Advances in Mechanical Systems Engineering 2019
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Introduction to Computational Materials Science

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Purpose of this lecture

- ✓ The purpose of this lecture is to introduce you some our works using computational material science (CMS).
- ✓ CMS involves computational tools and numerical simulation methodologies for solving materials related problems.
- ✓ Using CMS, we investigate:

① **Microstructure** evolutions in materials at different length scales

② **Deformation behavior of materials** and mechanical properties

③ Other material properties (electronic, magnetic, thermal properties, and etc.)

Research interest

Structural materials for mechanical structures

Steel

Tokyo sky tree

Aluminum alloy

Audi A8 (all aluminum body)

http://www.audi.co.jp/jp/brand/ja/models/a8/a8.html

Nickel-based super alloy

Jet turbine

Target length-scale

In order to understand physical behavior of materials, we need to study physical phenomena in several length-scales.

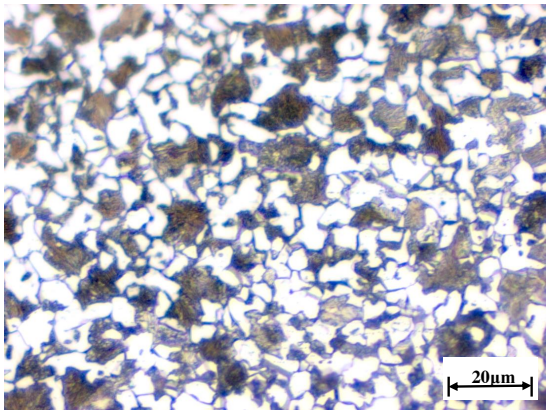
Macro-scale

http://www.mazda.co.jp/cars/axela/

Car
(4 m)

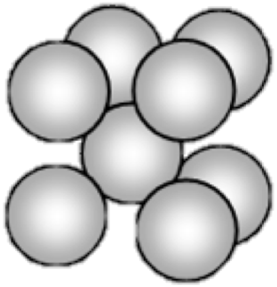
Meso-scale

Micro-scale



Crystal grains
(10^{-6} ~10^{-5} m)

Nano-scale



Atom
(10^{-10} m)

Hair
(10^{-4} m)

Human
(1~2 m)

10^{-12} m (pico)

10^{-9} m (nano)

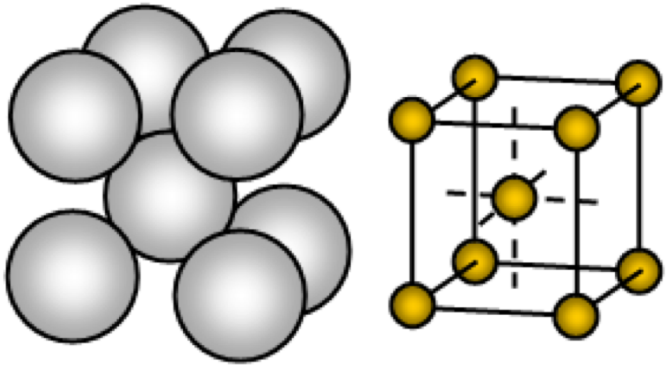
10^{-6} m (micro)

10^{-3} m (milli)

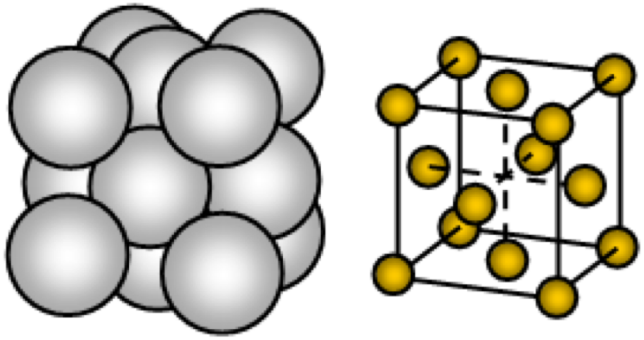
10^{0} m

Crystal structure

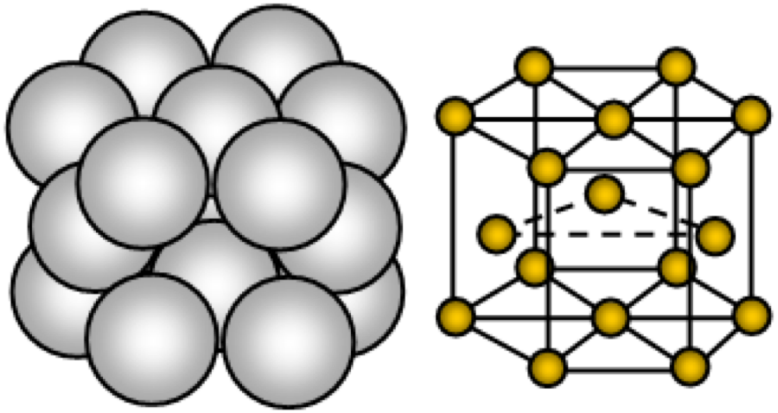
In metals, atoms consists of crystal structures as follows:



Body Centered Cubic; BCC
(Fe, Mo, Nb, Cr, etc.)



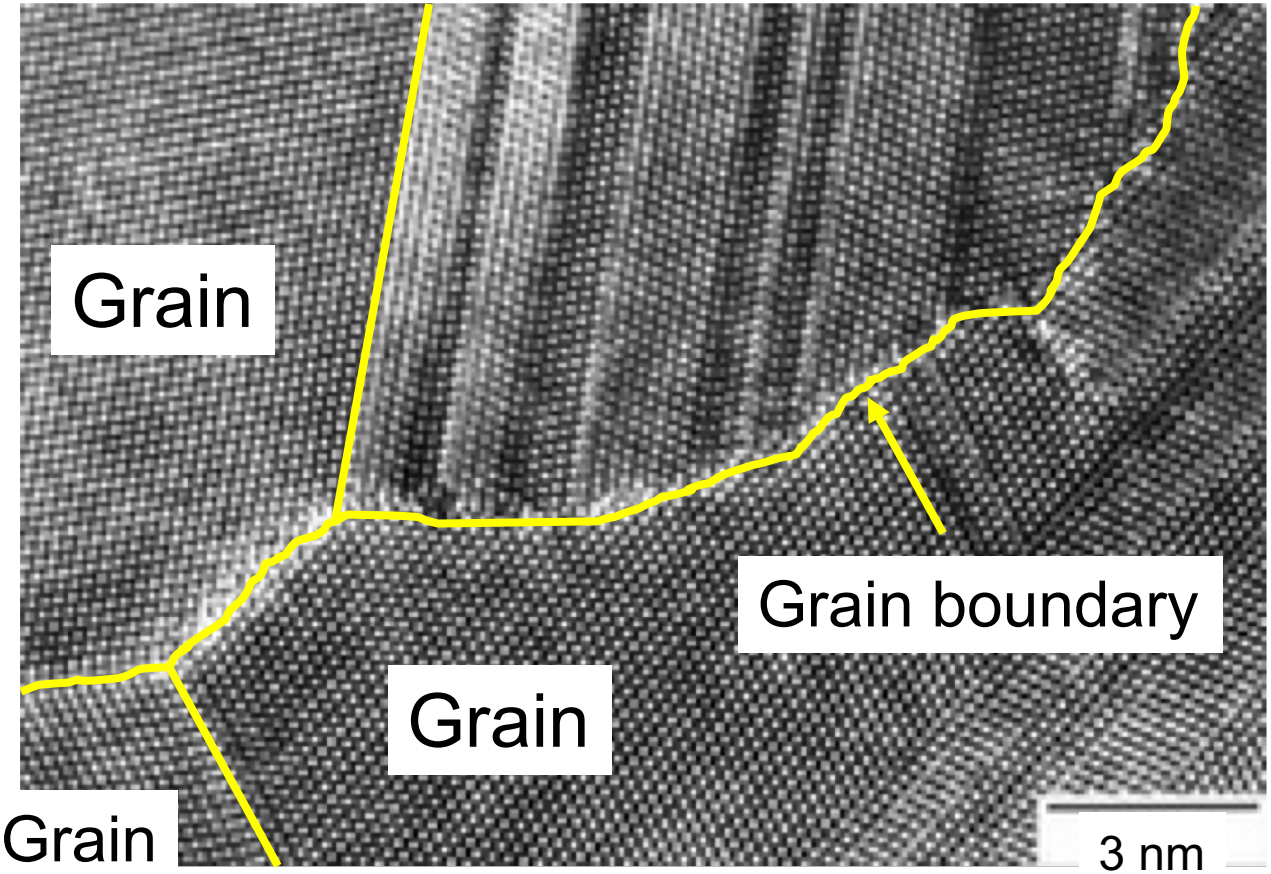
Face Centered Cubic; FCC
(Al, Au, Cu, Ag, etc.)



Hexagonal Close Packed; HCP
(Mg, Ti, Zr, Zn, etc.)

Crystal grain & grain boundary

Crystal grain is a periodic and repeated arrangement of atoms.
Grain boundary is a boundary between neighboring grains.



Grain boundary in silicon observed by transmission electron microscopy (TEM)
(http://www.msre.kumamoto-u.ac.jp/~mice/eng/projects/2008.php)

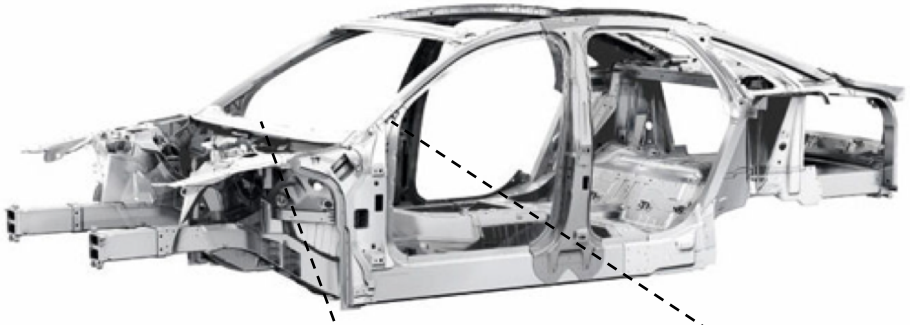
Transmission electron microscopy
http://www.hitachi-hightech.com

Microstructure at different scales

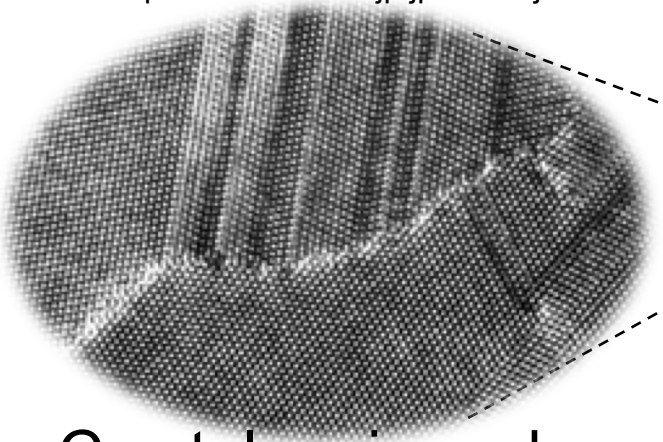
In order to design mechanical structures, we need to understand material behavior in several length-scales.

Audi A8 (Aluminum body)

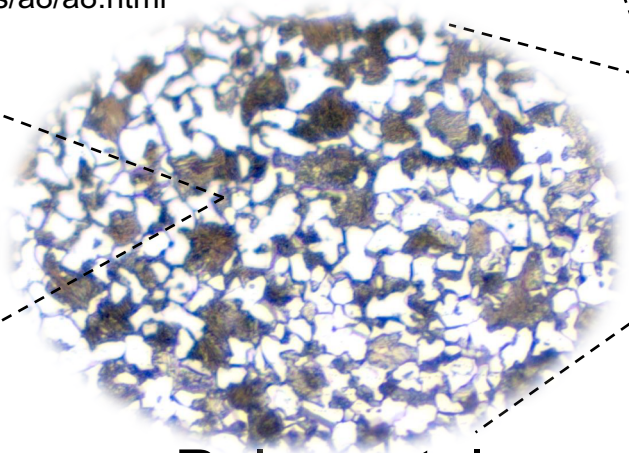
http://www.audi.co.jp/jp/brand/ja/models/a8/a8.html



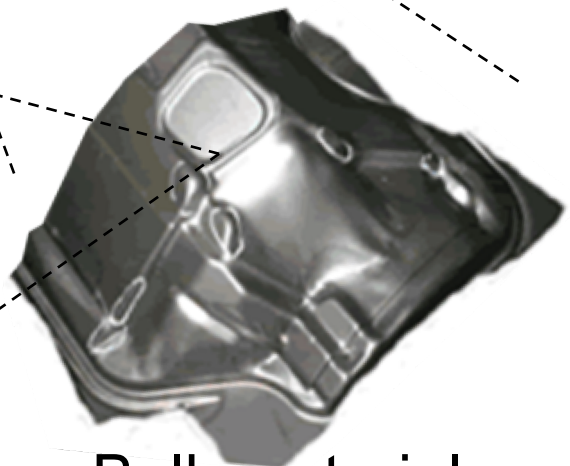
Audi space frame



Crystal grain and grain boundary (nanometer scale)

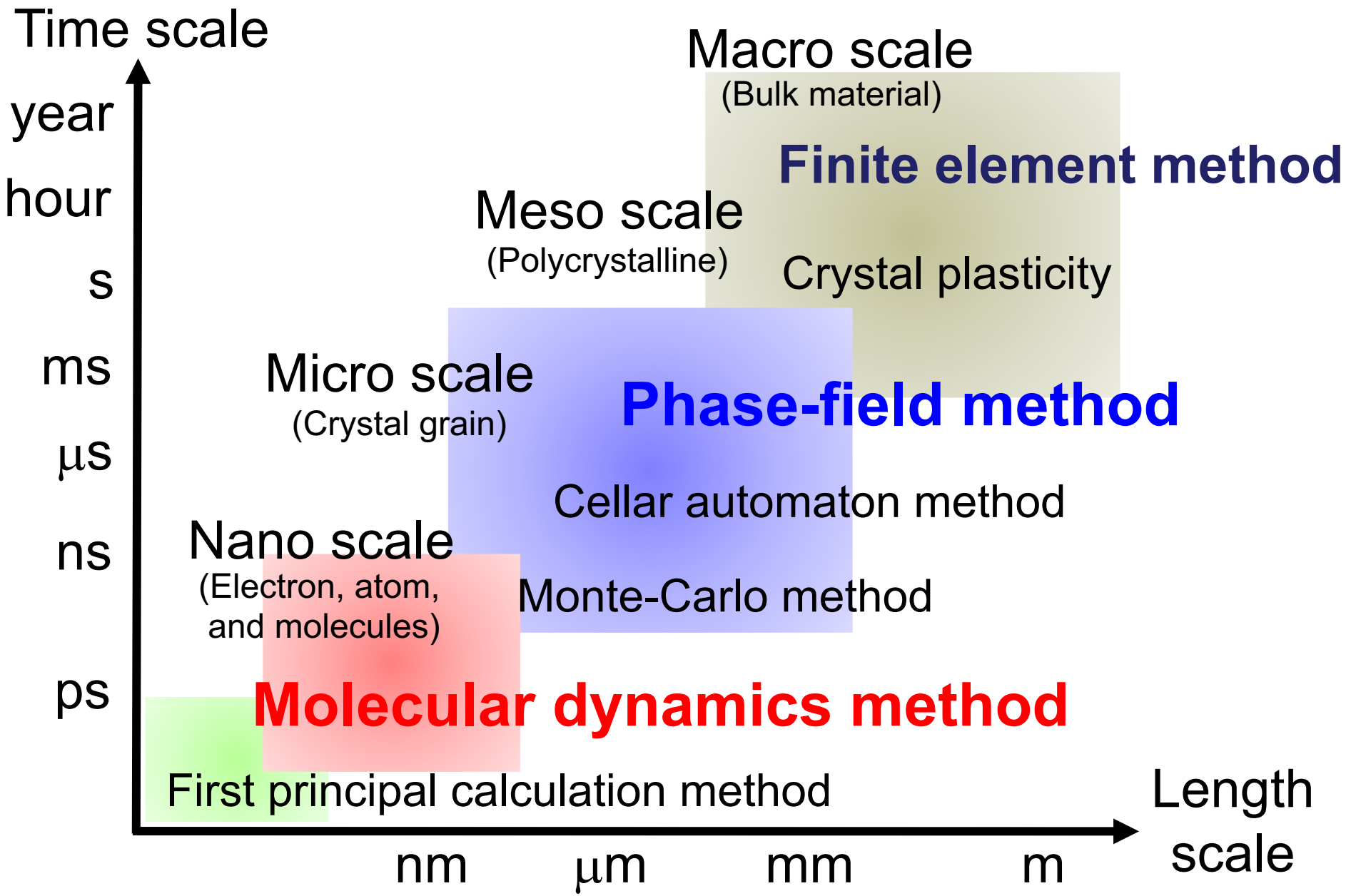


Polycrystal (micrometer scale)



