Dec. 23, 2015
工学と現代数学の接点を求めて(1)
@阪大基礎工

材料の強さと階層性

Shigenobu Ogata
(尾方成信)
Graduate School of Engineering Science, Osaka University
(大阪大学　基礎工学研究科)

Collaborators

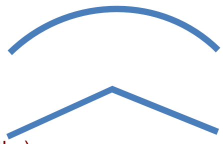
- Prof. Hajime Kimizuka (Osaka Univ., JAPAN)
- Prof. Ju Li (MIT, USA)
- Dr. Akio Ishii (Osaka Univ., JAPAN)
- Prof. Yunjiang Wang (Inst. Mech., CHINA)
- Prof. Masato Wakeda (Osaka Univ., JAPAN)
- Dr. Hideki Mori (Col. of Ind. Tech., JAPAN)
- Prof. Nobuhiro Tsuji (Kyoto Univ., JAPAN)
- Dr. Junping Du (Osaka Univ., JAPAN)
- Prof. Ting Zhu (Georgia tech., USA)
- Prof. Sidney Yip (MIT, USA)
- Prof. Dongsheng Xu (IMR, CHINA)

Outline

- はじめに（強さ？）
- 空間階層性への挑戦
- 時間階層性への挑戦
- まとめ

弾性変形と塑性変形の特徴

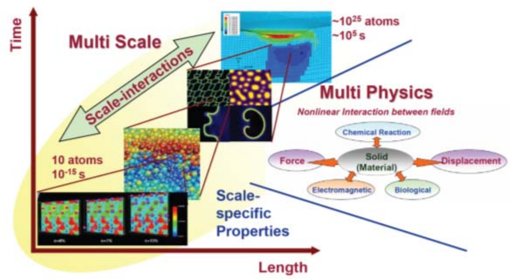
- **Elastic Deformation**
  - The most delocalized
- **Plastic Deformation**
  - Localized (characteristic lengths)



- **塑性変形の特徴は特徴サイズ（スケール）があること！**

塑性変形　（加工）

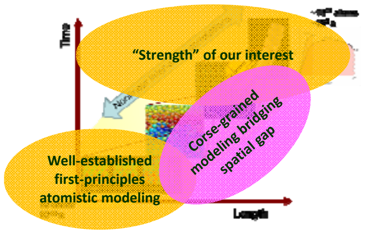
固体材料の時空間階層性



空間にして10^{10}、時間にして10^{20}程度のスケール幅がある

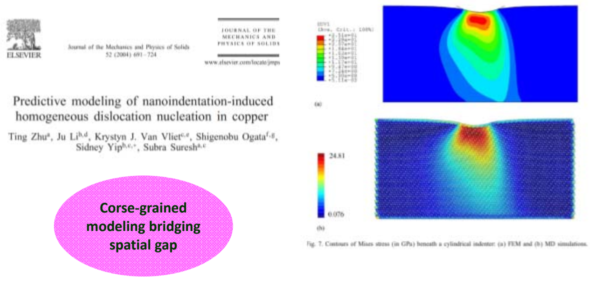
“強さ”が原理原則から予測できるか？

- Theoretical prediction of “strength” of structural materials is still big challenge



- Spatial and temporal multi-scale feature in structural materials
- Big scale gap between the first-principles scale and target scale of mechanical properties
- We need to establish smart models and/or modeling methods to bridge the gap

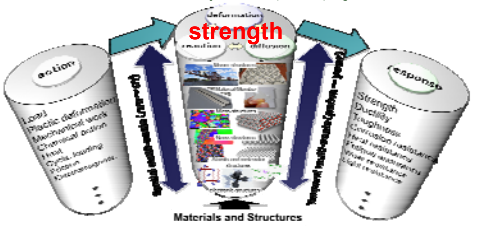
Nano-indentation (IPFEM)



原子・電子論からみた”強さ”とは

- 材料の力学的安定性 -

How much mechanically robust (stable) against various actions=“strength”



“strength” is relation btw action and response

“strength” should be dominated by

1) Deformation (dislocation, twin,..),
2) Diffusion (creep,...)
3) Reaction (aging, corrosion, ...)

in the multi-scale feature of materials and structures.

