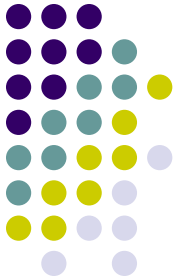


Modeling of Potential with Downfolding method

Atsushi M. Ito[1],

Yoshihide Yoshimoto[2], and Hiroaki Nakamura[1,3]

[1)] National Institute for Fusion Science

[2)] Graduate School of Engineering, Tottori University

[3)] Graduate School of Engineering, Nagoya University

Element for Plasma Material Interaction for Fusion

Tungsten（W）, Carbon（C）, Beryllium（Be）:

plasma facing material, divertor, first wall

Hydrogen（H, D, T）, Helium（He）:

Plasma particles, fuel for fusion, ash for fusion

Oxygen（O）, Nitrogen（N）:

impurity for PFM surface due to air.

Lithium（Li）:

Blanket for T breeding, future divertor

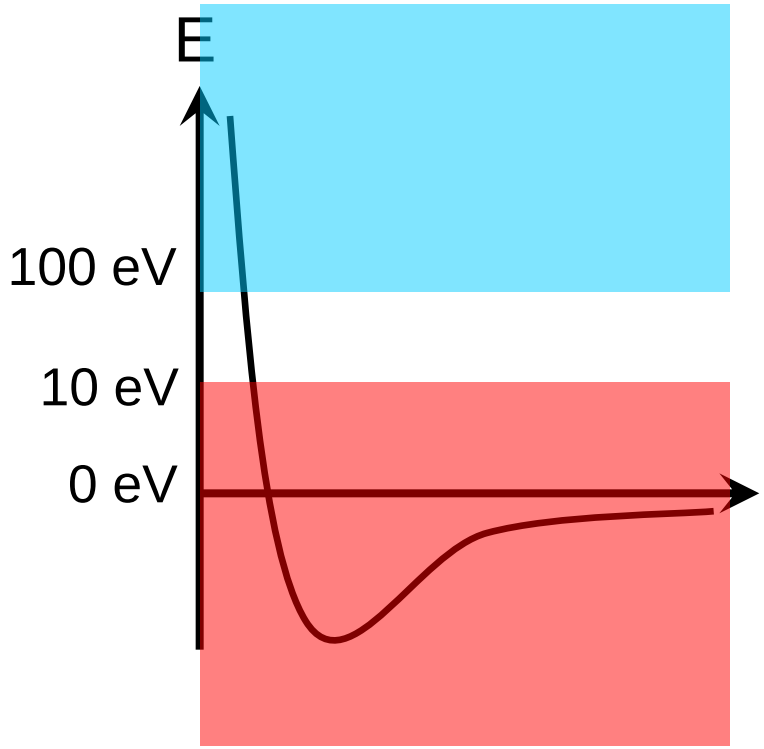
The others（Fe, Mo, V, Cr, Mo）:

Materials of devices, pipes, tiles, and so on.

Potential Model

MD, KMC and BCA,

needs inter atomic potential model



BCA calculates trajectory also based on potential model such as “Thomas-Fermi Potential with Moliere approximation” (>100eV).

Potential model for MD is optimized for low energy bonding (< 10 eV)

Potential model

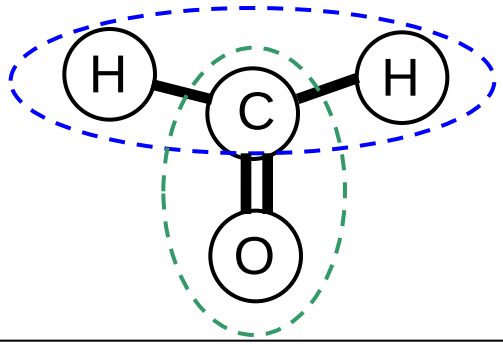
The simulation of potential model：

- There are many potentials for a single element
- There are some potentials for two kinds of elements.
- There are few potentials for more than three kinds of elements.

