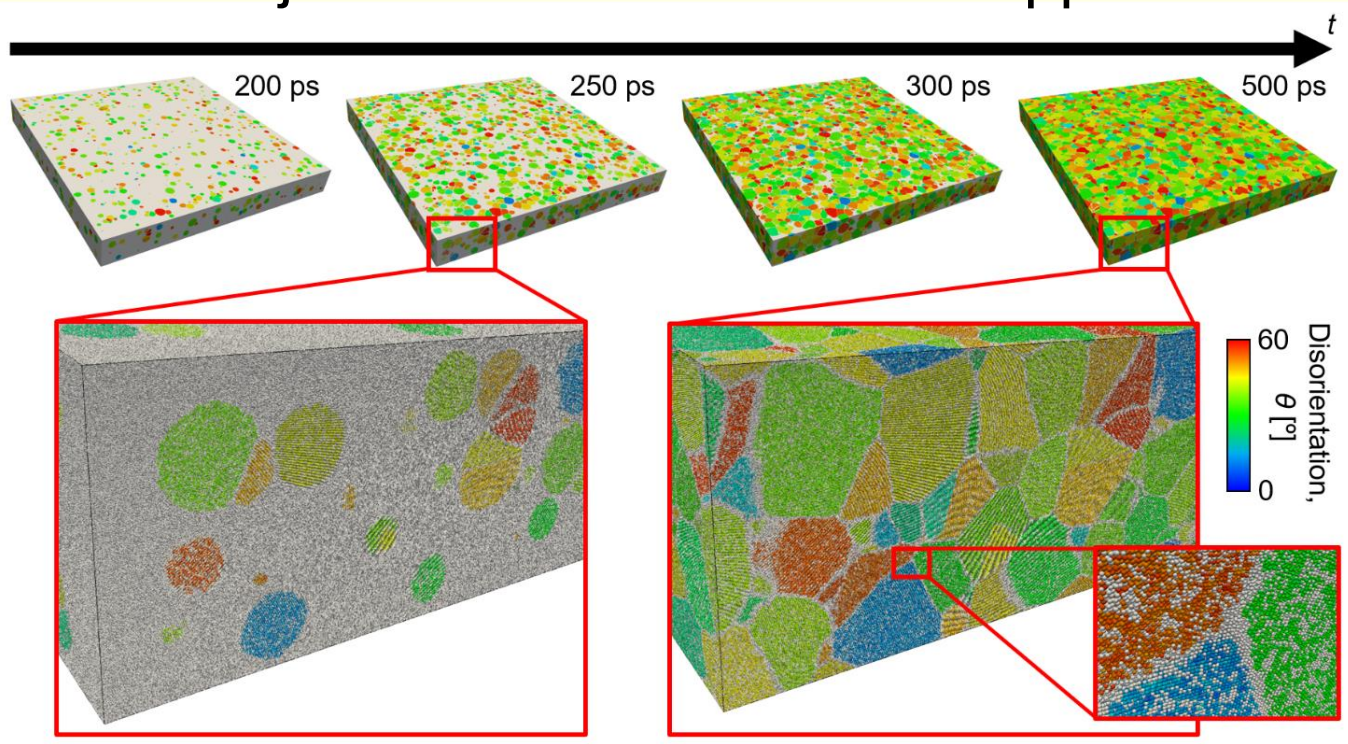
Sep 4, 2020
37th CMD workshop
@ online

Large-scale molecular dynamics simulation in conjunction with data-driven approach



(10,368,000,000 iron atoms, 78h/500ps using 256GPUs)

* A version for distribution

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mse.t.u-tokyo.ac.jp

Outline

1. Brief introduction of molecular dynamics (MD) simulation

2. Large-scale MD simulation of microstructure formation
   - Remaining problems in PFM and the role of MD
   - Large-scale MD simulation of nucleation and solidification
   - Evolution of multi-scale modeling

3. Inter-scale modeling: share of information
   - Conversion of atomistic configuration into phase-field profile
   - MPF simulation of grain growth starting from MD configuration

4. Cross-scale modeling: utilization of shared information
   - What is data-assimilation(DA)? - Bayes' theorem -
   - Concept of data assimilation between MD and PFM
   - On-the-fly estimation of solid-liquid interfacial properties by DA

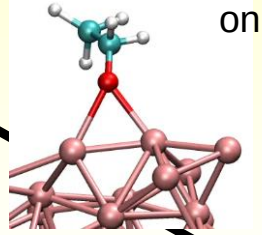
5. Summary with some ongoing works

Materials modelling laboratory
– modelling for materials design –

What is desired
for materials modelling?

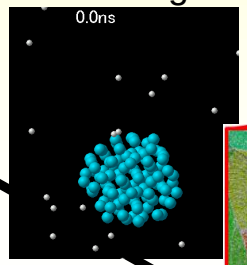
New materials design
from computational simulations

EtOH dissociation
on Fe cluster *1



Ab initio MD
（electronic）

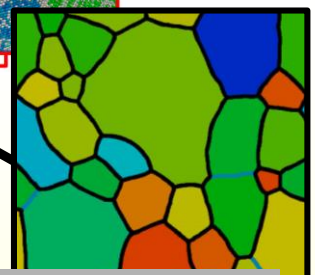
CNT growth*2



Classical MD
（atomistic）

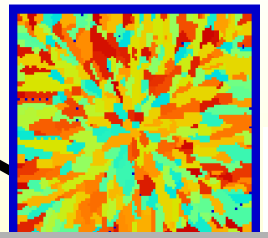
Nucleation and solidification
(10B atoms)*3

Grain growth*4



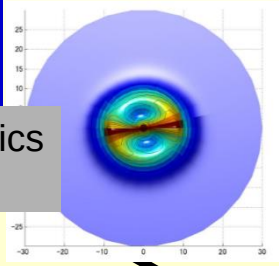
Phase-field method
（Meso-scale）

Microstructure formation



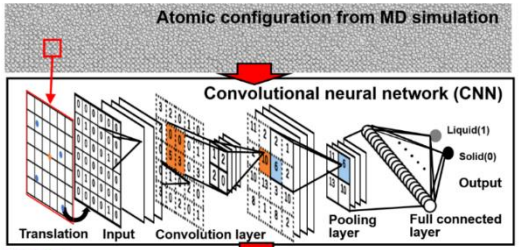
Continuum dynamics
（macro）

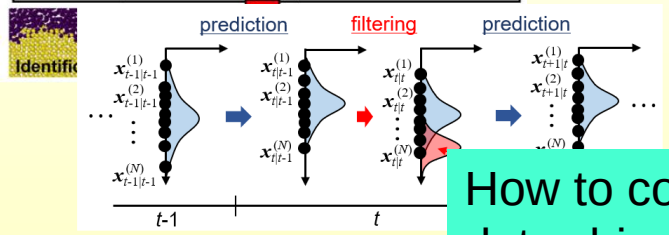
Heat and mass
transformation



*1CPL 731 (2019) 136619
*2CPL 382 (2003) 381
*3MSMSE 27 (2019) 054002
*4CMS, 152 (2018) 118.
*5CMS, 184 (2020) 109880.

Convolutional Neural Network*5





Bayesian inference

How to collaborate with
data-driven approach?

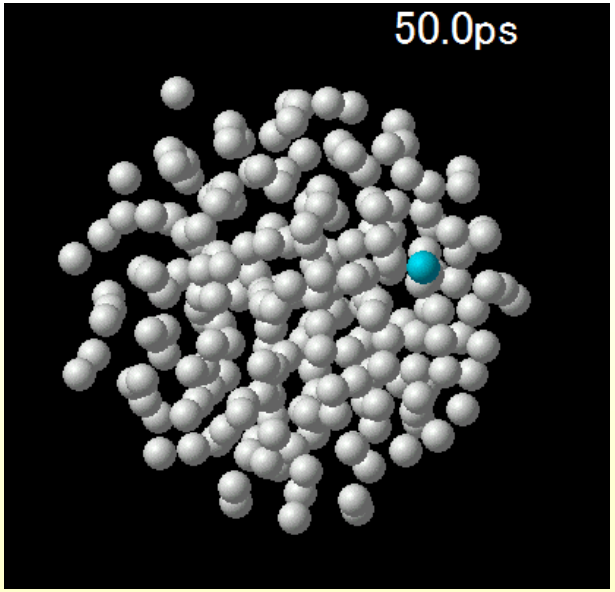
Molecular dynamics (MD) simulation

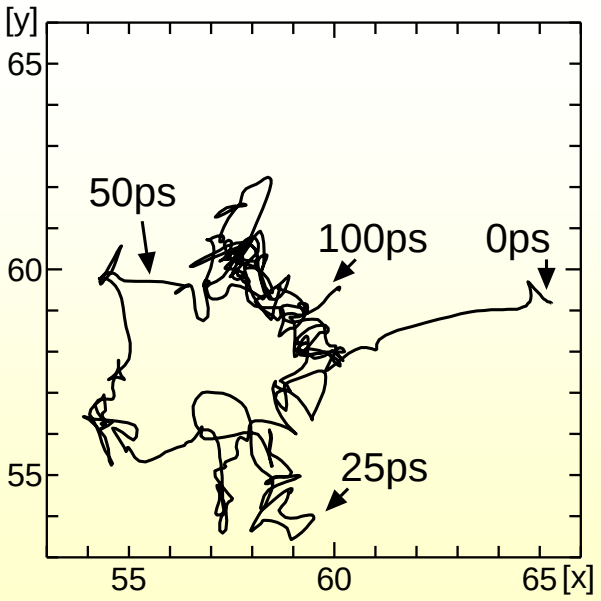
In the MD simulation, trajectories of all atoms in materials are determined by numerically solving Newton's equations of motion for a system of interacting atoms.

Governing equation: Newton's second law of motion $$m\frac{d^2\mathbf{r}}{dt^2} = \mathbf{F}$$

MD simulation is an deterministic method, in which position and velocity of all atoms at every time step is determined explicitly, when initial position and velocity and as well as the force acting on all atoms is defined.

例）Snapshot of Ar_{216} cluster at 50 K and trajectory of sky-blue atom during 100 ps.





Force acting on atoms

1. Force from (time-independent) Schrödinger equation $\hat{H}\psi = E\psi$
   →*ab initio* MD

Under adiabatic approximation, the electronic state (wave functions) are calculated by *ab initio* method. Then, the Hellmann–Feynman force is derived from the wave function.

$$\mathbf{F} = \left\langle \psi^* \left| \frac{\partial \hat{H}}{\partial \mathbf{r}} \right| \psi \right\rangle$$

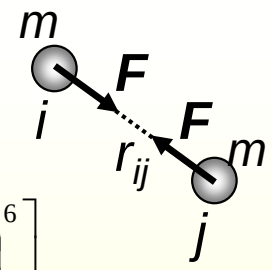
2. Force from the interatomic potential (force field)
   →classical MD

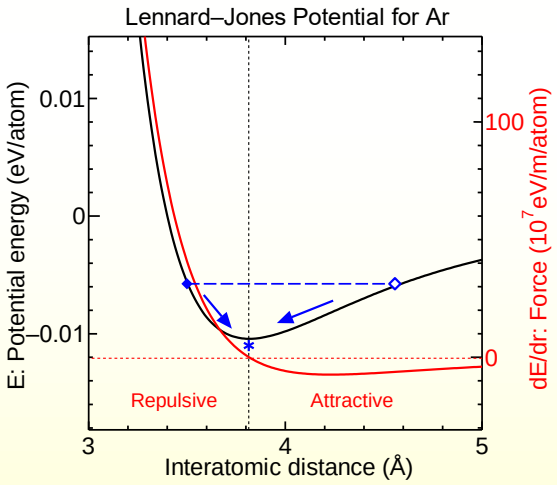
The interaction between atoms are approximated by the potential function (the force-field).

Ex) Lennard-Jones potential

$$\phi(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right]$$

$$f_{ij} = -\frac{\partial\phi(r_{ij})}{\partial r_{ij}} = 24\frac{\varepsilon}{r_{ij}}\left[2\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right]$$





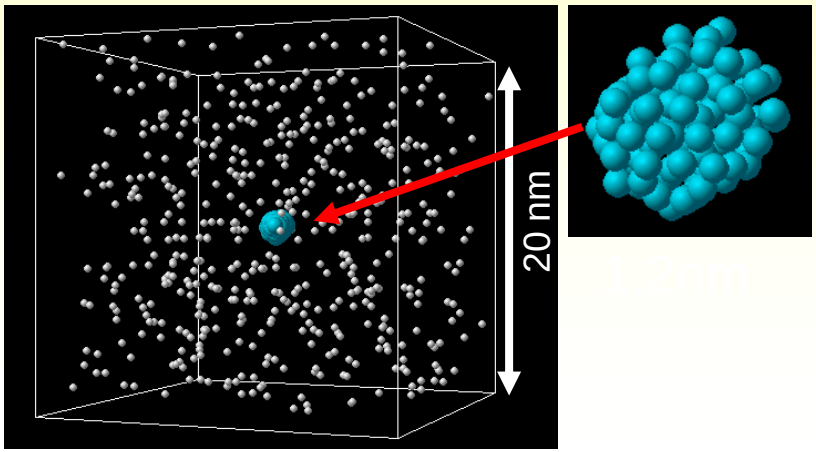
The force is derived from the differential of the potential.

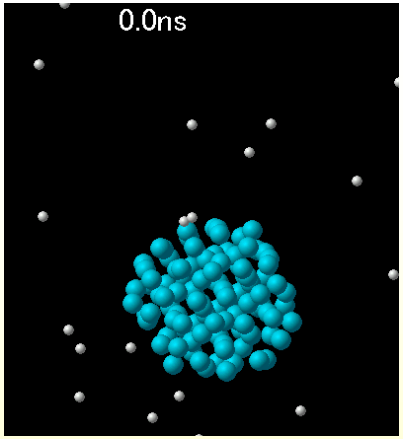
Position and velocity are derived from the Newton's equations of motion even if the force is given.
It is same process both for ab initio and classical MD.

$$m\frac{d^2\mathbf{r}}{dt^2} = \mathbf{F}$$

Modelling of metal-catalyzed growth of carbon nanotube and graphene

Carbon cap formation on Ni cluster



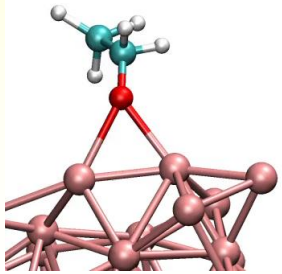


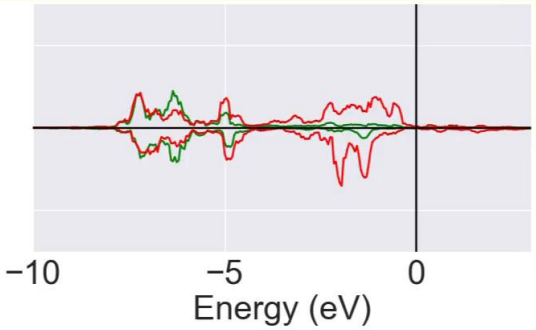
Classical MD

Y. Shibuta, S. Maruyama,
Chem. Phys. Lett, 382 (2003) 381.

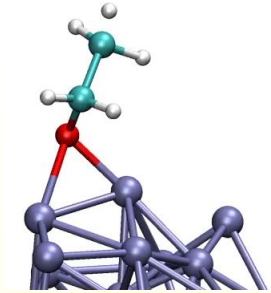
Precursor (EtOH) dissociation on transition metal (Fe, Co) cluster

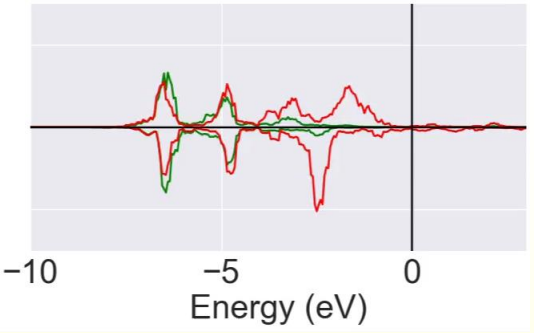
on Fe cluster





on Co cluster





Ab initio MD

S. Fukuhara, M. Misawa, F. Shimojo, Y. Shibuta,
Chem. Phys. Lett. 731 (2019) 136619.

A proper method should be chosen depending on the purpose of the study.

