

Get your feet wet!

Introduction to nanoHUB



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Overview

- What is nanoHUB
- nanoHUB Apps and Tools
- MSE Community
- Simulation Examples

What is nanoHUB?



An open-access cyberinfrastructure

National Science Foundation
EEC 1227110

Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the National Science Foundation



A wide-angle, low-perspective shot of a modern library. The image shows a long, central aisle flanked by tall, multi-tiered metal bookshelves. The shelves are densely packed with books of various colors and sizes. The ceiling is high and features a series of skylights that allow natural light to filter into the space, creating a bright and airy atmosphere. The overall design is industrial and functional, emphasizing the vastness of the collection.

A library of STEM resources

A wooden toolbox filled with various tools, including a hammer, level, saw, and brushes, with the text "A Toolbox of Simulation Apps" overlaid. The toolbox is made of light-colored wood and has a black interior. The tools are organized in compartments. On the left, there are several brushes and a small bottle. In the center, there is a blue level, a red saw, and a yellow Stanley PowerLock. On the right, there is a hammer, a black handle, and a white corrugated tube. The toolbox is placed on a wooden deck.

A Toolbox of Simulation Apps

A photograph of a cluttered workshop. In the foreground, a long wooden workbench is supported by metal legs. On the left side of the workbench, there are large stacks of light-colored lumber. The workbench surface is covered with various items, including a box of tissues, a black plastic crate, and several white plastic containers. Underneath the workbench, there are stacks of white PVC pipes and other plumbing materials. In the background, there is a wooden door, a window, and a large open doorway leading to another room. The walls are covered with various items, including a grid of colorful letters and numbers. A fire extinguisher and a large metal container are visible near the doorway. The floor is made of light-colored tiles.

An App Development Workspace

A historical printing press workshop. In the center is a wooden galley with a grid of compartments, labeled 'CENTAUR' on its side. To the right is a large black metal press labeled 'ALBION PRESS HENRY MAKER WATTS LONDON'. The background features shelves with books and a wooden cabinet with many small compartments. A lamp is visible in the upper left corner.

A Publishing Platform



A Scientific Community

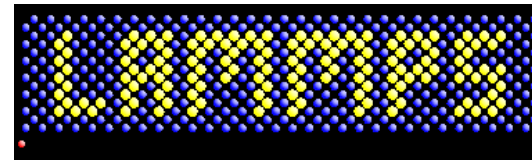
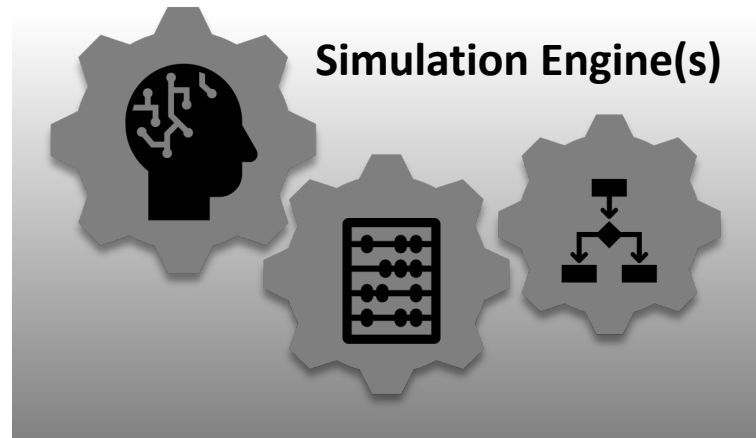
1.9 M annual users worldwide

HUB usage 2016-01-01 00:00:00

nanoHUB Simulation Engines, Apps, and Tools

Input deck: formatted text

```
units metal  
dimension 3  
boundary p p p  
atom_style atomic
```



SeqQuest Electronic Structure Code



Example nanoHUB App: Nanomaterial Mechanics Explorer


<https://nanohub.org/tools/nanomatmech>

nanoHUB App

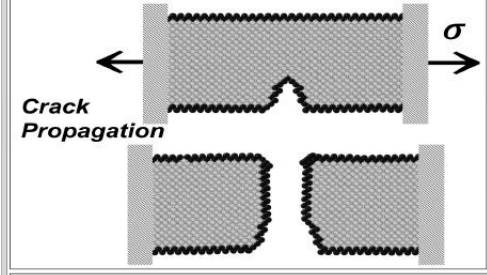
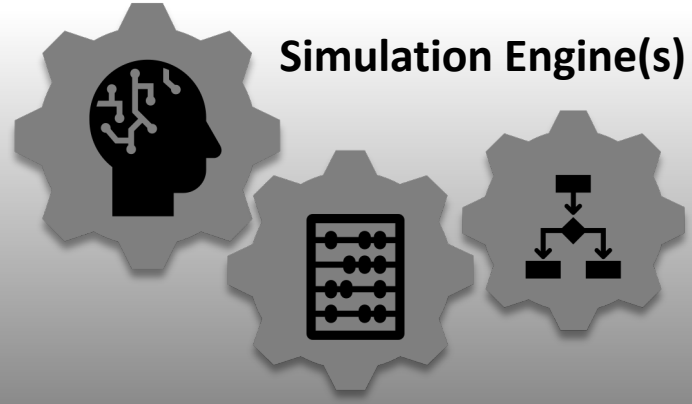
Input 1

Input 2

Input 3



Simulation Engine(s)