Linking “materials science” and “mechanics” (links btw different scales and fields) is necessary for understanding and engineering the “strength”

Outline

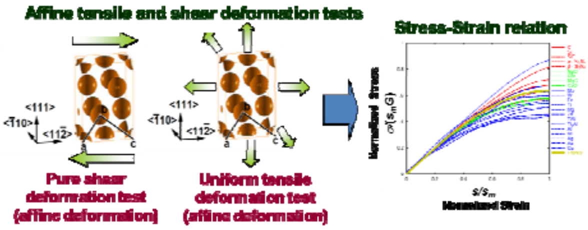
- はじめに
- 空間階層性への挑戦
- 時間階層性への挑戦
- まとめ

理想強度から強さへ

11

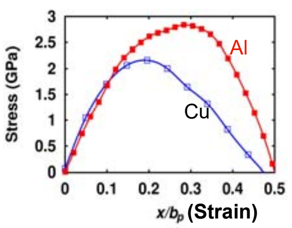
Ideal strength (first-principles calculation)

Using non-empirical DFT(Density Functional Theory), the stress-strain relations are estimated for 22 materials



Ogata, Science (2002), PRB (2004)

Ideal strength (Al vs. Cu)



Cu is 32% softer than Al
At equilibrium, Cu has
80% stiffer bulk modulus,
25% stiffer pure shear modulus.
Why does Cu lose to Al?

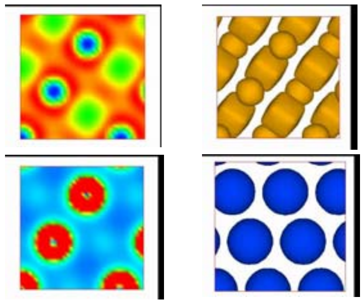
The apparent reason is Al offers a much longer deformation range before softening than Cu, by 50%! Cu starts out stiffer, but ends up significantly softer under pure shear (by 32%).

Ideal Strength and Strain of Cu and Al Ogata, Science (2002)

FCC (111)[112] pure shear by DFT using primitive cell

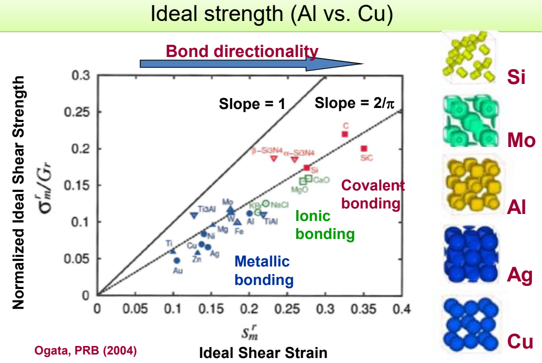
※Pure shear condition: stress components, excluding the applying shear stress component, keep to be zero during shear deformation test

Ideal strength (Al vs. Cu)



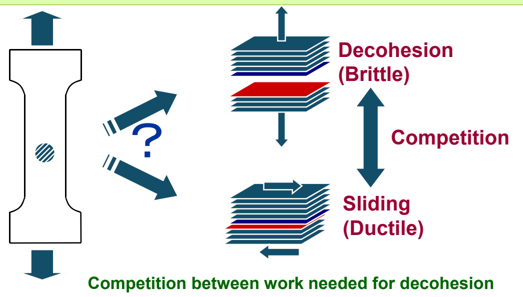
Ogata, Science (2002)

Ideal strength (Al vs. Cu)



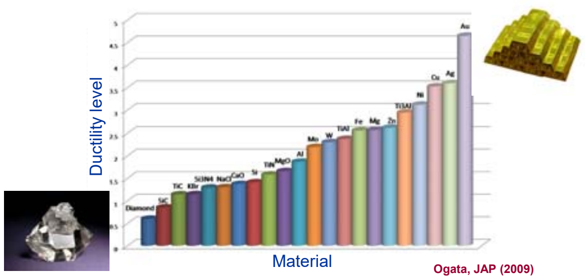
Ogata, PRB (2004)

Can we predict intrinsic ductility?



Competition between work needed for decohesion and sliding of adjacent atomic planes determines the intrinsic ductility

Yes, we can.



