Web-Based Visualization and Simulation Tools for Nanotechnology Education

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The purpose of our presentation is to discuss both the use of web-based visualization and simulation tools which are freely available through the internet.

These tools can be used to enhance students understanding of abstract nanoscience concepts which can also be utilized by the instructor to teach and design difficult concepts without buying the equipment.

These tools include 21 RAIN (remote access instruments in nanotechnology) nodes for accessing visualization instruments and over 500 simulation tools available through NanoHUB which allows students to simulate and understand nanotechnology related areas.
Order of Presentation

➢ Motivation
➢ Impact on Nanotechnology Education
➢ Human Vision Acuity
➢ Visualization Options
➢ Imaging Techniques
➢ Novel Properties at Nano scale
➢ Online Visualization & Simulation Tools
➢ Remote Accessible Instruments for Nanotechnology (RAIN)
➢ NanoHUB
➢ Conclusion
➢ Q & A…Comments
Exponential Convergence of Nanotechnology, Robotics and Artificial Intelligence (AI)
Exponential Convergence of Nanotechnology, Robotics and Artificial Intelligence (AI)

Modern AI Theory of Evolution

- Computer (Number Cruncher) - Computation (1950’s)
- Basic Robot (Special Purpose) - Repeated Tasks (1990’s)
- Programmable Robot (Foundational AI) - Machine Learning (2010’s)
- Human-Like (Augmented AI) - Deep Learning (2030’s)
- Super Human-Like (Strong AI) - Conscience? (2040’s+)
An Integrated Human and Robot Society

Manager

A Party

Entertainment

... and they praise my intelligence, but it's all artificial!
Visualization and Simulation

“I hear and I forget. I see and I remember. I do and I understand.”
Visualization and Simulation

“The purpose of computing is insight, not numbers.”
--- R. W. Hamming

**Motivation**

- Demands of Global Marketplace: Graduates who have sound knowledge of fundamental principles underlying the design and operation of complex systems.

- However, incorporation of such learning processes, including state-of-art technological tools and equipment, requires considerable time and financial resources.

- Keeping curricula and labs current with the rapid change of technology pose another challenge for academia.
Motivation

• Development of new products based on nanotechnology requires visualization coupled with interfacial interactions, and measurement at the nanoscale.
• It is predicted that the general need for measurement tools for the emerging field of nanotechnology applications is expected to create a multibillion-dollar market within the next decade.
• Visualization of physical phenomena can confirm hypothesis
• Observation provides opportunities for study without damaging the sample.
• Objects under study may be too small for our hands to handle or manipulate
• Our students are motivated by “seeing for themselves”!
Visualiztion and Simulation Impact

➢ Simulations are recognized as an efficient and effective way of teaching complex and dynamic engineering systems.

➢ A simulation-based teaching environment enables students to acquire experience and consider their previous results.

➢ Simulation has been shown to be effective in improving teaching and learning of various subjects.

➢ By reducing practical learning time for students, and for schools and programs, simulation reduces costs for practice oriented educational methodology.
Visualization and Simulation

Impact

➢ Enhance students understanding of the properties of matter at the nanoscale which differ from bulk material.
➢ Help instructors improve teaching of abstract concepts of nanoscale phenomena.

➢ Understand the benefits and application of visualization at the nanoscale.

➢ Increase knowledge in the field of nanotechnology and STEM education.

➢ Understand the use of remotely accessible instruments for visualization of nanoscale samples.
At about 300 mm (12”), a person with 20/20 vision is able (at best) to resolve objects separated by not more than about 0.089 mm (0.0349”) under normal lighting conditions.

To see smaller objects, we use magnification systems including single convex lenses (magnifying glasses) and more complex vision enhancement systems such as optical microscopes.
Limits in Visualization

➢ Optical Microscopy Resolution Limits

\[ \sigma = \frac{k \lambda}{NA} \]

\( \sigma \) = minimum feature size
\( \lambda \) = wavelength of light used
\( NA \) = Numeric Aperture (lens)
\( k \) = Constant (about 0.5)

➢ Shorter wavelengths of light and higher numerical aperture lenses are difficult to produce!