Bulk material (meter scale)

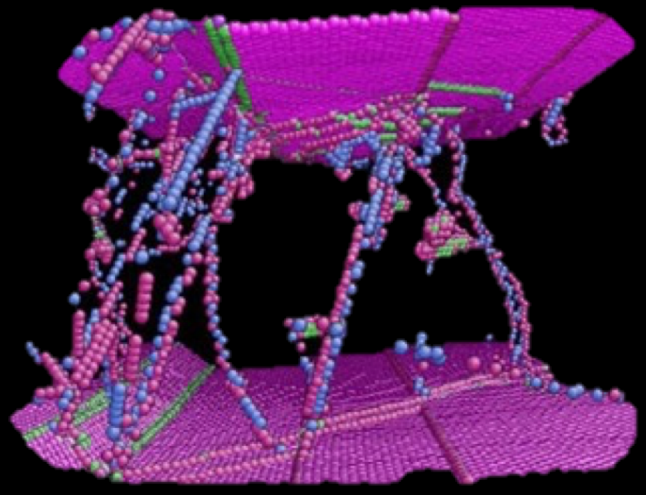
Numerical simulation methods



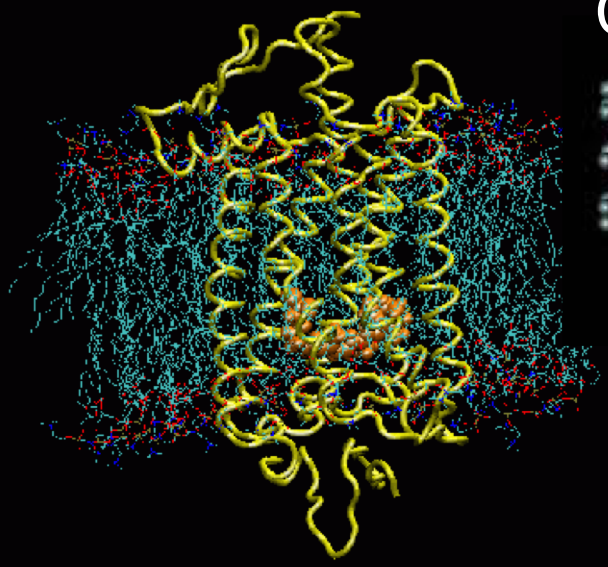
Molecular dynamics

Molecular dynamics (MD) is a computational method to predict and simulate **the movement of atoms** under a force contributed by other atoms.

Using MD, you can investigate

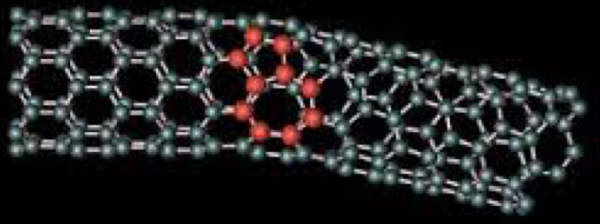


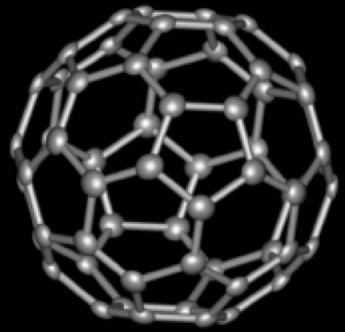
Crystal grains in metals



Proteins
Biomolecules

Carbon nanotubes





Fullerene

Principal of molecular dynamics

In MD, movement (velocity and acceleration) of all atoms in a system is calculated by calculating the forces acting on the atoms based on classical equations of motion (**Newton's second law**).

$$m\boldsymbol{a}(t) = \boldsymbol{F}(t)$$

$$\downarrow$$

$$m\frac{d^2\boldsymbol{r}(t)}{dt^2} = \boldsymbol{F}(t)$$

m : Mass of atom
$\boldsymbol{a}$: Acceleration (Vector value)
$\boldsymbol{F}$: Force (Vector value)
t : Time
$\boldsymbol{r}$: Coordinate of atom (Vector value)

✓ *Solve 2nd-order differential equation with respect to position of atom.*

Principal of molecular dynamics

In order to calculate the movement of atom, we need to calculate the atomic force using the following equation:

Atomic force applying to atom *i*

$$\boldsymbol{F}^i(t) = -\mathrm{grad}\boldsymbol{U} = -\nabla U(\boldsymbol{r}^i)$$

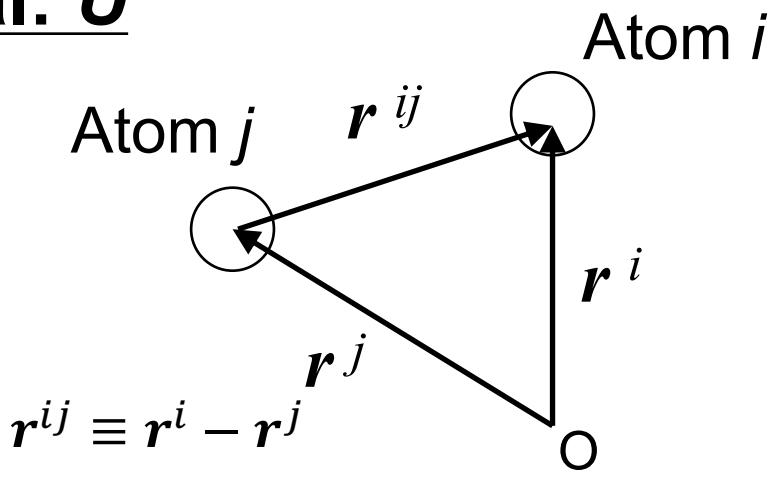
$$\nabla = \left(\frac{\partial}{\partial r_x}, \frac{\partial}{\partial r_y}, \frac{\partial}{\partial r_z}\right)$$

Potential energy of atom *i*

The most fundamental potential energy is

Two-body interatomic potential: *U*

$$U(\boldsymbol{r}^i) = \frac{1}{2}\sum_{j\neq i}^{N}\sum_{i=1}^{N}\Phi(\boldsymbol{r}^{ij})$$



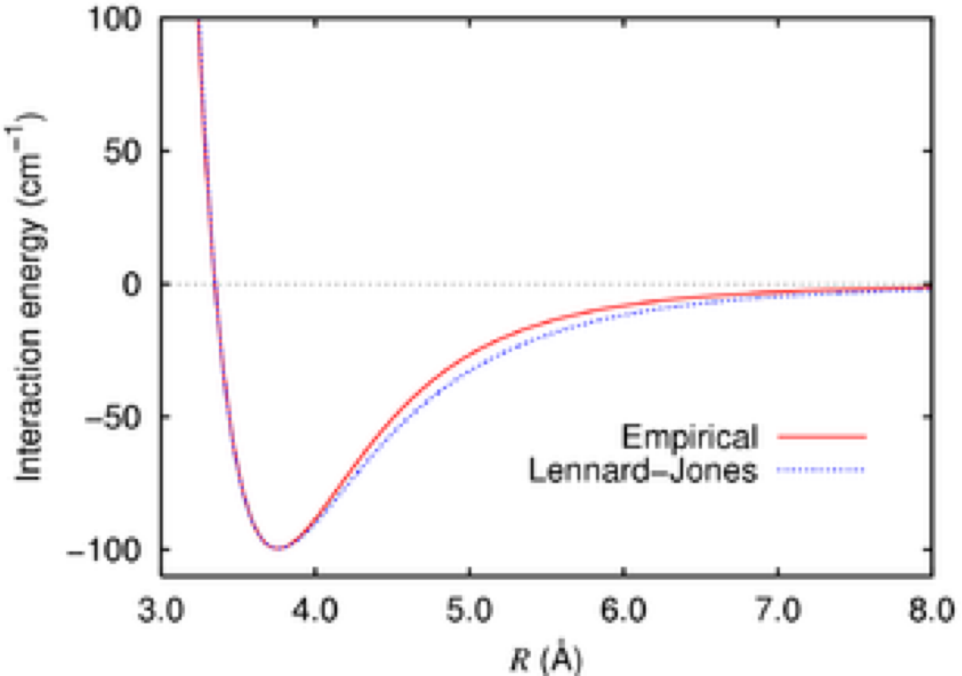
- A vector from atom *j* to atom *i* :
- Total number of atoms: *N*

Lennard-Jones (LJ) Potential

- LJ potential is the most classical potential energy function which is a good approximation of atoms interacting by **the van der Waals force**.
- LJ potential is widely used for various materials, especially rare gas atoms like Ar and Ne.

$$\Phi(\boldsymbol{r}^{ij}) = 4\epsilon\left\{\left(\frac{\sigma}{\boldsymbol{r}^{ij}}\right)^{12} - \left(\frac{\sigma}{\boldsymbol{r}^{ij}}\right)^{6}\right\}$$

Repulsive term Attracting term



Embedded Atom Method (EAM) potential

M. S. Daw and M. I. Baskes, PRL, 50 (1983), 1285.

The Embedded Atom Method (EAM) potential is a modern potential which is good for modelling and simulating metallic materials.

Total energy $$U = \sum_i F(\bar{\rho}_i) + \frac{1}{2}\sum_{i \neq j} \phi(r_{ij})$$

Many body

2-body

Combined electron density $$\bar{\rho}_i = \sum_j \rho(r_{ij})$$

An embedded function describing the energy embedded to an atom *i* in the combined electron density which is contributed from each of its neighboring atoms *j* by amount $r(r_{ij})$.

The pair potential function representing the energy in bond *ij* which is due to the short-range electro-static interaction between atoms.

Finnis-Sinclar (FS) potential

The one of the most popular EAM potential is the Finnis-Sinclair (FS) potential for simulating metallic materials.
The parameters of the EAM potentials can be available from the database.

Total energy $$U = \sum_i F\left(\bar{\rho}_i\right) + \frac{1}{2}\sum_{i \neq j} \phi\left(r_{ij}\right)$$

Embedded function $$F\left(\bar{\rho}_i\right) = -A\sqrt{\rho_i}$$

Combined electron density $$\bar{\rho}_i = \sum_j \rho\left(r_{ij}\right)$$

Partial electron density function $$\rho_i = \left(r - d\right)^2 + \frac{\beta\left(r-d\right)^3}{d}$$

for r < d, otherwise 0.

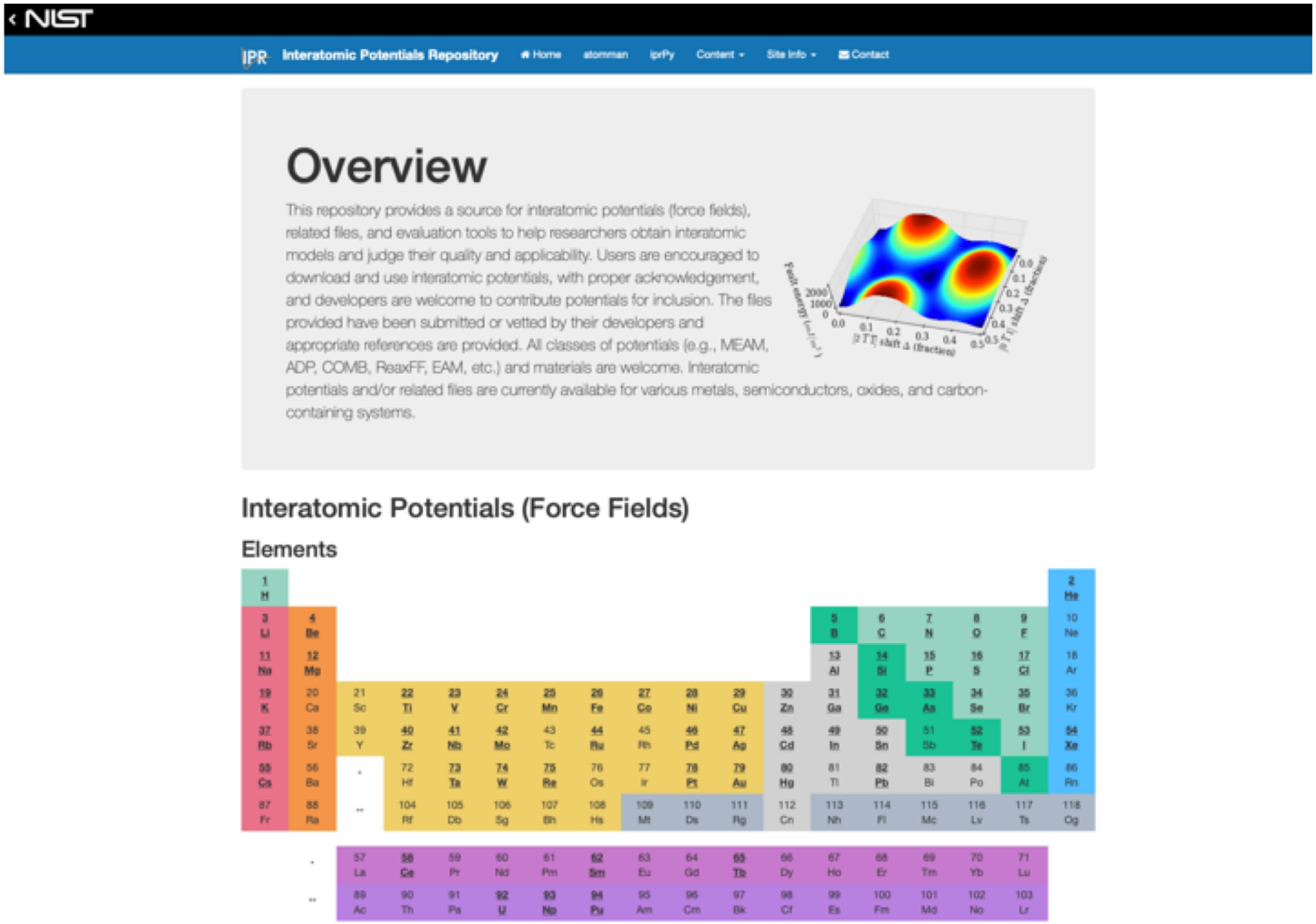
Pair potential function $$\phi_{ij}\left(r_{ij}\right) = \left(r - c\right)^2\left(c_0 + c_1 r + c_2 r^2\right)$$

for r < c, otherwise 0.

M. W. Finnis and J. E. Sinclair, Phil. Mag. **A50** (1984), 45.

Potential energy database

Parameters for many interatomic potential energy can be available from database developed in National Institute of Standards and Technology (USA)



LAMMPS

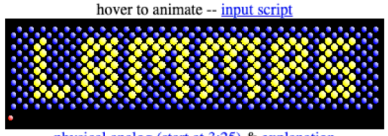
LAMMPS is a popular open-source code which has been widely used for molecular dynamics simulation.

Large-scale Atomic/Molecular Massively

LAMMPS Molecular Dynamics Simulator

***lamp**: a device that generates light, heat, or therapeutic radiation; something that illumines the mind or soul* -- www.dictionary.com

hover to animate -- input script



physical analog (start at 3:25) & explanation

NEW The 2019 LAMMPS Workshop and Symposium was held Aug 13-15 in Albuquerque, NM --- program and talk/poster PDFs here

Big Picture	Code	Documentation	Results	Related Tools	Context	User Support
Features	Download	Manual	Publications	Pre/Post processing	Authors	Mail list
Non-features	GitHub	Developer guide	Pictures	Pizza.py Toolkit	History	IRC channel
Packages	SourceForge	Tutorials	Movies	Offsite LAMMPS packages & tools	Funding	Workshops
FAQ	Latest features & bug fixes	MD to LAMMPS glossary	Benchmarks	Visualization	Open source	Contribute to LAMMPS
Wish list	Report bugs & request features	Commands	Citing LAMMPS	Related modeling codes		.

LAMMPS is a classical molecular dynamics code with a focus on materials modeling. It's an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator.

LAMMPS has potentials for solid-state materials (metals, semiconductors) and soft matter (biomolecules, polymers) and coarse-grained or mesoscopic systems. It can be used to model atoms or, more generically, as a parallel particle simulator at the atomic, meso, or continuum scale.