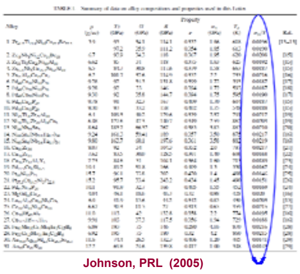
Ogata, JAP (2009)

金属ガラスの変形のサイズ依存性

18

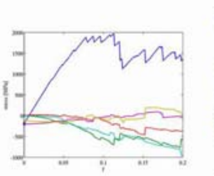
2% yield strain of metallic glasses

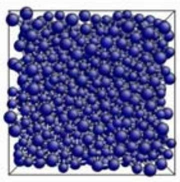
Experiments

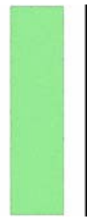


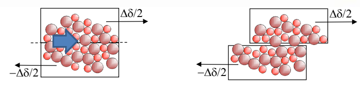
Johnson, PRL (2005)

Plaston in glasses (shear transformation zone; STZ)









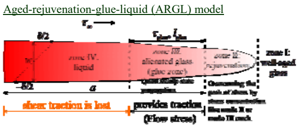
Ogata, Shimizu, Li, Wakeda, Shibutani, Intermetallics (2006)

Inelastic Displacement coloring

Collective motion of ~100 atoms is unit of shear deformation
→ STZ can be a plaston

Shear banding is collective motion of STZs

Aged-rejuvenation-glue-liquid (ARGL) model

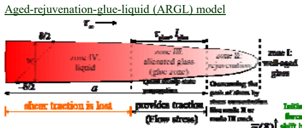


Shimizu, Ogata, Li, Acta Mater. (2006)

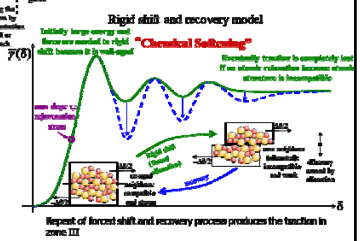
Shear banding could be a collective motion of many STZs. However, looking at the individual STZ does not provide valuable insights. → SB is plaston

What happens in glue zone (zone III)

Aged-rejuvenation-glue-liquid (ARGL) model



Shimizu, Ogata, Li, Acta Mater. (2006)



2% yield strain of metallic glasses

Aged-rejuvenation-glue-liquid (ARGL) model
(MD analysis)

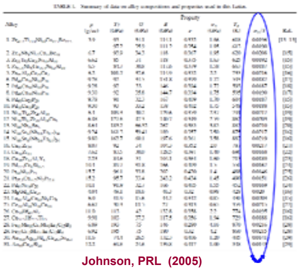
	ρ	E	B	μ	ν	$2\tau_{glue}/E$
binary LJ system[a] [23]	1.2	39	60	15	0.38	2.4%
$Cu_{50}Ag_{50}$[a] [24]	9.6	50	85	12	0.44	2.1%
$Cu_{46}Zr_{54}$[a] [25]	6.9	38	89	12	0.44	2.0%
$Zr_{52.5}Cu_{17.9}Ni_{14.6}Al_{10}Ti_5$[b] [26]	7.0	71	153	27	0.12	1.9%

[a] $T = 0.2$, [b] $T = 300$K, unit of ρ in g/cm³, E, B, and μ in GPa.

The shear stress corresponding to 2% strain is necessary for the shear band propagation.

Shimizu, Ogata, Li, Acta Mater. (2006)

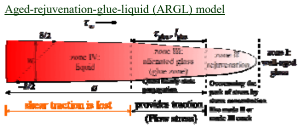
Experiments



Johnson, PRL (2005)

Melting by shear band propagation

Aged-rejuvenation-glue-liquid (ARGL) model



Hypothesis: The experimentally measured ε_y corresponds to quasi steady-state propagation of glue zone (zone III):
$E\varepsilon_y/2$(stress corresponding to ε_y) = τ_∞ = τ_{glue} (traction at zone III)

Propagation of the glue zone can only be quasi steady state: no matter how small the heat injection rate $h = \tau_{glue}\dot{\delta}$ is, it will eventually melt.