Crack Propagation

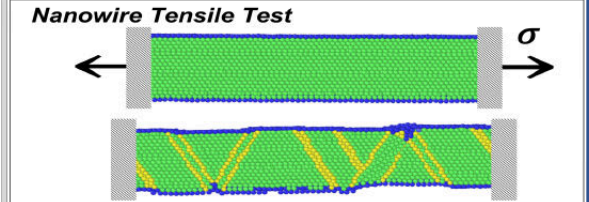
σ

Phase

T_c




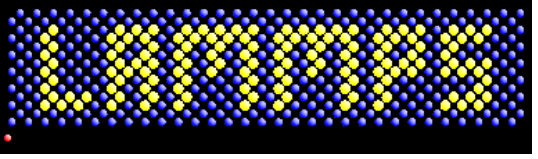
Nanowire Material and Orientation

| |
|---------------------|
| Copper [110] |
| Aluminum [100] |
| Copper [100] |
| Copper [110] |
| Copper [111] |
| Copper [112] |
| Nickel [100] |

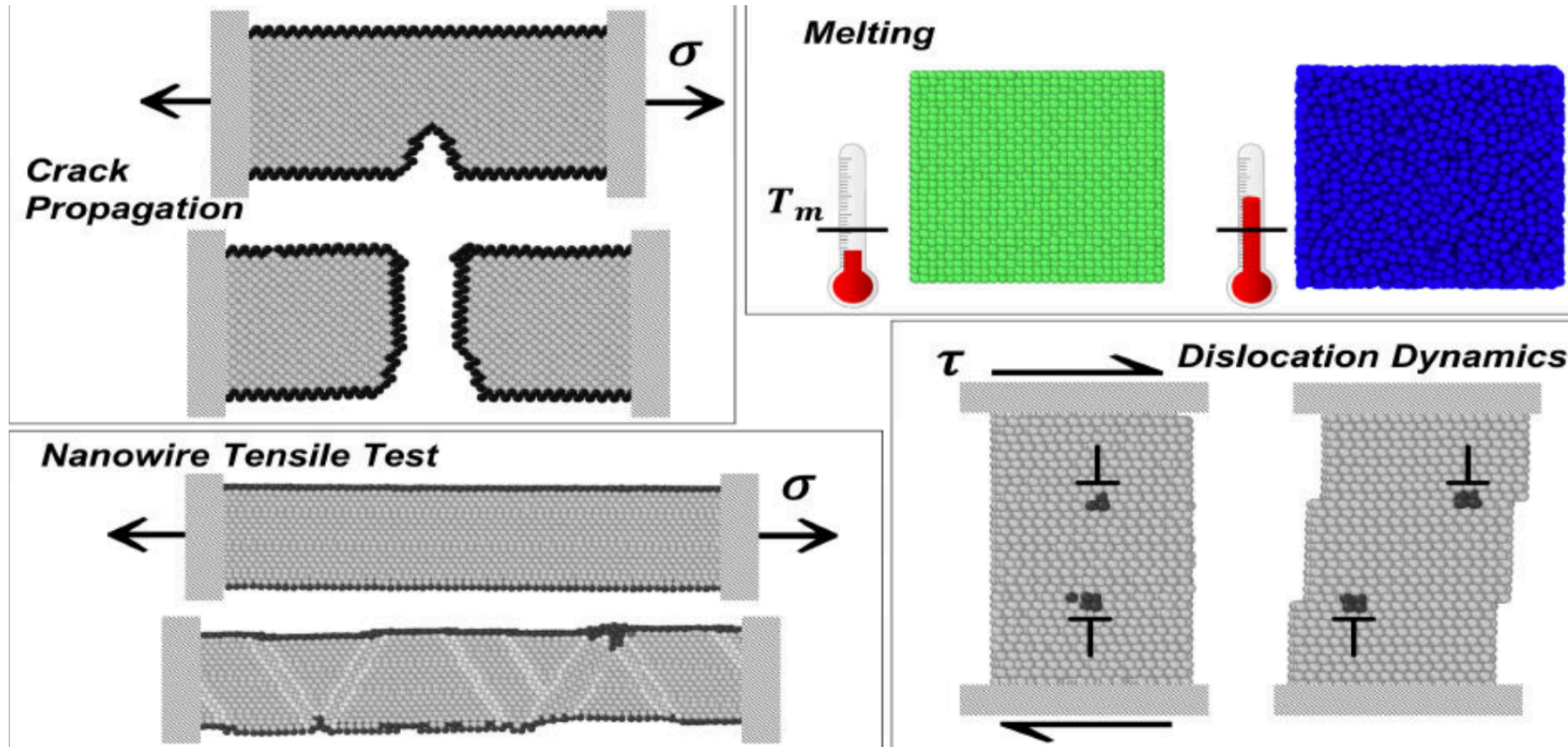


Nanowire Tensile Test

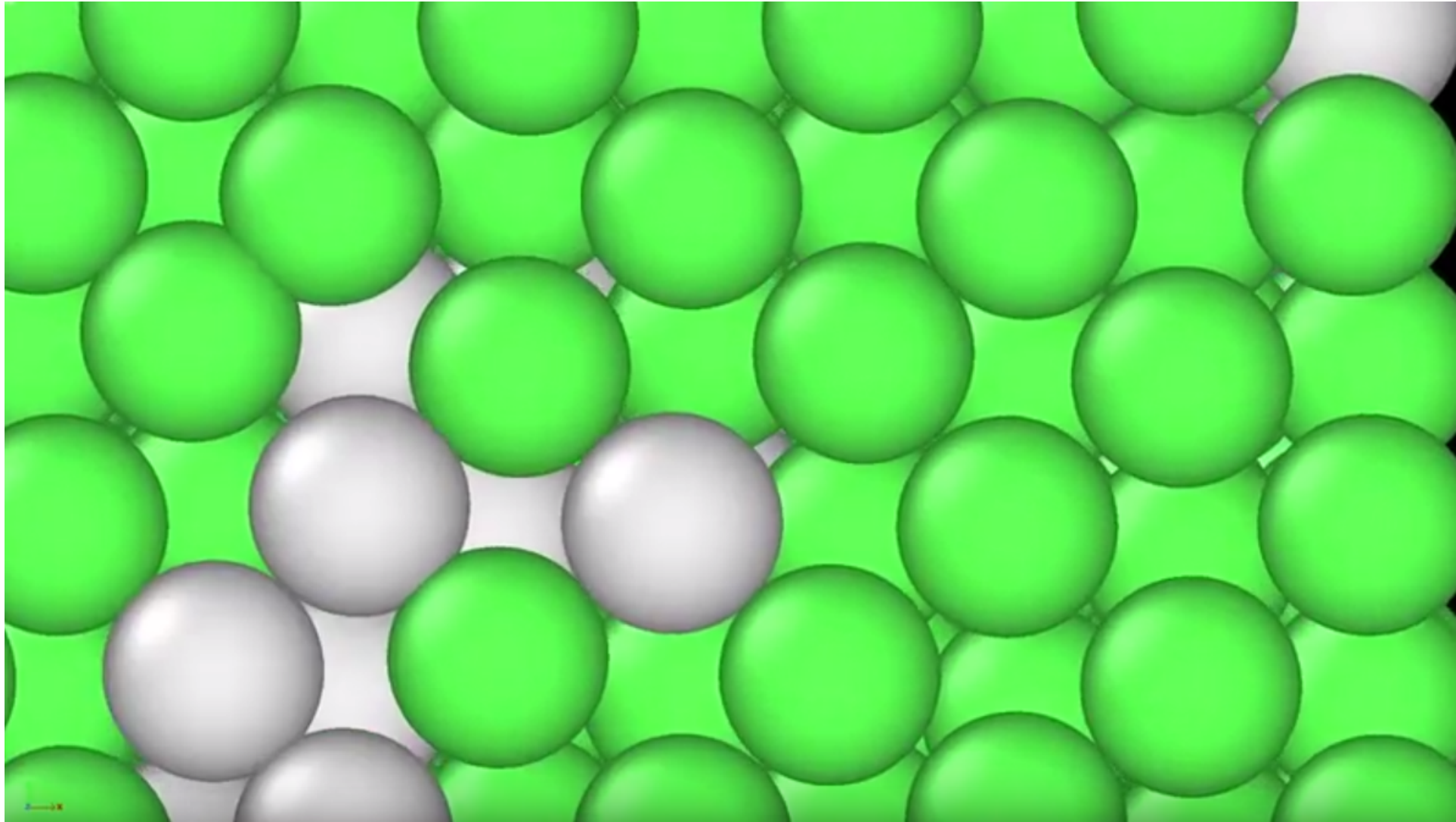
σ



Nanomaterial Mechanics Explorer: Melting