Potential for many kinds of elements cannot be composed of potentials for two kind of elements.

Exam.）Using C-H potential U_{CH} and C-O potential U_{CO} simultaneously,

in CH_2O, U_{CH} calculates energy as a CH2 molecule because it cannot treat the effect from O atom. Similarly, U_{CO} calculate only the energy as a CO molecule.



Purpose

Purpose of this work：

To create the potential model which treat all element in PWI of nuclear fusion.

- It can treat simultaneously more than three elements.
- It can treat simultaneously metal metallic bond, covalent bond and ionic bond.
- Good accuracy（less than 0.1 eV/atom）

The present work：

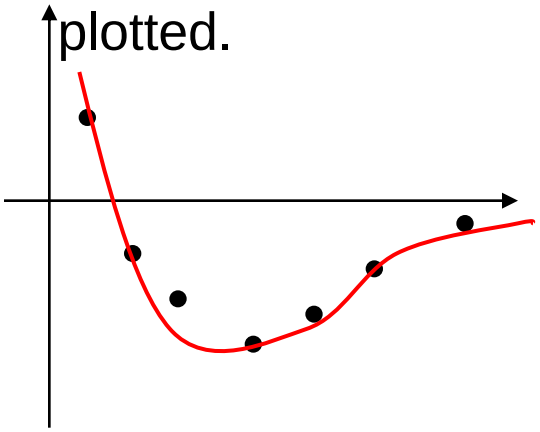
To start creating the potential model by using “downfolding method”.

- AFS potential for W is optimized.
- AFS potential extended to W-He system.

Way of potential model creation

Two body potential

1. Energy is calculated by ab-initio method, and plotted.



2. Create a fitting curve as a unction of potentil.

- It is simple because of one degree of freedom.
- This way is difficult for many degree of freedoms

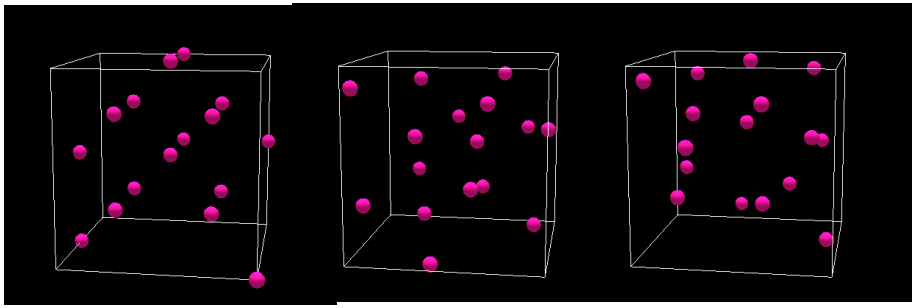
Many body potential

1. Function of potential should be initially given from viewpoint of physics and chemistry.
   - Function form（exp, power …）
   - Degree of freedom
   - Meaning parameters
   - Ignored term
   - (Fast calculation in computer)
2. Parameters are determined to be close to reference energy, which is estimated by ab-initio calculaton and experiments.

Downfolding method (Y. Yoshimoto, J.Chem.Phys.,**125**(2006)184103)

1. Function form of potential model $U_{\mathrm{MD}}(\{r\},\{a\})$ and temporary parameters $\{a\}_0$ are determined.

2. N sample structures are created by MD simulation which simulates your target phenomena.



3. The energy for the N samples $E_{\mathrm{FP}}(\{r\})$ are calculated by ab-initio method.

   →In this work, OpenMX is employed, (DFT, numerical orbital, LDA).

   →plane wave is better (VASP, PHASE)

4. Parameters $\{a\}$ is optimized by using .

Downfolding method (Y. Yoshimoto, J.Chem.Phys.,**125**(2006)184103)

- Sample structures are obtained by the MD which simulates target phenomena.