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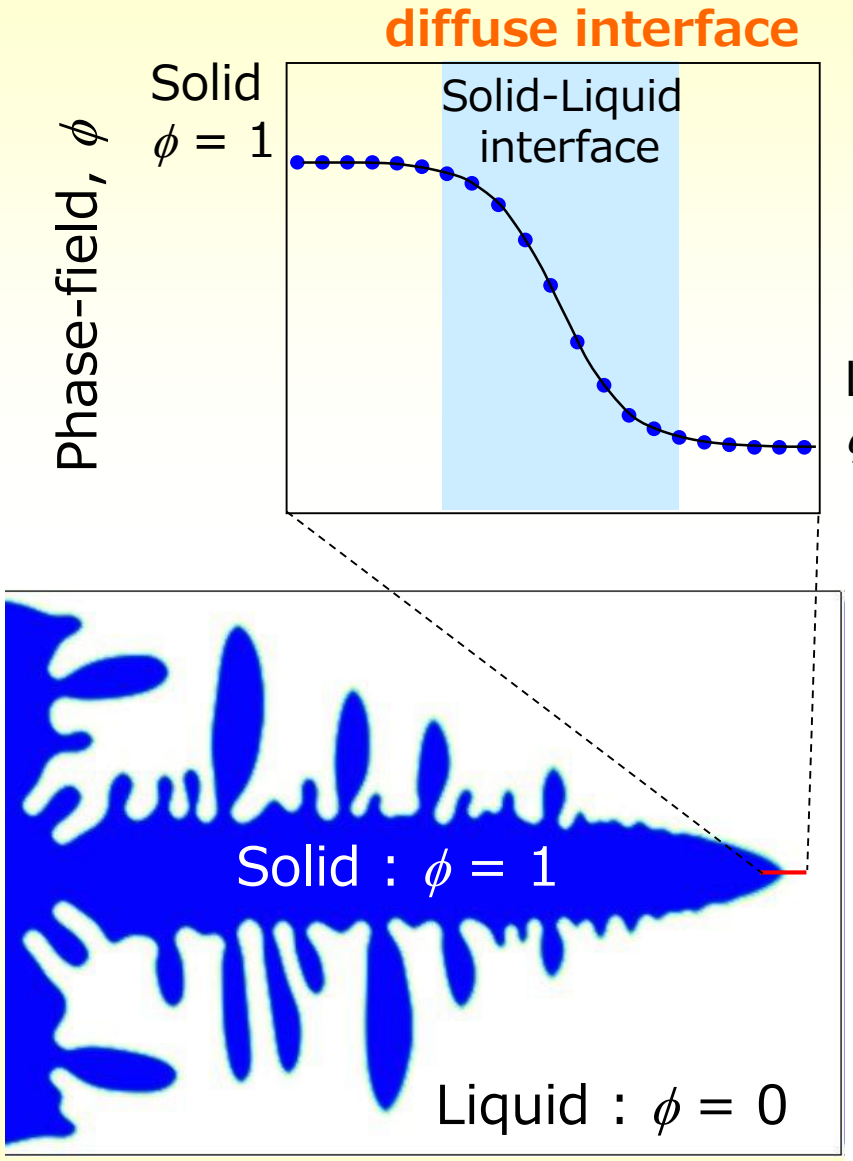
5. Summary with some ongoing works

Phase-field model



Phase-field, ϕ

$$\frac{\partial \phi}{\partial t} = \varepsilon^2 \nabla^2 \phi + f(\phi, c)$$

Driving force, Gibbs-Thomson effect

Concentration, c

$$\frac{\partial c}{\partial t} = \nabla M(\phi) \nabla \mu(\phi, c)$$

Diffusion in bulks, Stefan condition

Temperature, *T*

$$\frac{\partial T}{\partial t} = \cdots$$

Velocity, *v*

$$\frac{\partial v}{\partial t} = \cdots$$

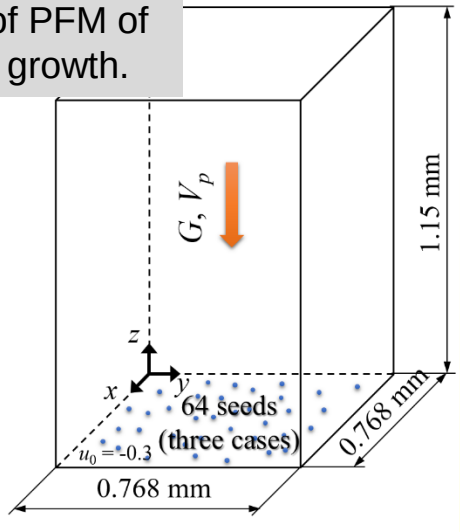
Remaining problems in PFM and the role of MD

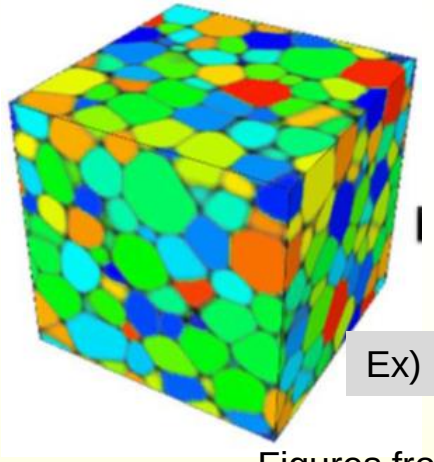
Now, PFM can treat large-scale 3D simulation of solidification and grain growth

Remaining problems in PFM

1. There is no explicit way to treat a nucleation event.
   →Nuclei specified in advance as having a random (or a particular) distribution or forcibly formed in line with an assumption
2. It is not easy to treat the anisotropy in grain boundary properties.
   →Mostly the approximate model (such as Read-Shockley) employed.

Ex) Initial condition of PFM of competitive dendrite growth.





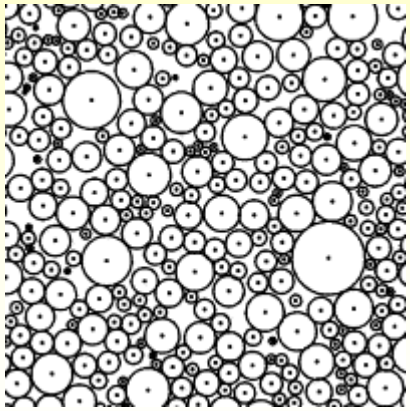
Ex) Multi-PFM of grain growth

Figures from Prof. T. Takaki (KIT)

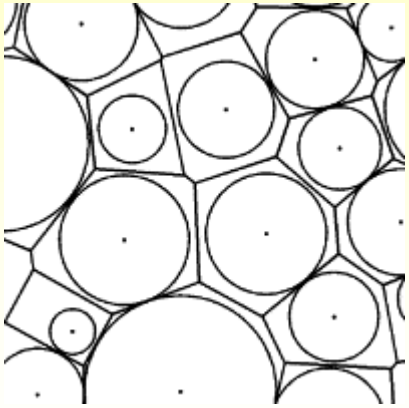
Can we treat these problems by MD simulation?

- Spontaneous nucleation occurs when an enough spatiotemporal scale is given.
- The anisotropy in grain boundary properties is inherently taken into account.

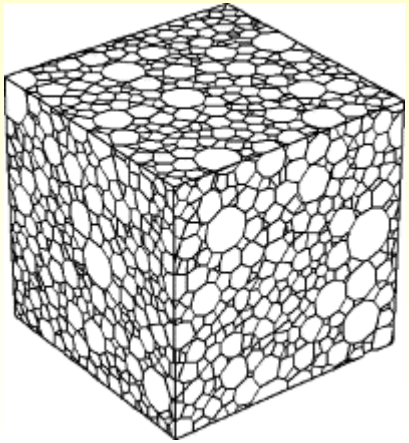
Polycrystalline microstructures by Laguerre-Voronoi tessellation



Log-normal distribution

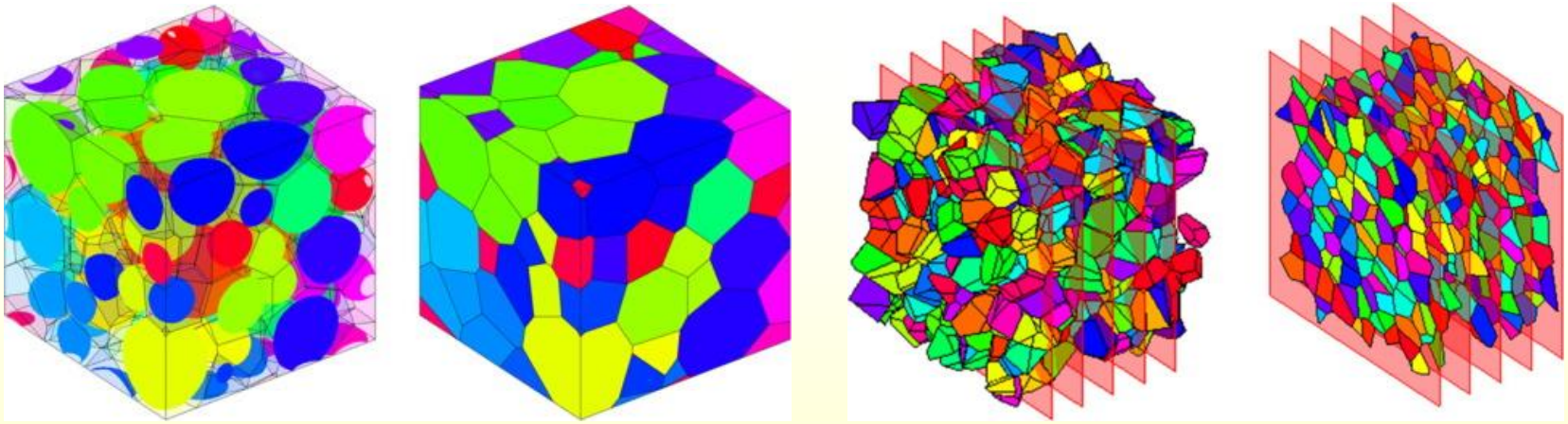


Voronoi division



Polycrystalline microstructure

Z. Fan, Y. Wu, X. Zhao, Y. Lu, Comp. Mater. Sci. 20 (2004) 301.

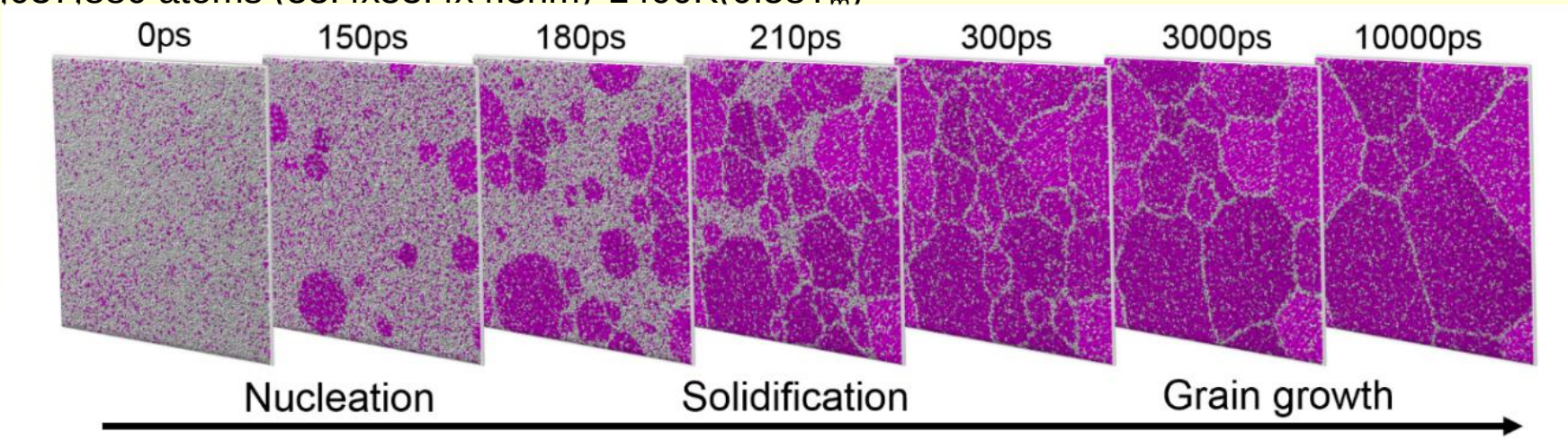


S. Falco, J. Jiang, F. De Cola, N. Petrinic, Comp. Mater. Sci. 136 (2017) 20.

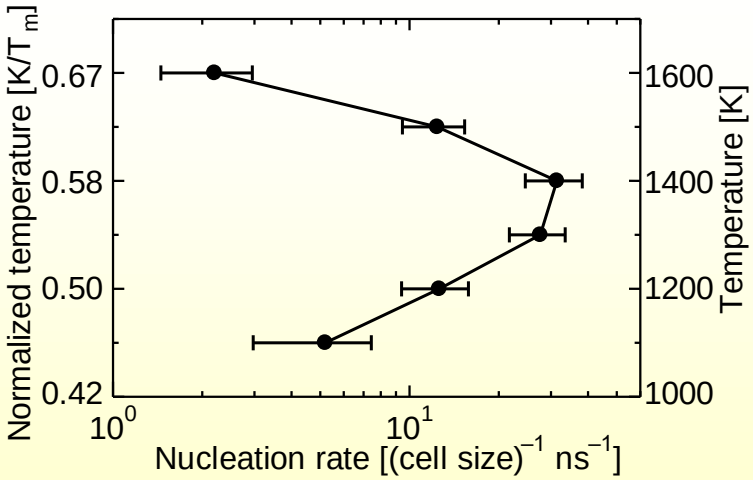
How to include the orientational relationship between grains?
How to express the anisotropy in grain boundary properties?

Homogeneous nucleation and microstructure evolution in million-atom MD simulation (quasi-2D)

1,037,880 atoms (53.4x53.4x4.3nm) 1400K($0.58T_m$)



Nucleation rate



Classical nucleation theory for homogeneous nucleation

$$I = I_0 \exp\left(-\frac{16\pi}{3}\frac{\sigma_{SL}^3}{(\rho\Delta s_f \Delta T)^2 k_B T}\right)$$

Two competing effects in the exponent result in the nose shape

Thermally activated homogeneous nucleation occurs in MD simulations without any inducing factor.