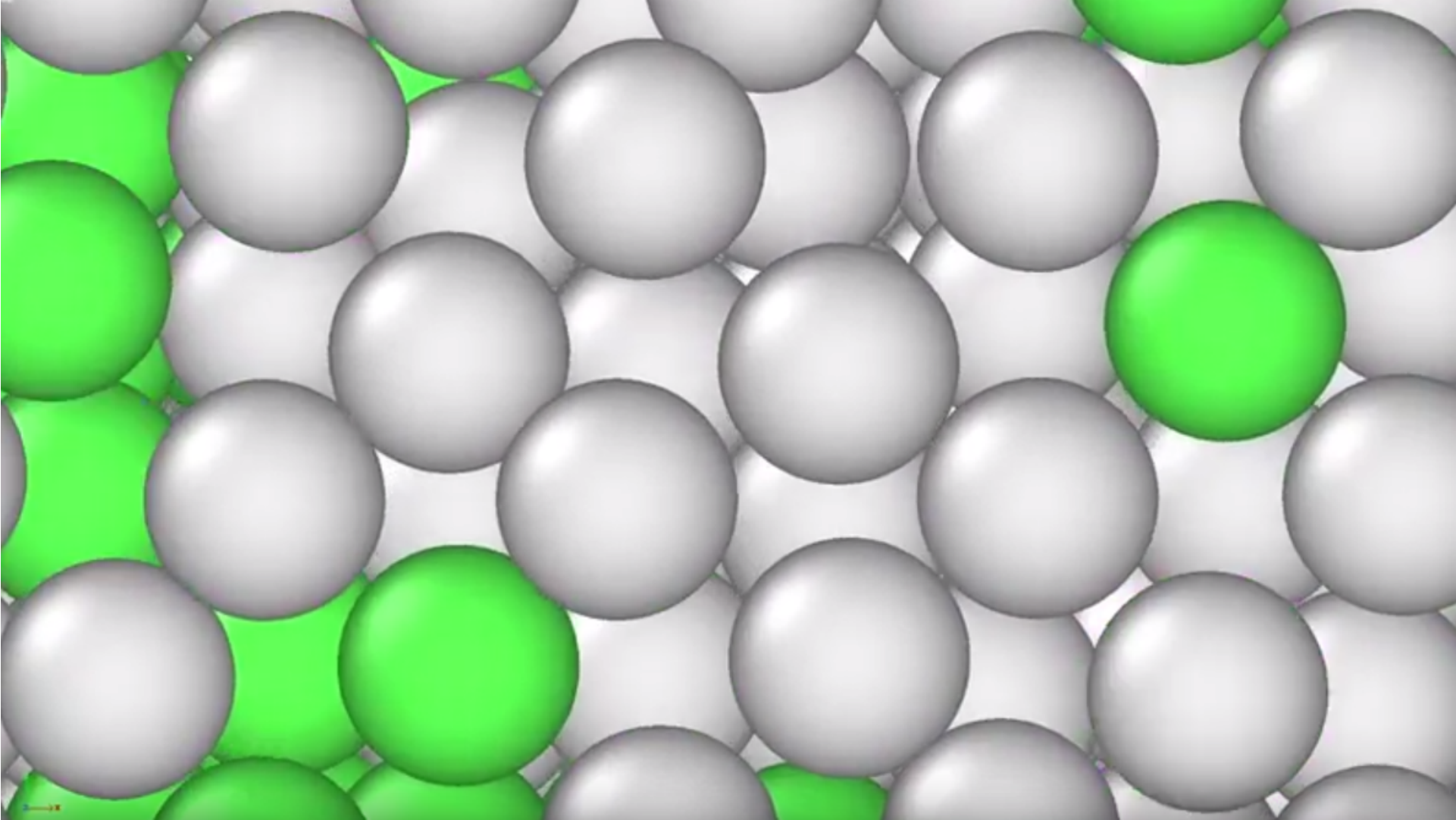


What repeating pattern do you see?

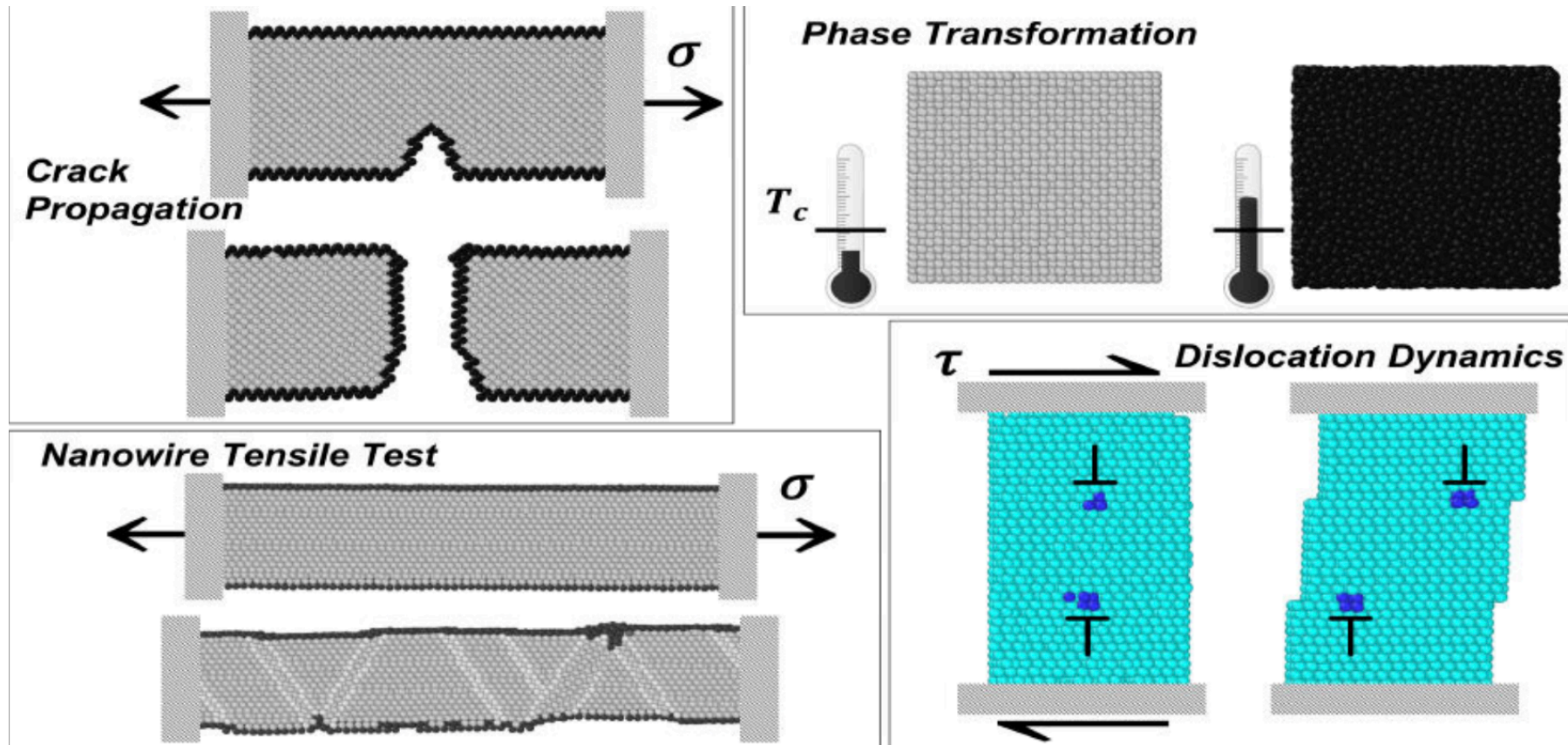


Could you extend this image to make it larger? Would you know where to place the next atoms? How do you know?