  → optimal parameters should be converted for each phenomenon.

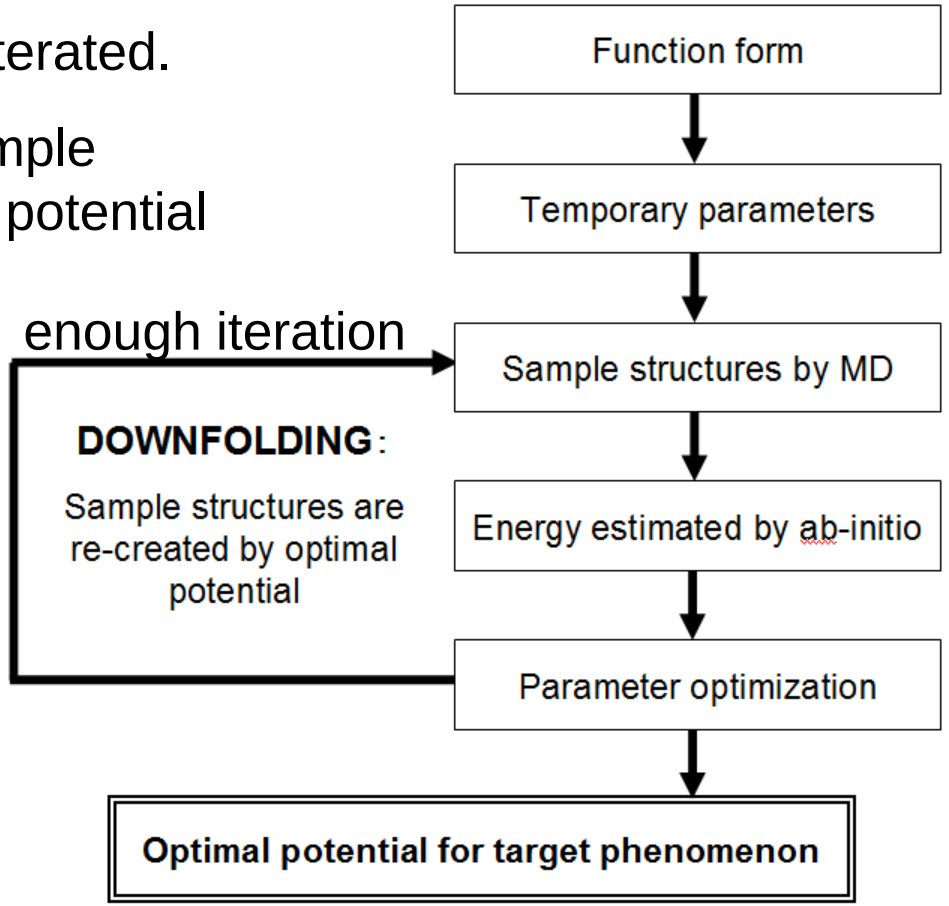
- MD sampling and optimization are iterated.

  → Probability of occurrence of sample structures are close to real with potential optimization

exam1）If MD simulates at constant temperature, potential become good for structures in the temperature.

exam2）If MD is multi-canonical MD, potential is optimized for wide range temperature.

exam3) If MD is PMI(injection), potential is optimized for it.



Parameter optimization by nonlinear least-squares method

Parameters a_i of potential $U_{\mathrm{MD}}(\{r\},\{a\})$ are optimized by using nonlinear least-squares method.

The diference with reference energy $E_{\mathrm{FP}}(\{r\})$ is defined by

$$\Phi = \frac{1}{N}\sum_{\{r\}}^{N}\left(U_{\mathrm{MD}}(\{r\};\{a\}) - E_{\mathrm{FP}}(\{r\})\right)^2$$

Parameters a_i are selected so that $\Phi \to 0$.