Y. Shibuta, K. Oguchi, T. Takaki, M. Ohno, Scientific Reports, 5 (2015) 13534.

Billion-atom MD simulation by multi-GPU parallel computation

nature COMMUNICATIONS

ARTICLE

DOI: 10.1038/s41467-017-00017-5 OPEN

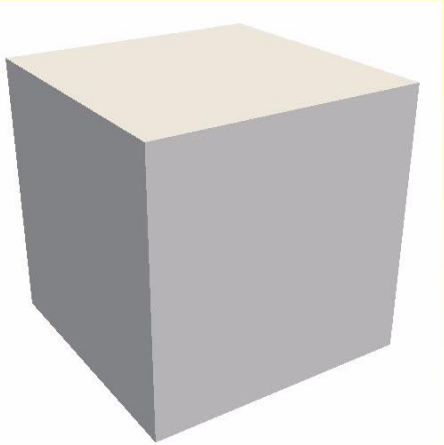
pure Fe (FS potential)

Y. Shibuta, S. Sakane, E. Miyoshi, S. Okita, T. Takaki, M. Ohno

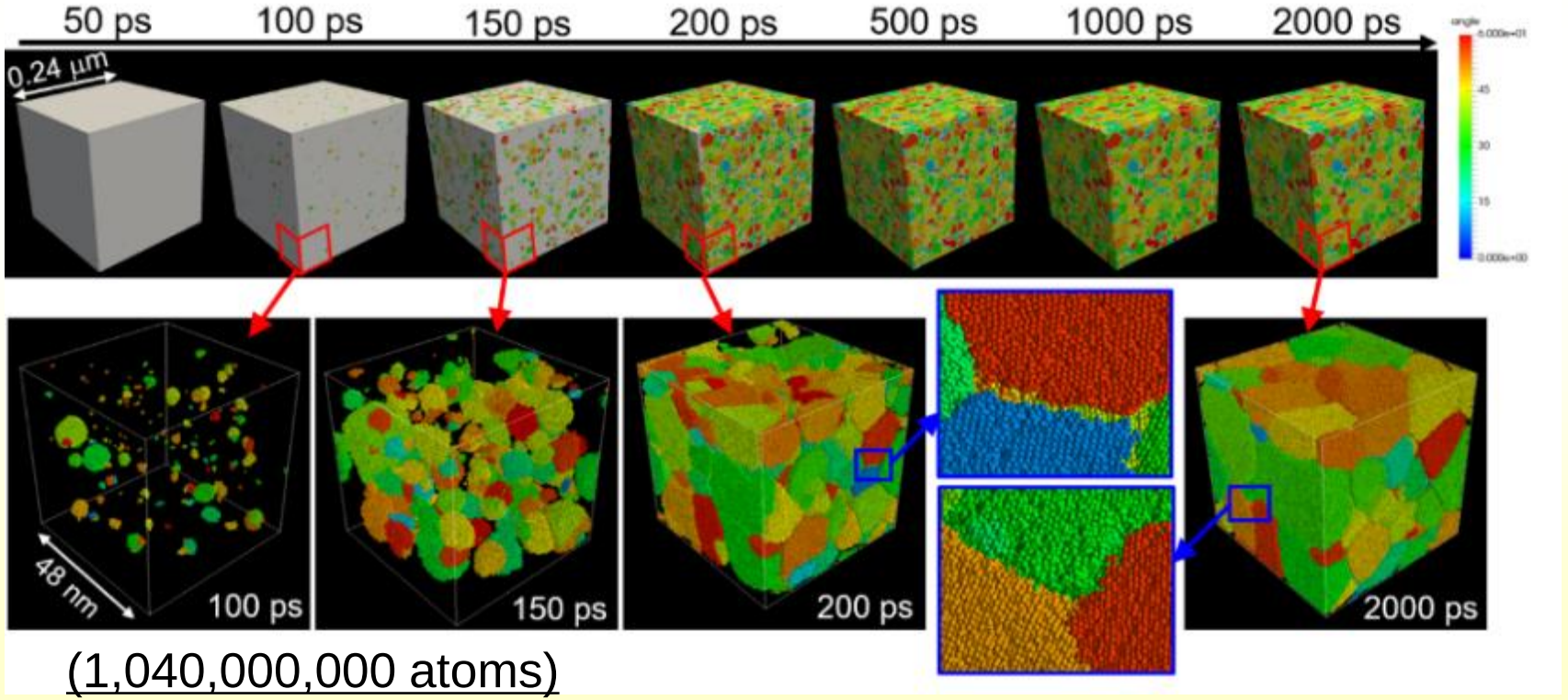
Nature Communications, 8 (2017) 10.

Heterogeneity in homogeneous nucleation from billion-atom molecular dynamics simulation of solidification of pure metal

Yasushi Shibuta[1], Shinji Sakane[2], Eisuke Miyoshi[2], Shin Okita[1], Tomohiro Takaki[3] & Munekazu Ohno[4]



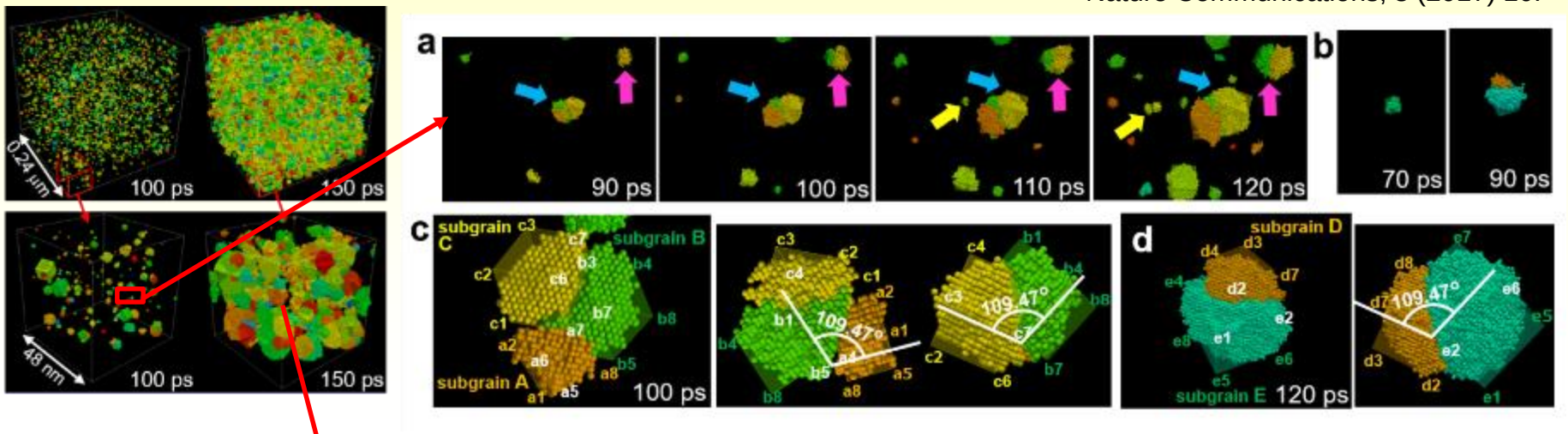
TSUBAME2.5
512GPU
(c.a.10ps/1h)

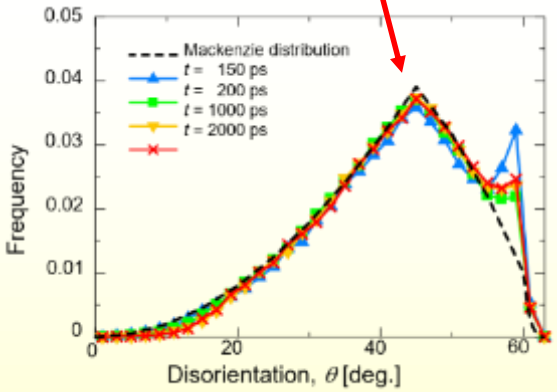


(1,040,000,000 atoms)

Heterogeneity in homogeneous nucleation

Y. Shibuta, S. Sakane, E. Miyoshi, S. Okita, T. Takaki, M. Ohno
Nature Communications, 8 (2017) 10.

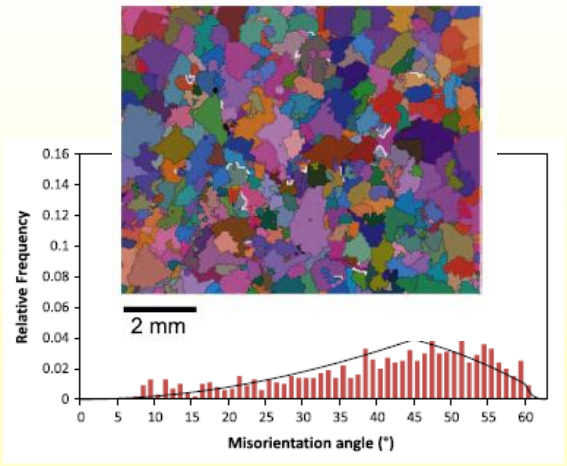




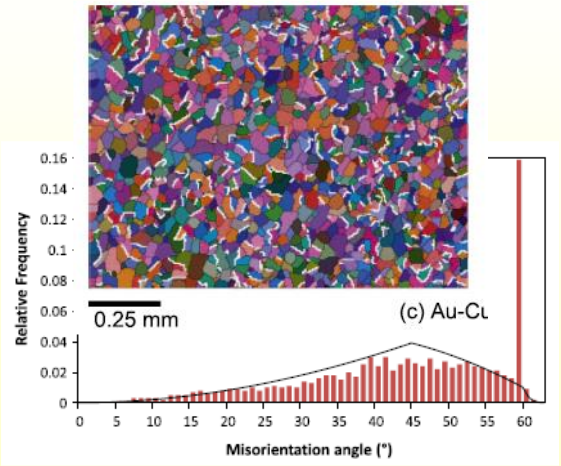
Orientational relationship between neighbor grains

Peak around 60° appears

From experiments: the origin of peak from fine microstructure, abundant twin boundary



Au-Cu-Ag



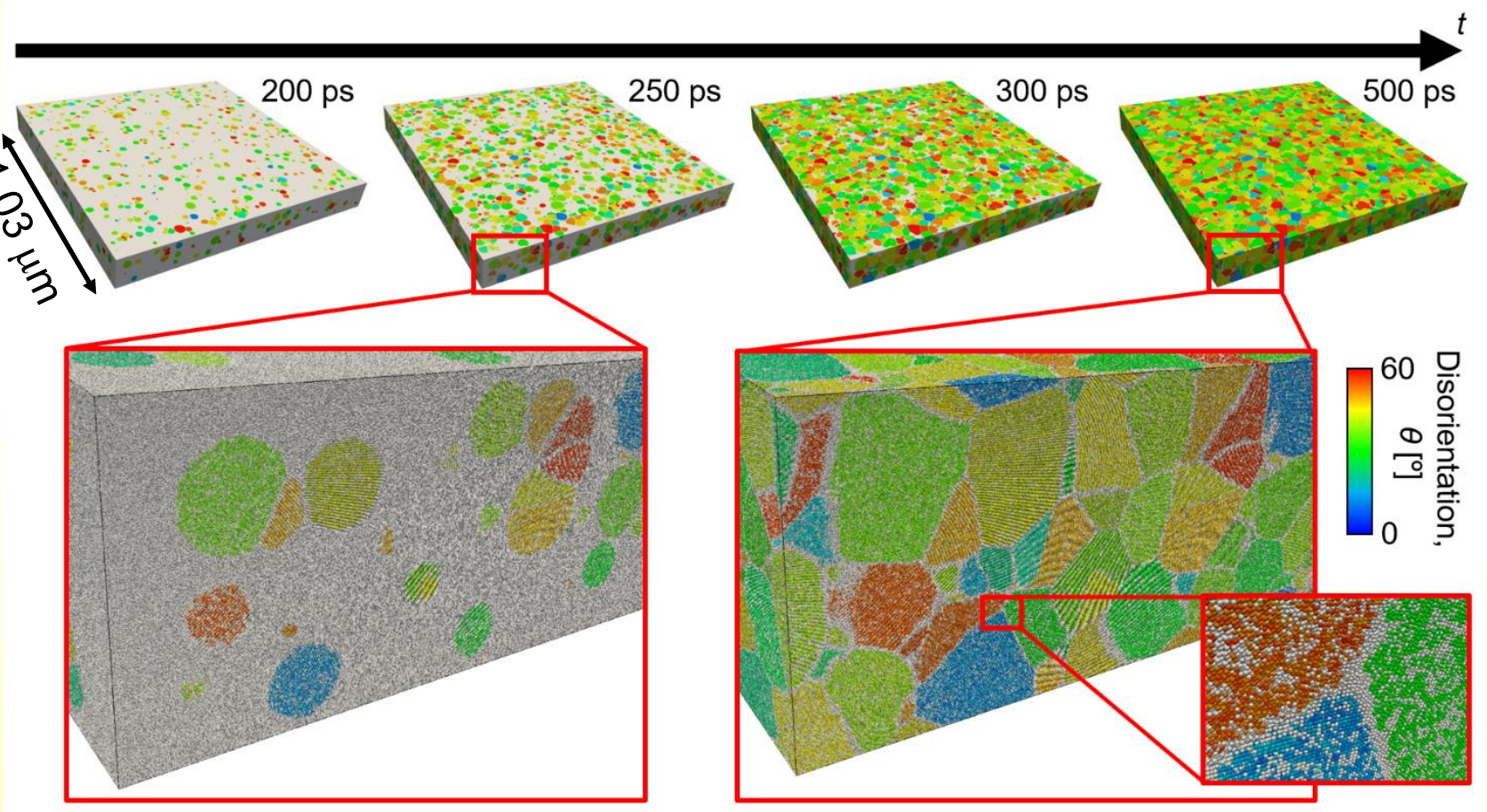
Au-Cu-Ag + 200ppm Ir

G. Kurtuldu, A. Sicco, M. Rappaz, Acta Mater 70 (2014) 240.

Micrometer-scale MD simulation of microstructure formation

Y. Shibuta, S. Sakane, E. Miyoshi T. Takaki, M. Ohno, Model. Simul. Mater. Sci. Eng., 27 (2019) 054002.

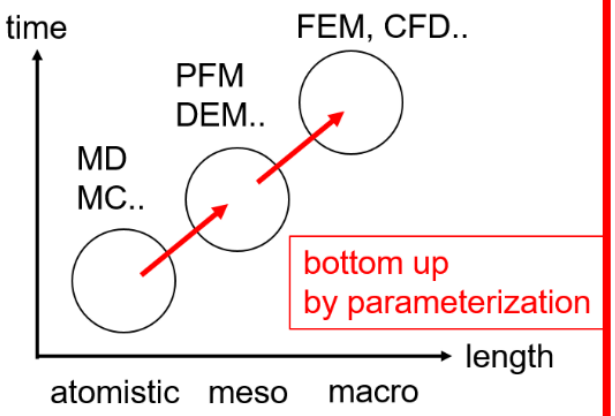
10,368,000,000 iron atoms in 1.03 x 1.03 x 0.11 μm^3
FS potential (pure iron)
78h/500ps using 256GPUs(P100 on TSUBAME3.0)



Evolution of multi-scale modeling

"Advent of cross-scale modeling: high-performance computing of solidification and grain growth"
Y. Shibuta, M. Ohno, T. Takaki, Advanced Theory and Simulations, 1 (2018) 201800065.

