2022 UB Workshop in Computational Sciences

How to engineer a super-bouncy ball?

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What is MS&E

Physics

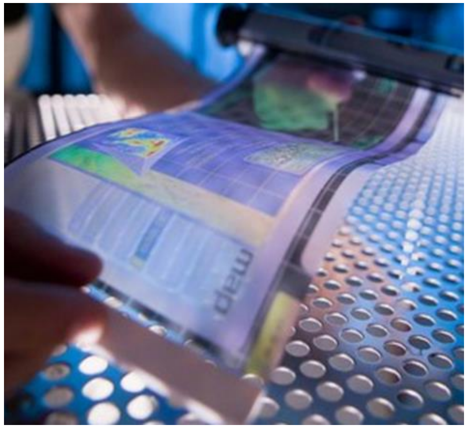
Chemistry

Mathematics

Computer Science

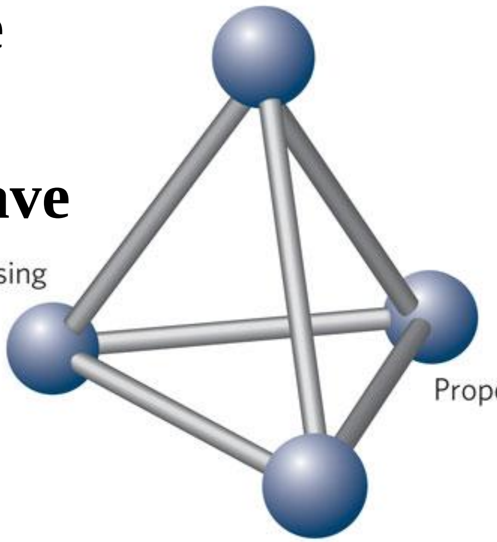
Metals, ceramics, polymers, semiconductors,… Or "stuff"

New stuff



What is Materials Engineering?

- Materials Science & Engineering is a relatively new, interdisciplinary field
  - Foundation from chemistry, physics, math
  - Core materials include metals, ceramics, semiconductors, and polymers
- Structure/properties/processing/performance pyramid
  - Science = understand why materials behave the way they do
  - Engineering = controlling properties for applications



http://www.nature.com/nmat/journal/v11/n7/fig_tab/nmat3367_F2.html

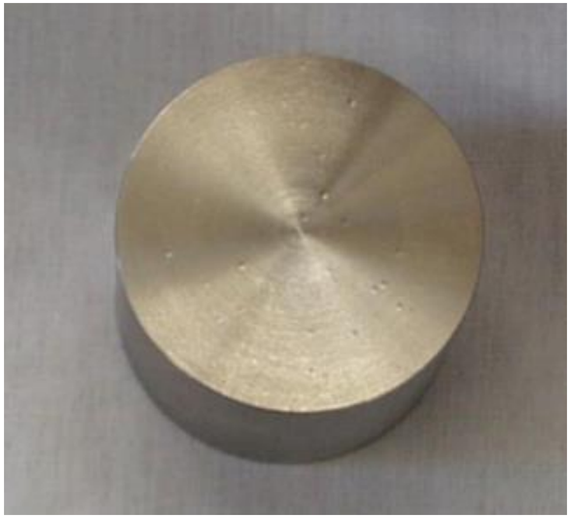
Demo 1

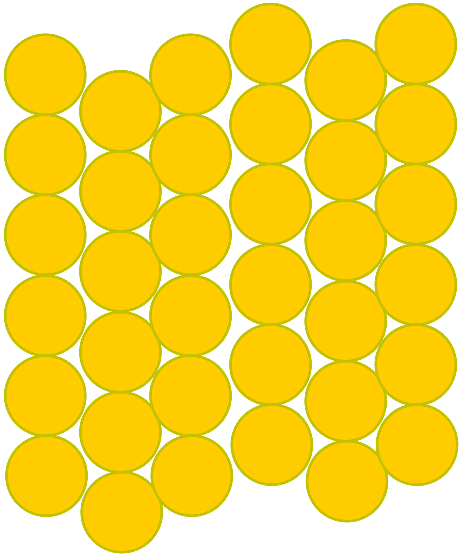
Specially engineered metal

Steel

If I drop the ball, what will happen?