What do you notice is different about the white atoms?



Nanomaterial Mechanics Explorer: Dislocation Dynamics



Visualization of Edge Dislocations From a Textbook

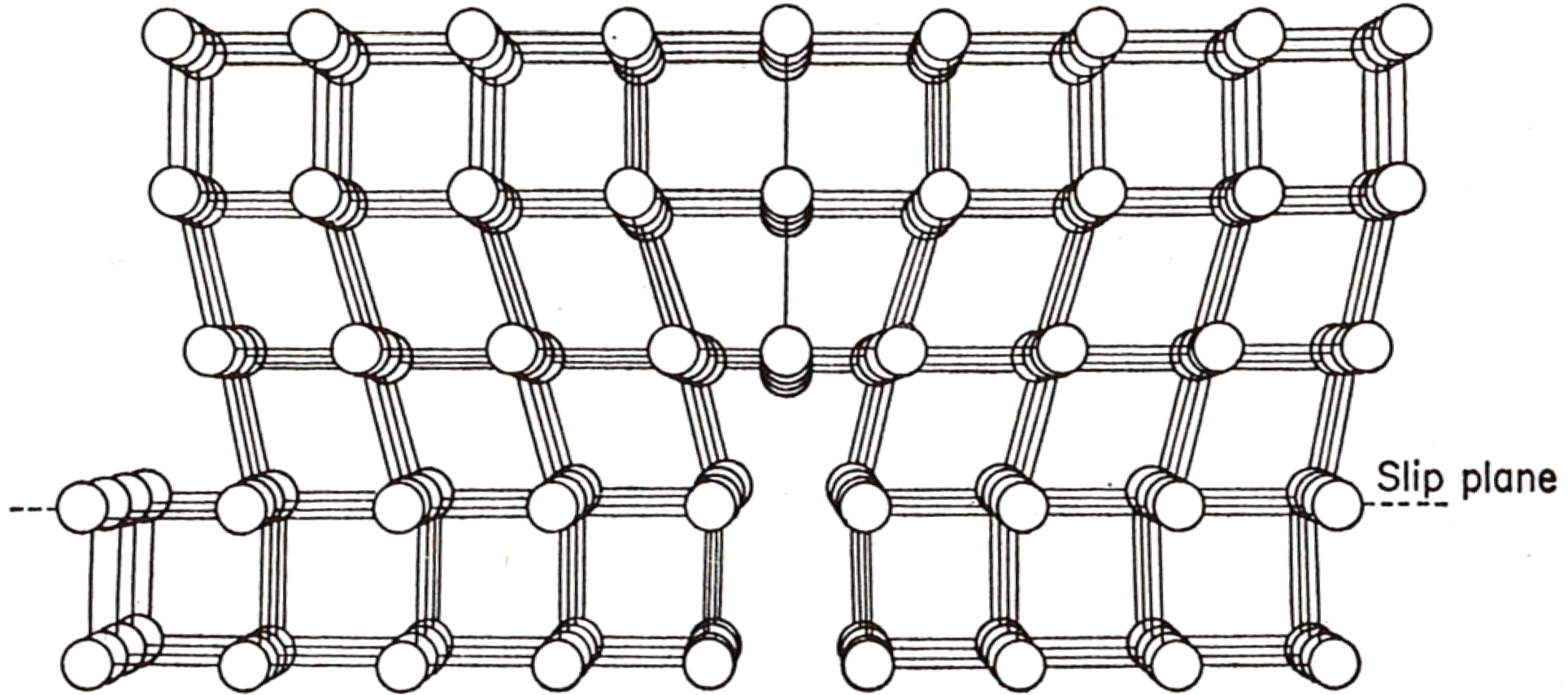
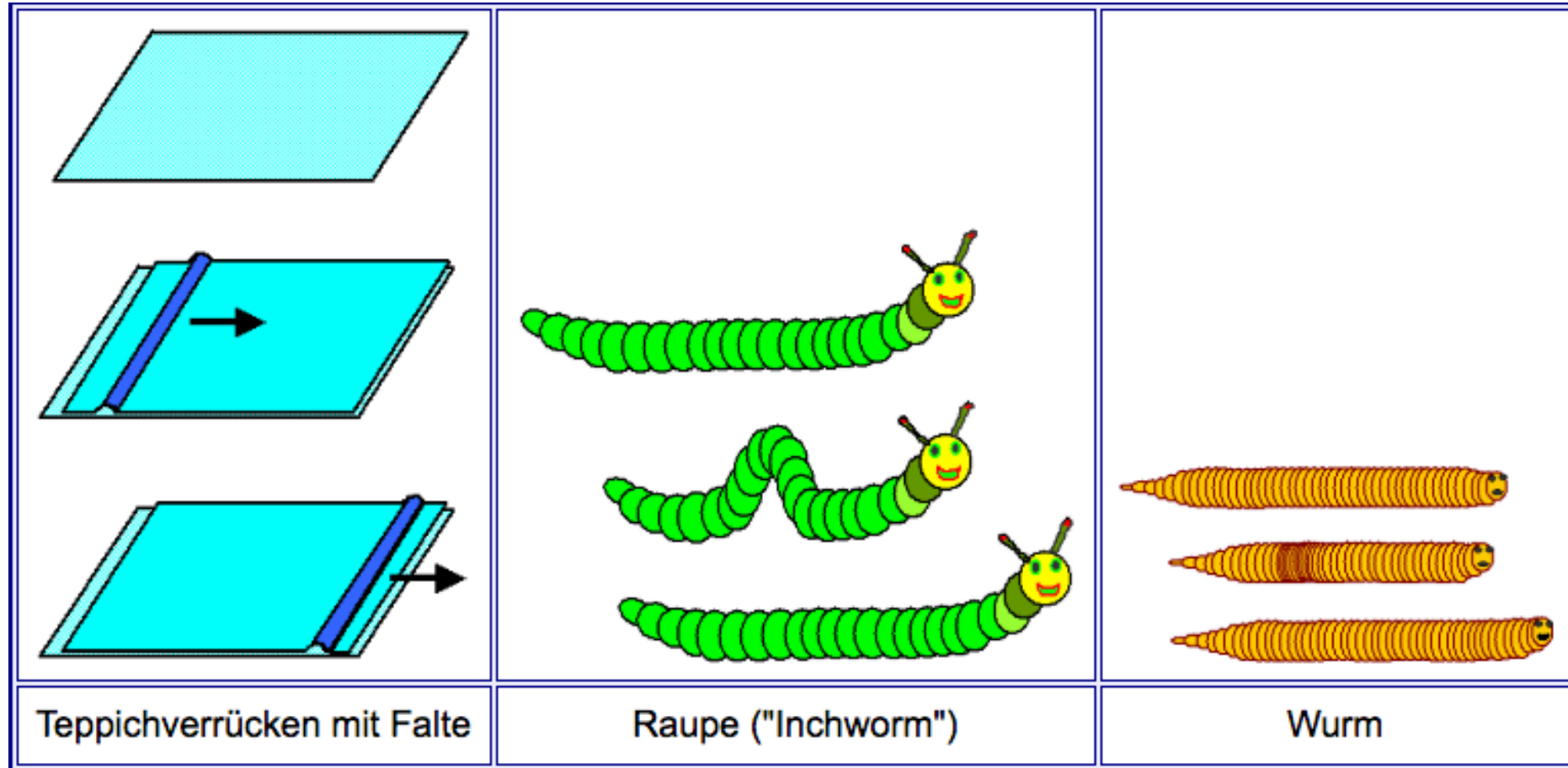