1. multi-scale modeling

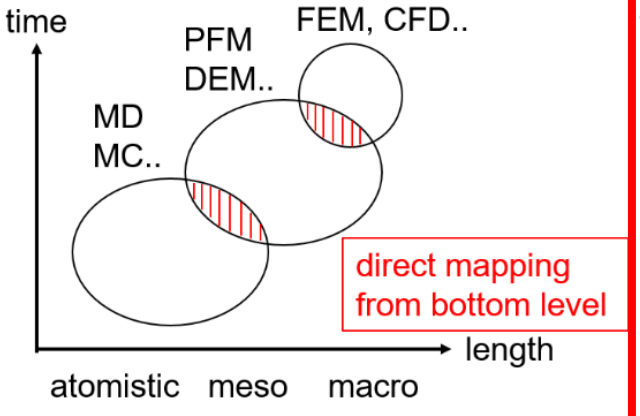


・Parameterization

Ab initio (Electronic)
↓
MD/MC (Atomistic)
↓
PFM (Continuum)

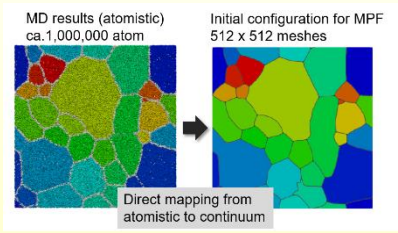
Averaged "static" information

2. Inter-scale modeling

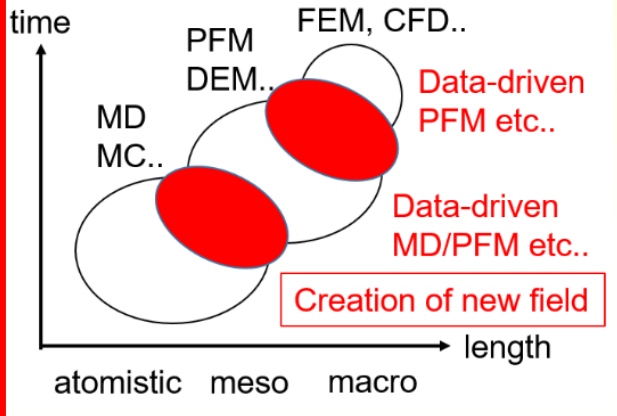


・share of information
・validation of models

Ex) direct comparison between MD and PFM

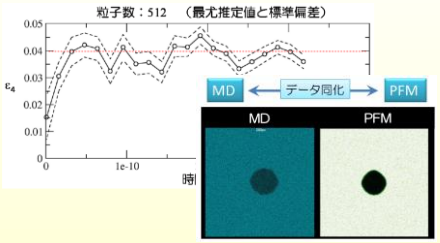


3. Cross-scale modeling



・utilization of shared information

Ex) Data-driven MD/PFM



"On-the-fly" use of information

ADVANCED THEORY AND SIMULATIONS

Outline

1. Brief introduction of molecular dynamics (MD) simulation

2. Large-scale MD simulation of microstructure formation
   - Remaining problems in PFM and the role of MD
   - Large-scale MD simulation of nucleation and solidification
   - Evolution of multi-scale modeling

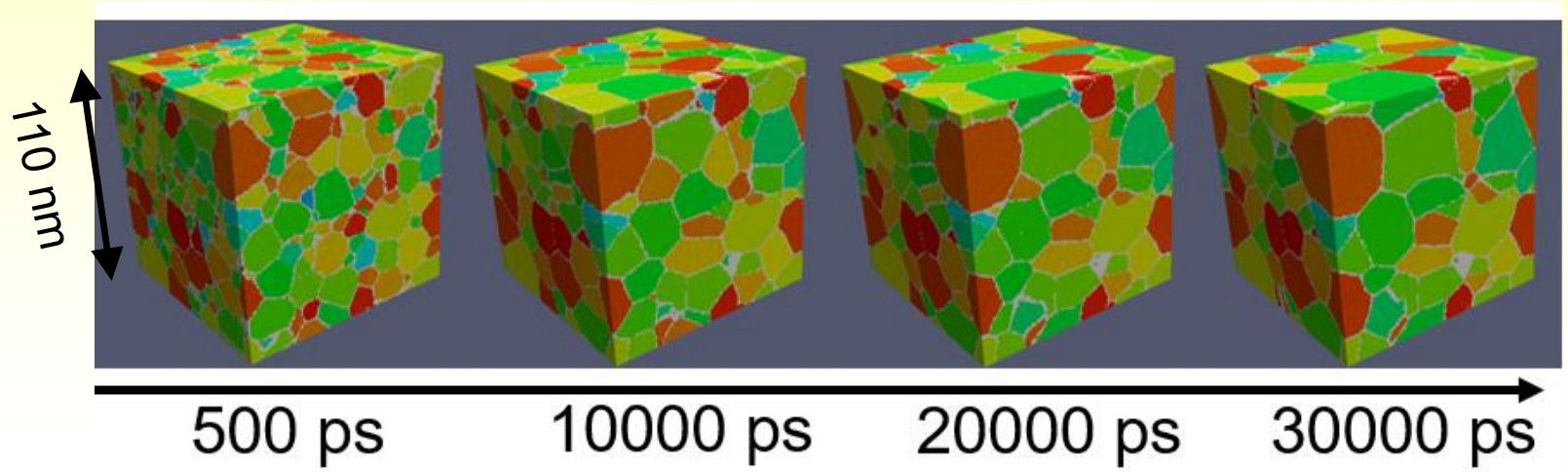
3. Inter-scale modeling: share of information
   - Conversion of atomistic configuration into phase-field profile
   - MPF simulation of grain growth starting from MD configuration

4. Cross-scale modeling: utilization of shared information
   - What is data-assimilation(DA)? - Bayes' theorem -
   - Concept of data assimilation between MD and PFM
   - On-the-fly estimation of solid-liquid interfacial properties by DA

5. Summary with some ongoing works

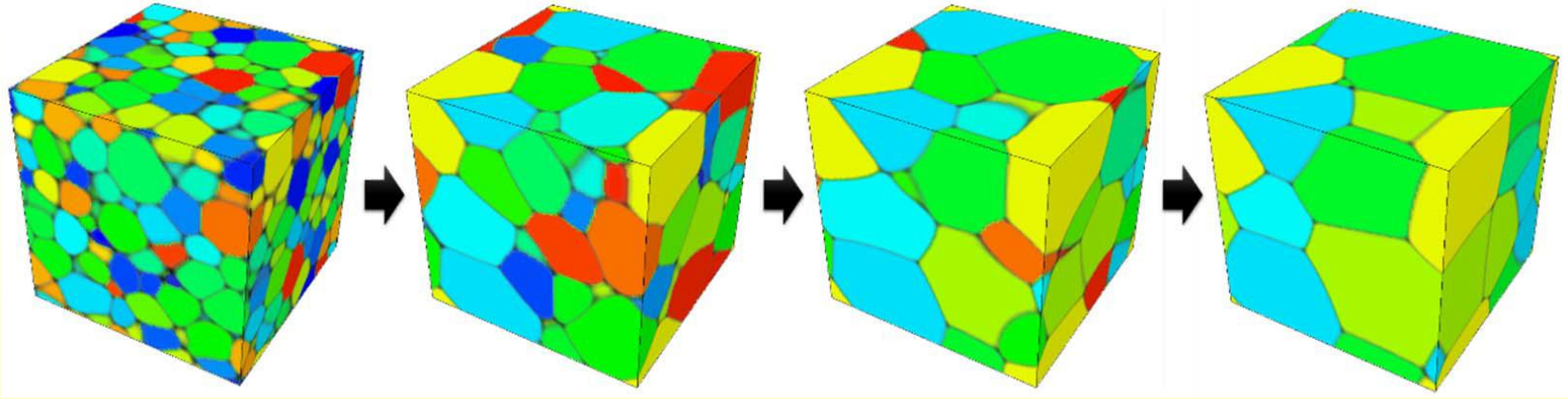
Connection between MD and PFM

Our large-scale MD (113,246,208 atoms)（50days by 128GPU）



S. Okita, E. Miyoshi, S. Sakane, T. Takaki, M. Ohno, Y. Shibuta, Acta Mater. 153 (2018) 108.

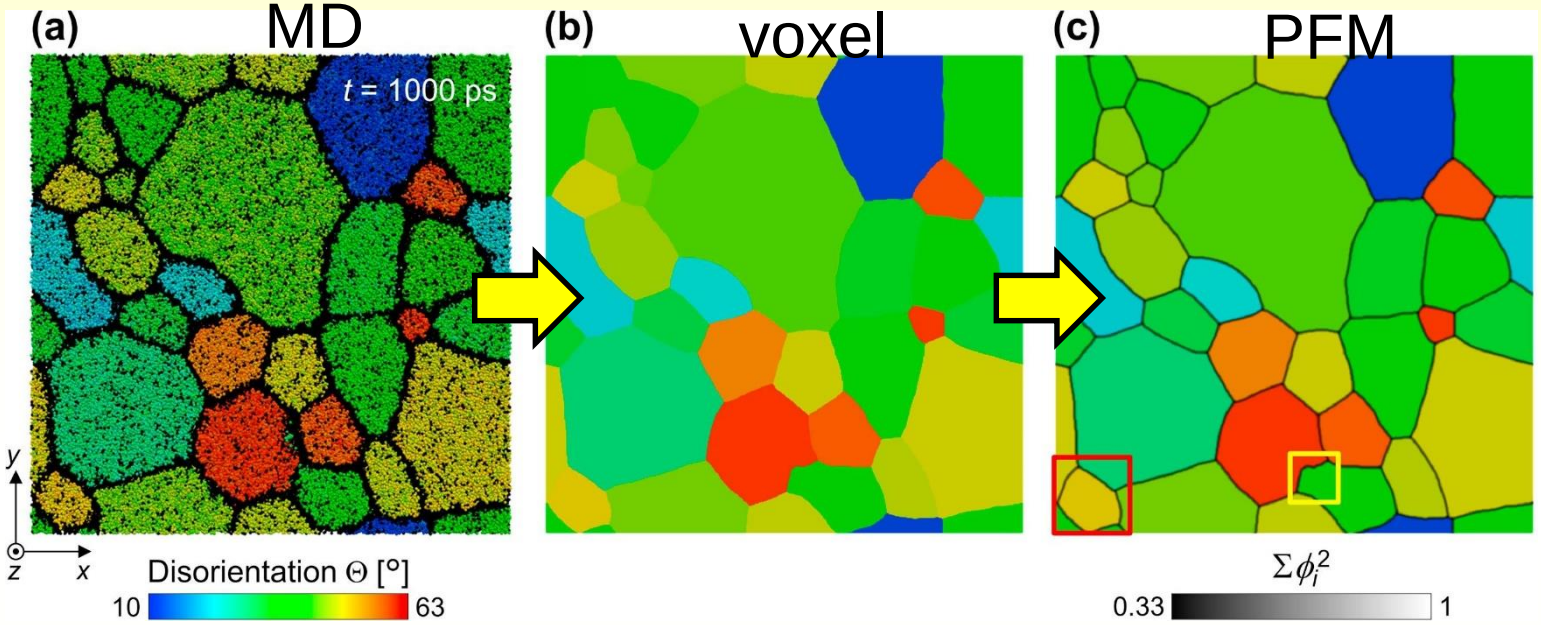
Multi-phase-field simulation（less than 1day by 1GPU）

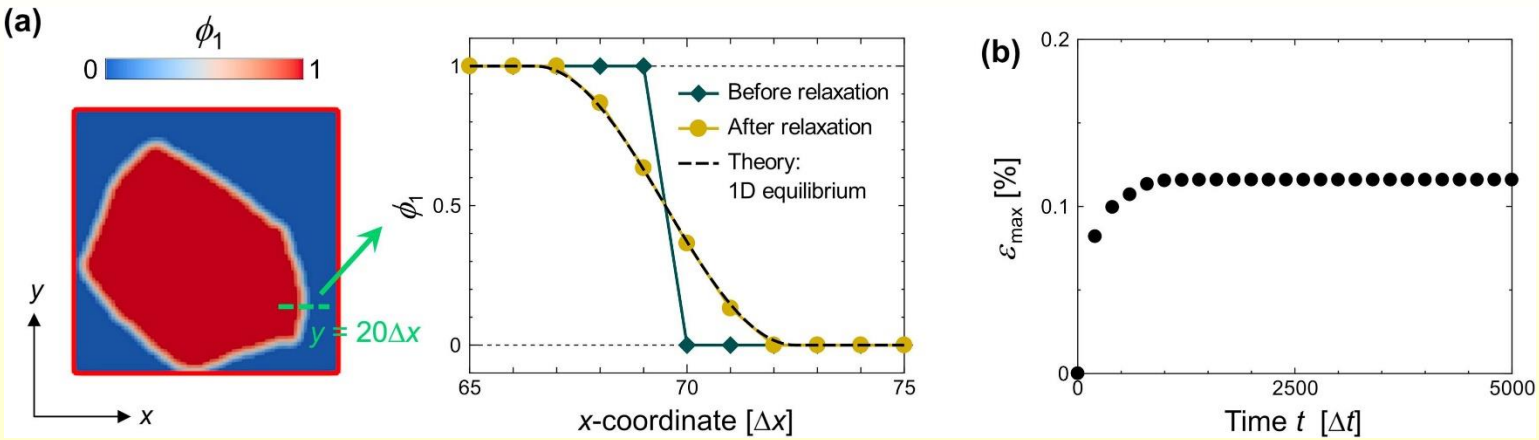


e.g. E. Miyoshi and T. Takaki: Computational Materials Science, 120 (2016) 77.
E. Miyoshi and T. Takaki: Computational Materials Science, 112 (2016) 44.

Bridging MD and PFM for grain growth prediction

E. Miyoshi, T. Takaki, Y. Shibuta, M. Ohno, Comp. Mater. Sci. 152 (2018) 118.





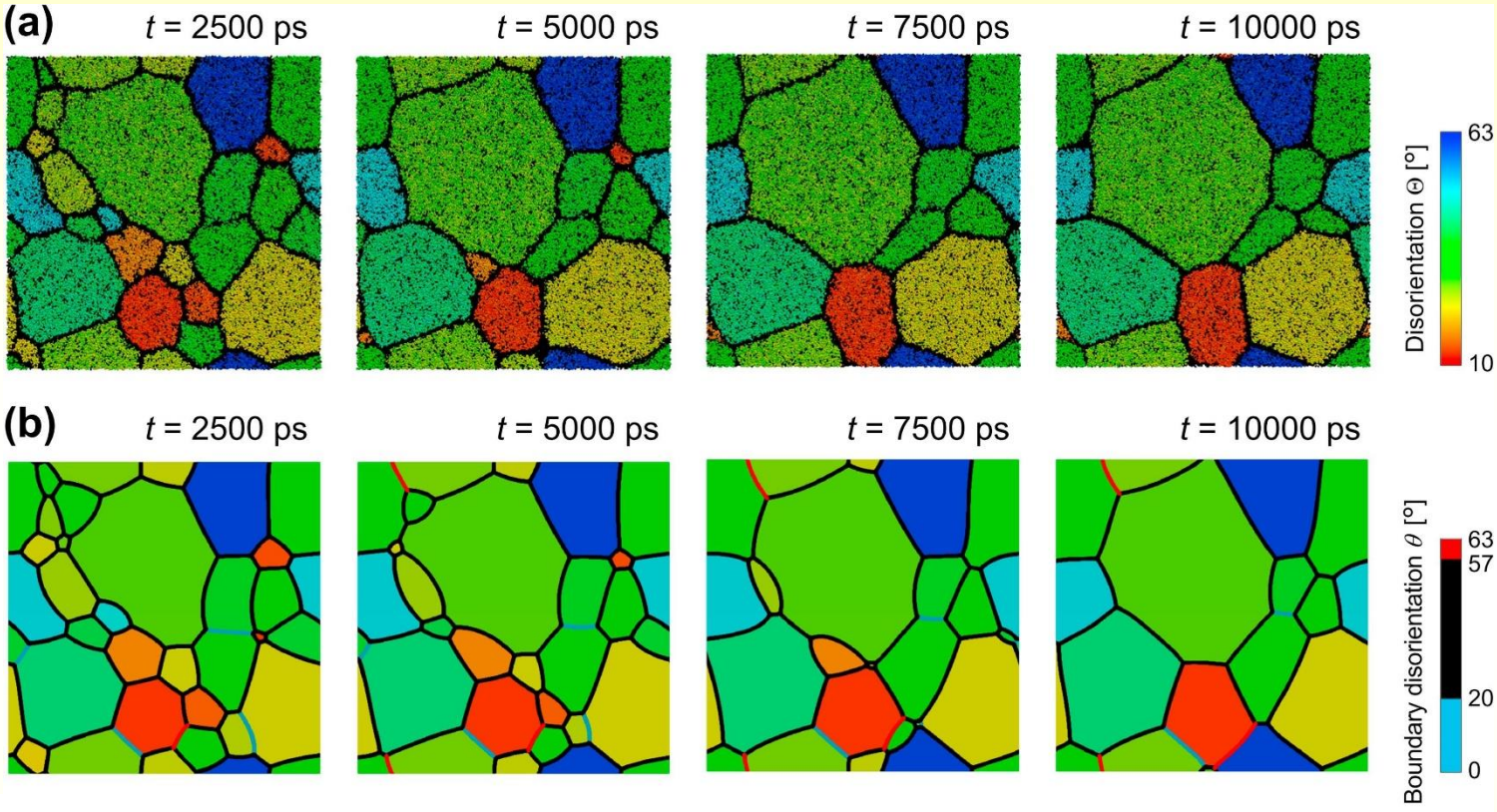
Atomistic configuration from MD is converted into phase-field profile.