Heated zone width $\propto \sqrt{\alpha t}$

Heat injected $= ht$

Temperature increase $c_V(T - T_{env}) \propto \frac{ht}{\sqrt{\alpha t}}$

Time needed to reach melting point T_g :

$$t_{incubation} \propto \frac{\alpha c_V^2 (T_g - T_{env})^2}{h^2}$$

Plug in $\tau_{glue} \sim 0.01E$, $\dot{\delta} \sim c_S = \sqrt{\mu/\rho}$,
thermal diffusivity α, heat capacity c_V for Zr-based BMGs,
$t_m \sim 100$ ps, $l_{glue}^{max} \sim 100$ nm
If we take $\dot{\delta} = 0.1c_S$, then $t_{incubation} \sim 10$ ns, $l_{glue}^{max} \sim 1\ \mu$m

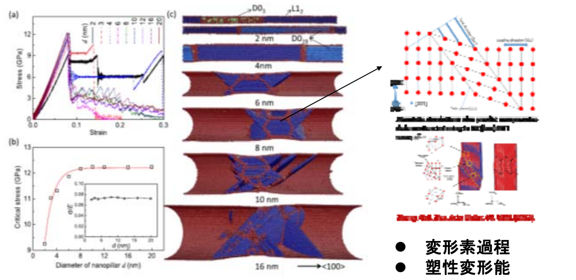
1μm以上進展しないと融解に至らず割れにつながらない →

それ以下のサイズでは延性的塑性変形挙動

ナノワイヤーの変形のサイズ依存性

25

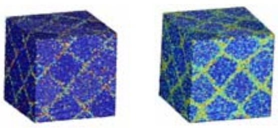
Size-dependent deformation mechanism transition



- 変形素過程
- 塑性変形能

Wang, Gao, Ogata, APL (2013)

バルクナノメタルの
強度と変形のサイズ依存性

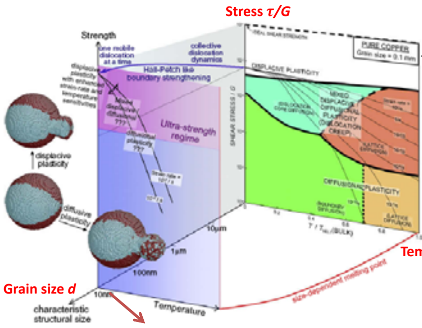


27

クリープ現象の粒径依存性

Yunjiang Wang[2] and Shigenobu Ogata[1]
1 Graduate School of Engineering Science, Osaka University
2 Chinese Academy of Science, Institute of Mechanics

Deformation-Mechanism (Weertman-Ashby) Maps



Space of map
- Stress
- Temperature
- Strain rate

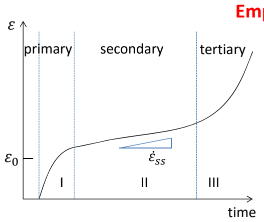
+
- **Grain size**

Need deformation-mechanism map at nanoscale.

T. Zhu, J. Li / Progress in Materials Science 55 (2010) 710–757

29

Fundamentals of Creep



Time-dependent strain subject to external stress at elevated temperature

Define the minimum strain rate as creep rate

Empirical Mukherjee-Bird-Dorn equation

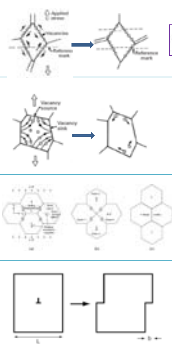
$$\dot{\varepsilon} = \frac{AD_0Gb}{k_BT}\left(\frac{b}{d}\right)^p\left(\frac{\sigma}{G}\right)^n \exp\left(-\frac{Q}{k_BT}\right)$$

A. K. Mukherjee et al., Trans. ASM 62, 155 (1964).

- $\dot{\varepsilon}$: steady-state creep-rate
- A: constant related to T, σ, d
- D_0: diffusion coeffecience
- G, b: shear modulus, burger's vector
- d: grain size; T: temperature; σ: stress
- P, n: grain size, and stress exponent
- Q: activation energy
- k_B: Boltzmann constant

30

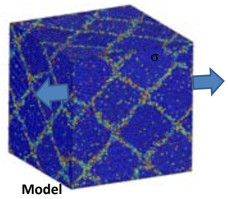
Proposed Fundamental Mechanisms Responsible for Creep



Creep Mechanisms	Schematics	Equation	Reference
Coble (Grain boundary diffusion)		$\dot{\varepsilon}_C = A_C D_{gb}\frac{Gb}{kT}\left(\frac{\delta}{b}\right)\left(\frac{b}{d}\right)^3\left(\frac{\sigma}{G}\right)$	*Coble, JAP, 1963*
Nabarro-Herring (Lattice diffusion)		$\dot{\varepsilon}_{NH} = A_{NH}\frac{D_l G b}{kT}\left(\frac{b}{d}\right)^2\left(\frac{\sigma}{G}\right)$	*Nabarro, 1948; Herring, JAP, 1950*
Grain boundary sliding		$\dot{\varepsilon} = A_{GBS} D_{b0}\frac{Gb}{k_BT}\left(\frac{b}{d}\right)^3\left(\frac{\sigma}{G}\right)^2$	*Lüthy, MSE 1979*
Dislocation • climb • sliding • forest interaction • ………..		$\dot{\varepsilon} = b\rho v$	*Orowan equation*