Then, the following time evolution equation of parameter a_i;

$$\frac{da_i}{dt} = -c\frac{\partial \Phi}{\partial a_i} = -c\left(U_{\mathrm{MD}} - E_{\mathrm{FP}}\right)\frac{\partial U_{\mathrm{MD}}}{\partial a_i}$$

*) If the function form of $U_{\mathrm{MD}}(\{r\},\{a\})$ is better, Φ becomes close to 0.

*) Pay attention for Φ are trapped in local minimum. We can MD for parameter $\{a\}$ space Hamiltonian to find good initial parameter.

$$H(\{p_a\};\{a\}) = \sum_i \sum \frac{p_{a,i}^{\ 2}}{2m_i} + \Phi(\{r\};\{a\})$$

Case1）W single element system

Embedded Atom Method（EAM）potential (AFS potential[3,4]) is optimized by downfolding method.

$$U_{\mathrm{AFS}}(\{r\}) = \frac{1}{2}\sum_{i,j} V(r_{ij}) - A\sum_{i} \rho_i^{1/2}(\{r\})$$

$$V(r_{ij}) = \begin{cases} (r_{ij}-c)^2(c_0 + c_1 r_{ij} + c_2 r_{ij}^2) + B(b_0 - r_{ij})^3 \exp(-\alpha r_{ij}) & \\ \qquad\qquad \text{if } r_{ij} < b_0, & \\ (r_{ij}-c)^2(c_0 + c_1 r_{ij} + c_2 r_{ij}^2) \qquad \text{if } b_0 \le r_{ij} < c, & \\ 0 \qquad\qquad \text{else.} & \end{cases}$$

$$\rho_i(\{r\}) = \sum_{j \neq i} \phi(r_{ij})$$

$$\phi(r_{ij}) = \begin{cases} (r_{ij}-d)^2 + \beta(r_{ij}-d)^3/d \quad \text{if } r_{ij} < d, & \\ 0 \qquad\qquad \text{else.} & \end{cases}$$

[3] M. W. Finnis, et al., Phil. Mag. A50 (1984) 45-55.

[4] G. J. Ackland, et al., Phil. Mag. A56 (1987) 15-30.