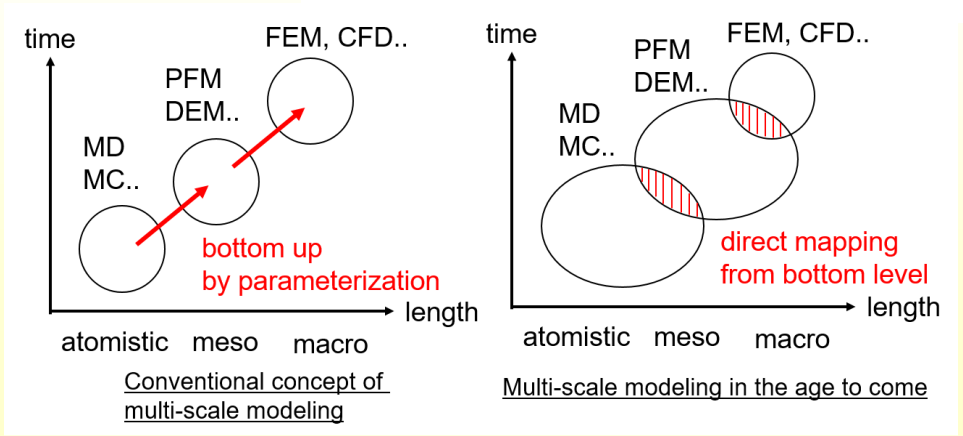
Bridging MD and PFM for grain growth prediction

E. Miyoshi, T. Takaki, Y. Shibuta, M. Ohno, Comp. Mater. Sci. 152 (2018) 118.

MD (atomistic)

MPF (continuum)





Conventional multiscale modeling:

Averaged values from smaller system are extracted as parameters and transfer to larger system.

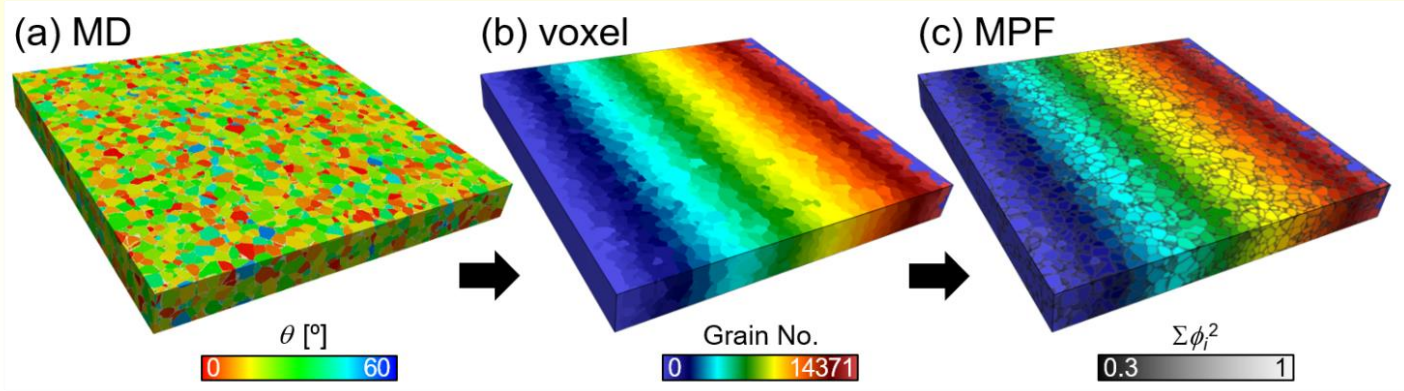
New concept of multiscale modeling:

Direct mapping from bottom level

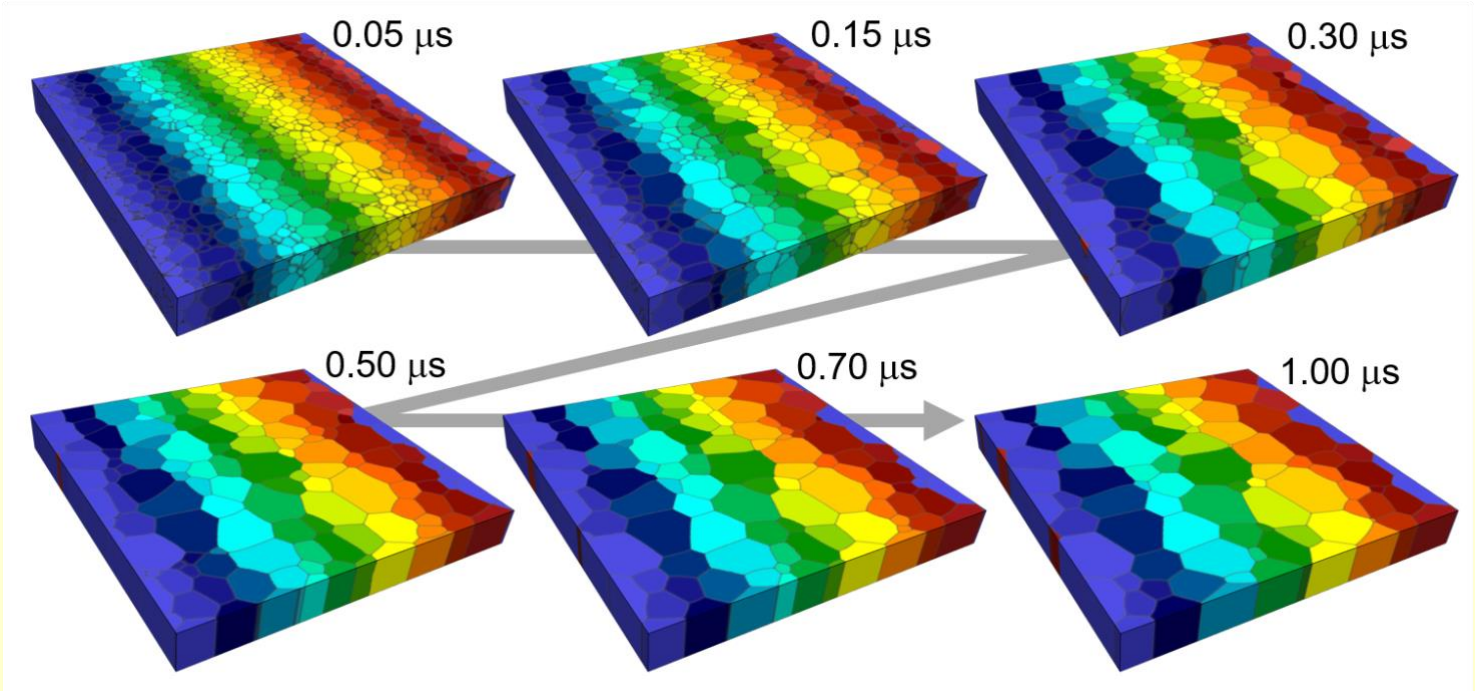
MPF simulation of grain growth starting from MD configuration

Y. Shibuta, S. Sakane, E. Miyoshi T. Takaki, M. Ohno, Model. Simul. Mater. Sci. Eng. 27 (2019) 054002.

Conversion of atomistic configuration into phase-field profile



Subsequent grain growth by MPF



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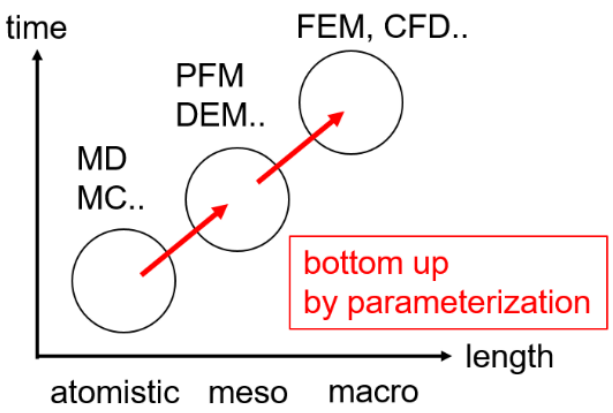
5. Summary with some ongoing works

Evolution of multi-scale modeling

"Advent of cross-scale modeling: high-performance computing of solidification and grain growth"
Y. Shibuta, M. Ohno, T. Takaki, Advanced Theory and Simulations, 1 (2018) 201800065.

1. multi-scale modeling

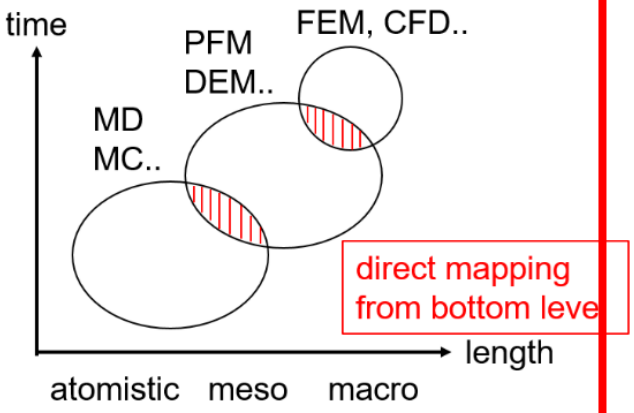


・Parameterization

Ab initio (Electronic)
↓
MD/MC (Atomistic)
↓
PFM (Continuum)

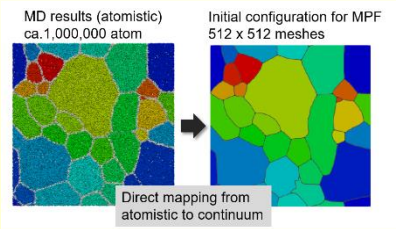
Averaged "static" information

2. Inter-scale modeling

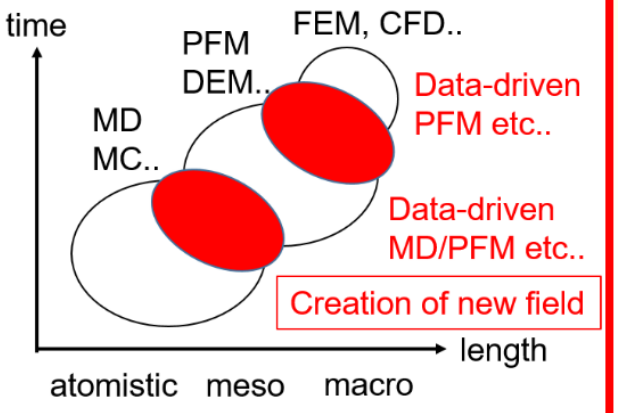


・share of information
・validation of models

Ex) direct comparison between MD and PFM

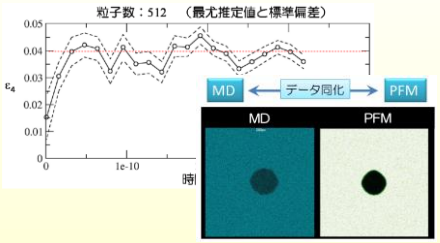


3. Cross-scale modeling



・utilization of shared information

Ex) Data-driven MD/PFM



"On-the-fly" use of information

ADVANCED THEORY AND SIMULATIONS

What is data-assimilation?

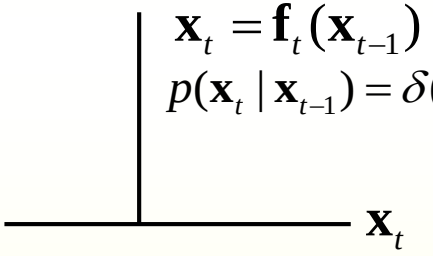
If the simulation model covers all observed phenomena completely,
the simulation can reproduce the observation exactly. However, it is impossible..

Therefore, the system noise is added to have a range in the answer
in order to compensate the incompleteness in the simulation model
or the numerical error due to the discretization of time differential.

→ called a system model

Simulation model

$$\mathbf{x}_t = \mathbf{f}_t(\mathbf{x}_{t-1})$$
$$p(\mathbf{x}_t \mid \mathbf{x}_{t-1}) = \delta(\mathbf{x}_t - \mathbf{f}_t(\mathbf{x}_{t-1}))$$

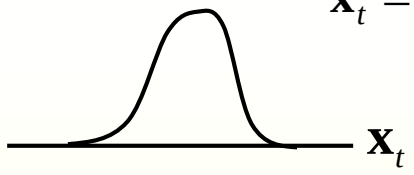


- Deterministic
- Delta function
  as probability distribution

System model

$$p(\mathbf{x}_t \mid \mathbf{x}_{t-1})$$
$$\mathbf{x}_t = \mathbf{f}_t(\mathbf{x}_{t-1}) + \mathbf{v}_t$$

$\mathbf{v}_t$: system noise



- probabilistic
- having a range
  as probability distribution

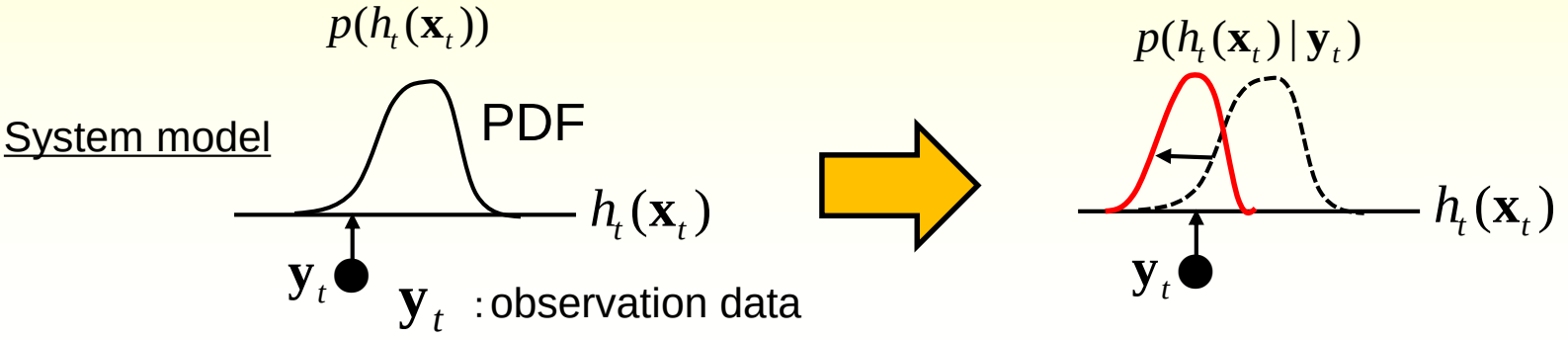
$p(A \mid B)$ is the conditional probability: probability of A given B.

Here, $p(A,B) = p(A \mid B)\,p(B)$

↑ joint probability for A and B

What is data-assimilation?

Moreover, we want to increase the accuracy of simulation results by importing observation data (i.e., data assimilation).



Comparison with observation data

Assimilation into observation data

In the system model, there is a probability function distribution (PDF) for the answer.
It is possible to increase the accuracy by revising the PDF.

This is basic concept of data assimilation. But how to assimilate?

Bayesian inference!

Practically, several filtering techniques are proposed:
Particle filter, Kalman filter, Ensemble Kalman filter, etc.

Bayes' theorem

$p(A,B) = p(A \mid B)\,p(B) = p(B \mid A)\,p(A)$ derives the following relation.

Thomas Bayes
(1702-1761)

Bayes' theorem

likelihood

prior probability
Probability of A

$$p(A \mid B) = \frac{p(B \mid A)\,p(A)}{p(B)}$$

posterior probability
Probability of A given B

Very simple but very important theorem
→implying the derivation of cause (distribution) from the effect (observation)

For example, assuming A as cause and B as effect,

$$p(cause \mid effect) = \frac{p(effect \mid cause)\,p(cause)}{p(effect)}$$

"From an effect obtained from the observation,
we can know the probability of the cause."

Bayes' theorem: example

From 意味が分かるベイズ統計学: 一石賢, ベレ出版, 2016

Let us consider an airplane accident assuming following three reasons.

	Event probability	Probability to cause accident
Human error	0.6	0.02
Maintenance error	0.3	0.03
Error in control tower	0.1	0.01

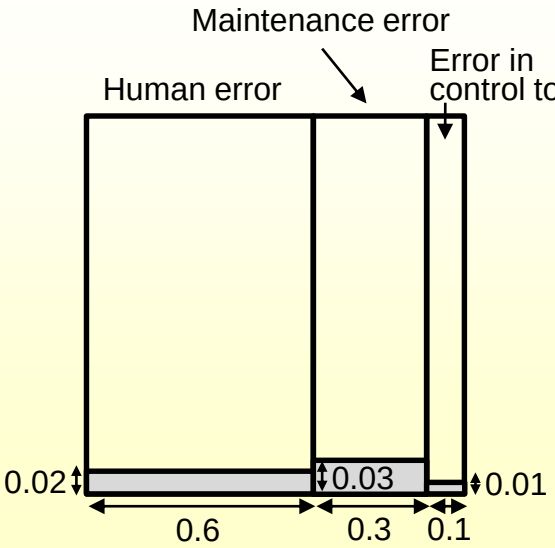
When one accident happens, what probability is it for the cause as “Error in control tower”?