FIG. 4.5. An edge dislocation (after Goldman).

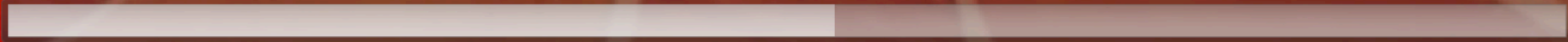
Visualizations of Edge Dislocations

From an Online Textbook

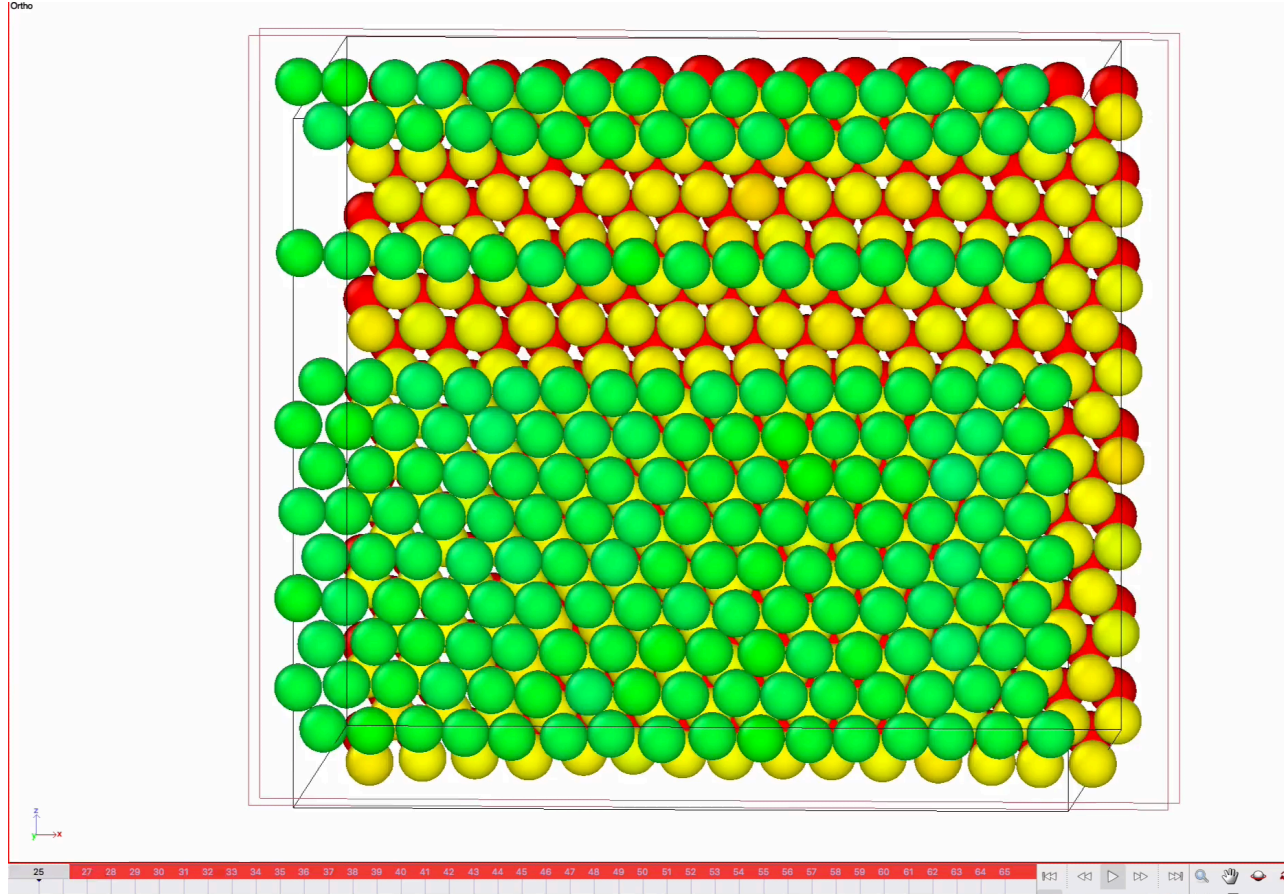


© H. Föll (MaWi 1 Skript)

https://www.tf.uni-kiel.de/matwis/amat/mw1_ge/index.html