LAMMPS runs on single processors or in parallel using message-passing techniques and a spatial-decomposition of the simulation domain. Many of its models have versions that provide accelerated performance on CPUs, GPUs, and Intel Xeon Phis. The code is designed to be easy to modify or extend with new functionality.

LAMMPS is distributed as an open source code under the terms of the GPL. The current version can be downloaded here. Links are also included to older versions. All LAMMPS development is done via GitHub, so all versions can also be accessed there. Periodic releases are also posted to SourceForge.

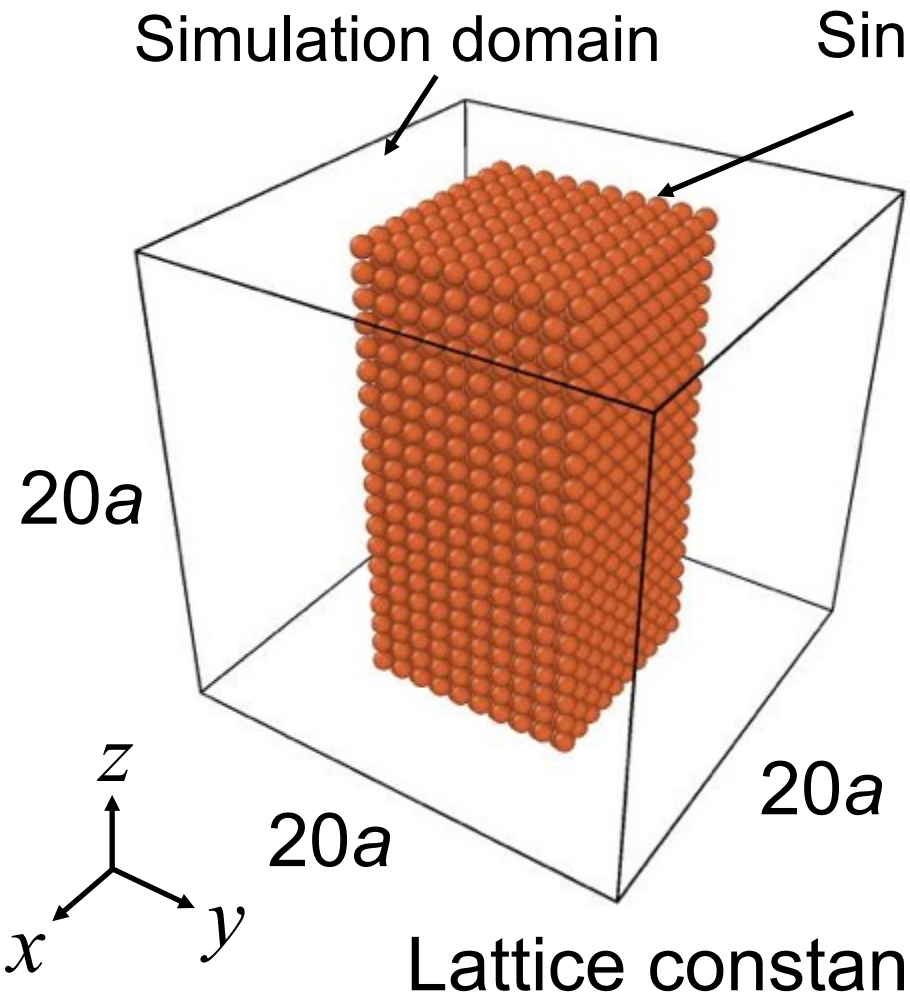
LAMMPS is distributed by Sandia National Laboratories, a US Department of Energy laboratory. The main authors of LAMMPS are listed on this page along with contact info and other contributors. Funding for LAMMPS development has come primarily from DOE (OASCR, OBER, ASCI, LDRD, Genomes-to-Life) and is acknowledged here.

The LAMMPS web site is hosted by Sandia, which has this Privacy and Security statement.

Please see: http://lammps.sandia.gov

Simple example

You can easily simulate uniaxial tensile deformation of single crystal iron using LAMMPS.



Lattice constant
a = 2.8665 Å

Orientation:
[100] // x axis
[010] // y axis
[001] // z axis

Interatomic potential:
Embedded atom method
Finnis-Sinclair potential

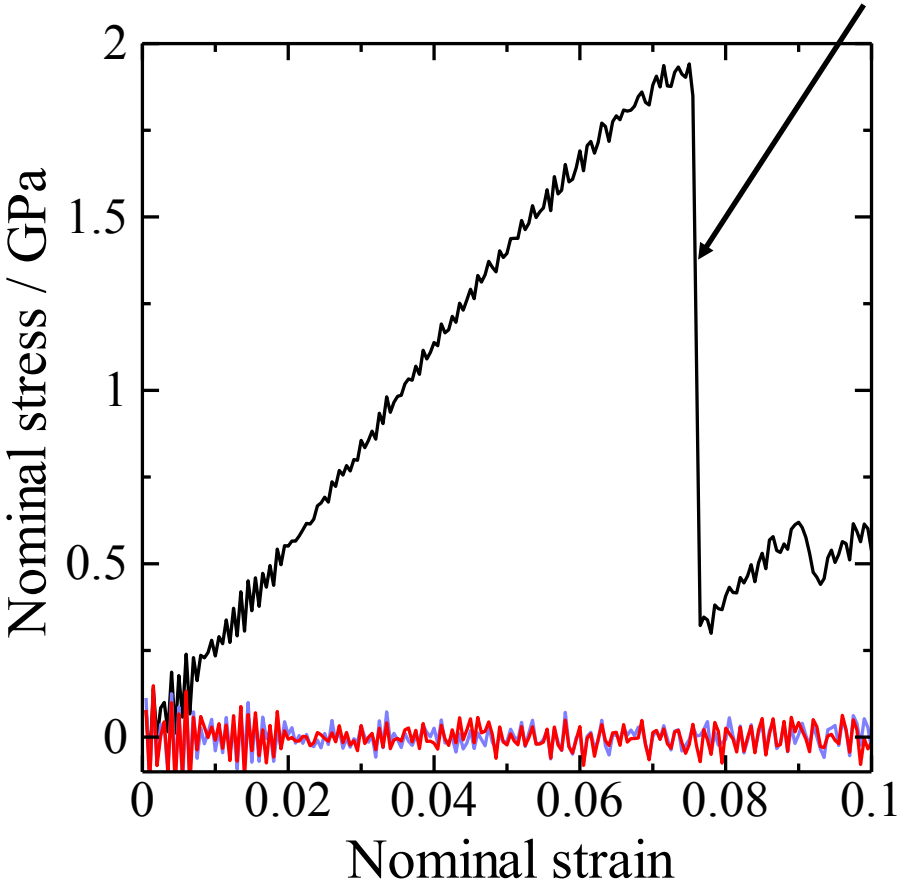
Temperature: 27 ℃

Tensile direction: z axis

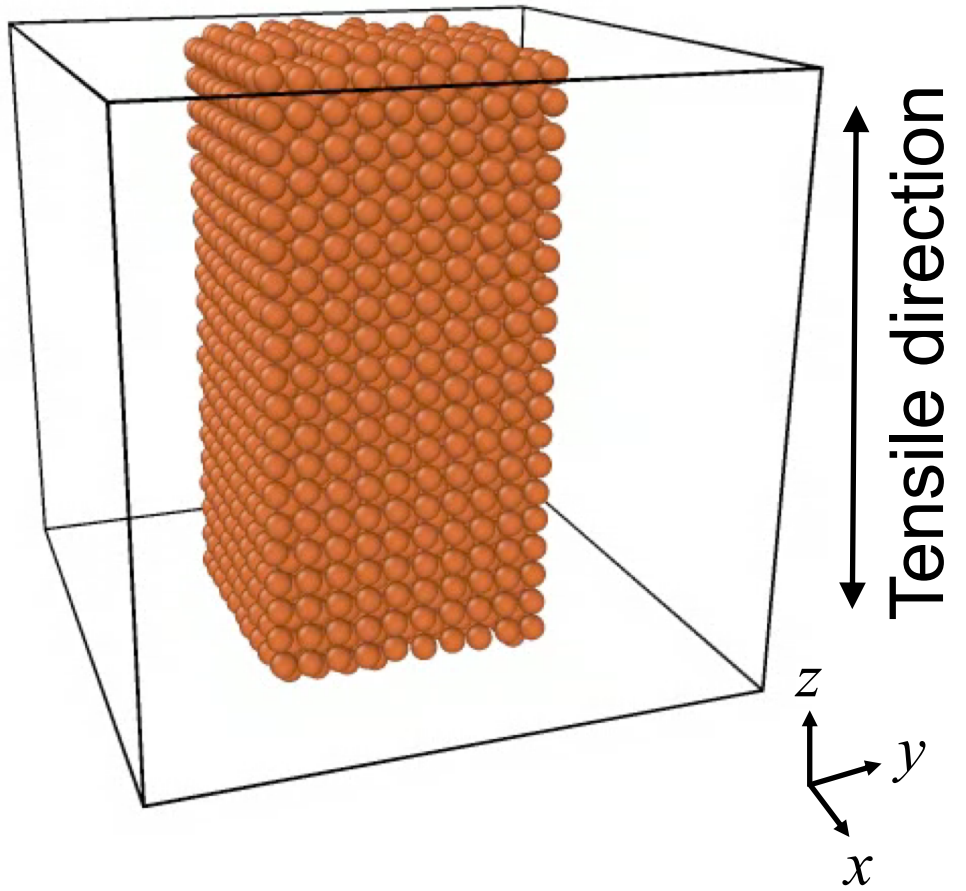
Time increment: 0.005 ps

Tensile deformation of single crystal iron

Sudden drop of stress corresponds to dislocation motion in iron.

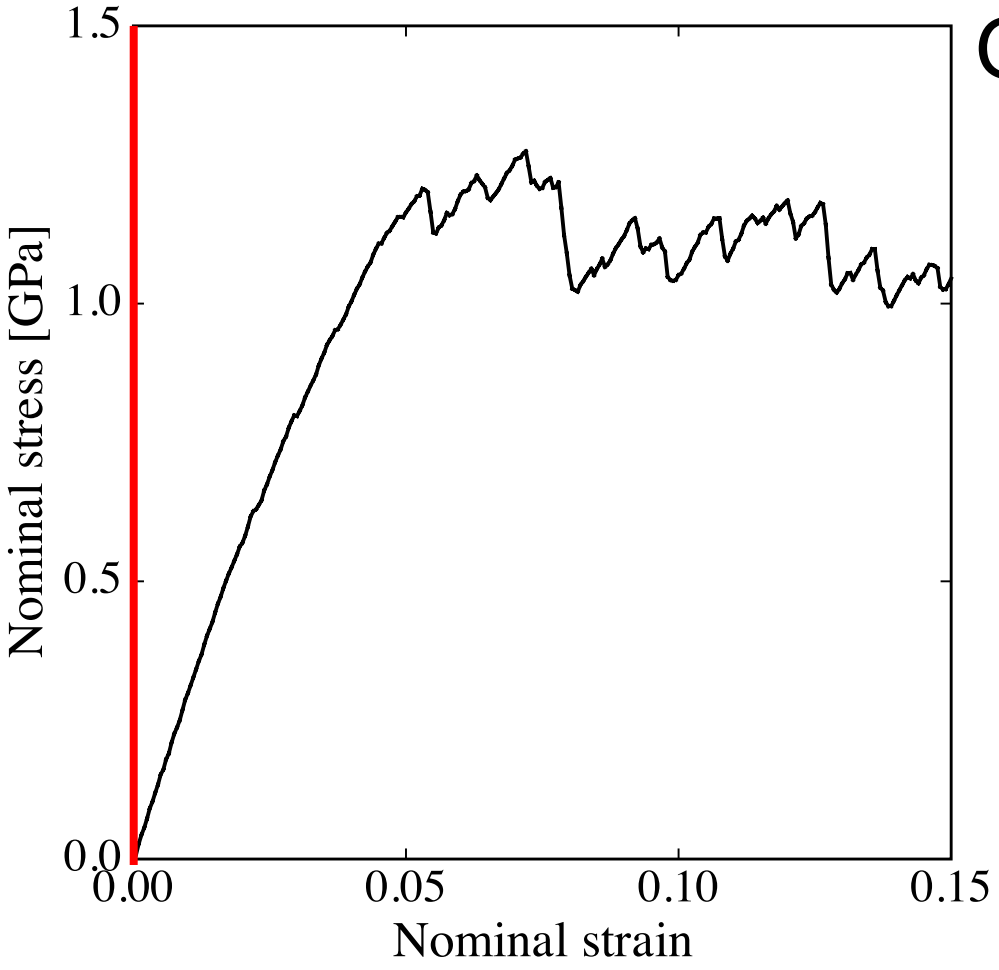


Nominal stress-nominal strain curves of a single crystal Fe calculated by MD simulation

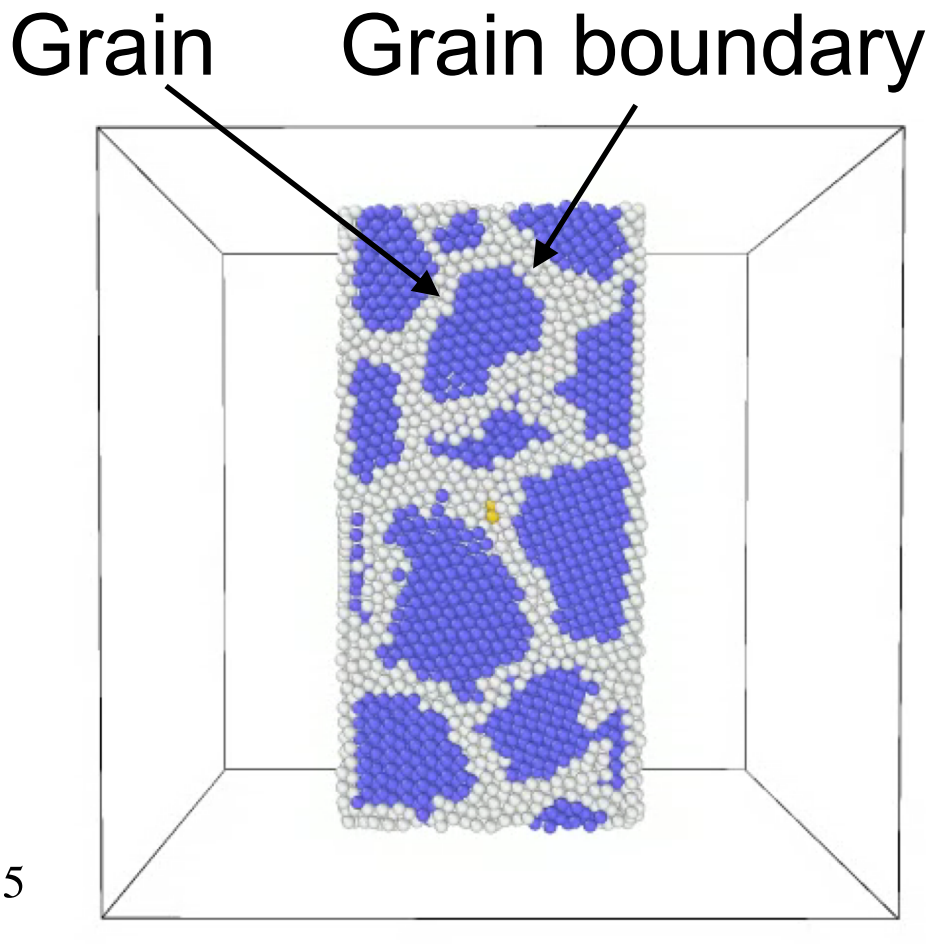


Deformation behavior of a single crystal Fe during uniaxial tensile deformation.