From Bayes' theorem

$$p(ect \mid acc.) = \frac{p(acc. \mid ect)\,p(ect)}{p(acc.)}$$

ect: error in control tower
Acc.: accident

$$= \frac{0.01 \times 0.1}{0.02 \times 0.6 + 0.03 \times 0.3 + 0.01 \times 0.1} \approx 0.045$$



Now

$$p(acc.) = p(acc. \mid hue)\,p(hue) + p(acc. \mid mae)\,p(mae) + p(acc. \mid ect)\,p(ect)$$

hue: human error
mae: maintenance error

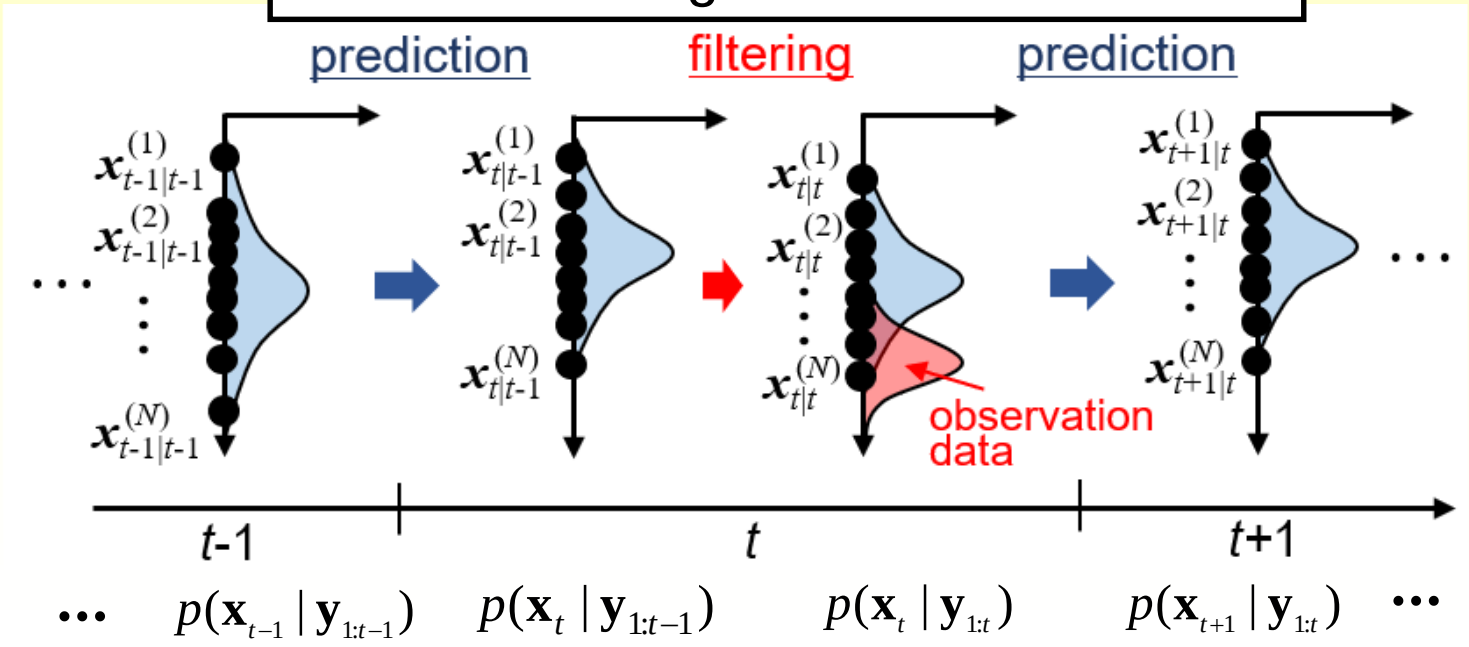
Here,

$$p(effect) = \sum_{cause} p(effect \mid cause)\,p(cause)$$

$$p(C_k \mid E) = \frac{p(E \mid C_k)\,p(C_k)}{p(E)} = \frac{p(E \mid C_k)\,p(C_k)}{\sum_{i=1}^{n} p(E \mid C_i)\,p(C_i)}$$

Bayes’ expansion formula

Schematic image of data assimilation



Predicted distribution: prediction of current state from observation data until t-1

$$p(\mathbf{x}_t \mid \mathbf{y}_{1:t-1}) = \int p(\mathbf{x}_t \mid \mathbf{x}_{t-1}) p(\mathbf{x}_{t-1} \mid \mathbf{y}_{1:t-1}) d\mathbf{x}_{t-1}$$

obtained by system model

$\mathbf{x}_t = \mathbf{f}_t(\mathbf{x}_{t-1}) + \mathbf{v}_t$ $\mathbf{v}_t$: system noise

Filtered distribution: prediction of current state from observation data until now (t)

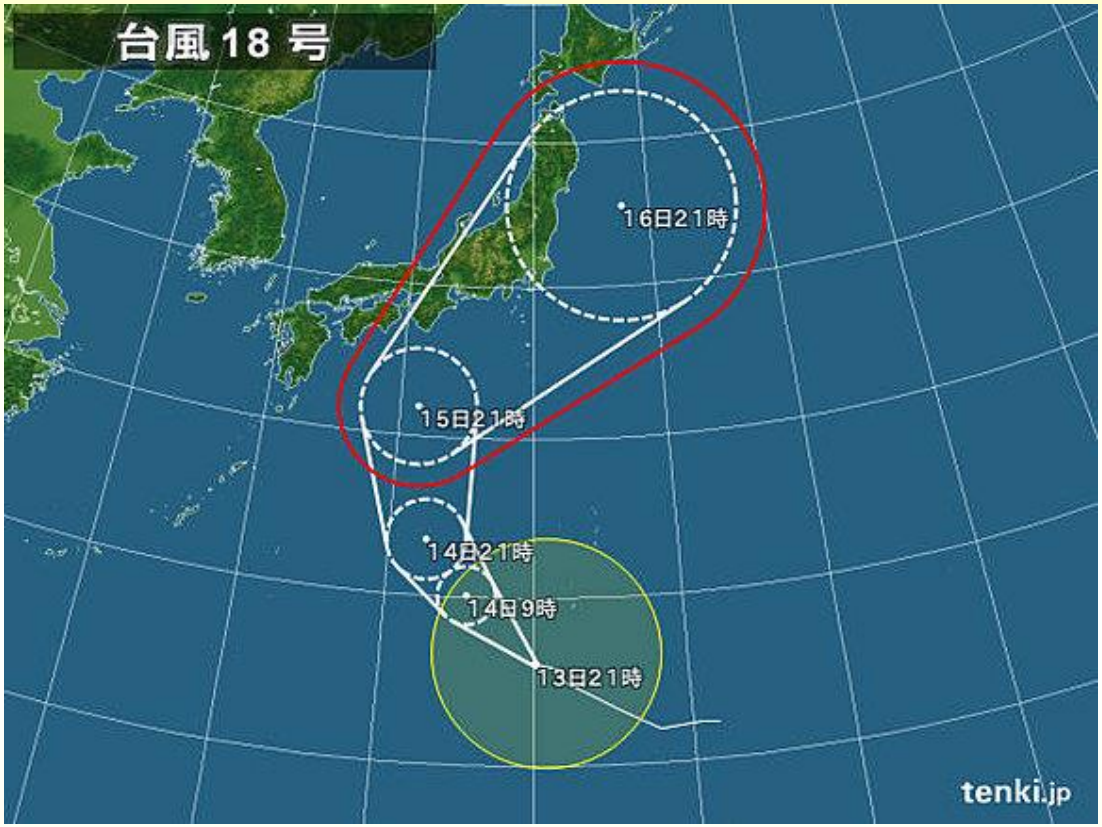
Likelihood

$$p(\mathbf{x}_t \mid \mathbf{y}_{1:t}) = \frac{p(\mathbf{y}_t \mid \mathbf{x}_t) p(\mathbf{x}_t \mid \mathbf{y}_{1:t-1})}{\int p(\mathbf{y}_t \mid \mathbf{x}_t) p(\mathbf{x}_t \mid \mathbf{y}_{1:t-1}) d\mathbf{x}_t}$$

Bayesian inference

Practically, several filtering techniques to define likelihood are proposed:
Particle filter, Kalman filter, Ensemble Kalman filter, etc.

Application example of data assimilation: weather forecast



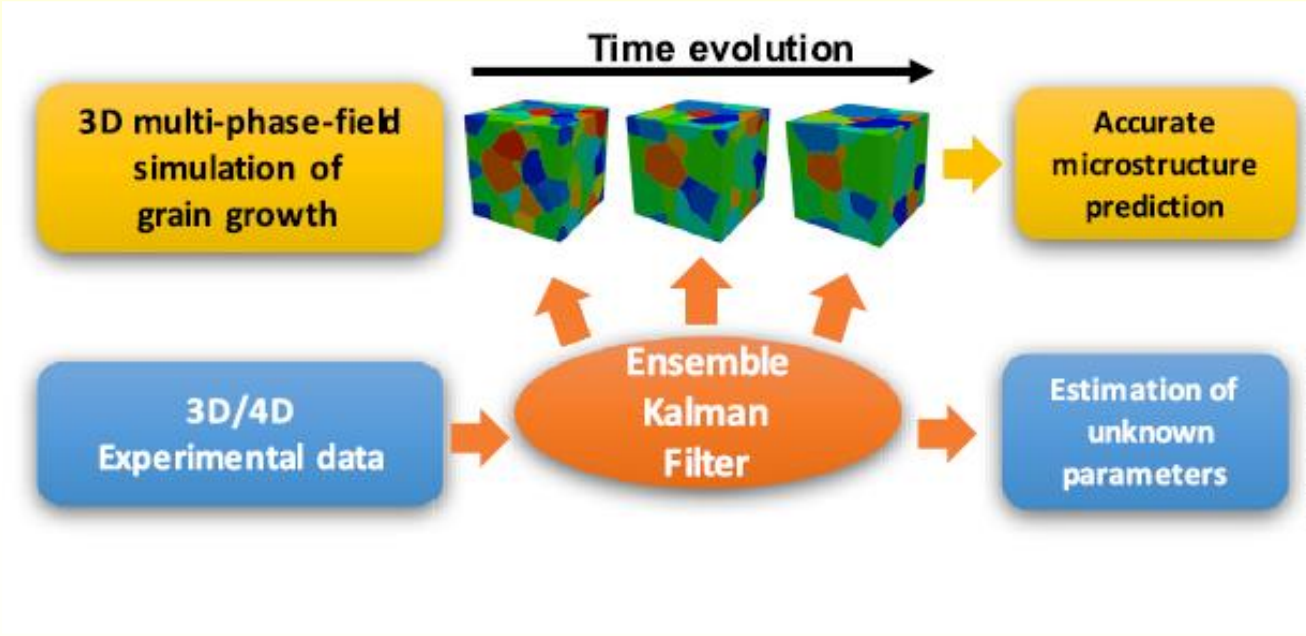
How is the weather forecasted?

Referred from tenki.jp web
(For Typhoon No. 18 at Sep, 2013.)

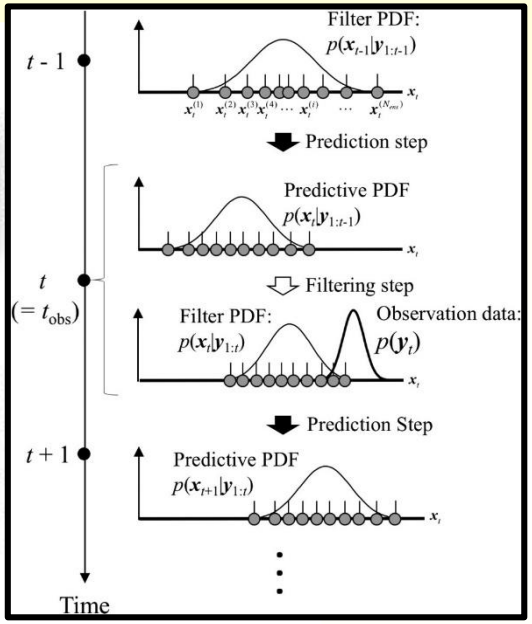
Forecast circle changes as the time goes.
→observation data is used for assimilation.

Interesting points
・Where the typhoon comes from now?
・Size of typhoon
Not so interesting (for most of people)
・Where and when the typhoon starts?
（i.e. the initial condition）
・model of forecast
（NS eq.? What difference scheme？）

Data assimilation for estimation of grain boundary properties



Schematic image of EnKF

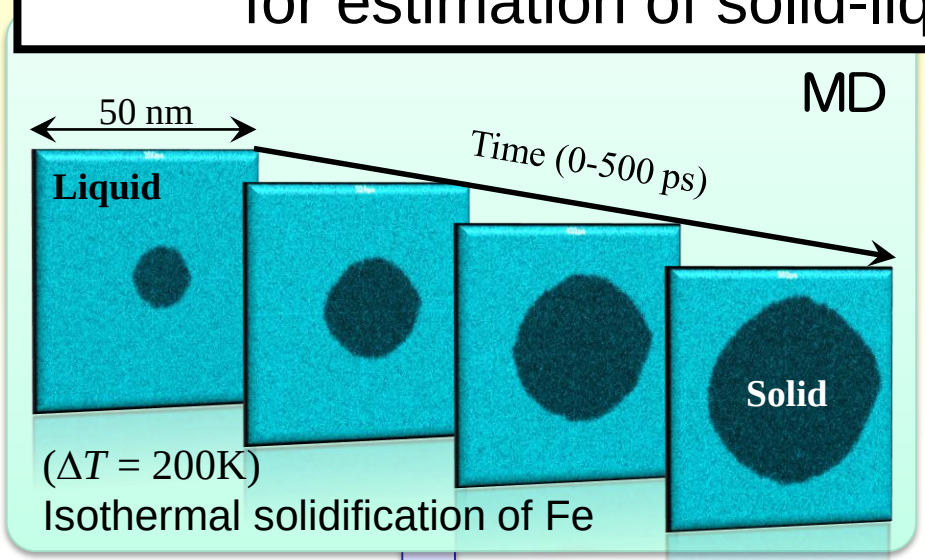


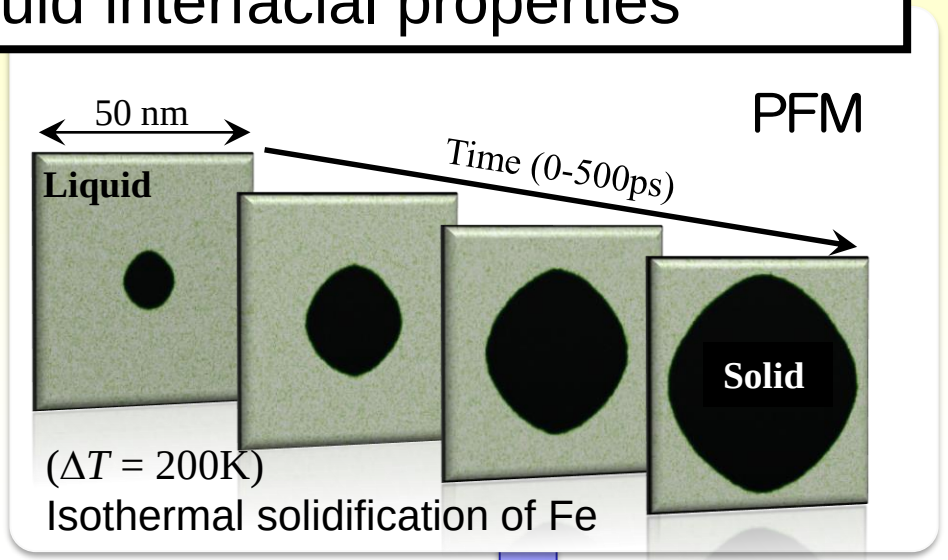
Parameter estimation for MPF simulation from 3D/4D experimental data.