➢ High Index of Refraction materials are difficult to produce.
Options in Visualization

➢ Observe the sample with shorter wavelengths of light or radiation
  – Need to convert the imaging result into something that we can visualize
    • X-Ray film
    • Scanning Electron Microscope

➢ Probe the sample physically
  – Need to be very, very careful
    • Mechanical feedback
    • Motion to vision conversion required
Imaging Techniques: Scales

- Proteins 10 nm
- Bacteria 1 µm
- Red Blood Cell 5 µm
- Human Hair 75 µm
- Si Atom Spacing 0.4 nm
- DNA 2 nm
- Virus 50 nm
- Cell 30 µm
- Ant 5 mm

Scale:
- 10^-10 to 10^-1 (Angstrom, Nanometer, Micron, Millimeter, Meter)

Methods:
- AFM
- TEM
- Near Field Optical
- Optical Microscope
- SEM
What Doors Open At The Nano-Scale?

New phenomena and opportunities become accessible
The Sources of the Unique Properties at Nano Scale

Small size

- High surface to volume ratio – unique environment of surface atoms
- Surface forces dominate over bulk forces (which depend on volume) – for example, gravity is not important!
- Importance of quantum mechanical effects
- Dominance of the wave properties of light
Size Effects

Electronic and vibrational states and transitions show deviations from those in the bulk.

Tunable new properties!!!
Structure of Nanoparticles

<20%  Surface to Volume Ratio  ~80%
Properties of Nanoparticles

➢ As the diameter of a material gets smaller new seemingly tunable properties can be observed.

➢ The energy states become discrete and quantum effects dominate.

- Conduction band
- Bulk Metal
- Large Metal Cluster
- Small Metal Cluster
Novel Properties

Physical properties of bulk materials change as dimension decrease below characteristic lengths.

- Optical properties
- Electrical properties
- Reactivity
- Geometric fluctuations
- Magnetic moment
Methods of Nanoscale Visualization

➢ **Optical Microscope**
  Suffers from diffraction effect on sample surfaces.
  Limited resolution at nanoscale.

➢ **Scanning electron microscope (SEM)**
  Require the use of electron beams at high vacuum environment
  and cannot be used for biological non conductive samples and
  samples under liquid.

➢ **Atomic Force Microscopy (AFM)**
  Uses sharp probe scanning over the sample while maintaining
  a very close spacing to the surface. A tool to measure both
  topography and force-related material properties at the
  nanoscale.
Visualization and Simulation at the Nanoscale

Visualization of processes can be achieved by using laboratory instruments, online simulation and remote access instruments.

Online Tool/Methods of Visualizations and Simulation at the Nanoscale:

- Remote Accessible Instruments for Nanotechnology (RAIN)
- NoanoHUB: www.nanohub.org
Online Tools/Methods of Visualizations and Simulation at the Nanoscale

Remote Accessible Instruments for Nanotechnology (RAIN)
NoanoHUB: www.nanohub.org

Benefits

• Saving on buying an expensive equipment
• Helps to train students before buying the equipment
• Introduce students to the field of nanotechnology
Remote Access

Remotely Accessible Instruments for Nanotechnology (RAIN) allows students to access and control microscopes, like FESEM-field emission scanning electron microscopes, and analytical tools, like EDS-energy (X-ray) dispersive spectroscopy, to look at nano-sized materials from the ease of classrooms, or even home computers, all across the country. Students control the tools over the Internet in real-time and with the assistance of an experienced engineer at the microscope advising over video conferencing software.
Learning through Visualization and Simulation at the Nanoscale
Remote Accessible Instruments for Nanotechnology (RAIN): Types of Tools

RAIN allows students to access and control microscopes and analytical tools, to look at nanosized materials from the ease of classrooms, or home computers, all across the country. Students control the tools over the Internet from 19 centers in real-time.