Tensile deformation of polycrystal crystal iron



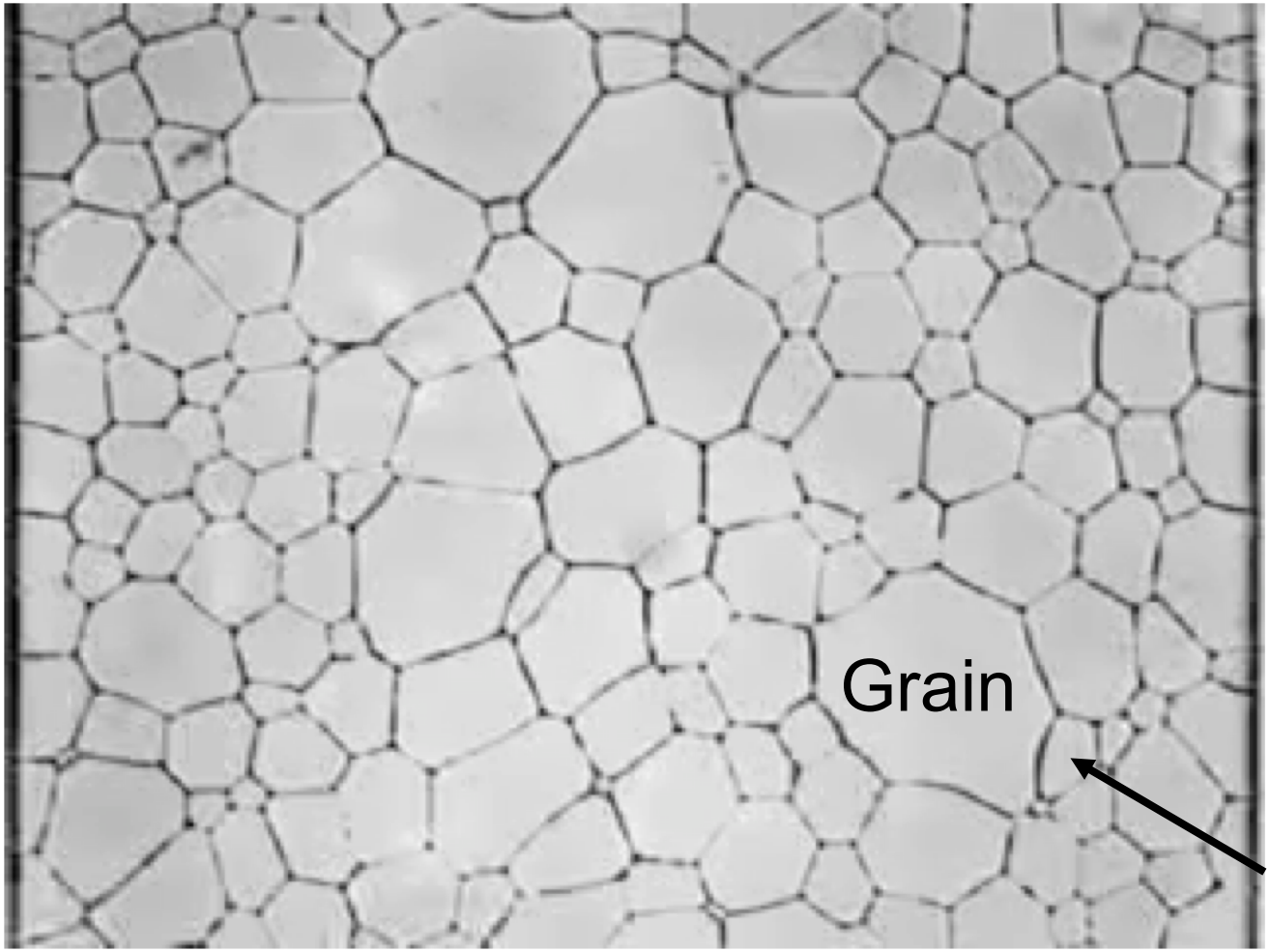
Nominal stress-Nominal strain curves of polycrystalline Fe calculated by MD simulation



Deformation behavior of polycrystalline Fe during uniaxial tensile deformation.

MD simulation in meso-scale

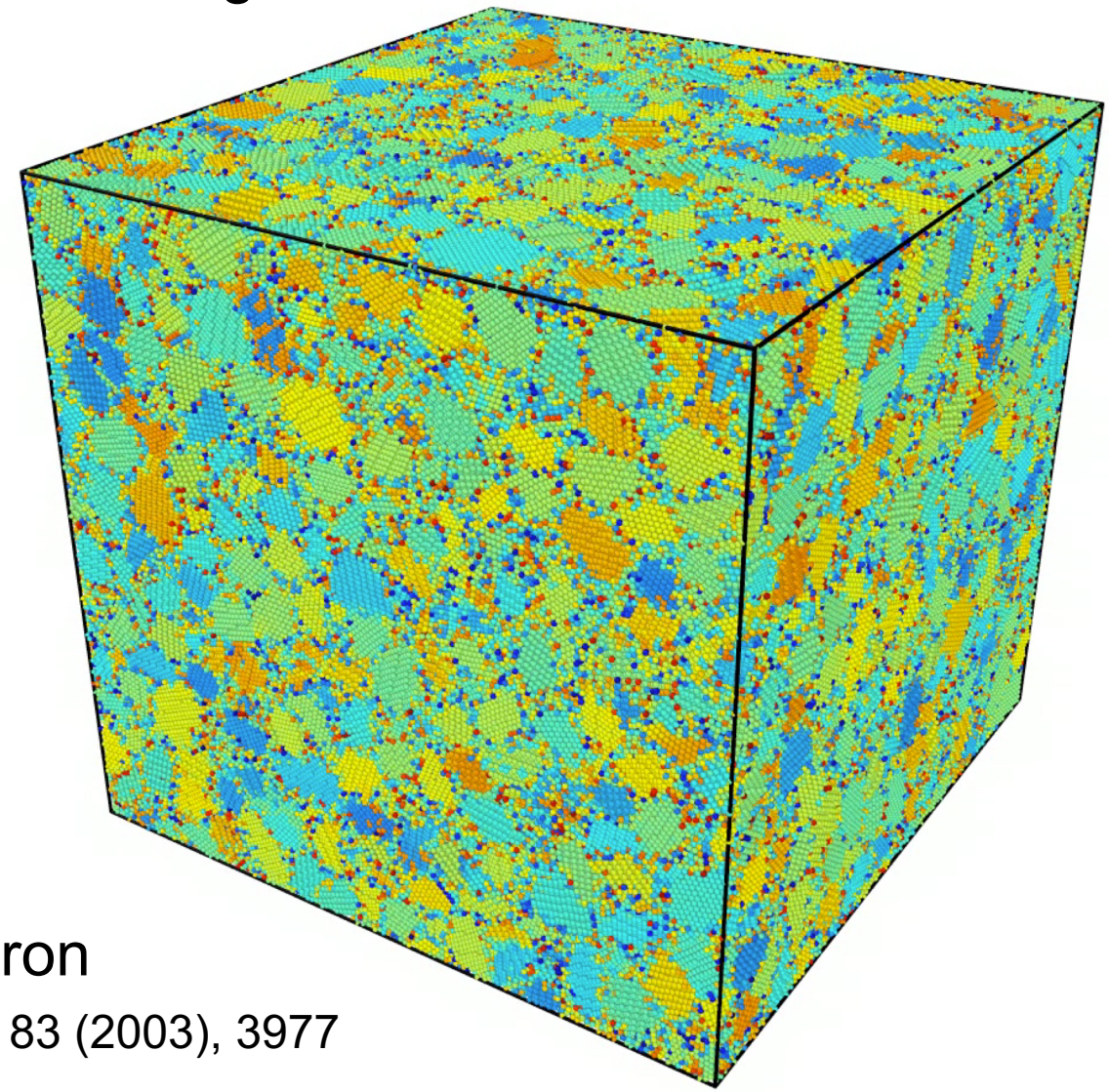
Polycrystalline grains grow with time at high-temperature.
Since size of crystal grain strongly affects strength of metals, it is very important to understand gran growth behavior.



http://www.ctcms.nist.gov/solidification/phasefield.html

MD simulation of grain growth

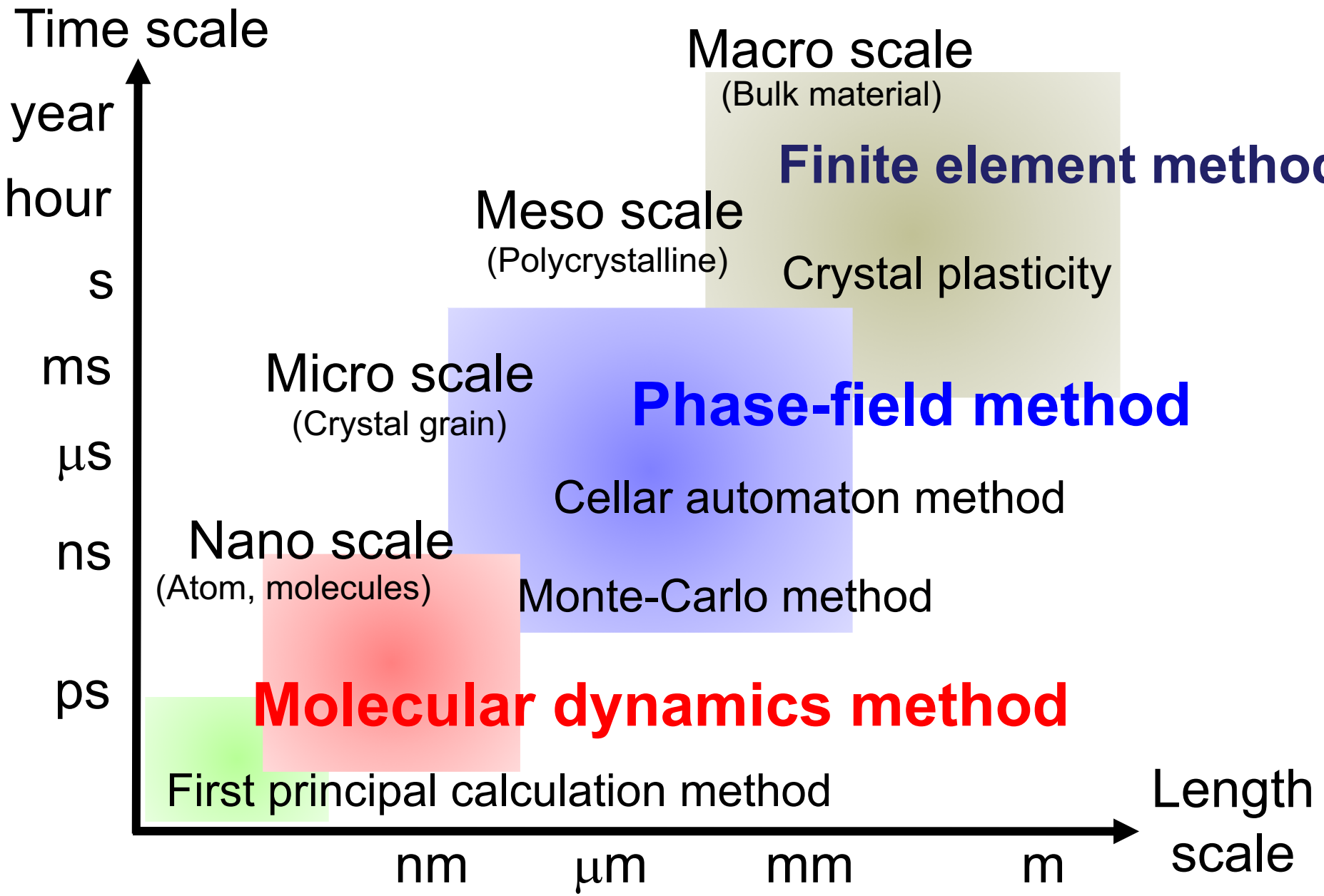
Using MD simulation, we can investigate not only the movement of atoms, but also the migration of grain boundaries and the variation of crystal orientation.



- ✓ LAMMPS (6 GPUs)
- ✓ 3,078,458 atoms
- ✓ 1200 K
- ✓ 2.45 ns
- ✓ FS potential for pure iron

Mendelev et al, Phil. Mag. A, 83 (2003), 3977

Various simulation methods



What is phase-field method?

Phase-field method is a numerical technique for investigating **microstructure evolutions** (solidification, grain growth, and phase transformation) **in meso-scale** on the basis of total free energy minimization theory (the second law of thermodynamics).

Phase-field method is a **coarse-grained model** for simulating microstructure evolutions in ***much longer time scale*** (typically order of 10^{-6} s) than that in MD simulation.

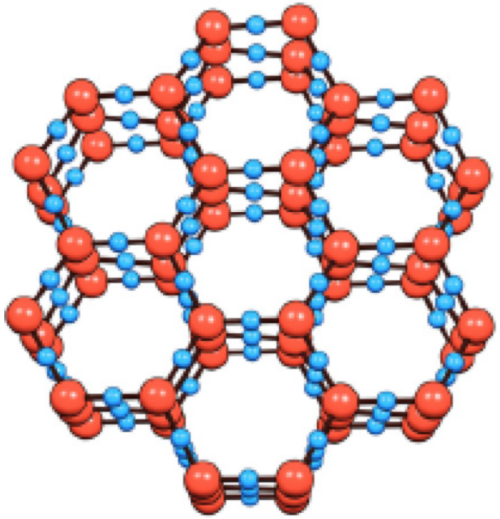
Snow crystals

Snow crystal shows “dendrite” structure.

http://www.snowcrystals.com/photos/photos.html

Why Hexagons?