Ensemble Kalman filter-based data assimilation for three-dimensional multi-phase-field model: Estimation of anisotropic grain boundary properties
A. Yamanaka, Y. Maeda, K. Sasaki, Mater. Des. 165 (2019) 107577

Can we estimate interfacial parameters PFM dynamically from MD data?

Concept of data assimilation between MD and PFM for estimation of solid-liquid interfacial properties

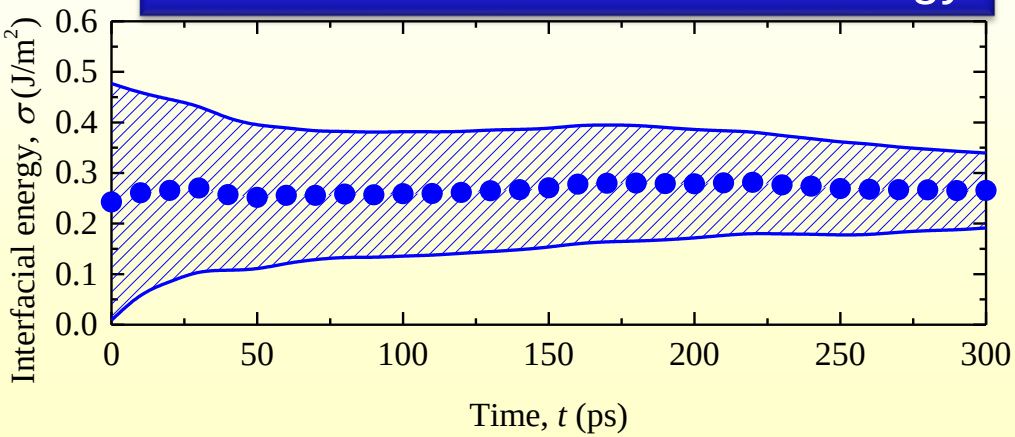




Data assimilation (EnKF)

M. Ohno et al.
Phys. Rev. E 101
(2020) 052121.

Estimation of SL interfacial energy

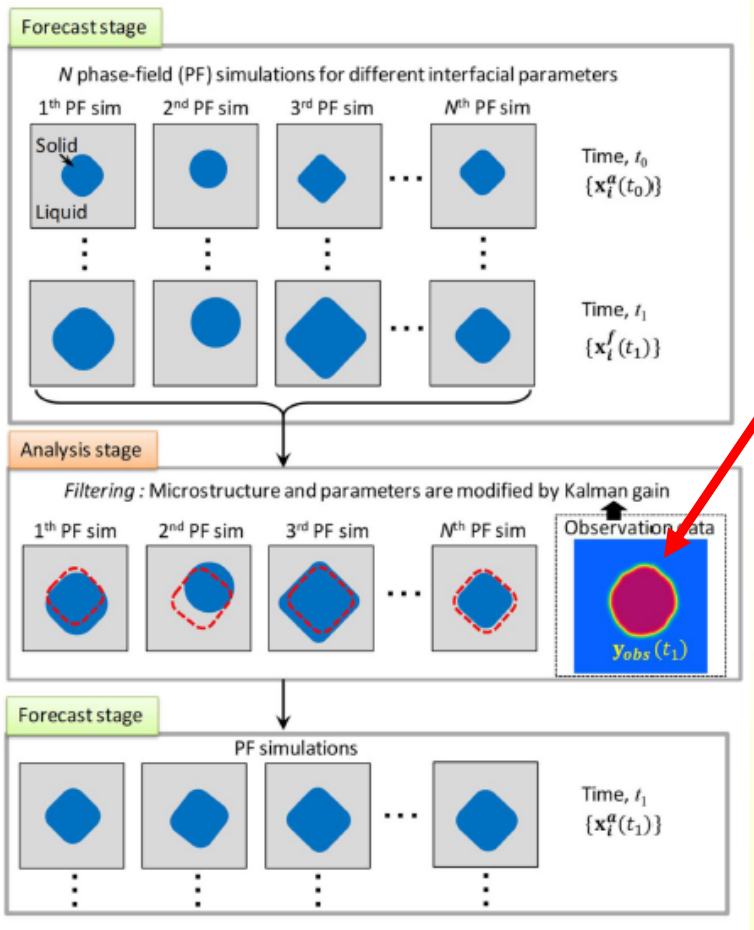


* Time-variable properties during microstructure formation can be estimated from MD profile.
* Prior knowledge is not required for estimation of time-variable properties

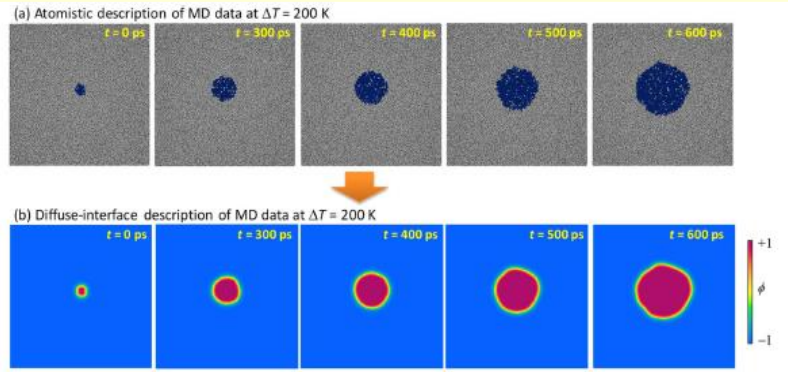
New concept of collaboration between MD and PFM
~ cross-scale modeling

Bayesian inference of interfacial properties out of equilibrium

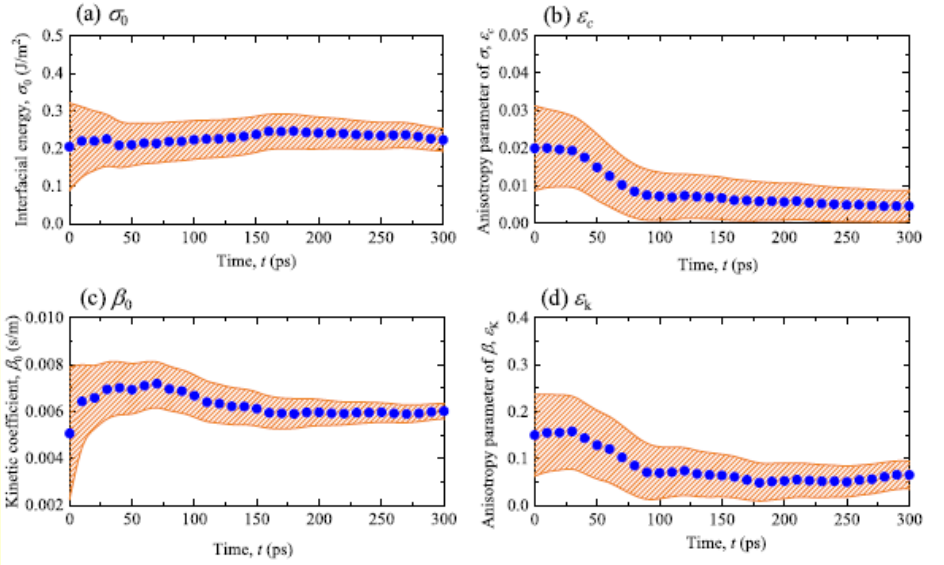
Data assimilation based on Ensemble Kalman filter (EnKF)



MD results employed as observation data



Simultaneous estimation of solid-liquid interfacial energy, interfacial mobility and their anisotropy



M. Ohno, Y. Oka, S. Sakane, Y. Shibuta, T. Takaki, Phys. Rev. E 101 (2020) 052121.

Procedure of on-the-fly parameter estimation

Y, Nagatsuma, in graduation thesis, The University of Tokyo, 2020 (unpublished)

A simple phase-field model (PFM)

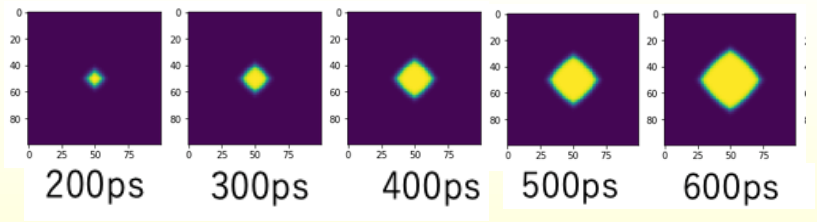
$$\frac{\partial \boldsymbol{\phi}}{\partial \boldsymbol{t}} = \boldsymbol{M_\phi}\left[\nabla(\boldsymbol{a}^2\nabla\boldsymbol{\phi}) - \frac{\partial}{\partial \boldsymbol{x}}\left(\boldsymbol{a}\frac{\partial \boldsymbol{a}}{\partial \boldsymbol{\theta}}\frac{\partial \boldsymbol{\phi}}{\partial \boldsymbol{y}}\right) + \frac{\partial}{\partial \boldsymbol{y}}\left(\boldsymbol{a}\frac{\partial \boldsymbol{a}}{\partial \boldsymbol{\theta}}\frac{\partial \boldsymbol{\phi}}{\partial \boldsymbol{x}}\right) + 4\boldsymbol{W}\boldsymbol{\phi}(1-\boldsymbol{\phi})(\boldsymbol{\phi} - 0.5 + \boldsymbol{\beta})\right]$$

$$a(\theta) = \bar{a}[1 + \zeta cos\{k(\theta - \theta_0)\}]$$

Data assimilation based on Ensemble Kalman filter (EnKF)

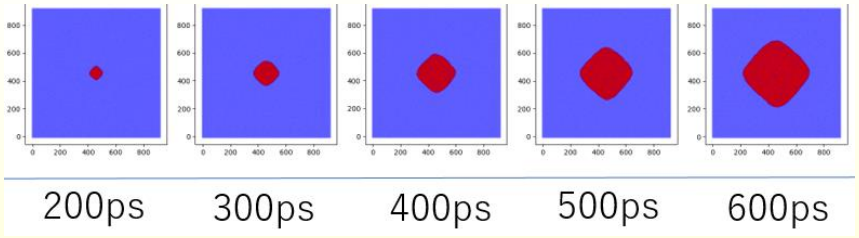
Anisotropy parameter ζ, inclination of solid crystal θ_0, change in the driving force, β are simultaneously estimated.

1. Parameter estimation using synthetic observation data (Twin experiment)



Observation data prepared by PFM simulation with known parameters with some random noises
- true value of parameter known in advance

2. Parameter estimation using MD data as observation data



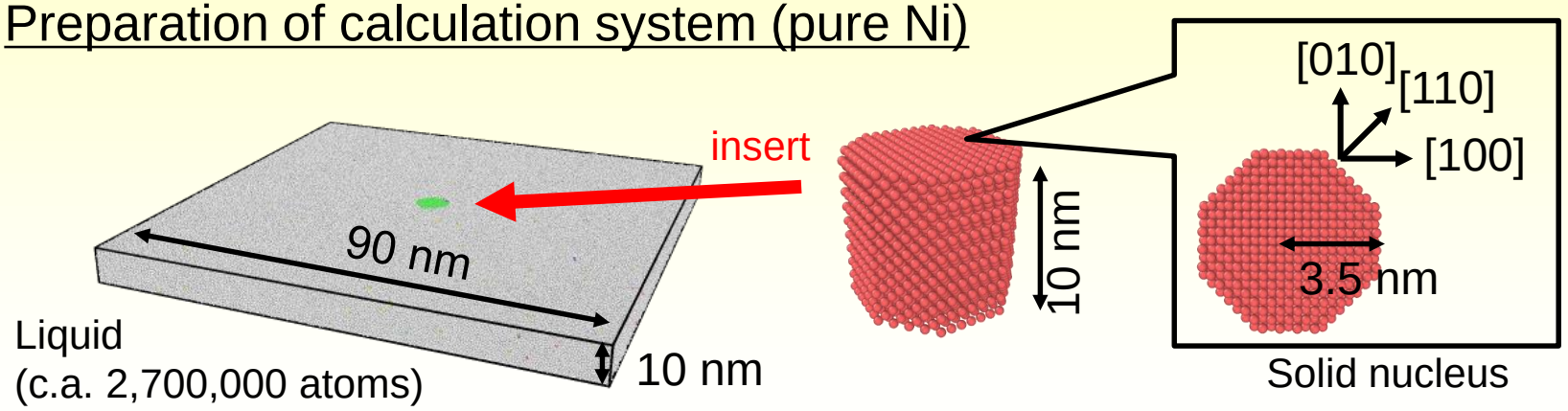
MD data used as the observation data
- true values of parameters unknown in advance

On-the-fly parameter estimation

Preparation of MD data for single Ni crystal growth

Y, Nagatsuma, in graduation thesis, The University of Tokyo, 2020 (unpublished)

Preparation of calculation system (pure Ni)

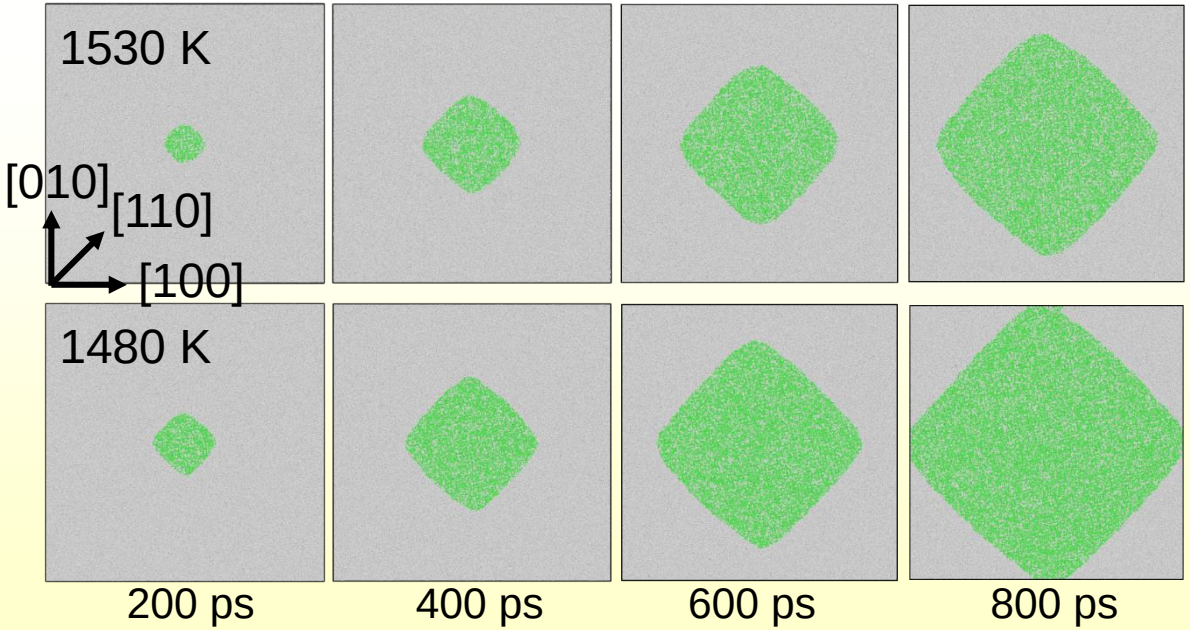


Calculation condition and snapshots of MD results

Interatomic potential:
EAM* by Zope & Mishin

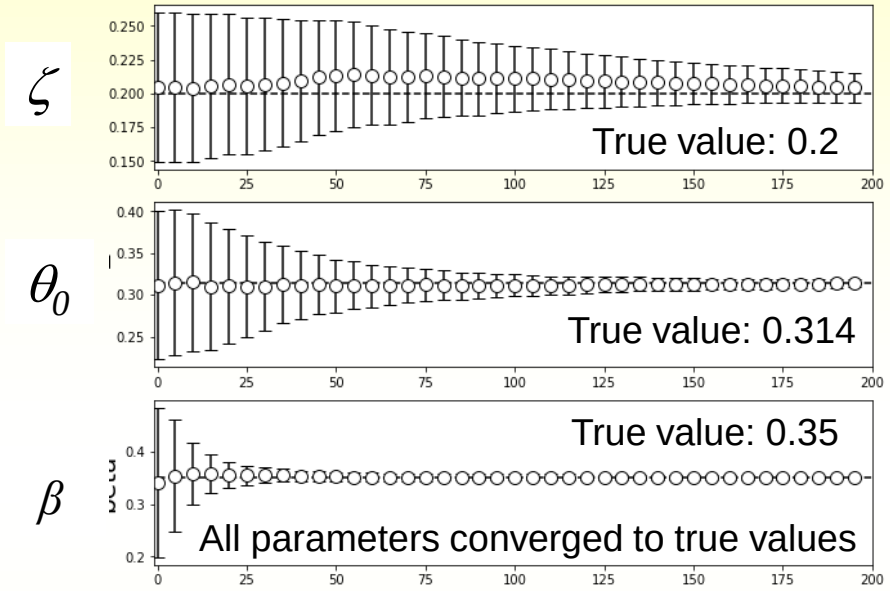
*R.R. Zope & Y. Mishin,
Phys. Rev. B 68, 024102 (2003).