- Atomic Force Microscope (AFM)
- Optical Microscope
- Confocal Microscope
- Scanning Electron Microscope (SEM)
- Energy Dispersive Spectroscopy (EDS)
- Profilometer
- Ultraviolet–visible Spectrophotometer
- Molecular Analyzer
- Fourier Transform Infrared Spectroscopy (FTIR)
- X-ray fluorescence (XRF)
- Fabrication Tools
**RAIN Network Instruments**

nano4me.org/remoteaccess

<table>
<thead>
<tr>
<th>RAIN Site</th>
<th>Remote Access Instruments</th>
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<tbody>
<tr>
<td>Arizona State University</td>
<td>SEM</td>
</tr>
<tr>
<td>Erie Community College</td>
<td>SEM/EDS</td>
</tr>
<tr>
<td>Forsythe Tech Community College</td>
<td>AFM</td>
</tr>
<tr>
<td>Northcentral Technical College</td>
<td>SEM, AFM, Flex AFM</td>
</tr>
<tr>
<td>North Seattle College</td>
<td>Confocal Microscope, AFM, Profilometer, SEM/EDS</td>
</tr>
<tr>
<td>Oakton Community College</td>
<td>SEM/EDS, Flex AFM, Profilometer</td>
</tr>
<tr>
<td>Pasadena City College</td>
<td>SEM/EDS</td>
</tr>
<tr>
<td>Pennsylvania State University</td>
<td>FESEM/EDS, SPM/AFM, Profilometer, UV-vis</td>
</tr>
<tr>
<td>Salt Lake Community College</td>
<td>SEM, AFM/SPM</td>
</tr>
<tr>
<td>University of Texas at San Antonio</td>
<td>SEM/EDS</td>
</tr>
</tbody>
</table>

Source: Dr. Cakmak, Penn State.
Remote Accessibility of Nanotechnology Instruments

Atomic Force Microscope (AFM)
- Forsyth Tech Community College - (Nanosurf Flex Scan head AFM)
- Northcentral Technical College - (Nanosurf easyScan 2)
- North Seattle College - (Nanosurf easyScan 2)
- Oakton Community College - (Nanosurf easyScan 2 FlexAFM)
- Pennsylvania State University - (Bruker Innova)
- Salt Lake Community College - (Agilent 5400 AFM/SPM & Nanosurf easyScan 2)

Scanning Electron Microscope (SEM)
- NCI-SW at Arizona State University - (Phenom Pro)
- CABOCES - (Phenom ProX & JEOL-JSM-6010PLUS/LA)
- Erie Community College - (JEOL JSM-6010LA)
- Northcentral Technical College - (Hitachi TM 3030)
- Oakton Community College - (Hitachi TM 3000)
- North Seattle College - (Aspex EXplorer)
- Pasadena City College - (Phenom ProX)
- Pennsylvania State University - (ZEISS 55 Ultra FESEM)
- Research Triangle Nanotechnology Network - (FEI Quanta 200 Field Emission Gun)
- Salt Lake Community College - (Hitachi TM3000)
- SUNY Polytechnic Institute - (Hitachi TM3000 w/ x-ray (EDS))
- University of Texas at San Antonio - (Hitachi S5500 STEM)
- SCME at University of New Mexico - (Phenom ProX)

Optical Microscope
- Pennsylvania State University - (Leitz Ergolux)
Step 1
**Watch Videos:** To get the most out of your remote access session, we suggest that teachers and students learn about the technology used to view things at the nano-scale level. Our recommended videos can be viewed in the classroom, or assigned as homework.

Step 2
**Complete the Remote Access Request Form:** This is where you request a remote test session (if this is your first time running remote access with us) and a live session; select the instruments and topic areas you’d like to focus on; and provide your lab instructor with other important information such as your class' interests and knowledge level.

Step 3
**Run a remote test session**
This is used to check your audio, video, and Internet connections. It takes about 20 minutes.
Step 1
Before you start remote access, you’ll need to:
1. Install Video Conferencing Software
   Based on the instrument and partner site you requested, you will need either Zoom or Team Viewer. Both are free to download and use.

2. Set up your computer. You need:
   - Webcam
   - Microphone
   - Speakers
   - A projector or large display is recommended, but not required

Step 3
Choose your samples: You can use in house samples or send your own to the remote access site you selected when scheduling your session. Based on your remote access request (step 2), a remote access manager will reach out to you regarding in house sample availability and to provide address information for any samples you wish to mail in.

Step 4
Run a live session
- This is where you will have live remote access to the lab equipment.
- This can take anywhere from 15 minutes to 2 hours.