31

Atomistic MD Simulations of Creep Deformation



Calculation details:

- Copper with 16 grains
- random grain orientation
- Mishin EAM potential
- NσT ensemble
- Periodic boundary condition

σ(GPa)	T (K)	d (nm)
0.066	720	8
↓	840	10.7
	960	
	1080	13.3
3.49	1200	16.0

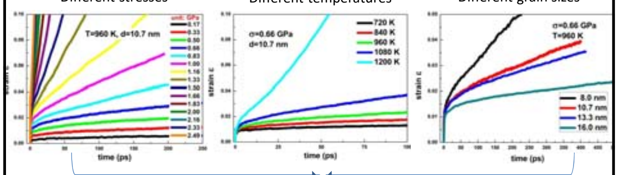
$\dot{\varepsilon}$ creep rate

$$\dot{\varepsilon} = A(T,\sigma,d)\sigma^n\frac{1}{d^P}\exp\left(-\frac{Q}{k_BT}\right)$$

Correlating steady-state creep-rate with different (T,σ,d) conditions, determining (n, P, Q)

32

Creep at different stresses, temperatures, and grain sizes

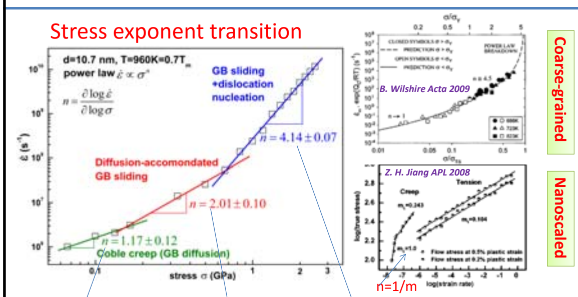


$$\dot{\varepsilon} = A(T,\sigma,d)\sigma^n\frac{1}{d^P}\exp\left(-\frac{Q}{k_BT}\right)$$

$$(n, P, Q)$$

33

Transition of Creep Mechanisms



$\dot{\varepsilon} = \left(A_C\frac{\delta}{k_BT}\frac{D_{GB}}{d^3}\right)\sigma^1$ $\quad\dot{\varepsilon} = \left(\frac{A_{GBS}D_{Gb}}{G}\frac{b}{k_BT}\left(\frac{b}{d}\right)^3\right)\sigma^2$ $\quad\dot{\varepsilon} = \left(Ad^{-P}\exp\left(-\frac{\Delta Q}{k_BT}\right)\right)\sigma^{n\geq4}$

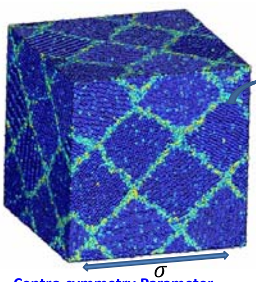
Coble creep (GB diffusion) — GB sliding — Dislocation Power-law creep

Wang, Ogata, PRB, (2011).

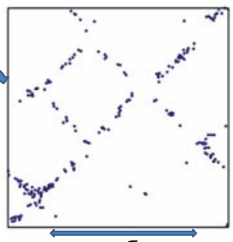
34

Creep at Low Stress

Creep at 166 MPa, 840 K, 2 ns
GB diffusion and sliding



Centro-symmetry Parameter

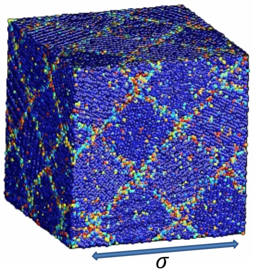


Displacement>$\sqrt{2}/2a_0$, Nearest Neighbor

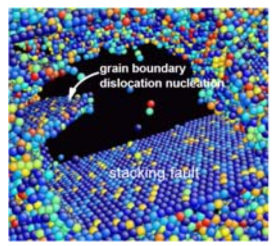
35

Creep at High Stress

Creep at 1.16 GPa, 960 K,
GB dislocation nucleation



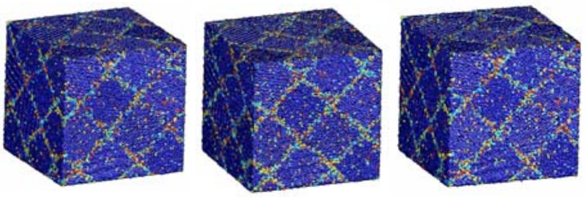
Centro-symmetry Parameter



Creep deformation of a nanocrystalline metal.