Using LAMMPS
Visualization: OVITO
(using a-CNA)
T = 1530 and 1470 K

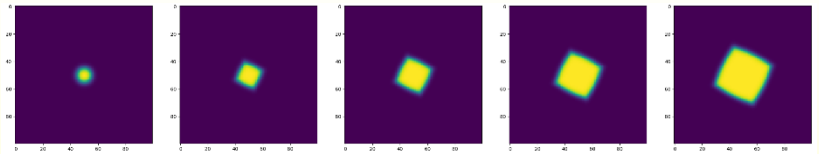


Simultaneous estimation of three parameters (ζ, θ_0, β)

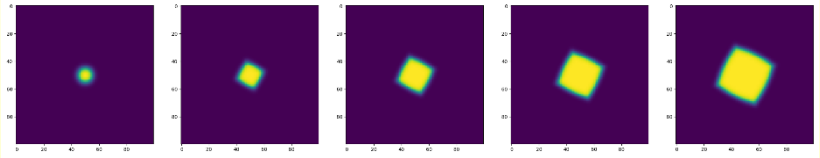
Synthetic observation data from PFM (twin experiment)



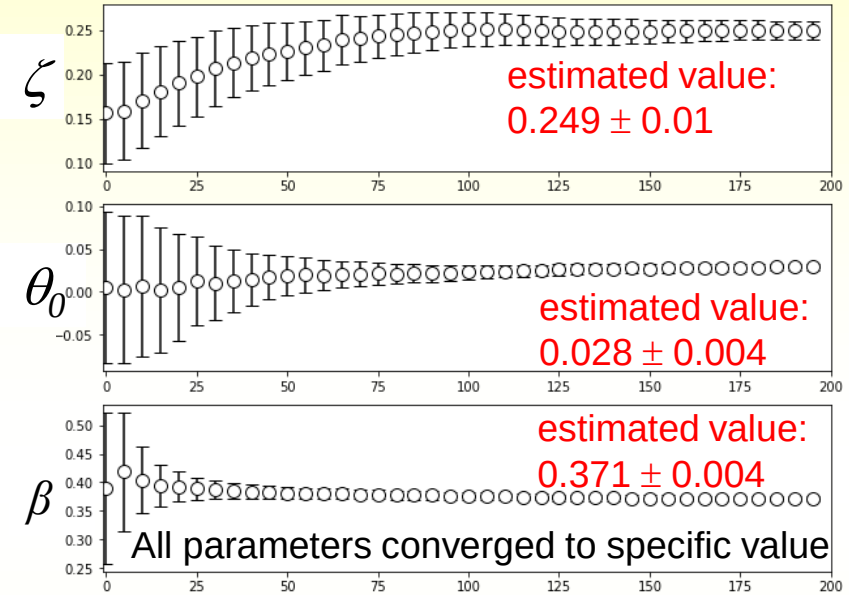
Observation data



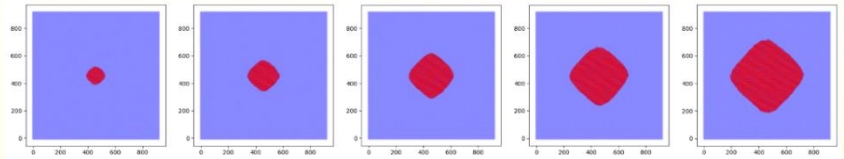
Estimated result



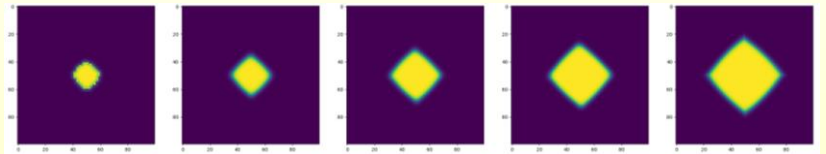
MD data as observation data



Observation data



Estimated result



Succeeded to estimate three parameters simultaneously.

Y, Nagatsuma, in graduation thesis, The University of Tokyo, 2020 (unpublished)

Outline

1. Brief introduction of molecular dynamics (MD) simulation

2. Large-scale MD simulation of microstructure formation
   - Remaining problems in PFM and the role of MD
   - Large-scale MD simulation of nucleation and solidification
   - Evolution of multi-scale modeling

3. Inter-scale modeling: share of information
   - Conversion of atomistic configuration into phase-field profile
   - MPF simulation of grain growth starting from MD configuration

4. Cross-scale modeling: utilization of shared information
   - What is data-assimilation(DA)? - Bayes' theorem -
   - Concept of data assimilation between MD and PFM
   - On-the-fly estimation of solid-liquid interfacial properties by DA

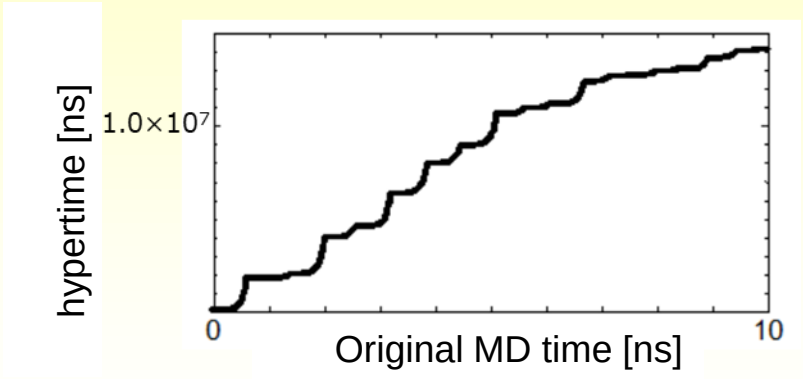
5. Summary with some ongoing works

Collective variable-driven hyper dynamics (CVHD) for acceleration of diffusion MD at room temperature

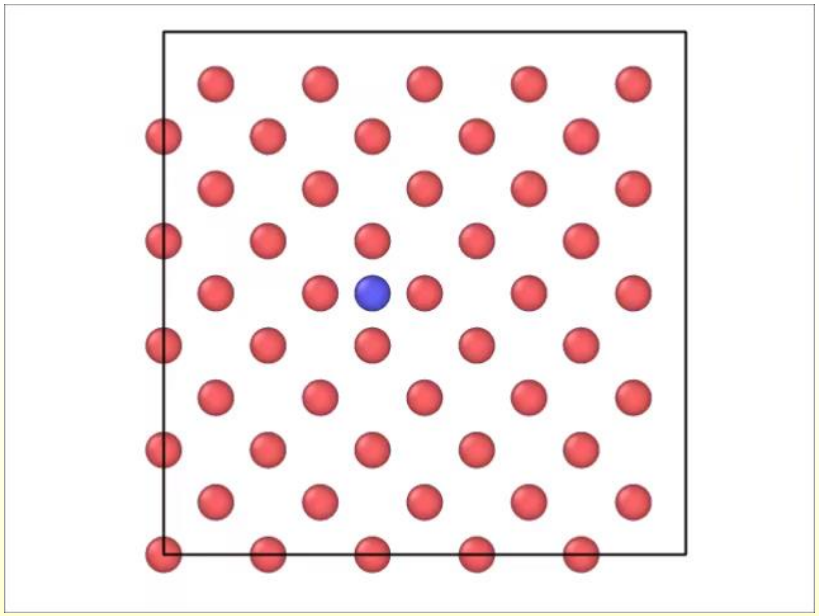
Calculation condition
Interatomic potential：EAM*

*T. T. Lau et al., PRL. 98 (2007) 215501

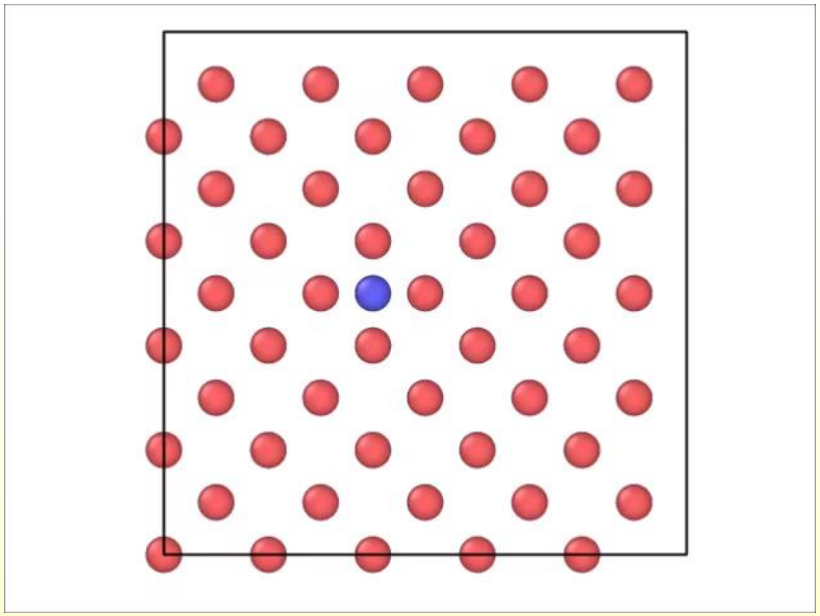
Fe：250 atoms　C：1 atoms
300 K, NVT const.
CV: bond length



MD(10ns)



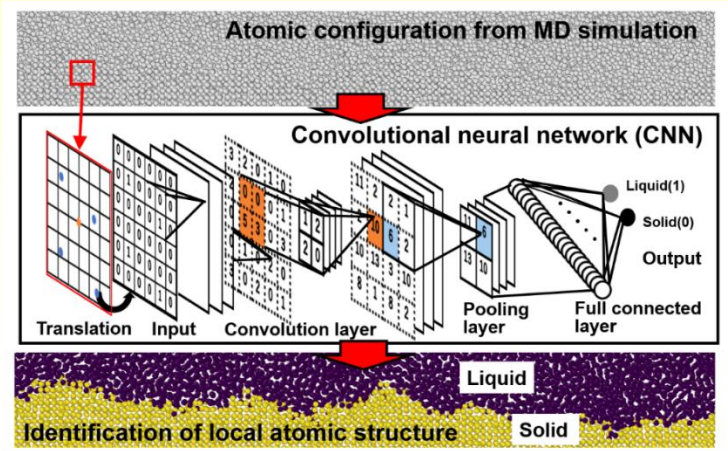
MD＋CVHD(1.4×10^{7}ns)



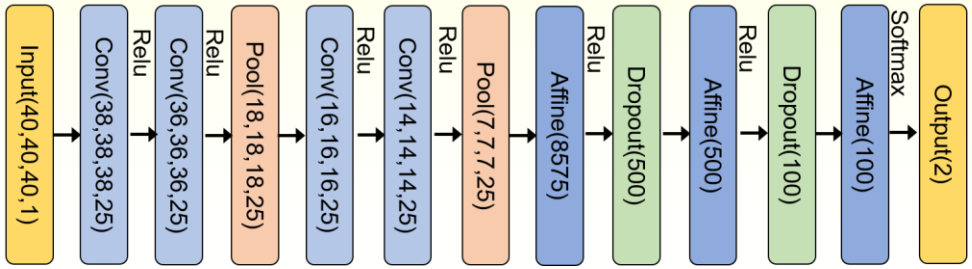
S. Fukuhara, K.M. Bal, E.C. Neyts, Y. Shibuta, Comp. Mater. Sci., 177 (2020) 109581.

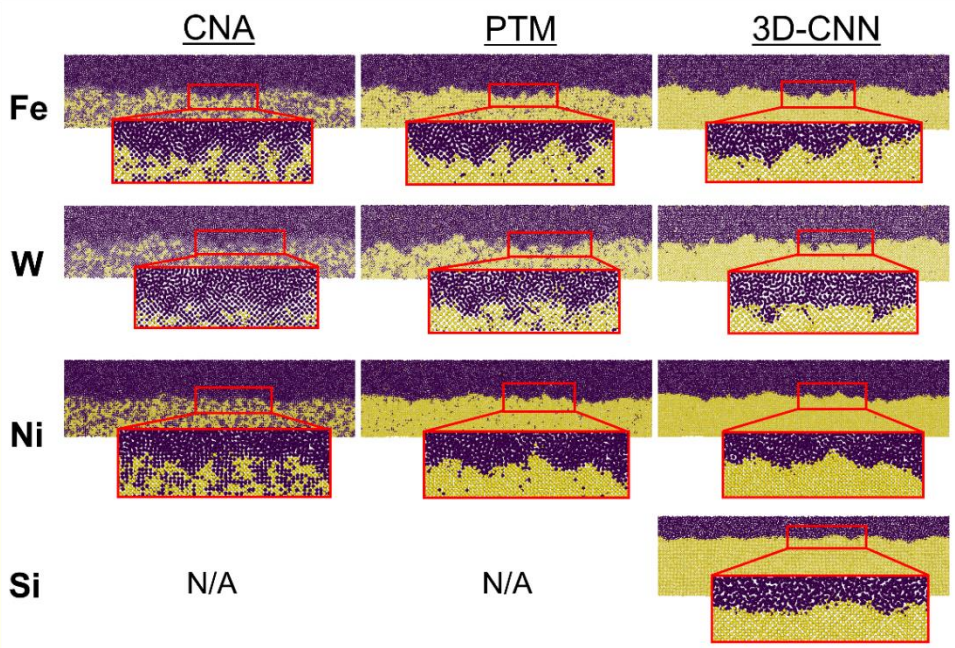
Keyword: metadynamics, hyperdynamics

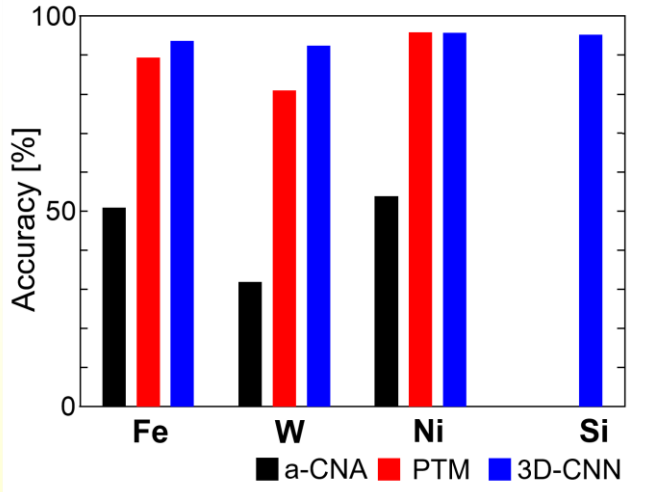
Machine learning approach to automated analysis of atomic configuration of MD simulation



Local atomic structures of solid-liquid biphasic system are identified by 3D convolutional neural network (CNN).







Accuracy of 3D-CNN is more than 90% for all structures.

T. Fukuya, Y. Shibuta, Comp. Mater. Sci., 184 (2020) 109880.

Summary

Based on large-scale MD simulations on microstructure formation,
Several new trials on multi-scale modeling are introduced.

Inter-scale modeling: share of information

- Direct mapping of atomistic configuration into phase-field profile
- PFM simulation staring from the microstructure by MD simulation

Cross-scale modeling: utilization of shared information

- On-the-fly estimation of SL interfacial properties based on data assimilation

Data-driven technique is opening new stage of multi-scale modeling

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