Step 5
Give us feedback!
Help us show the NSF that remote access is a valuable resource.
Web-Based Visualization and Simulation Tools for Nanotechnology Education

Simulation

Simulation offers a number of other advantages
(a) allowing the user to modify system parameters and observe the outcomes without any harmful side effects
(b) eliminating component or equipment faults that affect outcomes
(c) supporting users progress at their own pace in discovery and understanding of concepts and issues,
and (d) enhancing the presentation of “dry” concepts by integrating theory and practice
Web-Based Visualization and Simulation Tools for Nanotechnology Education

Nanohub.org

- Computing Cloud located at Purdue University
- 500+ simulation tools
- 1.4 million users Worldwide
- 5500 resources
SIMULATE
explore the powerful tools at your fingertips

Workspace
Development workspace

nanoDDSCAT
Calculate scattering and absorption of light by targets with arbitrary geometries and complex refractive index.

Crystal Viewer Tool
Visualize different crystal lattices and planes

MOSFet
Simulates the current-voltage characteristics for bulk, SOI, and double-gate Field Effect Transistors (FETs)
NanoDDSCAT

Calculate scattering and absorption of light with arbitrary geometry and complex Refractive Index

1. Target
NanoDDSCAT

Calculate scattering and absorption of light with arbitrary geometry and complex Refractive Index

2. Spectrum Calculation
NanoDDSCAT

Calculate scattering and absorption of light with arbitrary geometry and complex Refractive Index

3. Field
NanoDDSCAT
Calculate scattering and absorption of light with arbitrary geometry and complex Refractive Index
4. Process and Simulate
NanoDDSCAT
Worldwide Usage
Crystal Viewer

Visualize different crystal lattices and planes
Crystal Viewer
Visualize different crystal lattices and planes
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Visualize different crystal lattices and planes
Crystal Viewer

Worldwide Usage

12,167
Jun 2019

Users By Organization Type

<table>
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<tr>
<th>Type</th>
<th>Users</th>
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</thead>
<tbody>
<tr>
<td>Unidentified</td>
<td>6,913 (56.79%)</td>
</tr>
<tr>
<td>Educational</td>
<td>4,805 (39.6%)</td>
</tr>
<tr>
<td>Industry</td>
<td>181 (1.49%)</td>
</tr>
<tr>
<td>National Lab</td>
<td>102 (0.84%)</td>
</tr>
<tr>
<td>Educational</td>
<td>9 (0.07%)</td>
</tr>
<tr>
<td>Unemployed</td>
<td>49 (0.4%)</td>
</tr>
<tr>
<td>Government Agency</td>
<td>40 (0.33%)</td>
</tr>
<tr>
<td>Military</td>
<td>9 (0.07%)</td>
</tr>
</tbody>
</table>

Users by Country of Residence

<table>
<thead>
<tr>
<th>Country</th>
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</tr>
</thead>
<tbody>
<tr>
<td>UNITED STATES</td>
<td>2,852 (22.08%)</td>
</tr>
<tr>
<td>INDIA</td>
<td>426 (10.17%)</td>
</tr>
<tr>
<td>PAKISTAN</td>
<td>305 (7.28%)</td>
</tr>
<tr>
<td>KOREA, REPUBLIC OF</td>
<td>118 (2.82%)</td>
</tr>
<tr>
<td>GERMANY</td>
<td>114 (2.72%)</td>
</tr>
<tr>
<td>COLOMBIA</td>
<td>83 (1.98%)</td>
</tr>
<tr>
<td>CHINA</td>
<td>81 (1.93%)</td>
</tr>
</tbody>
</table>
Simulate the current-voltage characteristics for Bulk, SOI, and double-gate Field Effect Transistors (FETs).
MOSFET

Simulate the current-voltage characteristics for Bulk, SOI, and double-gate Field Effect Transistors (FETs)
MOSFET

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Simulate the current-voltage characteristics for Bulk, SOI, and double-gate Field Effect Transistors (FETs)
MOSFeT Worldwide Usage
Web-Based Visualization and Simulation Tools for Nanotechnology Education

Target Audience & Curricula

**Targeted Students**
- 4 year degree program in engineering and engineering technology
- 2 year Associate degree in engineering and engineering technology
- K-12

**Suggested Courses**
- Introduction to Nanotechnology
- Introduction to Semiconductor Manufacturing
- Material Science
- STEM courses
- Undergraduate research and Independent study
- Micro electro mechanical systems (MEMS)
Sample Student Projects
Visualization Tool for Quantum Dots
Quantum dots (QDs) are very small (order of several nanometer) confined structures made of metal and semi-conductors. Their optical and electronic properties differ from the bulk material and can emit light of certain frequencies if light or electricity is applied to them. The frequency of emission can be tuned by changing the size, shape and material of the dots. It has many potential applications in LEDs, transistors, solar cell, diode lasers and others.