Permanent deformation on steel





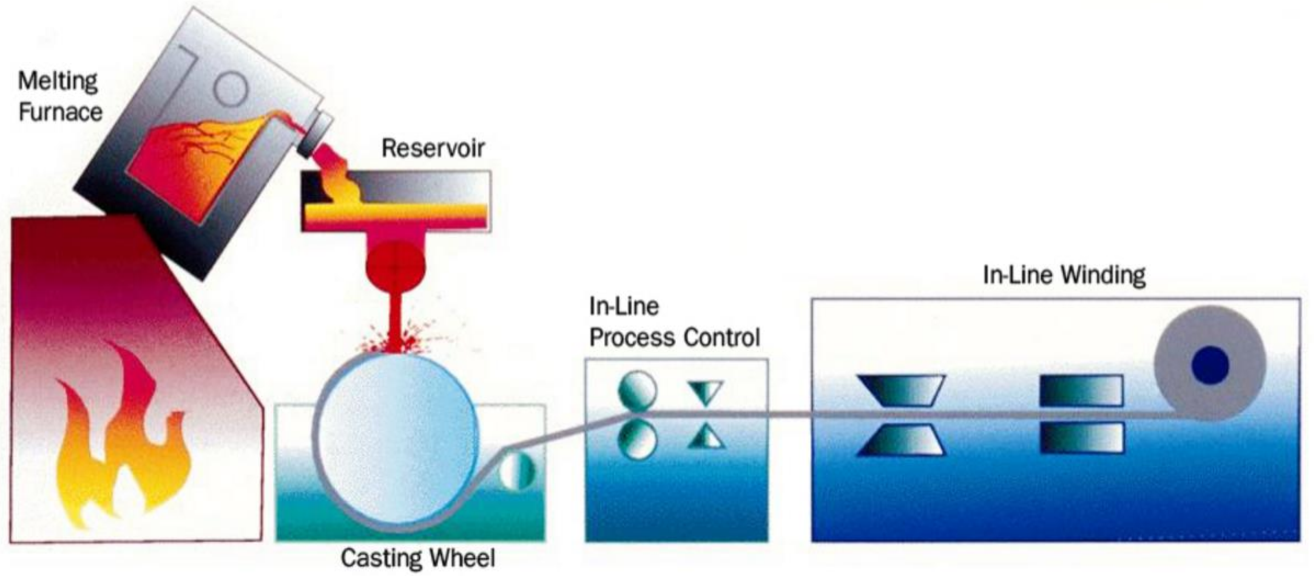
Planes of atoms that can slip easily past one another

↓

Plastic deformation that absorbs energy

How to prevent deformation?

Materials processing technique: melt and quench



Super-fast quench: cool down from melts rapidly (as fast as a million degrees per second!)

What does super-fast quench do?

Let's use high-performance computing (HPC) cluster to answer this question – because we cannot really see what happens to materials from a super-fast quench! (the two pieces of metals look almost the same)

- Step 1: Copy files from the shared folder on the cluster to your Windows desktop using WinSCP
- Step 2: Copy the above files to your own working space on the cluster
- Step 3: Start the calculation and wait for the results
- Step 4: Visualize the results