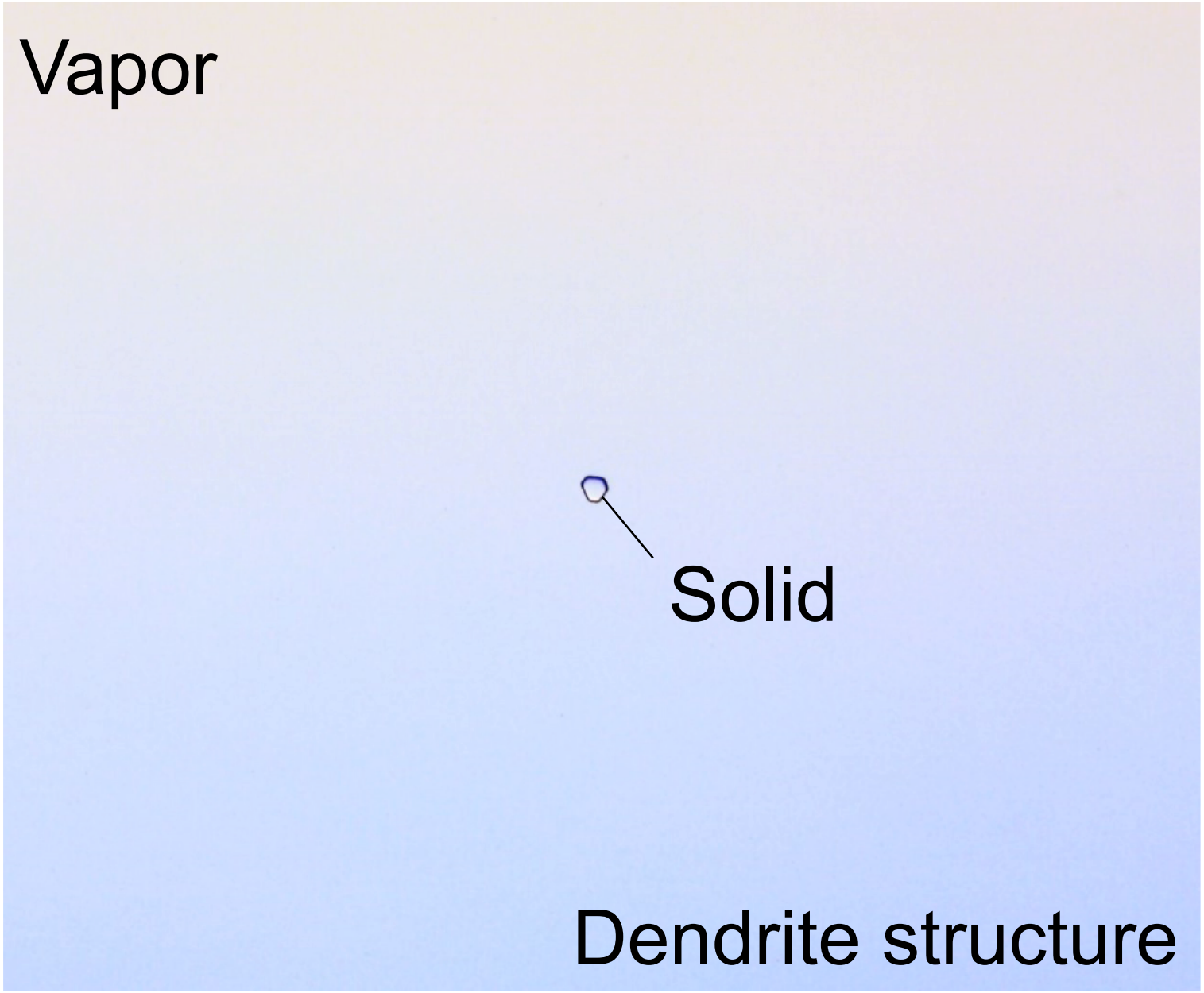
Crystal structure



Red ：O atom

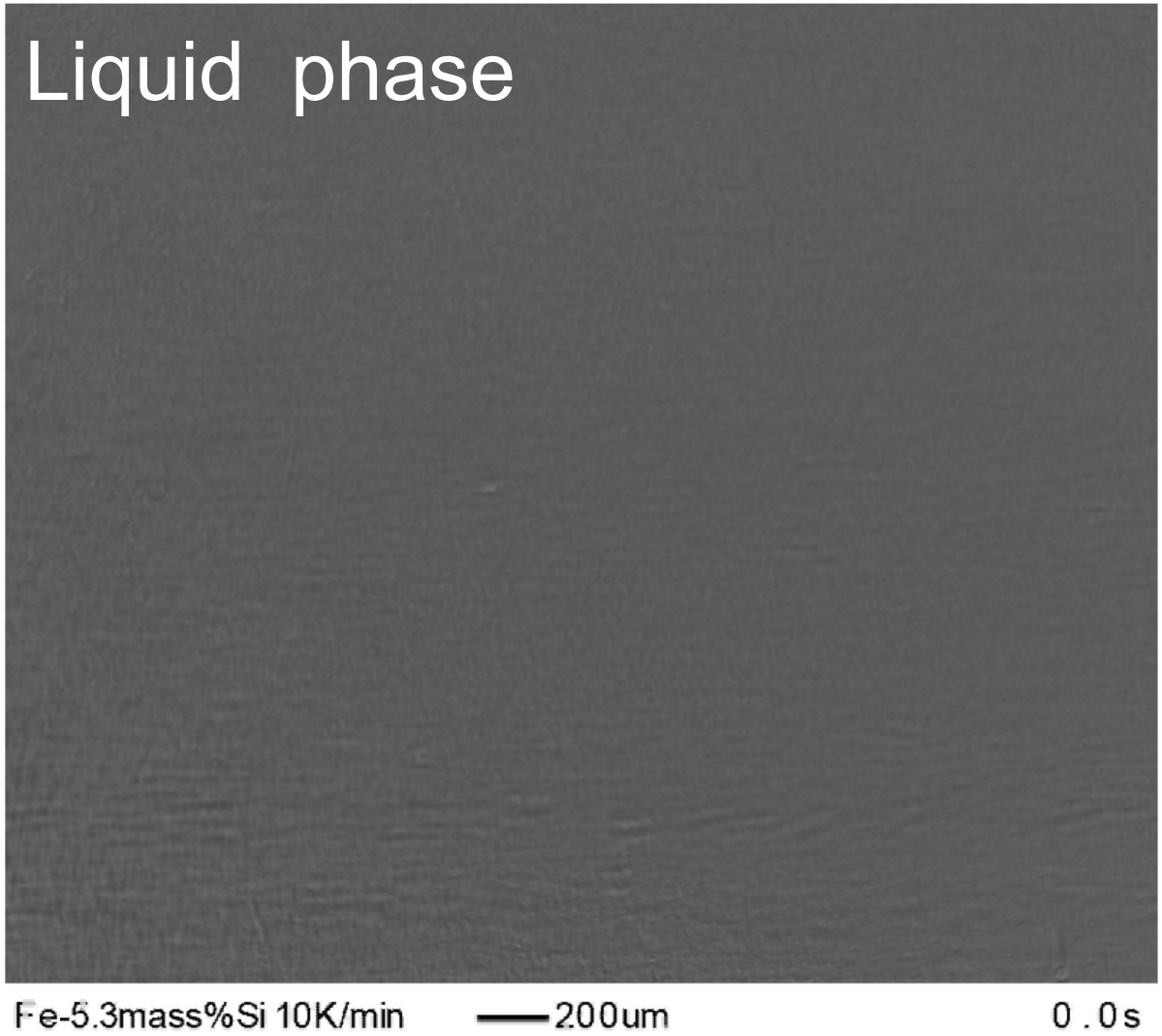
Blue：H atom

Solidification in vapor

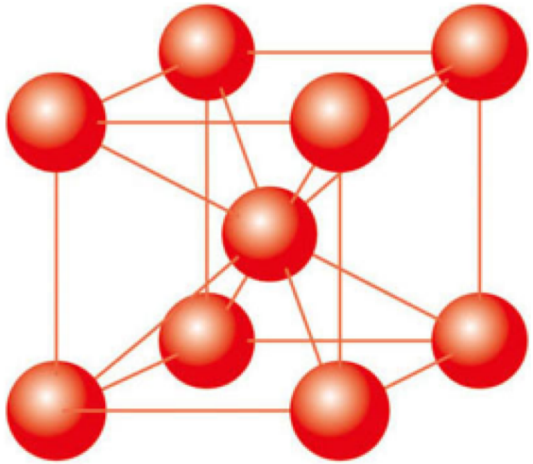


Solidification in alloys

Dendrite structure can be observed in alloys.



BCC structure



In-situ observation of dendrite in Fe-Si alloy using X-ray tomography

Courtesy of Prof. Yasuda (Kyoto University)

Phase-field method

The second law of thermodynamics

We assume that solidification proceeds so that total Gibbs free energy of the system decreases monotonically with time.

Total Gibbs free energy of a system

$$G = \int_V \left\{ g\left(\phi, \nabla\phi, c, \nabla c\right) \right\} dV$$

$$= \int_V \left\{ \underbrace{g_{chem}\left(\phi, c\right)}_{\text{Chemical term}} + \underbrace{g_{double}\left(\phi\right) + g_{grad}\left(\nabla\phi, \nabla c\right) + \cdots}_{\text{Interfacial terms}} \right\} dV$$

$\phi\left(\boldsymbol{x}, t\right)$: Non-conserved order parameter describing migration of solid/liquid interface

$c\left(\boldsymbol{x}, t\right)$: Conserved-order parameter describing diffusion of solute atom

Governing equations

Time evolution equation of solid/liquid interface

$$\frac{\partial \phi}{\partial t} = -M_{\phi} \frac{\delta G}{\delta \phi}$$

This equation is called as the time-dependent Ginzburg-Landau equation in physics or the **Allen-Cahn equation** in metallurgy.

S. M. Allen and J. W. Cahn, Acta Metallurgica, (1979), 27, pp.1085-1095.

Time evolution equation of solute diffusion

$$\frac{\partial c}{\partial t} = \nabla \cdot \left\{ M_c \nabla \left(\frac{\delta G}{\delta c} \right) \right\}$$

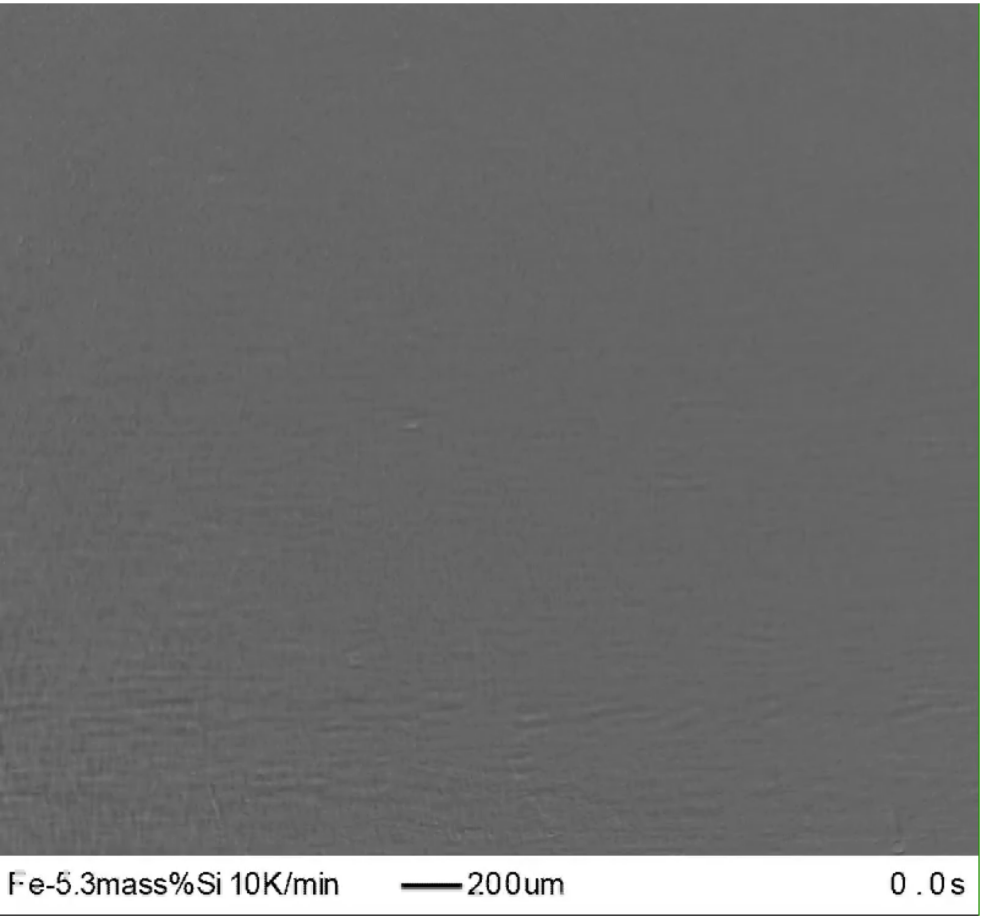
This equation is called as the **Cahn-Hilliard equation** in metallurgy.

J. W. Cahn and J. E. Hilliard, Journal of Chemical Physics, (1958), 28, pp. 258-267.

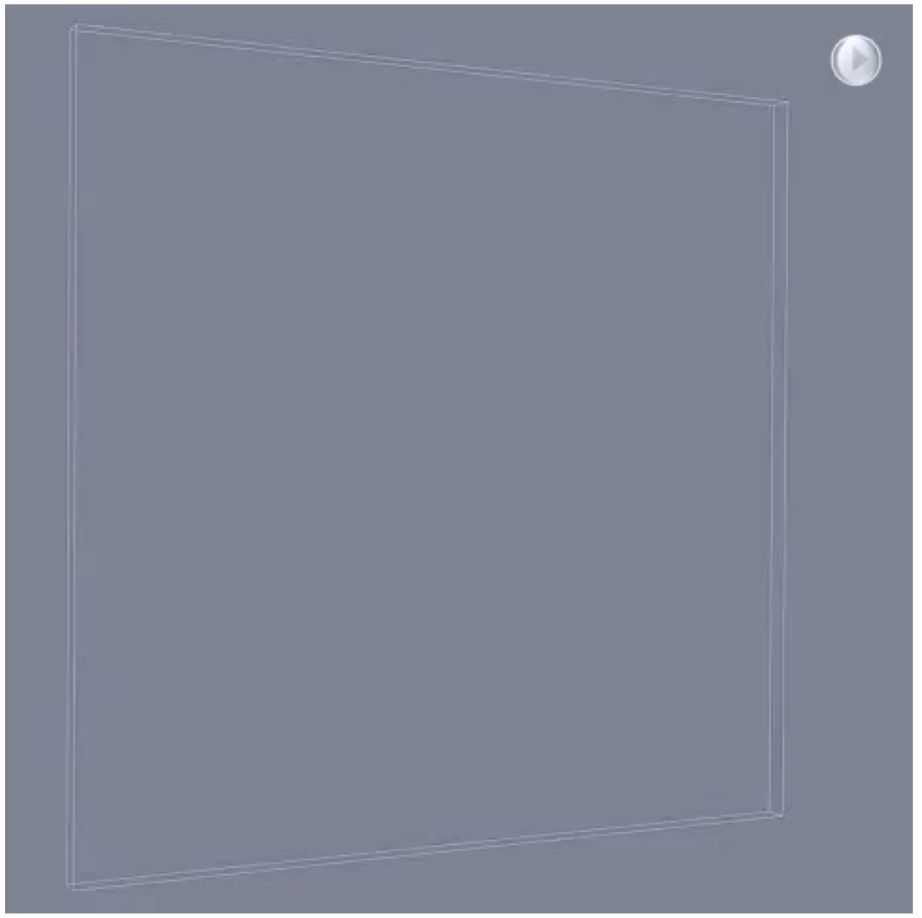
These two partial differential equations can be easily solved by numerical calculation, e.g. finite different method.

Experiment vs. Simulation

Experimental



Phase-field simulation

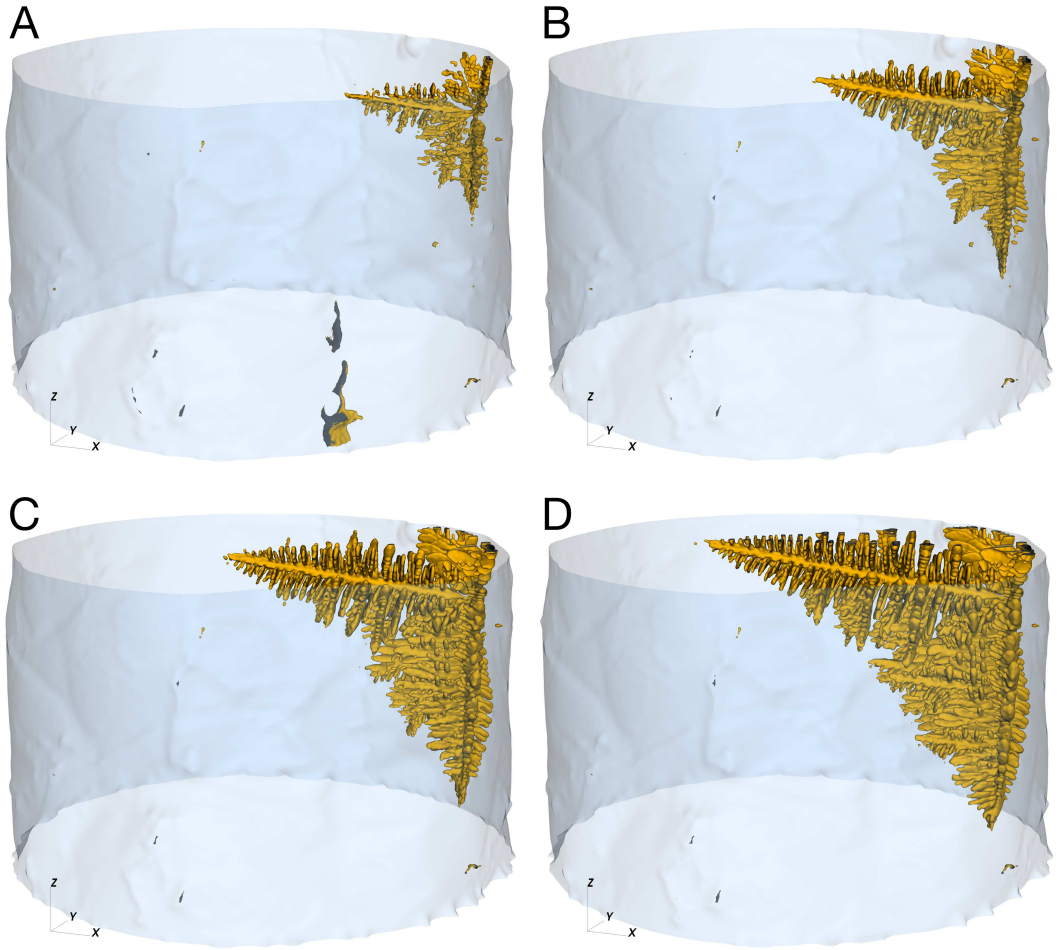


Courtesy of Prof. Yasuda (Kyoto University)

The growth of dendrites simulated by the phase-field method is very similar to that observed experimentally.

In-situ observation

Most recently, three-dimensional dendrite structure can be observed using the state-of the art X-ray tomography technique.