By completing the quantum dot lab (https://nanohub.org/resources/qdot) users will understand.
1. The 3D confinement of carriers in a QD.
2. Desirable effects of geometry of QD on the states of carrier.
3. Study light absorption.
Visualization of digital video discs (DVDs), and BluRay DVDs

Objective: To study the nanoscale features and determine density of information by direct measurement of the patterns and tracks using NanoSurf EasyScan 2 AFM in the Intermittent contact (tapping mode).

Video data requires significantly more storage density and in order to accommodate the data, the pit and land sizes must be shrunk to smaller values. The spacing between tracks, width of tracks, their depth and reflectance vary according to the type of disc. Measuring the physical characteristics of the disc can help calculate the storage capacity of the disc. The smallest features of the DVDs are pits about 400 nm long, 320 nm wide, 120 nm deep, with a track pitch of 740 nm. BluRay DVD players provide high definition video for HDTV, requiring more data density. On Blu-ray the pits are written on about 300 nanometer wide tracks, which is less than half the width of a DVD as shown in the following figures.
Surface Morphology of PS/PMAA (polystyrene/ polymethylmethacrylate)

The PS/PMMA sample is a thin layer of a blend of two polymer solutions spread onto a piece of silicon wafer. PS (polystyrene), and PMMA (polymethyl methacrylate), when mixed together, separate into well-defined phases on the silicon. This thin film of self-organizing diblock copolymers allows high resolution patterning of ordered domains to be made in nanoscale dimensions over wafer-scale areas. AFM topographic imaging was used to monitor the surface roughness of PMMA/PS blends versus PMMA/PS copolymers. Phase imaging is used to detect the differences in surface morphology for the blend. It uses an intermittent mode and is a powerful technique for producing contrasts on heterogeneous samples.
Nanolithography of CD Using Veeco Caliber AFM

Atomic force microscopy, in addition to obtaining morphological image of a surface can also be used in the lithographical techniques to create nanoscale patterns on metals, semiconductors, and monolayer functionalized surfaces. This is obtained by applying force or voltage between the AFM probe and the surface or substrate. The typical radius of probe is 20-60 nm and the probe-substrate separation in close contact condition is less than 1 nm. Dip-pen lithography uses AFM tip to write chemical onto surfaces similar to a conventional fountain pen, with AFM tip as the pen and the substrate being the paper. AFM nanolithography is less expensive, faster and relatively simpler than traditional methods of achieving features of similar dimension like electron beam lithography or focused ion beam milling lithography. Nanolithography is both a fabrication and imaging tool, as the patterned areas can be imaged with clean or -link coated tips. AFM mages of pre and post nanolithography on a simple CD in the lab using Veeco/Bruker Caliber AFM are given below:
Conclusion

- Enhanced teaching/learning of nanoscale phenomena
- Enrichment of STEM component
- Supporting the Nanotechnology Workforce development
- NanoHUB is an excellent simulation tool for introducing and analyzing nanotechnology phenomena at all educational levels at no cost.
- RAIN provides free online remote access to real world Nanotechnology tools.
“The future belongs to those who prepare for it.”
— Ralph Waldo Emerson
References


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6. Remote Accessible Instruments for Nanotechnology (RAIN) http://www.nano4me.org/remote access

7. nanoHUB nanoHUB.org https://nanohub.org/resources/crystal_viewer

8. https://www.facebook.com/nanotechnology.rain

9. https://nanohub.org/search/?terms=nano+visualization+tools


Acknowledgement

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Thanks....Any Comments...Questions?

To know what you know and what you do not know, that is true knowledge.

--- Confucius

The art of knowing is knowing what to ignore.

--- Rumi