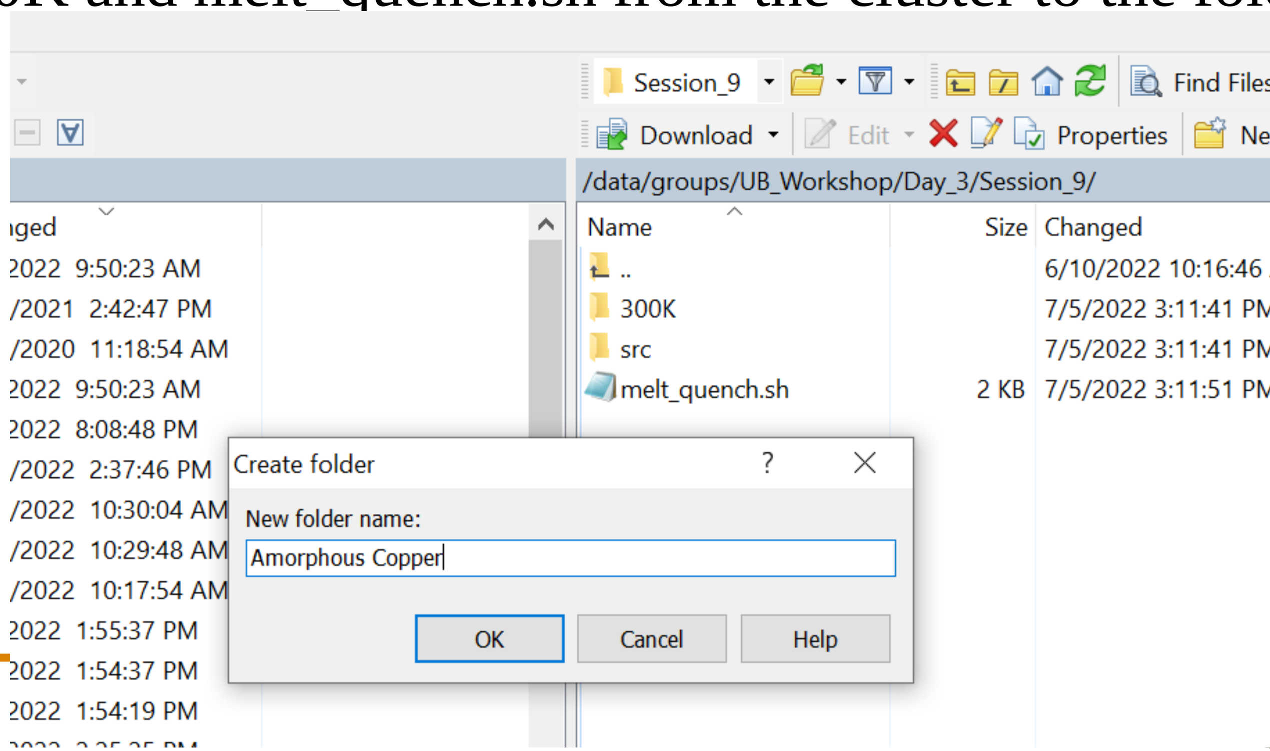
Melt-quench on HPC

- Step 1: Copy files from the shared folder on the cluster to your Windows desktop using WinSCP

➢ Files are located under /data/groups/UB_Workshop/Day_3/Session_9/Cu

➢ Create a folder on your desktop

➢ Drag the files (300K and melt_quench.sh from the cluster to the folder you just created



Melt-quench on HPC

- Step 2: Copy the above files to your own working space on the cluster

- Drag the folder you created in the previous step to your working directory on the cluster. (for example, /data/users/yourusername/foldername)

- Make sure you have 300K and melt_quench.sh under your working directory:
  - ✓ use “cd foldername” command to go into your working directory
  - ✓ use “ls” command to list the content of the directory)

```
(base) [yingma@king Amorphous Copper]$ ls
300K   melt_quench.sh
```

Melt-quench on HPC

- Step 3: Start the calculation and wait for the results

Start the calculation by command " sbatch melt_quench.sh "

Check the status by "squeue –u $USER".
- ➢ Each job takes about 50s to finish
- ➢ your job may be in the queue before it gets started