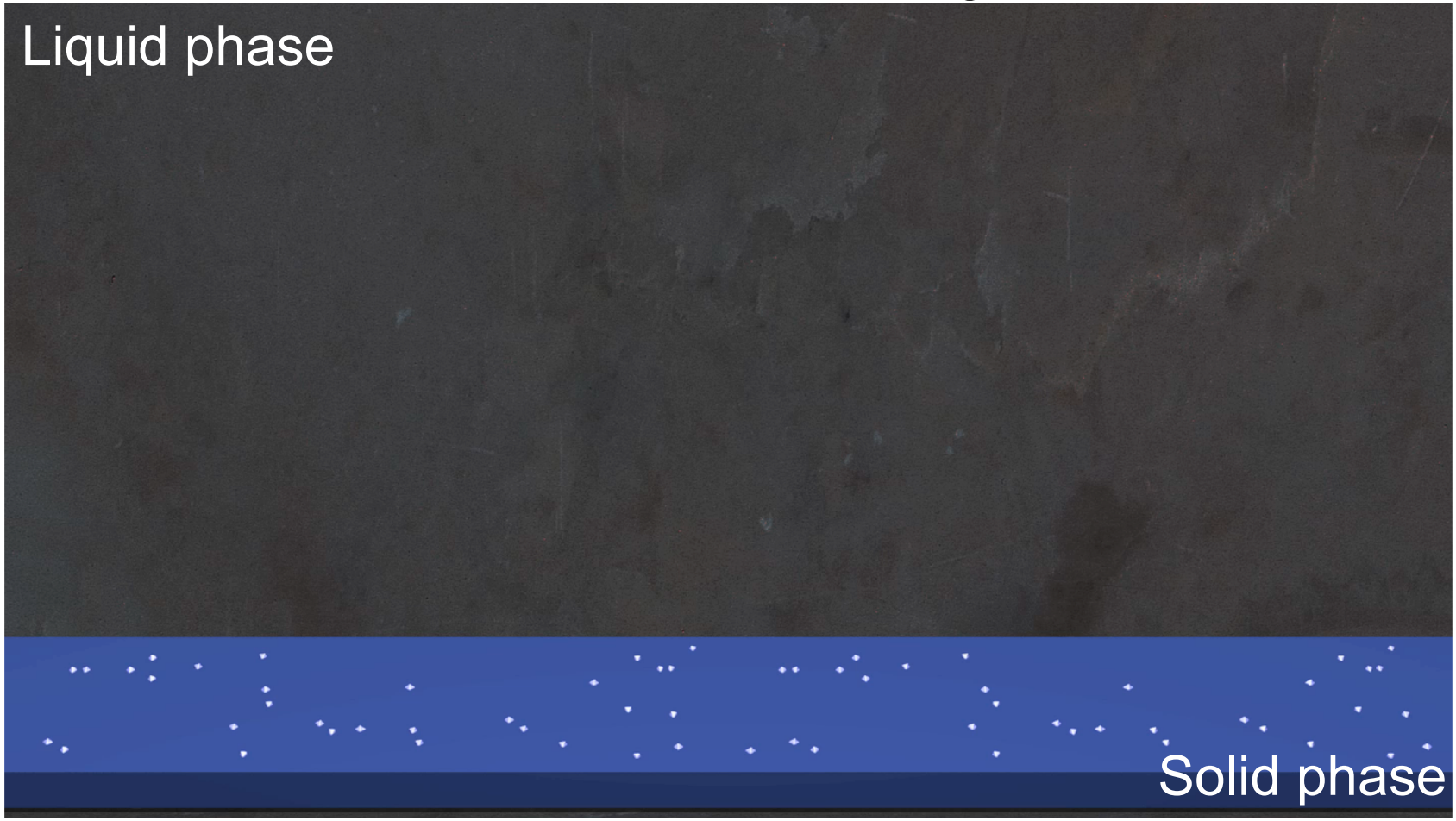


4D observation of dendritic solidification in Al-Cu alloy

J.W. Gibbs, K.A. Mohan, E.B. Gulsoy, P. W. Voorhees et al., *Scientific Reports,* 5 (2015), 11824

Large-scale simulation

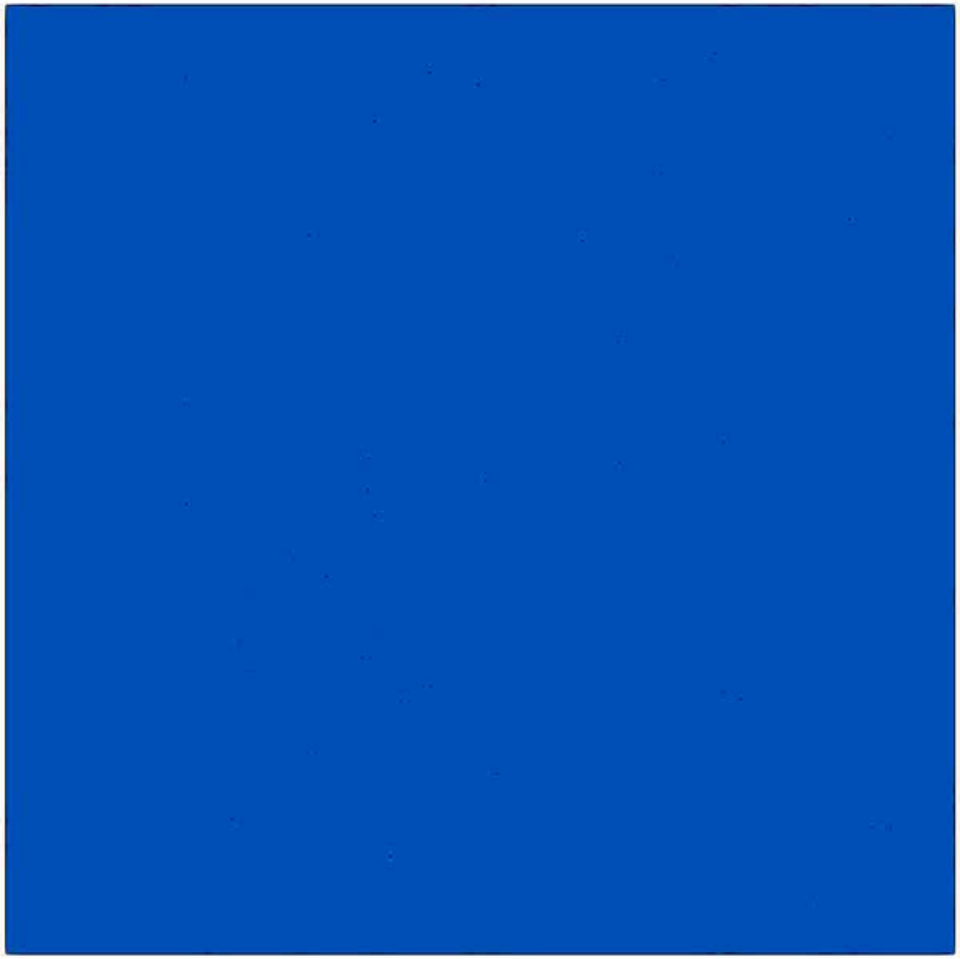
Extreme large-scale phase-field simulation of
Al-Si dendritic solidification using **4000GPUs**

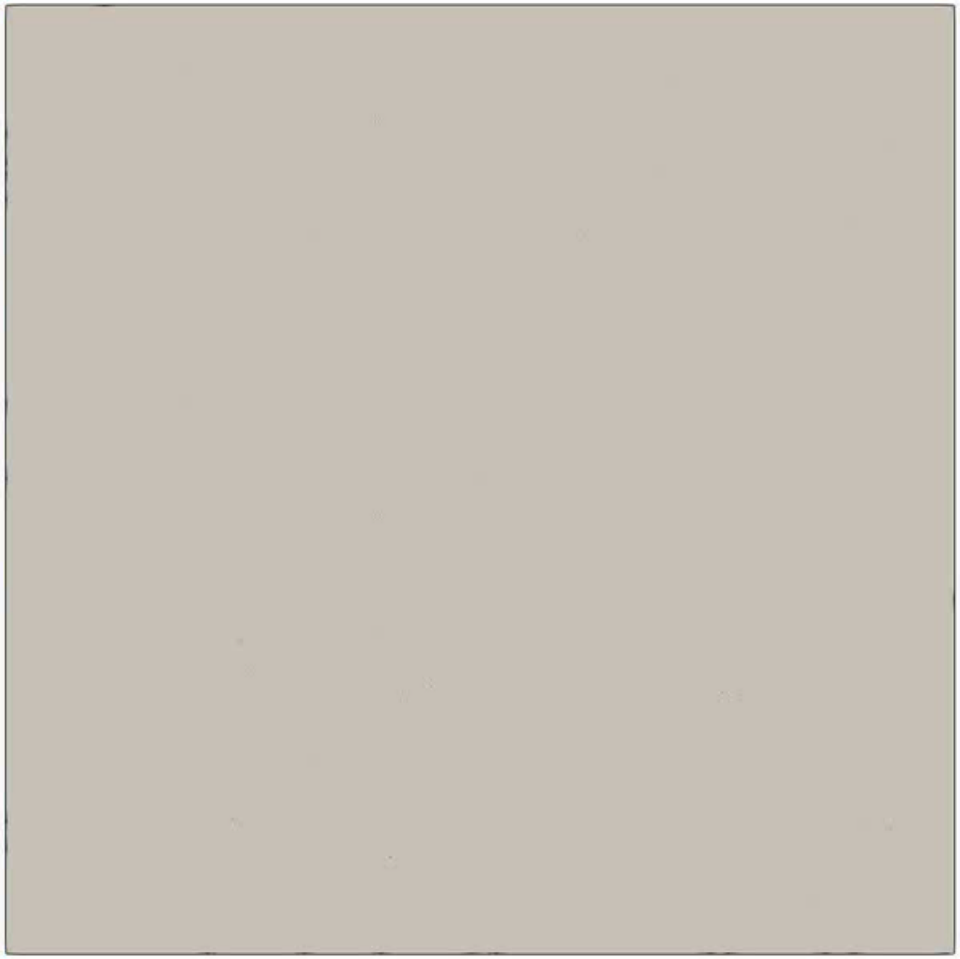


T. Shimokawabe, T. Aoki, T. Takaki, A. Yamanaka et al., Peta scale Phase-Field Simulation for Dendritic Solidification on the TSUBAME 2.0 Supercomputer, Proceedings of Supercomputing 2011, (2011)

Phase-field with fluid dynamics

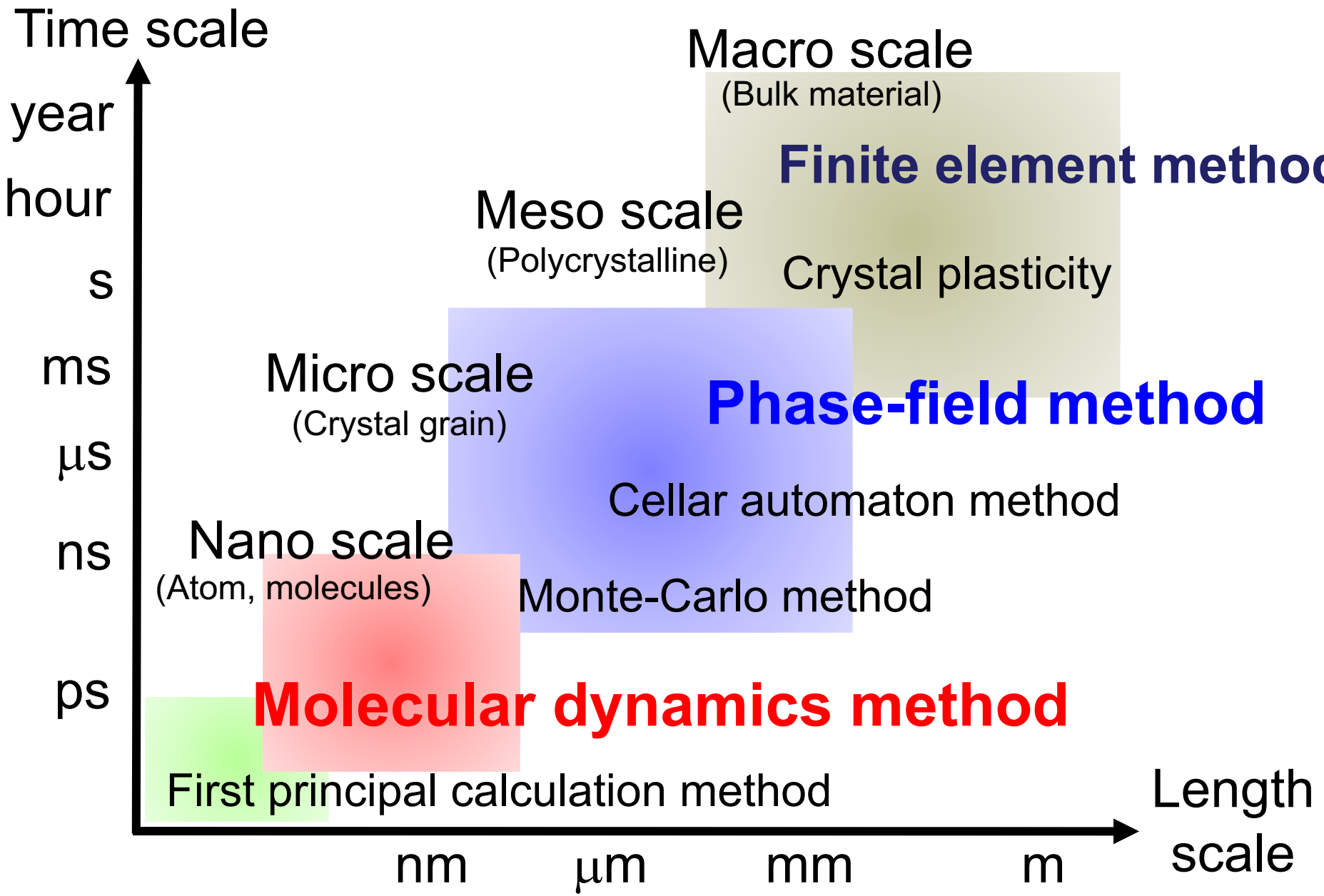
Free falling of growing dendrites with fluid flow





Courtesy of Prof. T. Takaki (Kyoto Institute of Technology)

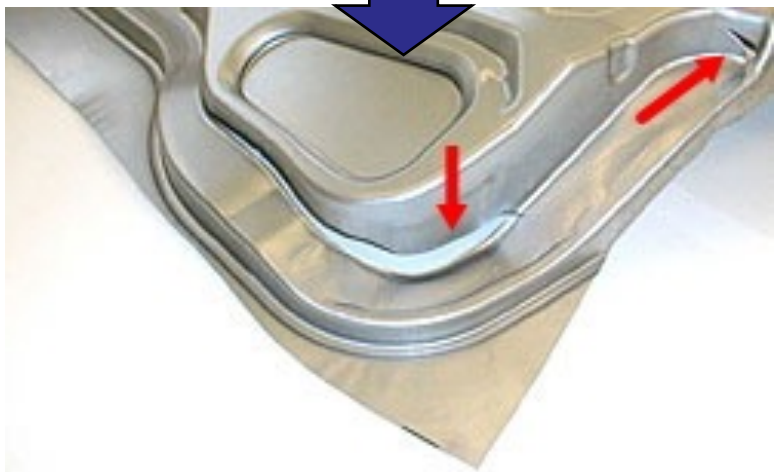
Various simulation methods



Deformation of aluminum alloy

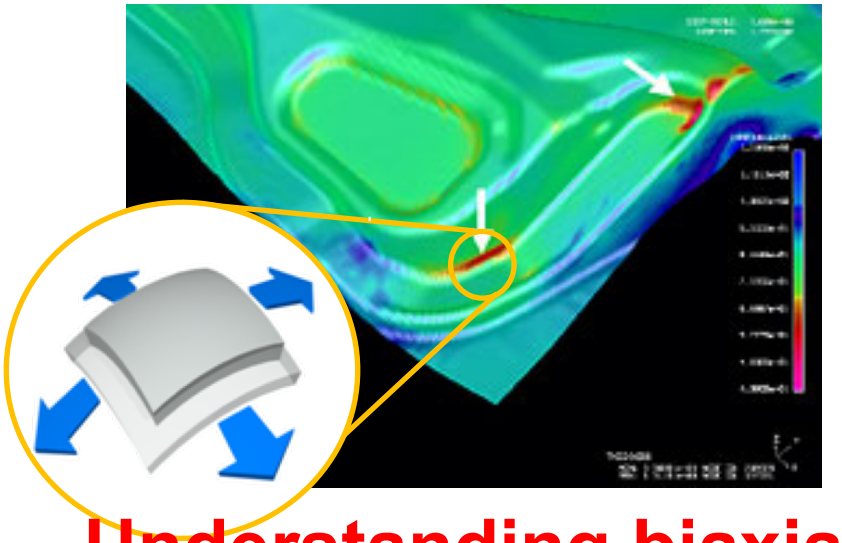
Reduction of car body weight

Aluminum alloy sheet



http://www.jstamp.jp/products/nv/function.html#ware

Forming failure

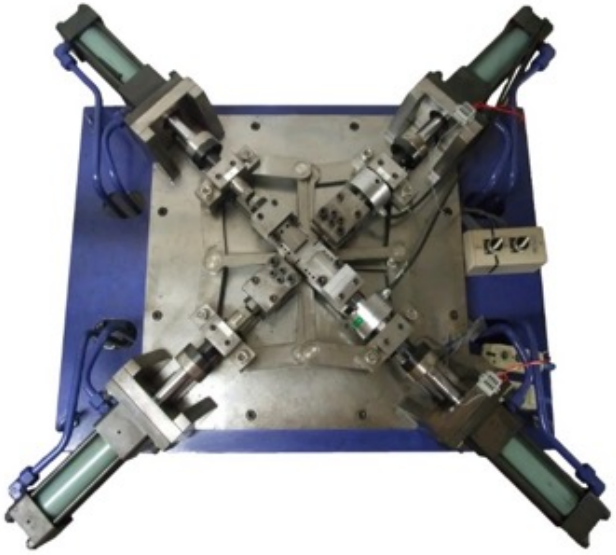


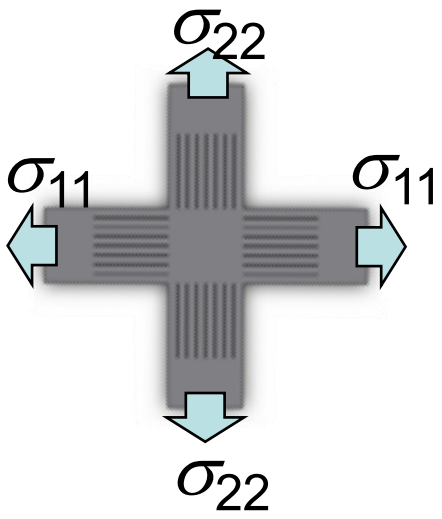
Understanding biaxial deformation behavior

