine

Quantum Science



@Earl Zubroff

Artificial Intelligence



Internet of Things



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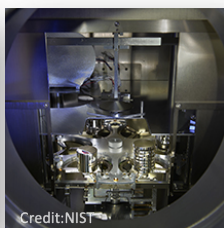
Infrastructure Resilience

NIST LABORATORY PROGRAMS



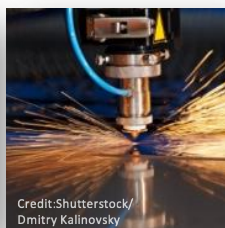
Credit: NIST

**Material
Measurement
Laboratory**



Credit: NIST

**Physical
Measurement
Laboratory**



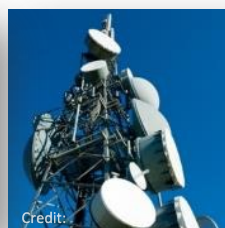
Credit: Shutterstock/
Dmitry Kalinovsky

**Engineering
Laboratory**



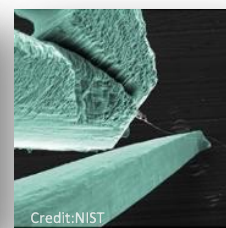
Credit: Shutterstock

**Information
Technology
Laboratory**



Credit: Shutterstock/
Italianestro

**Communication
Technology
Laboratory**



Credit: NIST

**Center for
Nanoscale
Science and
Technology**

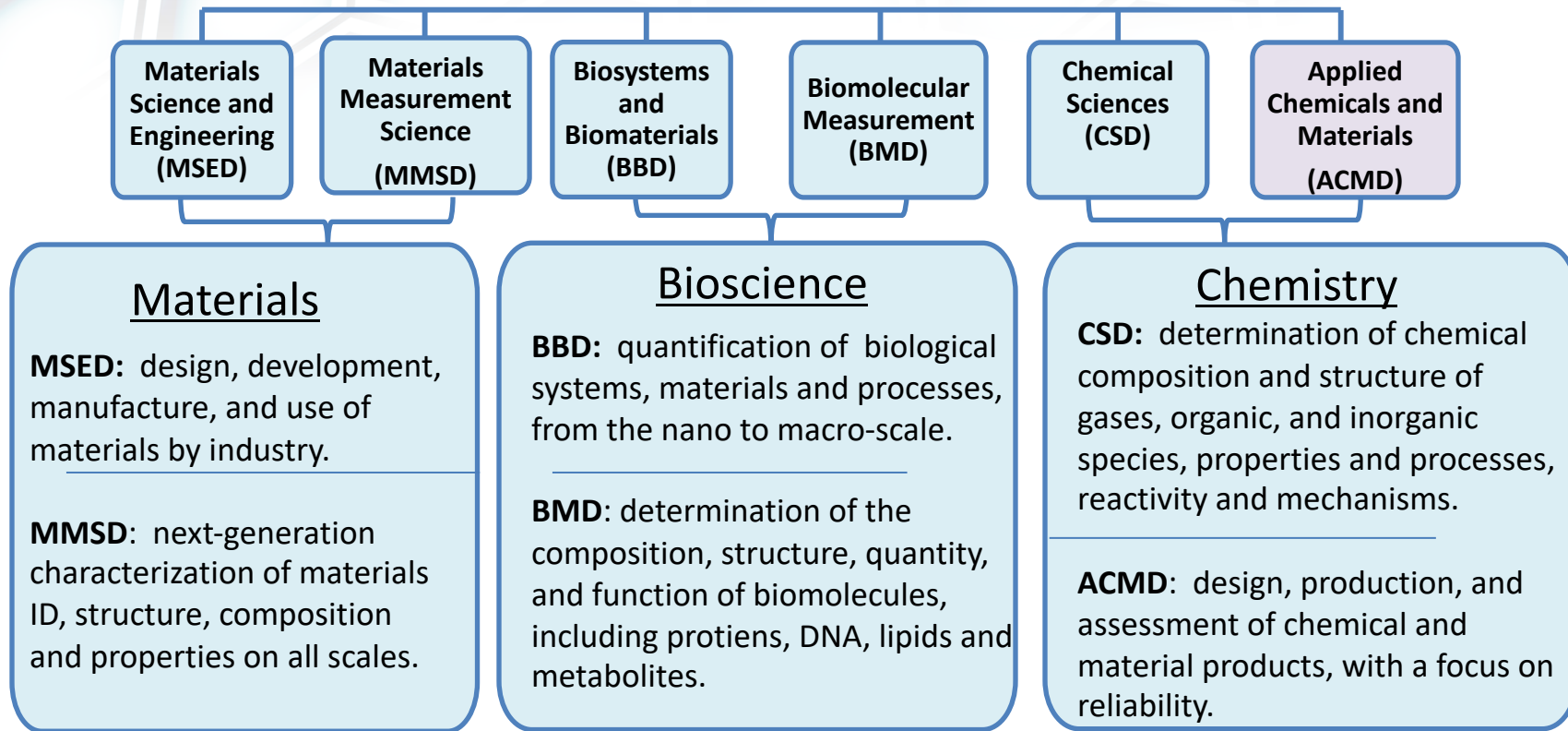


Credit: NIST

**NIST Center
for Neutron
Research**

Material Measurement Laboratory

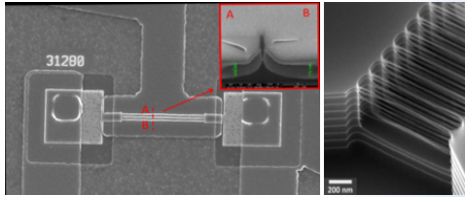
Measurement science, technology, standards, models and data that support...



NIST MATERIAL MEASUREMENT LABORATORY

Measurements of composition, structure & properties of matter...
...to advance technologies that serve all of humankind

Advanced Electronics



Reliable Materials for Buildings and Vehicles

Assessment of Soil, Water and Air Quality



Accurate Measurement of Materials, Chemicals & Biological Substances



Clean Alternative Fuels



Science-based DNA and Physical Forensics



Trustworthy Medical Tests and Diagnoses

NIST Products and Services

Collaborations

- 2600 Associates and Facility Users

Measurement Research

- 2,200 publications per year
- 8,000 attendees at 69 technical conferences

Standard Reference Data

- 100 different types
- 6,000 units sold per year