Wang, Ogata, PRB, (2011).

36



$\sigma = 66 - 167$ MPa, n= 1, grain boundary diffusion

$\sigma = 167 - 664$ MPa, n= 2, diffusion-accommodated grain boundary (GB) sliding

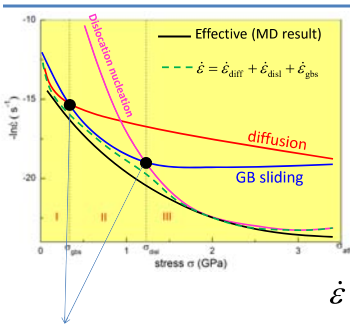
$\sigma = 664$ Mpa-2.49 GPa, n= 4.2, diffusion-accommodated dislocation activity

Diffusive → Displacive

Coble GBS Dislocation

37

Constitutive Equation for Nanocreep



Rate-controlling processes:

- GB diffusion (Coble creep)

$$\dot{\varepsilon}_{diff} = \frac{\delta D_{b0}}{d^3}\exp\left(-\frac{Q_{GB}}{k_B T}\right)\sinh\left(\frac{\sigma\Omega_{diff}}{k_B T}\right)$$

- GB sliding

$$\dot{\varepsilon}_{gbs} = \varepsilon^{T}\frac{3\delta}{d}\nu_{gbs}\exp\left(-\frac{Q_{GB} - \tau\Omega_{gbs}}{k_B T}\right)$$

- Dislocation nucleation

$$\dot{\varepsilon}_{disl} = \frac{b}{d}\nu_{disl}\exp\left(-\frac{Q_{disl} - \tau\Omega_{disl}}{k_B T}\right)$$

$$\dot{\varepsilon} = \dot{\varepsilon}_{diff} + \dot{\varepsilon}_{disl} + \dot{\varepsilon}_{gbs}$$

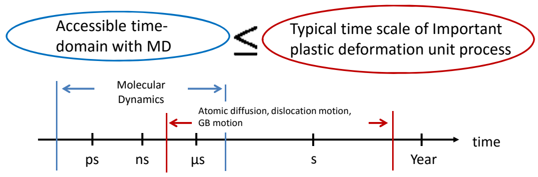
Wang, Ogata, PRB, (2011).

38

Outline

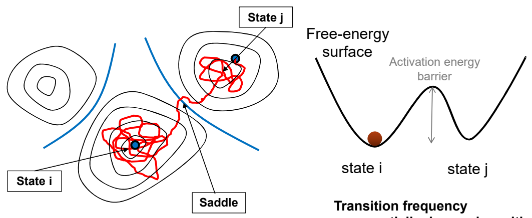
- はじめに
- 空間階層性への挑戦
- 時間階層性への挑戦
- まとめ

DIFFICULTY OF MD SIMULATION OF INFREQUENT EVENTS FOR MATERIALS PLASTIC DEFORMATION



Need to overcome the time scale issue of MD

GENERAL STRATEGY OF ACCELERATED MD METHODS



Free energy surface with many local minima

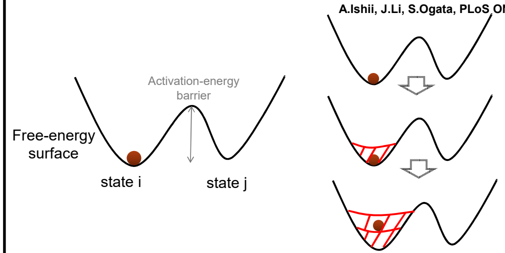
Transition frequency exponentially decreasing with increasing the energy barrier

Strategy: Making the escape from state i happen sooner without knowing about the escape path and the shape of the free energy surface.

ADAPTIVE BOOST MOLECULAR DYNAMICS METHOD

A.Ishii, S.Ogata, H.Kimizuka, J.Li, PRB (2012).

