Fitting UO_2 Interatomic Potential Using Micro-Genetic Algorithm

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1. Introduction

An atomistic computer simulation such as a first-principle method or classic molecular dynamics is becoming popular tools to understand high temperature phenomena in a UO_2 nuclear fuel with an improved computer performance. As the classical molecular dynamics (MD), which is based on simple Newton mechanics and interatomic potentials, can handle a large system, it is useful to investigate thermal behaviors [1,2,3]. Because the interatomic potential defines the forces between atoms, the accuracy in the MD results critically depends on the accuracy in the interatomic potential.

The traditional procedures for a construction of an interatomic potential consists of two steps: First, the interatomic potential function form should be determined by considering the material characteristics. Second, its parameters should be fitted by a comparison with reference values. The second fitting procedure is usually an effort-consuming trial and error method.

In this paper, a micro-genetic algorithm is implemented for improving the fitting procedure of a UO_2 interatomic potential, and the newly developed potential is compared with the potentials in the literatures.

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2. Methods and Results

2.1 Potential function and simulation condition

The general pair interatomic potential for UO_2 is a Morse type potential as follows, which is good for a semi-ionic system:

$$\phi_{ij}(r_{ij}) = \frac{z_i z_j e^2}{r_{ij}} + f_0(b_i + b_j)\exp\left(\frac{a_i + a_j - r_{ij}}{b_i + b_j}\right) - \frac{c_i c_j}{r_{ij}^6}$$
$$+ f_0 D_{ij}[\exp\{-2\beta_{ij}(r_{ij} - r_{ij}^*)\} - 2\exp\{-\beta_{ij}(r_{ij} - r_{ij}^*)\}]$$

where z is the effective partial electronic charge, r is the distance between atoms, r_{ij}^* is the bond length of anion-cation pair in vacuum, and other parameters are characteristic parameters of ion species.

Two well-known potential parameters' sets are shown in Table 1 and 2.

Table 1. Potential parameters used in reference [1]

Ion	z	a	b	c	f_0	D_{ij}	β_{ij}	r_{ij}^*
U	2.4	1.659	0.160	0	4.1860			
						(for U-O pair)		
O	-1.2	1.926	0.160	20		18.0	1.25	2.369

Table 2. Potential parameters used in reference [2]

Ion	z	a	b	c	f_0	D_{ij}	β_{ij}	r_{ij}^*
U	2.4	1.63	0.163511	0	4.07196			
						(for U-O pair)		
O	-1.2	1.91	0.163511	19.519		13.6765	1.65	2.369

The MD simulation for UO_2 was carried out at the system containing 3×3×3 CaF_2 type crystal structure unit cells (108 U atoms and 216 O atoms) as shown in Fig. 1. The larger system size make stable calculation results close to actual values, but take more time to calculate. Fig. 2 shows that 3×3×3 system size is enough for getting stable results.

The Moldy code was implemented for the MD simulation under the NPT ensemble (constant N-number of atoms, P-pressure, T-temperature). The time step (Δt) was 0.0002 ps and the number of time steps was 10000. The lattice parameters were obtained by averaging last 1000 time steps.

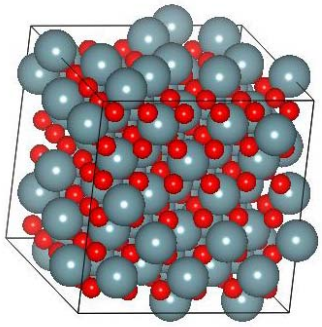

Fig. 1. MD simulation system for UO_2.
(Large sphere: U atom, small sphere: O atom)

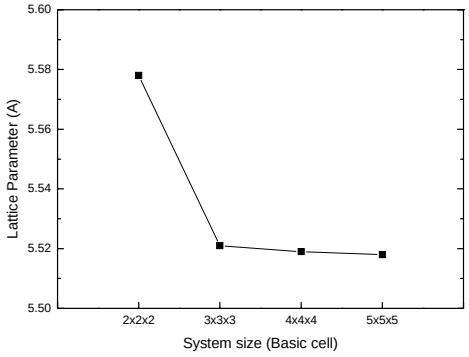

Fig. 2. Change of MD simulation results with system sizes at 1300K.

2.2 Micro-genetic algorithm

The genetic algorithm (GA) is a computer simulation technique for an optimization problem inspired by the evolutionary biology [4]. Based on the fitness of every individual, a new population at next generation, which is a set of candidate solutions, is created by the selection and recombination of individuals. The new population is then used in the next iteration of the algorithm. These procedures make a population of candidate solutions to evolve to better solutions. The micro-GA is a small population GA with re-initialization [5].

2.3 Developed interatomic potential

In this study, the population size of GA was 6 and the crossover probability was 0.4. The niching and mutation probability were excluded. The tournament selection and the elitism were implemented for making a new population at next generation. The fitness of an individual was evaluated by the comparison of calculated lattice parameter with observed one.

The interatomic potential parameters fitted in this study are summarized in table 3. The parameters were not adjusted by hand but obtained by an automatic GA. Fig. 3 shows the comparison of MD calculation results using the interatomic potentials in this study and literatures [1,2]. The interatomic potential of UO_2 fitted by GA agreed well with the experimental data and reproduced the lattice parameter better than those in literatures.

Table 3. Potential parameters obtained by genetic algorithm

Ion	z	a	b	c	f_0	D_{ij}	β_{ij}	r_{ij}^*
U	2.4	1.629	0.163511	0	3.70699			
						(for U-O pair)		
O	-1.2	1.932 5	0.165787	19.519		13.7961	1.65	2.369

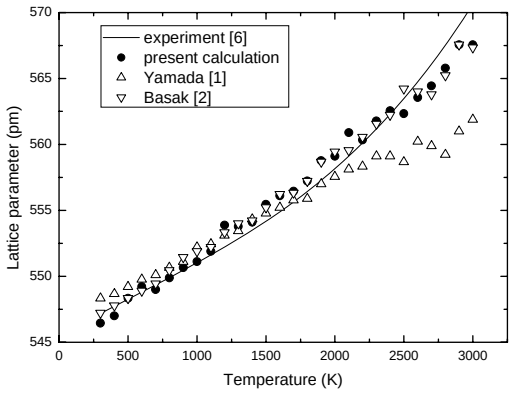

Fig. 3. Change in the lattice parameter of UO_2 with temperature

3. Conclusions

The micro-GA was implemented for improving the fitting procedure of UO_2 interatomic potential. The interatomic potential parameters automatically fitted by GA agreed well with the experimental data and other simulations results in the literatures. In the further study, the interatomic potentials of actinide oxides will be investigated by GA, which is established in the paper.

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