Case1）W single element system

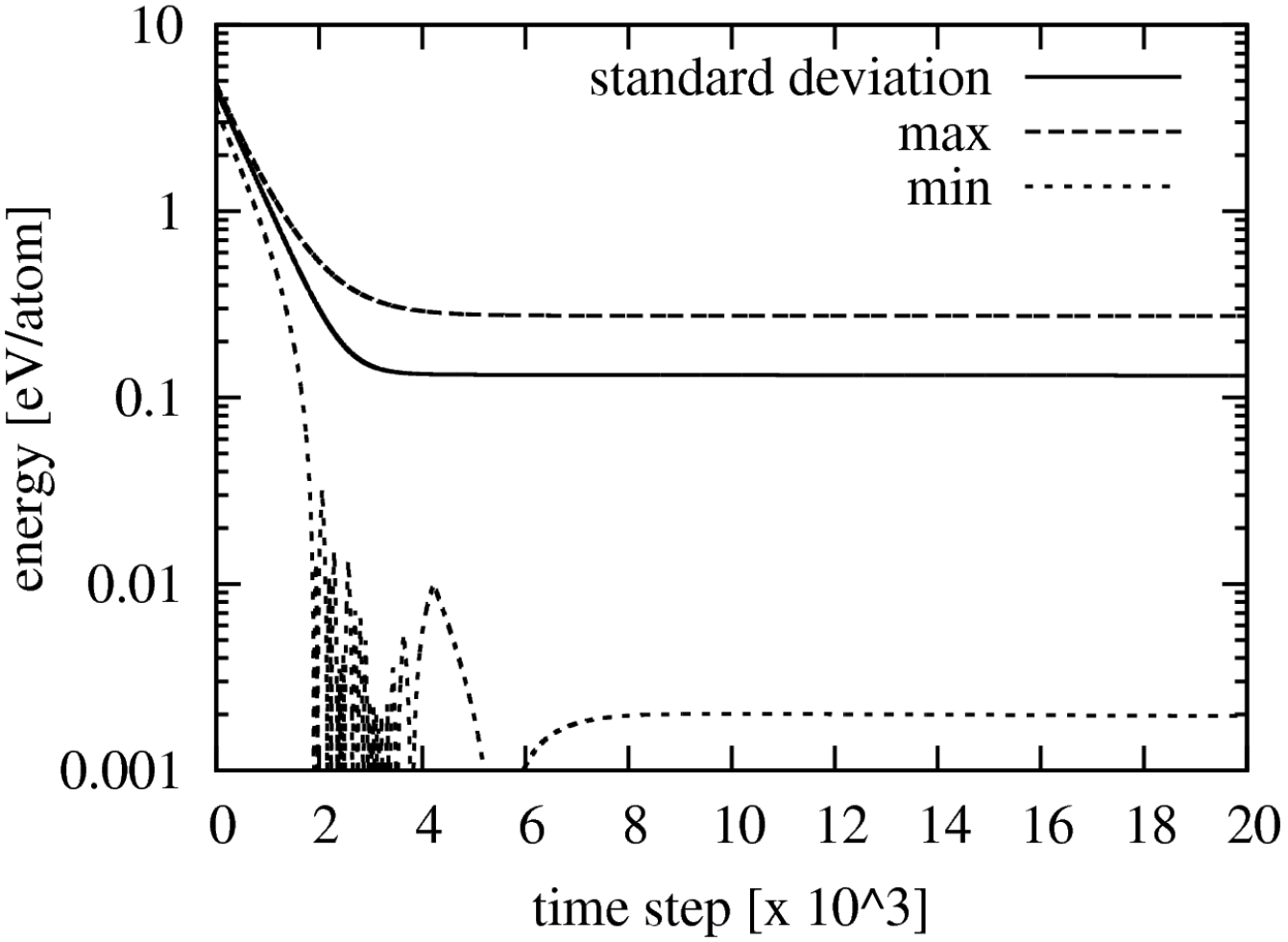
System has 16 W atoms. Reference energies are by OpenMX.