A.Ishii, J.Li, S.Ogata, PLoS ONE (2013).



- Add boost energy (ΔV) to the original free-energy surface.
- The boost energy is determined by an adaptive manner (no risk of over-boost)
- The boost energy is expressed by a smooth function (not so many Gaussians)
- $t_{i\to j} = t^{boost}_{i\to j}\langle\exp(\beta\Delta V)\rangle$: Hyperdynamics theorem

ADAPTIVE BOOST MOLECULAR DYNAMICS METHOD

Perform canonical MD sampling for certain MD steps and obtain the probability $\rho(A)$.

$$\rho(A) = \frac{\int \cdots \int \delta(\hat{A}(r,p) - A)\exp(-\beta H)drdp}{\int \cdots \int \exp(-\beta H)drdp}$$

Repeat these two procedures until certain transition occurs.

Calculate the boost energy $\Delta V(A)$ and add it onto the free energy surface $F(A)$.

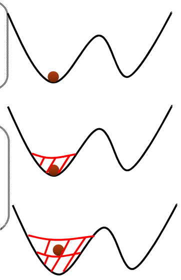
$$\Delta V(A) \equiv \frac{1}{\beta}\ln\rho(A) \Rightarrow F'(A) = F(A) + \Delta V(A)$$

Time scale conversion

$$t_{i\to j} = t^{boost}_{i\to j}\langle\exp(\beta\Delta V)\rangle$$

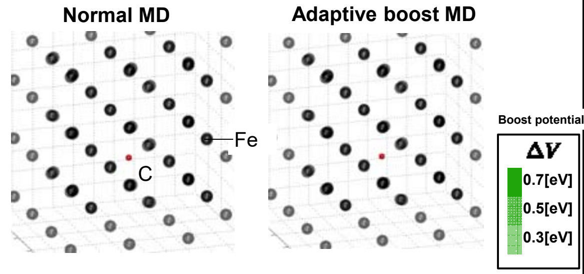
actual time ⇦ MD time

Voter, PRL (1997)



Ishii, Ogata, Kimizuka, Li, PRB (2012).

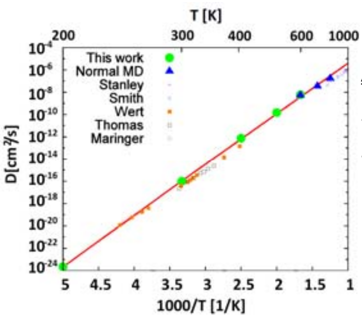
CARBON DIFFUSION DYNAMICS IN BCC AT 400K (NORMAL AND AB MD RESULTS)



- BCC (432 Fe atoms + 1 interstitial C atom) with PBC
- EAM interatomic potentials (Lau. et al. PRL 2007)

Ishii, Ogata, Kimizuka, Li, PRB (2012).

C DIFFUSIVITY IN BCC IRON



Activation enthalpy

- Adaptive Boost MD estimation ~ 0.89 eV
- Experiments: 0.77 ~ 0.90 eV

Ishii, Ogata, Kimizuka, Li, PRB (2012).

➢ With the aid of Adaptive Boost MD, diffusivity can be quantitatively analyzed even at low temperature for which no experimental data are available.

ACCELERATION FACTOR

$$t_{O\to O} = t^{boost}_{O\to O}\langle\exp((\beta\Delta V(A))\rangle$$

Acceleration factor

Temperature [K]	$t_{O\to O}$ [ns]	$t^{boost}_{O\to O}$ [ns]	$t_{O\to O}/t^{boost}_{O\to O}$
200	1.48×10^{16}	1.02×10^{-1}	1.45×10^{17}
300	3.24×10^{8}	5.64×10^{-2}	5.72×10^{9}
400	7.08×10^{4}	8.22×10^{-2}	8.78×10^{5}
500	2.48×10^{2}	8.12×10^{-3}	3.07×10^{4}
600	4.64	4.72×10^{-3}	9.78×10^{2}

まとめ

- 材料の強さの数理的理解と予測には時空間階層性への挑戦が不可欠である。
- 原子・電子論から見れば、材料の強さという概念は、外部からの刺激に対して発生する「反応、拡散、変形」という３つの材料応答形態の結果として評価される材料の力学的安定性という定義で一般化するのが自然である。

Thank you for your kind attention.