- 130 million data downloads per year

Standard Reference Materials

- 1,300 products available
- 33,000 units sold per year



Calibration Tests

- 24,000 tests per year

Laboratory Accreditation

- 800 accreditations of testing and calibrations laboratories per year

Standards Committees

- 400 NIST staff serving on 1,000 national and international standards committees

CENTER OF EXCELLENCE FOR ADVANCED MATERIALS RESEARCH

Center for Hierarchical Materials Design (CHiMaD)- led by Northwestern University

Consortium Members

- Northwestern-Argonne Institute of Science and Engineering
- Computation Institute (a partnership between the University of Chicago and Argonne)

Others closely involved include

- QuesTek Innovations
- ASM International



Northwestern University
Evanston, IL

Focus: developing the next generation of computational tools, databases and experimental techniques to enable “Materials by Design”

MATERIALS SCIENCE AND ENGINEERING

Division Function:

Provides the measurement science, standards, technology, and data required to support the Nation's need to design, develop, manufacture, and use materials.

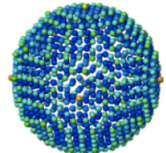
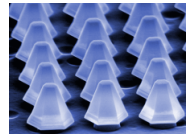
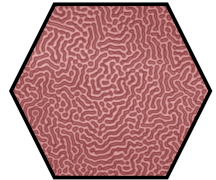
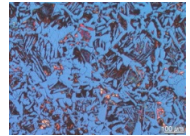
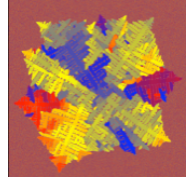
Division Chief: Mark VanLandingham

Groups:

- Polymers & Complex Fluids (Kate Beers)
- Functional Polymers (Chris Soles)
- Functional Nanostructured Materials (Albert Davydov)
- Mechanical Performance (Jon Guyer)
- Thermodynamics and Kinetics (Carrie Campbell)
- Polymer Processing (Dean DeLongchamp)

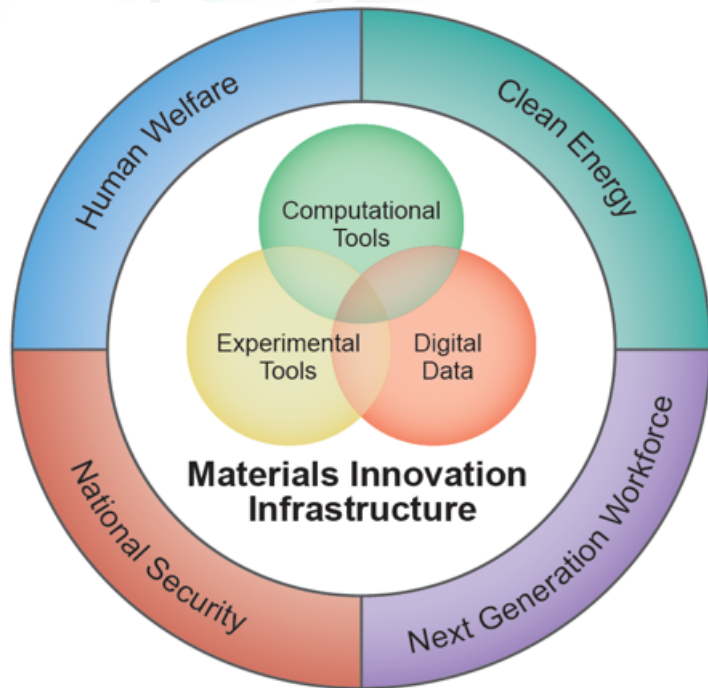
Capabilities:

- Metallurgical materials science (e.g. alloys, solidification, processing)
- Polymer & colloidal materials science (e.g. carbon nanotubes, nSoft)
- Microstructure, nanostructure (e.g. microscopy, scattering)
- Mechanical performance (NCAL, ballistic fibers)
- Materials data and computational tools (MGI)



The Materials Genome Initiative

Goal: to decrease time-to-market by 50% while <\$\$



Develop a Materials Innovation Infrastructure

Achieve National goals in energy, security, and human welfare with advanced materials

Equip the next generation materials workforce

Materials Genome Initiative for Global Competitiveness



INTERATOMIC POTENTIALS

Workshop history:

- Started in 2008 by Chandler Becker to bring together industry, government and academia to address the current state of the art and identify current needs and challenges.
- Held annually from 2008-2014
(<https://www.ctcms.nist.gov/potentials/activities.html>)
 - 2012: MGI focus
 - 2013: Testing and Validation focus
 - 2014: Materials for Gas Separations; Metal-Organic Frameworks
 - 2018: Potential Development and Workflow tools

•

Interatomic Potential Development and Tools at NIST

- Interatomic potential repository (IPR)
- Atomman
- iprPy
- PyFit-FF
- PINN potentials
- JARVIS-FF

Interatomic Potentials (Force Fields)

Elements

Alloy, Compound, Coarse-Grained and Fictional Potentials

The following is a list of all of the multi-element systems and non-element materials that we host potentials for. NOTE: be sure to read the potential descriptions! The multi-component potentials may not be applicable to the full composition range as they are often designed for specific compositions and/or composition ranges. Coarse-grained potentials reduce the simulation complexity by representing alloy compositions or molecules with a single particle type. Fictional potentials were purposefully fit to unrealistic target properties and therefore should not be used to accurately represent real materials.

Ag-Au-Cu	Ag-Au-Cu-Ni-Pd-Pt	Ag-Cu	Ag-Hf-Pd	Ag-Ni
Ag-TiO ₂	Al-Cu	Al-Cu-Ni	Al-Cu-Ni	Al-Cu-Fe-Mg-Si
Al-Cu-Ni	Al-Fe	Al-Ni	Al-Ni-Ni	Al-Ni
Al-Mg-Zn	Al-Mn-Pd	Al-Nb-Ti	Al-Ni	Al-NiO
Al-O	Al-Pb	Al-Sm	Al-Ti	Al-U
Al-Si	Al-Sr	Al-Sr	B-C-N	B-N
Be-O	Bi-Cu-Si-Fe-Al-K-Li-Na-Rb	C-Cu	C-Fe	C-Fe-Mn-Si
C-Fa-Ti	C-H-O	Co	Co	Co-Ni-Si-Sb-Ta-Zn

PyFit-FF



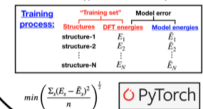
DFT data

Pre-processing

- atomic environment fingerprinting
- error/consistency checks
- matrix construction

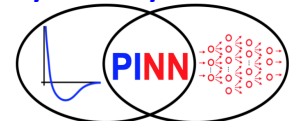
Training loop

L-BFGS (quasi-Newton method)

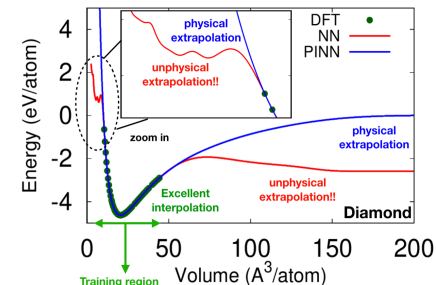


Interatomic potential

Physically informed



Neural Network potentials



www.ctcms.nist.gov/potentials

LOGISTICS

Schedule

Session interactions

Lunch

Notice! This site is currently under construction and testing. 

New! Please give us your feedback

Overview

This repository provides a source for interatomic potentials (force fields), related files, and evaluation tools to help researchers obtain interatomic models and judge their quality and applicability. Users are encouraged to download and use interatomic potentials, with proper acknowledgement, and developers are welcome to contribute potentials for inclusion. The files provided have been submitted or vetted by their developers and appropriate references are provided. All classes of potentials (e.g., MEAM, ADP, COMB, Reax, EAM, etc.) and materials are welcome. Interatomic potentials and/or related files are currently available for various metals, semiconductors, oxides, and carbon-containing systems.