Optimized parameter of AFS potential

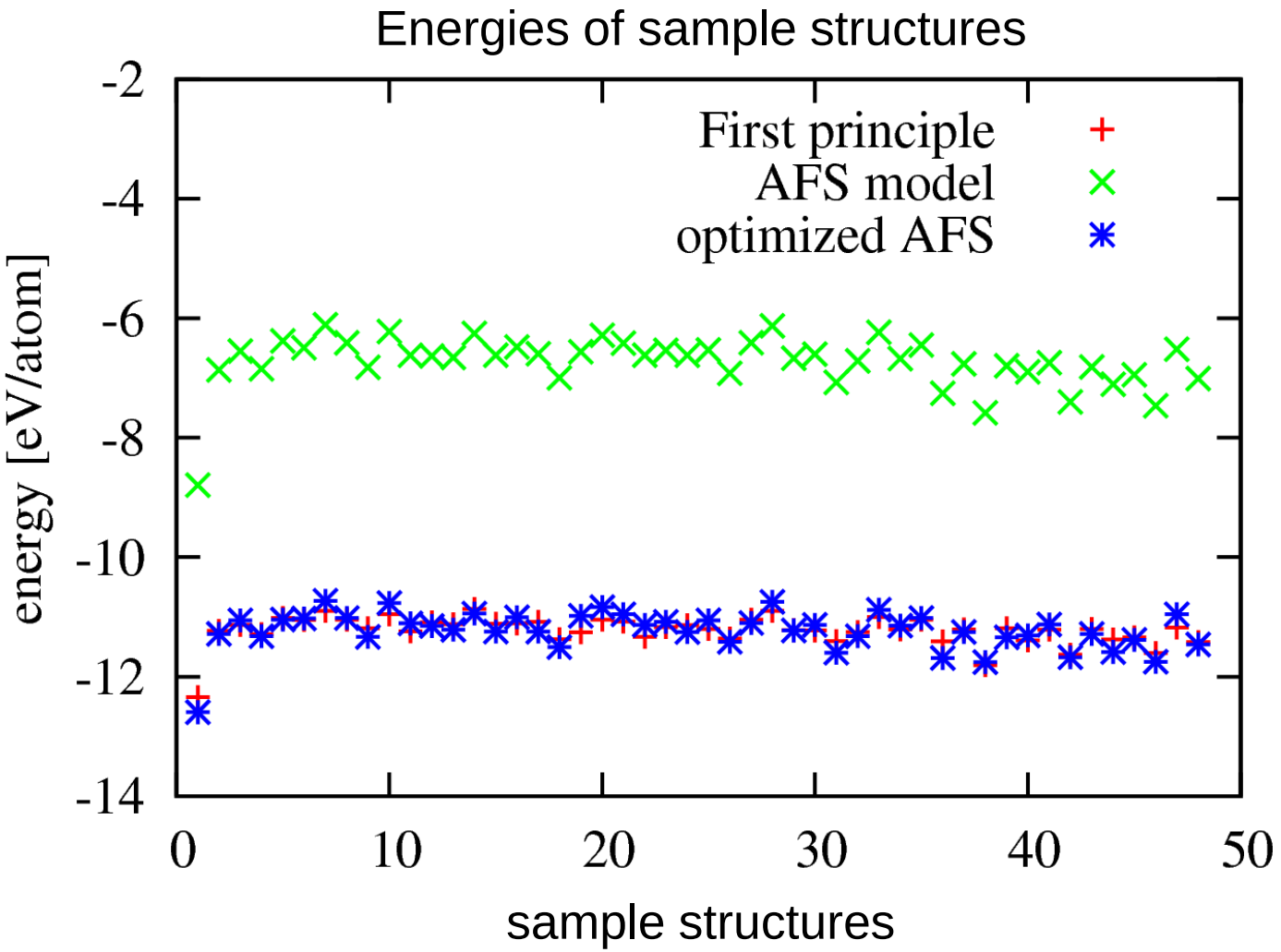
	AFS	Optimized AFS
c （fix）	3.25	3.25
c_0	47.1346499	47.0953
c_1	-33.7665655	-33.8642
c_2	6.2541999	6.00949
d （fix）	4.400224	4.400224
A	1.896373	2.01524
β	0.0	-0.0439063
B	90.3	90.2999
α	1.2	1.21896
b_0	2.7411	2.67707

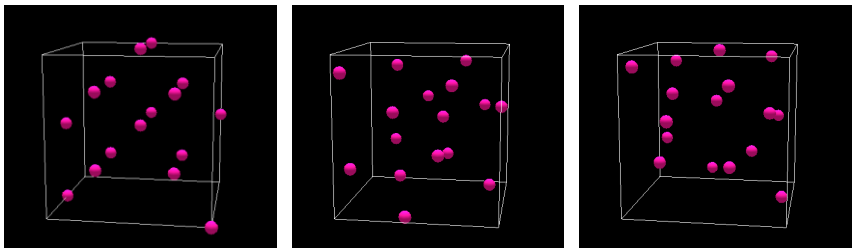
Case1）W single element system

Energy difference Φ with evolution time of parameter a



Case1）W single element system





Summary

- AFS potential is well optimized.
- W-He potential is good for almost sample（accuracy is 0.3 eV/atom）, but it need modify the function form for high energy structure.
- Anyway, downfolding is useful for potential creation.

Future problems

- What is good ab-initio calculation software? (VASP, PHASE, plane wave)
- What is good function forms

  → For metallic bond, covalent bond

  → Num. of parameters: O(element^{1}) is best. O(element^{3}) is bad.