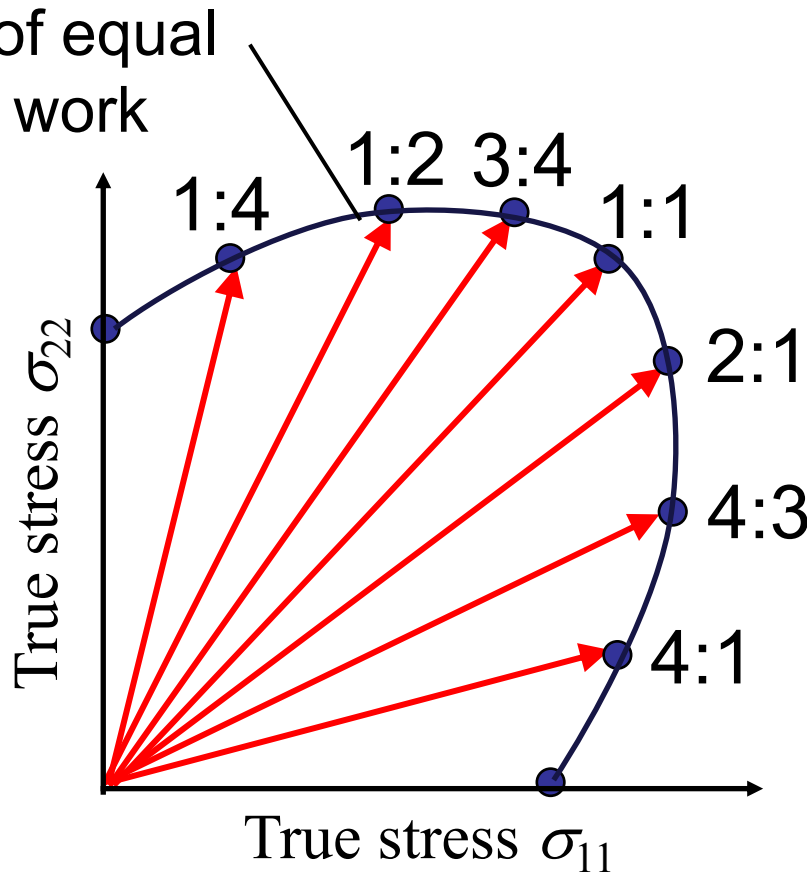
Biaxial tensile test

Biaxial tensile test using cruciform specimen is one of the effective experimental method to understand the biaxial deformation of sheet metals. But, it is time-consuming…

- High precision
- High reliability
- Expensive machine
- Time consuming



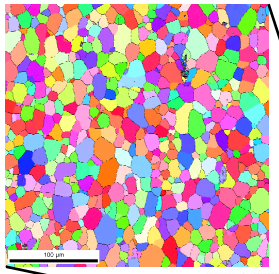


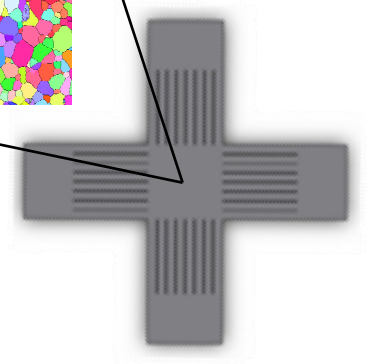


ISO 16842: 2014 - Metallic materials -- Sheet and strip – Biaxial tensile testing method using a cruciform test piec