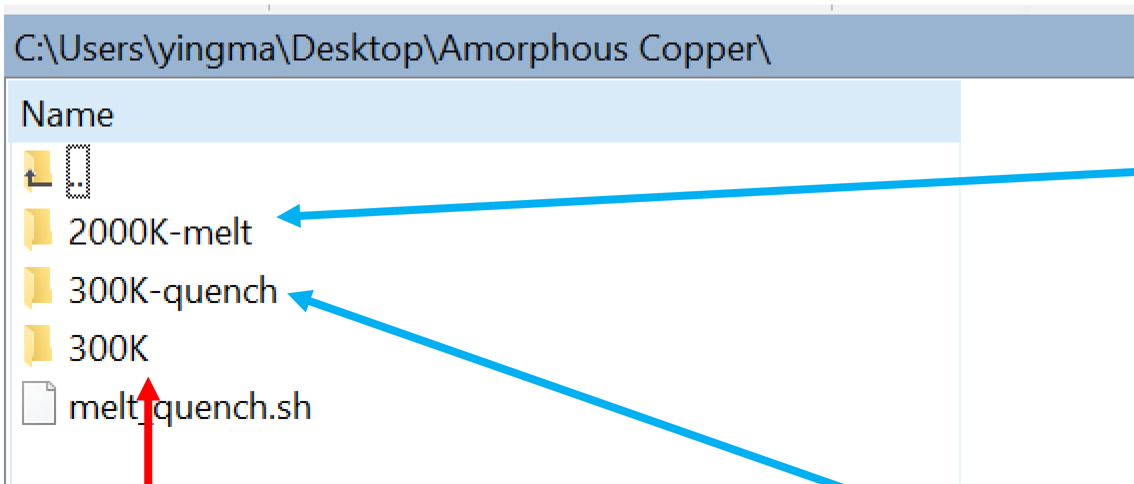
When your job finishes, you will see two additional directories, 2000K-melt and 300K-quench, and a few other files.

```
(base) [yingma@king Amorphous Copper]$ ls
2000K-melt  300K  300K-quench  melt_quench.sh  output  slurm.err  slurm.out
```

Melt-quench on HPC

- Step 4: Visualize the results

  Use WinSCP to copy 300K-quench and 2000K-melt, obtained from your calculation, to your local windows computer



Structure of melted copper (melting point: 1,984°F, or 1,085°C, or 1358 K)

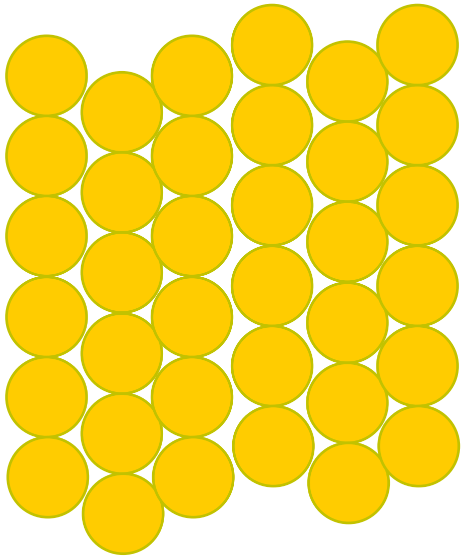
Structure of regular copper

Structure of super-fast quenched copper

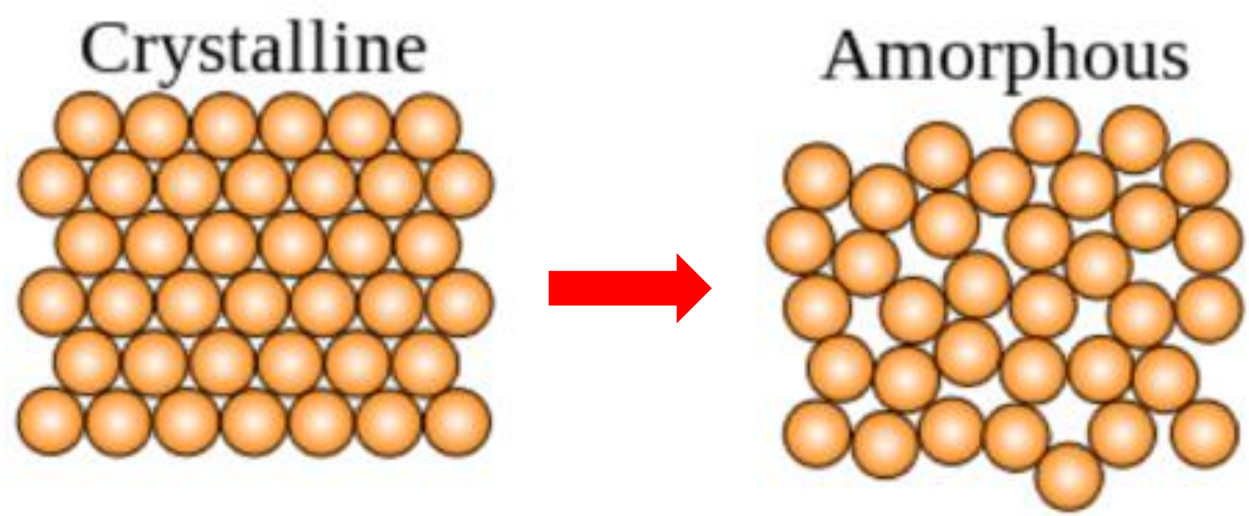
Use VESTA to open the file "REVCON" from each of the above folders. Do you see anything interesting?