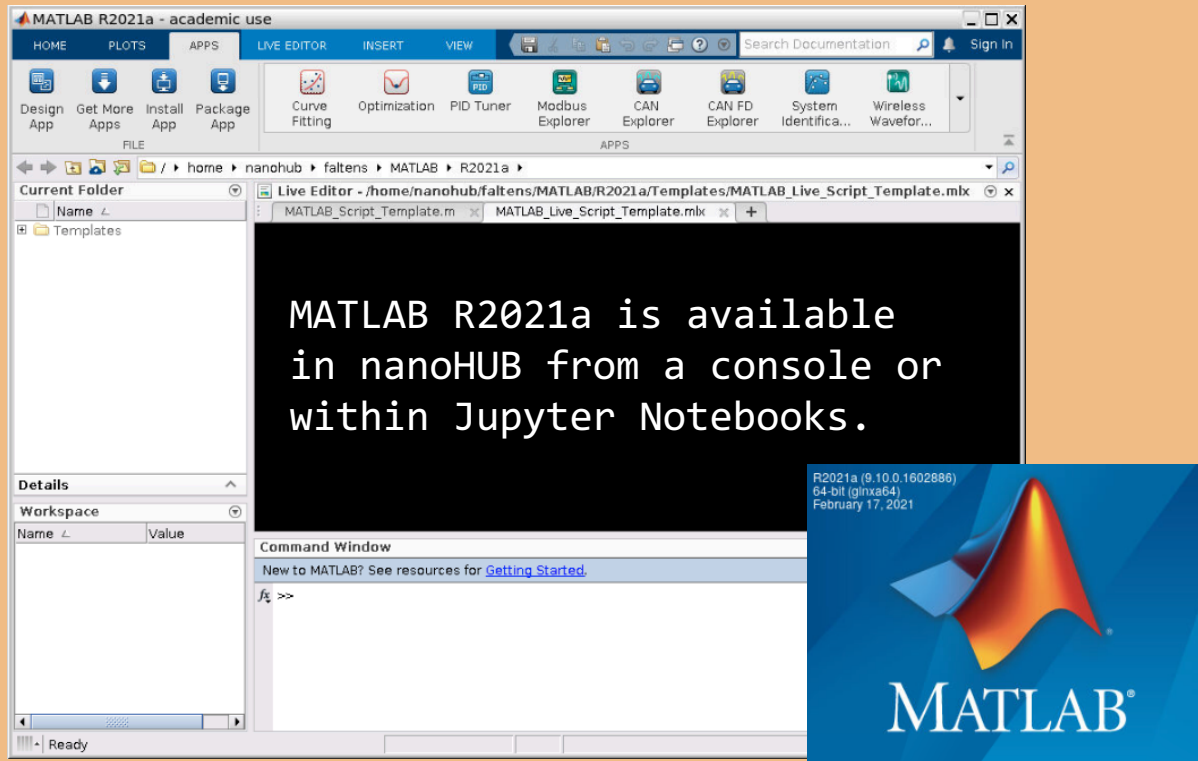
Visualization of Edge Dislocation from nanoHUB Simulation (+ Ovito)



[Video available on YouTube](#)

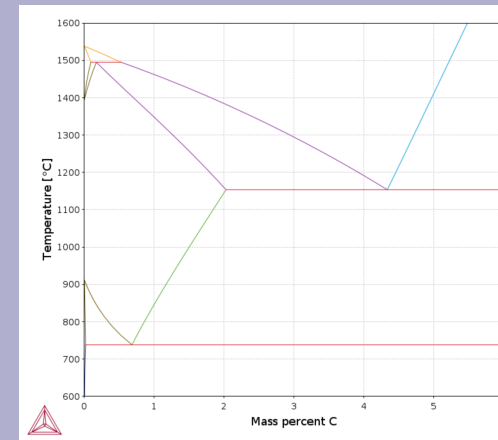
(Created from nanomatmech's dislocation dynamics simulation using advanced options. Download the dump files and visualize in Ovito.)