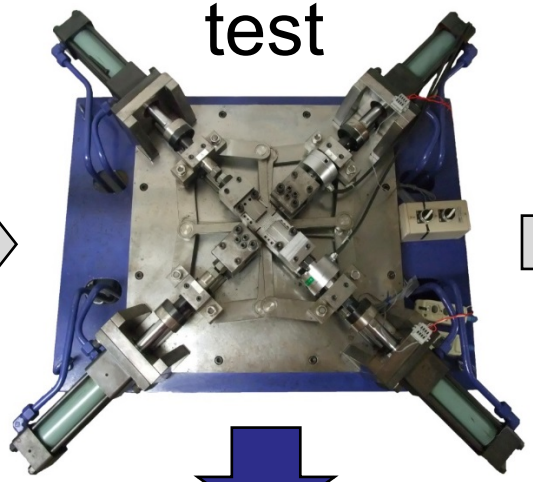
Numerical biaxial tensile test

Material information

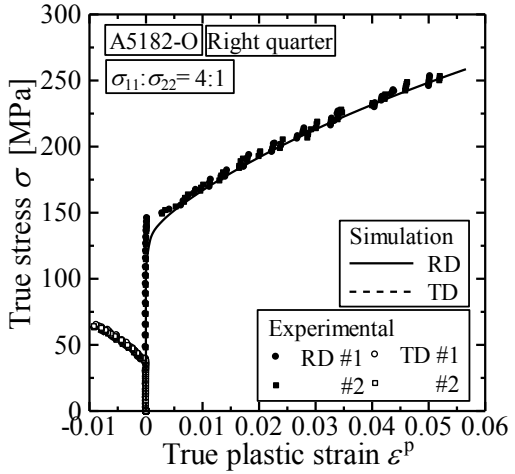




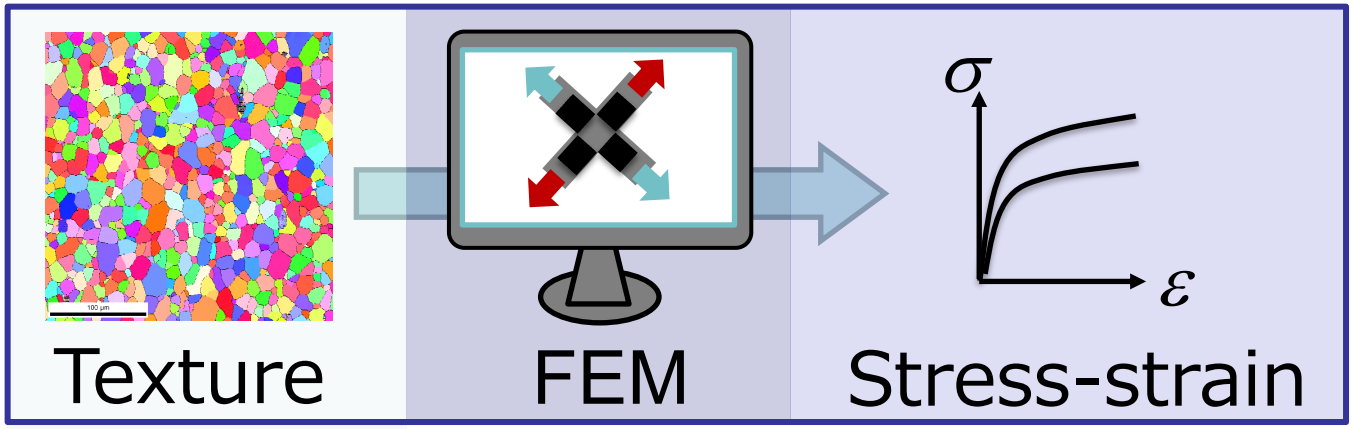
Biaxial tensile test



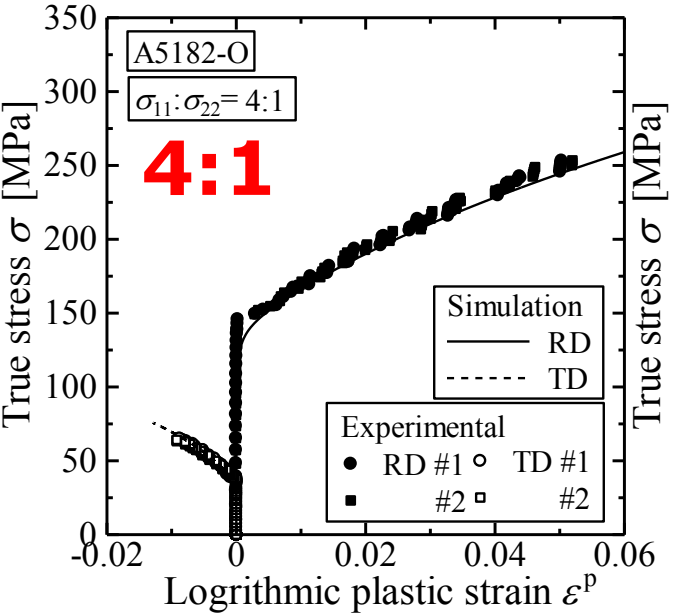
Stress-strain curve

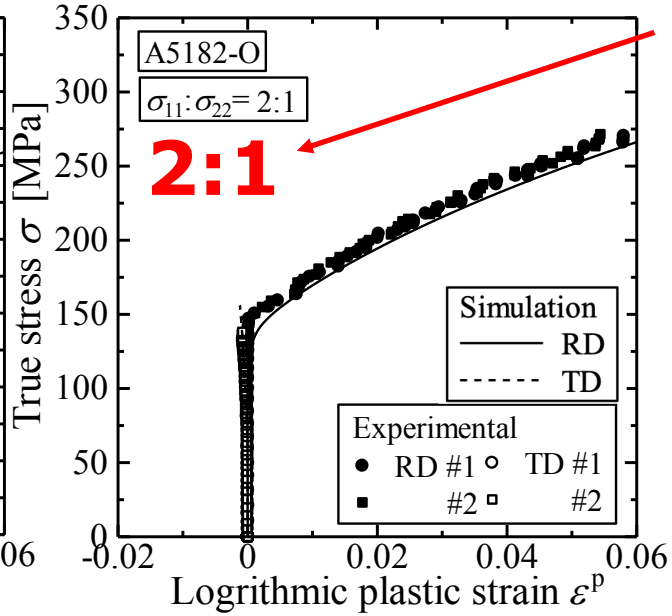


Numerical biaxial tensile test using finite element method

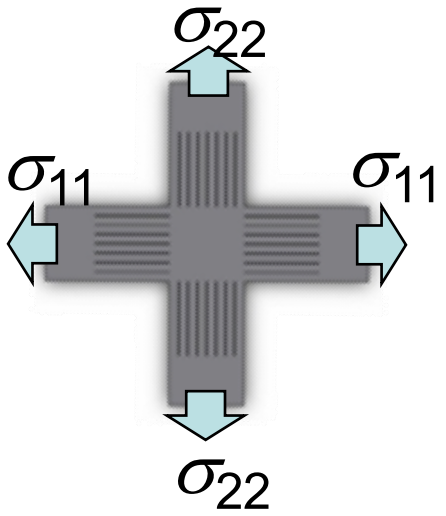


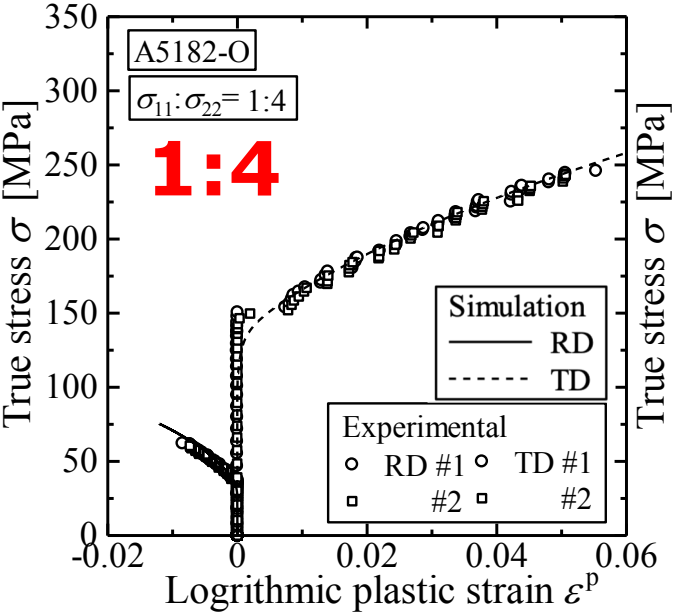
Experiments vs. Simulation

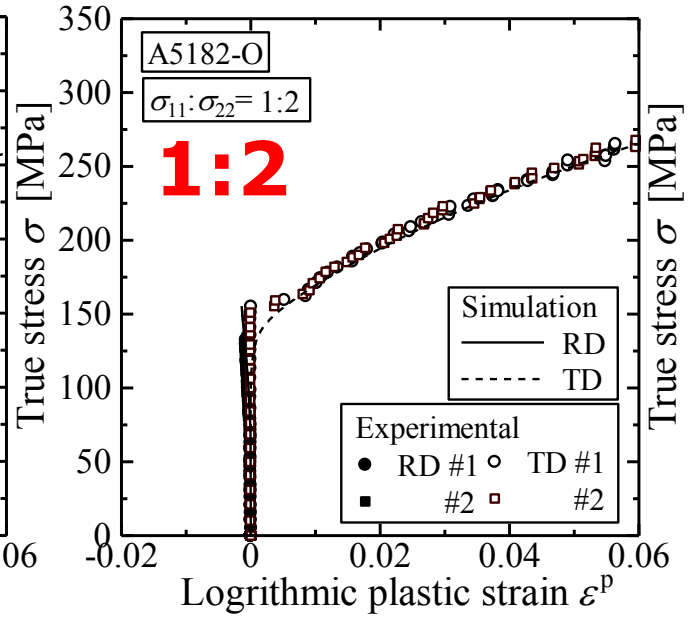


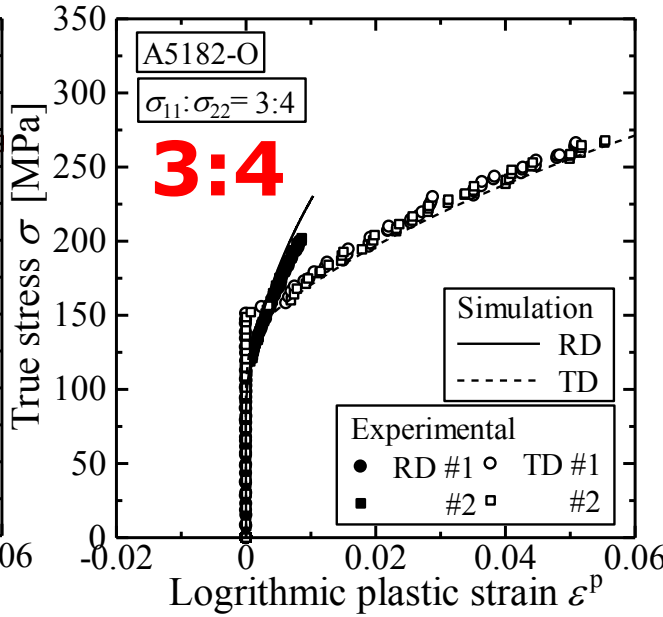


Stress ratio $\sigma_{11}:\sigma_{22}$



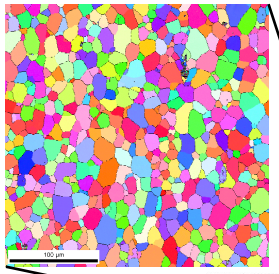


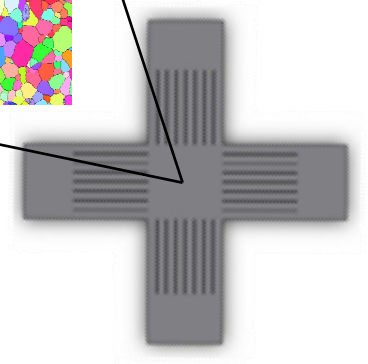




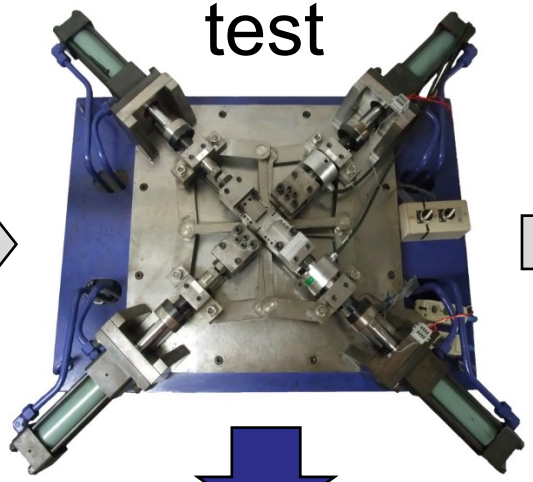
Numerical biaxial tensile test

Material information

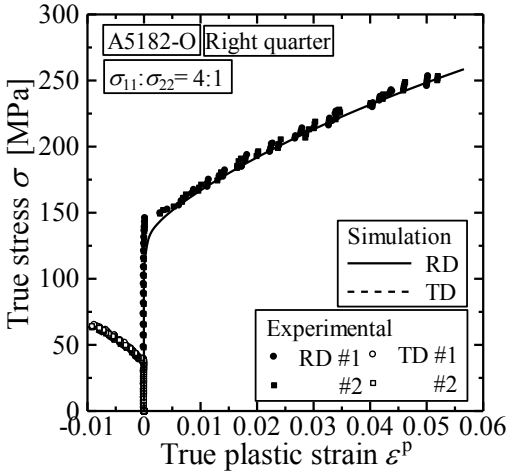




Biaxial tensile test



Stress-strain curve

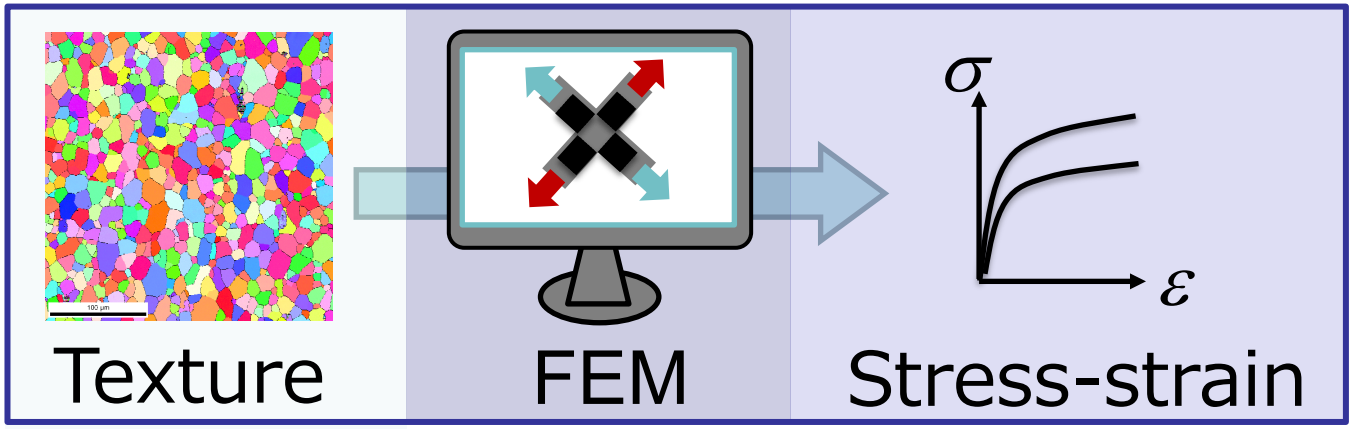


Numerical biaxial tensile test using finite element method

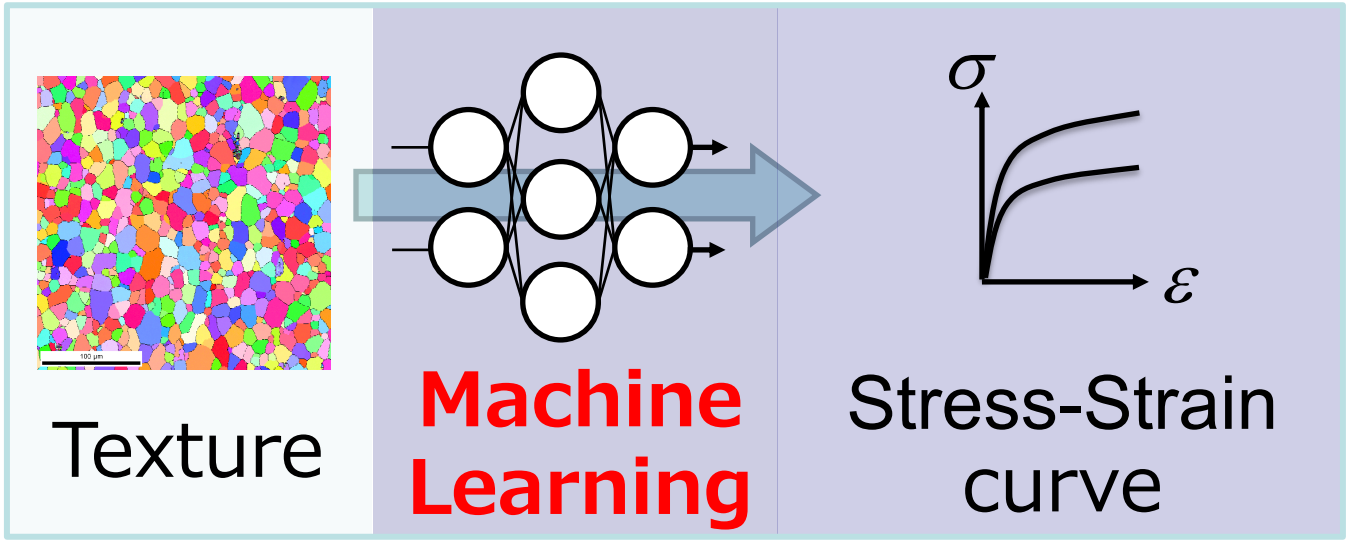
For numerical biaxial tensile test, special program (in-house source code) is required.

Machine learning

Numerical biaxial tensile test using finite element method



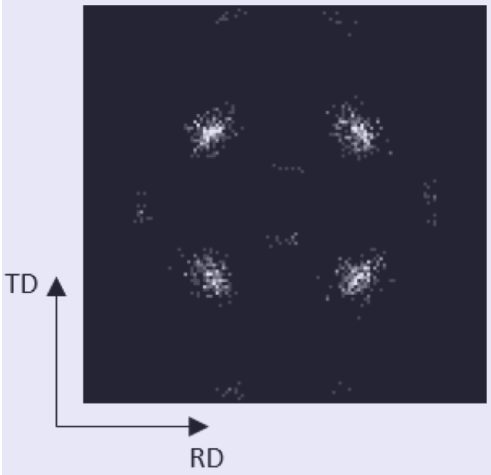
Training data



Deep learning using neural network (NN)

Input

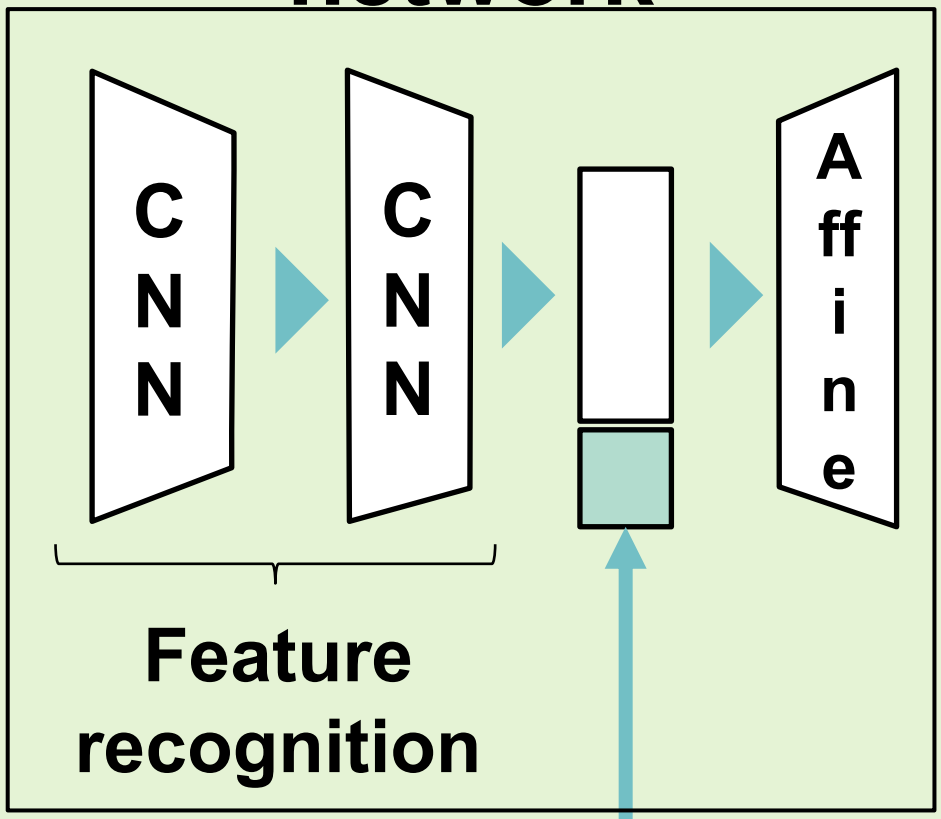
Image information of microstructure



Stress ratio

$\sigma_{RD} : \sigma_{TD}$

Convolution neural network



Output

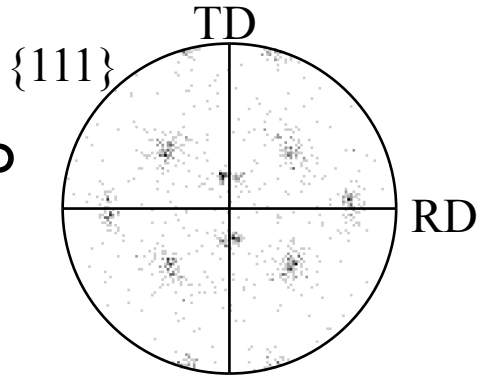
Stress -strain curve

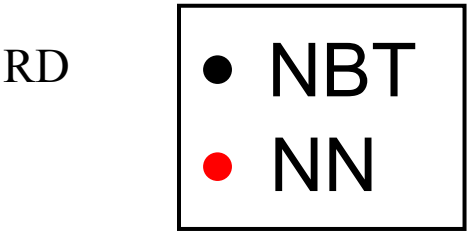
Verification of trained NN

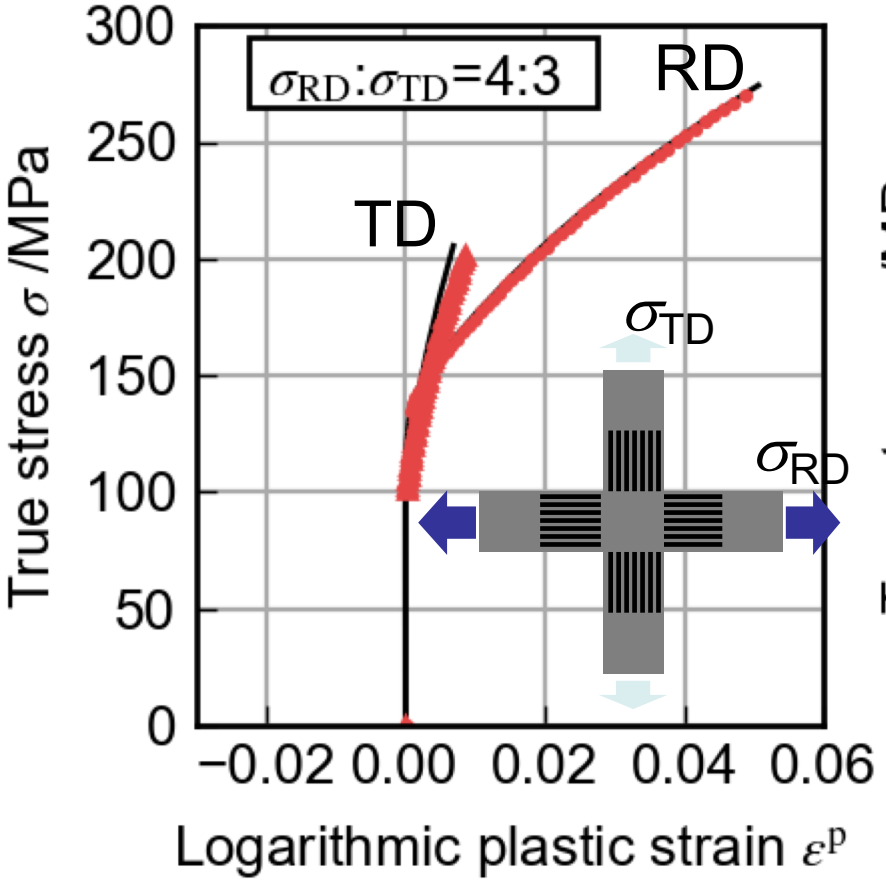
Verification data

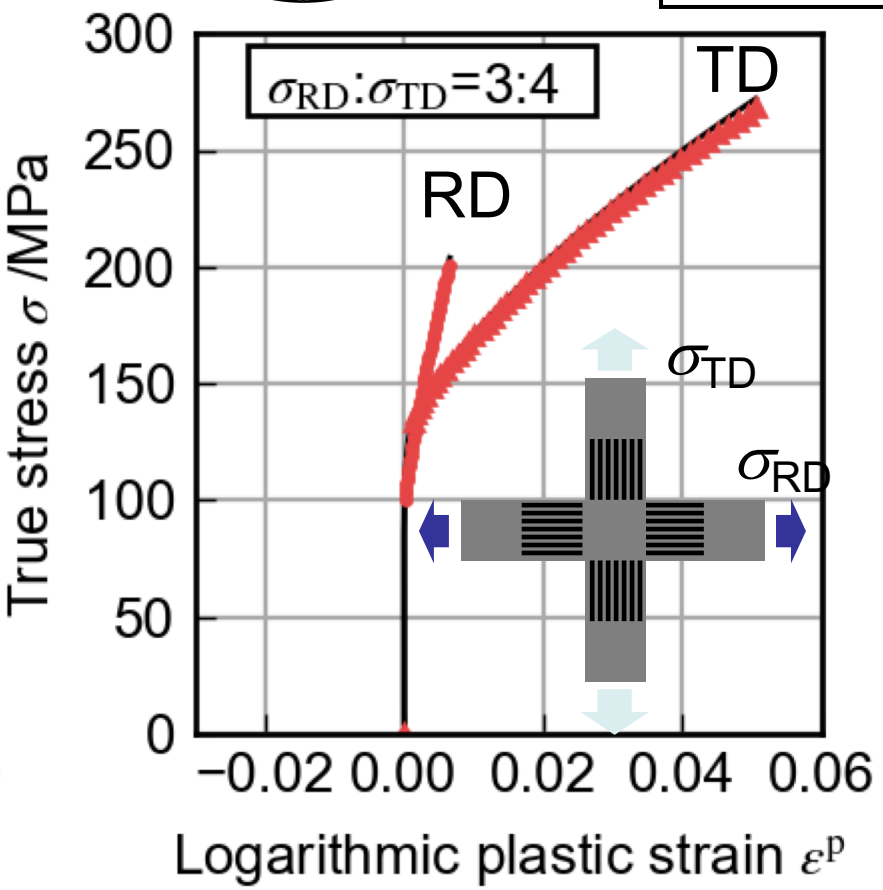
Cube: V_f = 24%, variance 6°

S: V_f = 46%, variance 6°









Summary

- Computational material science is now actively studied for efficient material design and development.

- In this lecture, molecular dynamics (MD), phase-field (PF) and finite element (FE) methods are introduce.

- MD, PF and FE methods are very powerful for predicting and simulating various phenomena in materials.