Eliminating the sliding of atoms

Strategy to prevent plastic deformation?



If we could make a material without sliding plane of atoms, we would expect much better elastic property!



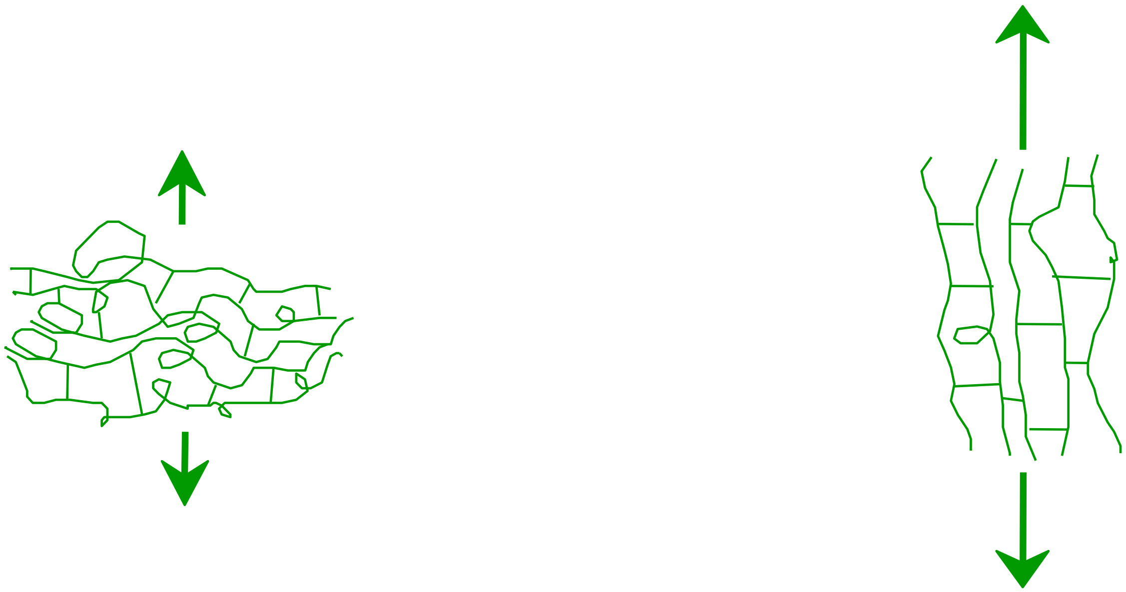
No planes of atoms

Commercial products

- Developed by a California Institute of Technology research team
- Commercial applications starting from 2003

Demo 2

Demo 2



The elasticity of rubbery materials comes from the stretching of the chain-like structure.

At very low temperatures, these chains refuse to move, leading to brittle failure.

Quick quiz

How to engineer a super-bouncy ball?

A. Make the ball bigger
B. Drop the ball from a higher position
C. Use a metal with an ordered atomistic structure, i.e., crystalline metal
D. Use a metal with a disordered atomistic structure, i.e., amorphous metal

Quick quiz

The racquetball becomes brittle at low temperature because:

A. The plane of atoms cannot slide any more
B. The chain-like structure cannot stretch any more
C. Liquid nitrogen seeps into the ball, which makes the ball brittle
D. Atoms from the ball dissolve in liquid nitrogen, leaving a brittle material behind

Take-away message

- **There are different types of materials, for example, metals, polymers, ceramics, and composites.**
- **Different materials exhibit different properties. Example of properties include elastic, electrical, optical, etc.**
- **Materials properties are determined by their structures: what atoms, molecules, and electrons are arranged in the materials.**
- **MSE is the subject that study the structure-property relation of materials. With an understanding of the structure-property relation, we can design new materials with better properties!**

Design materials with better properties: Materials Science

Design materials with better properties on an HPC:

Computational Materials Science

Design of record-breaking high-temperature superconductors
Design of super-hard materials
Design of high energy density battery materials
...

Many opportunities are waiting for you!