Example nanoHUB Tools

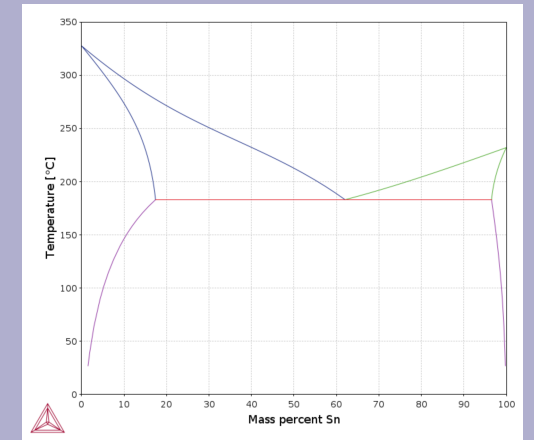


The academic version of Thermo-Calc is available to run in nanoHUB with no installation required.

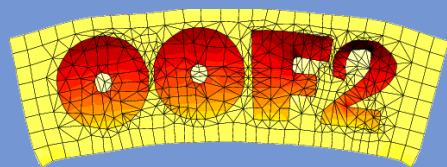
Fe-C Phase Diagram



Pb-Sn Phase Diagram



X11
Tools



Jupyter Notebooks, Jupyter Lab, and many custom Jupyter Apps are all available in nanoHUB



python™



GNU Octave

pymatgen

mendeleeev

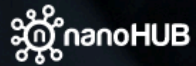


K Keras



Data Science and Machine Learning for MSE

<https://nanohub.org/groups/ml>



MENU

Data Science and Machine Learning

DISCOVERABILITY: VISIBLE JOIN POLICY: RESTRICTED CREATED: 09 SEP 2019



Login

Overview

Educational Material
and Training

Simulation Tools

Hands-on Data Science and Machine Learning Training Series

data science

machine learning

NCN Group - Machine Learning

neural networks

Organizers: Alejandro Strachan, Arun Mannodi Kanakkithodi, Saaketh Desai

This series of workshops introduces participants to important concepts and techniques in data science and machine learning in the context engineering and physical sciences applications. All workshops include hands-on activities, where participants apply the techniques to solve real problems using online resources at nanoHUB, no need to install any software.

Registration and online compute resources are free of charge.

Target audience: The workshops are designed for students, researchers, and industrial practitioners interested in exploring data science in a hands-on manner. The offerings assume little prior experience with machine learning and minimal programming experience. The Spring 2020 series contains introductory material.

Data Science and Machine Learning Modules for MSE

<https://nanohub.org/groups/mlmodules>

Hands-on Learning Modules on Data Science and Machine Learning in Engineering

Overview

Active learning → data science → machine learning → materials discovery → materials science → NCN Group - Machine Learning Modules

This series of modules introduces key concepts in data science in the context of application in materials science and engineering. The end to end modules include:

- ✓ **Recorded Lecture**
Introduces each topic and provides background material
- ✓ **Hands-on Tutorial**
Step-by-step instructions to perform interactive online activities and run interactive code
- ✓ **Homework**
Designed to help users explore the concepts using online models and simulations and adopt the code to problems of their interest

The modules are self-contained and modular, they are designed for easy incorporation into existing courses or for those interested in self-study. All interactive computing is performed using cloud computing in nanoHUB, there is no need to download or install any software. All resources are open and free.

Knowledge and Skills

DATA HANDLING

Data collection, completeness, and provenance:

Module 1

Module 2

Data storage and sharing:

Module 1

Module 2

Data querying, organization, and filtering:

Module 2

PREDICTIVE MODELING

Data visualization:

Module 2

Module 3

Digital representation and descriptors for materials:

Module 3

Simple regression models:

Module 4

Machine learning models for regression and classification:

Module 5

Random forests and decision trees:

Module 7

DECISION MAKING

Uncertainty quantification (coming soon):

Module 6

Active learning for design of experiments:

Module 7

nanoHUB Facilitates Many Connections

Materials Science
Community

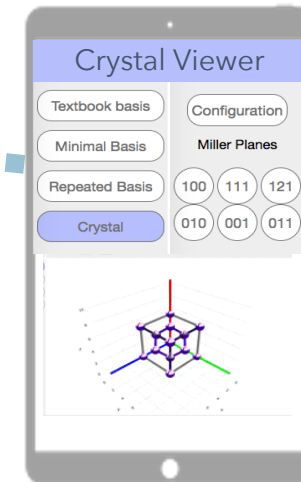


Compute Power

Coming soon!

Mobile & Embedded Apps

Web Apps & Tools



Data



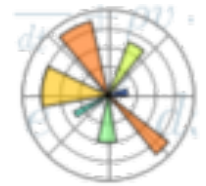
Jupyter Kernels, Libraries, & Packages in nanoHUB include...



pymatgen



mendeleeev



MSE Community



Please join!

Materials Group: <https://nanohub.org/groups/materials>

MSE Instructional Exchange Group (must prove that you are an MSE Faculty member):

<https://nanohub.org/groups/mseinstructionalexchange>

MSE Education Workshop Link

https://nanohub.org/groups/materials/mse_ed_june9_22