Performance of EAM and MEAM Potential for NiTi Alloys: A Comparative Study

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Abstract. NiTi alloys is one of the unique materials exhibiting shape memory effect. The martensitic transformation is the main reason for their behaviour, which is very sensitive to the heat treatment and the ratio of Ni-Ti atoms. The study of the NiTi alloys behaviour at the atomic level is indispensable to elucidate the mechanism of the martensitic transformation under the specific conditions. Molecular dynamics simulation is widely used in this kind of study. The results of the molecular dynamics simulation depend on the selection of the interatomic potential. This study is aimed to evaluate the performances of the standard EAM potentials of Zhou et al. and the modified EAM of Ko et al. by means of obtaining the more accurate lattice constant in comparison with the experimental value. These interatomic potentials are also tested to reproduce the recrystallization behaviour below the melting temperature. We found that the high accuracy of the lattice constant for NiTi alloy system could be achieved by employing MEAM potential of Ko et al. However, the EAM potential by Zhou et al. gives the rapid recrystallization of NiTi alloys at 1100 K. These results indicate that the MEAM potential of Ko et al. shows the better performance at low temperature simulation.

1. Introduction

NiTi alloys is one of the unique materials exhibiting shape memory effect (SME). This characteristic allows the NiTi alloys to transform to the other crystal structure and then return to its original structure under specific treatment [1,2]. The change in the structure of NiTi alloys is known as martensitic transformation, which is very sensitive to the heat treatment and the stoichiometry of Ni and Ti atoms [1].

NiTi alloys has been used in many applications, such as medical, military, and safety. This material has some distinguished properties such as biocompatible, water resistance, high electrical resistivity, very hard and tough, corrosion resistance, and many others [3-5].

The study of the behavior of NiTi alloys at the atomic level become indispensable to elucidate the mechanism of the martensitic transformation and to predict the structure of this material under specific condition. There are only few papers reported the computational study of NiTi alloys at high temperature [6,7] and high pressure [8] using molecular dynamics (MD) simulations. However, to the
best of our knowledge, the computational study of NiTi fabrication process at the temperature higher than the melting point has not been published.

It is widely known that the result of the MD simulation highly depends on the selection of the interatomic potential. Therefore, it becomes very important to evaluate the performance of the interatomic potential used in MD simulation. Recently, two interatomic potentials are developed for NiTi alloys, i.e. standard embedded-atom-method (EAM) potential by Zhou et al. [9] and modified EAM potential by Ko et al. [10]. This study is aimed to evaluate the performances of these two different potentials by means of obtaining the more accurate lattice constant in comparison with the experimental value. These interatomic potentials are also tested by using the MD simulations to reproduce the recrystallization behavior below the melting temperature. It has been found from our simulation that MEAM potential by Ko et al. [10] exhibits the better performance at low temperature.

2. Methods
In this section, the simulation details including the interatomic potentials and the simulation procedures used in this research are explained.

2.1. Interatomic potentials
We employed two types of potential in this simulation, i.e. the EAM [11,12] and the MEAM [13]. In the EAM type potential, the expression for the total energy of the system is [10]

$$E = \sum_i F_i(\bar{\rho}_i) + \frac{1}{2} \sum_{j \neq i} \phi_j(R_{ij})$$

(1)

Where is $F_i$ the embedding energy as the function of atomic electron density $\bar{\rho}_i$. Further, $\phi_j$ is the pair potential interaction between atoms $j$ and $l$ separated by a distance $R_{ij}$. In the standard EAM potential, the atomic electron density of atom $i$ is calculated from the sum of electron density of neighbouring atoms $j$,

$$\rho_i = \sum_{j \neq i} \rho_{ij}(R_{ij})$$

(2)

In order to account the directional character of bonding, MEAM potential introduce angular terms in the formulation of total atomic electron density. The total atomic electron density is obtained from the combination of partial electron density from different angular contribution with weighting factor $t^{(h)}$ in which $h = 1 – 3$. Each partial electron density is the function of atomic configuration and the atomic electron density $\rho^{a(h)}(h = 0 – 4)$,

$$\rho^{a(h)}(R) = \rho_0 \exp[-\beta^{(h)}(R/R_e - 1)]$$

(3)

Where $\rho_0$, $\beta^{(h)}$, and $R_e$ are atomic electron density scaling factor, decay lengths, and the nearest-neighbor distance in the equilibrium reference structure, respectively.

In our simulation of NiTi alloys, the EAM parameters have been generalized by Zhou et al. [9], while the MEAM parameters have been obtained from Ko et al. [10].

2.2. Simulation procedure
The Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) package [14] has been used to carry out the simulation. The total energies of the system have been calculated at some values of lattice constant. The system used in this calculation consist of $10 \times 10 \times 10$ unit cells of B2 crystal structure in $x$-, $y$-, and $z$-directions, respectively. It contains 2000 Ni and Ti atoms as shown in figure 1.
In order to evaluate the performance of the two interatomic potentials, we have also performed the MD simulation of the recrystallization of NiTi alloy below the melting temperature. This MD simulation has used two-phase system as the initial configuration. It has been obtained by adding a liquids structure on the top of crystal structure of NiTi alloy. The NPT Nosé-Hoover scheme [15,16] has been employed to control the pressure and the temperature of the system. The equations of motion have been numerically solved using Verlet algorithm, with the timestep of 1 fs. The simulation has been performed at the temperature of 1100 K. The equilibration has been done for 50000 MD steps. The structure of the system is investigated by using density profile analysis [17].

3. Results and Discussion

In this research, we compare the lattice constant of NiTi alloys at 0 K obtained from EAM [9] and MEAM [10] potentials. Further, we used these potentials to reproduce the recrystallization process of NiTi alloys at 1100 K to confirm their performance at high temperature.

3.1. Lattice constant of NiTi alloys

This calculation is aimed to obtain the most stable configuration of NiTi alloys using EAM and MEAM potentials. Figure 2 shows the plot of the energy $E$ of each atom for the B2 structure of NiTi alloys in some different lattice constants $a$. The lowest energy indicates that the most stable configuration has been achieved.
Figure 2. The energy $E$ of each atom as the function of lattice constant $a$. The line with solid and open circles represent the results from EAM potential of Zhou et al. and MEAM potential of Ko et al., respectively. The arrows point out to the lowest energy value at specific lattice constant obtained from each potential.

In figure 2, it is clearly seen that the most stable configuration of B2 structure of NiTi alloys are found at $a = 3.05 \text{ Å}$ and $a = 3.00 \text{ Å}$ for EAM potential by Zhou et al. [9] and MEAM potential by Ko et al. [10], respectively. The experimental value of the lattice constant of NiTi alloys in the B2 structure has been reported as $3.015 \text{ Å}$ [18]. In this case, the result from the MEAM potential by Ko et al. [10] is more accurate by approximately 0.7% than that of EAM potential by Zhou et al. [9]. We can also see in figure 2 that the lower energy is found by employing the MEAM potential for NiTi alloys. Thus, we can say that the MEAM potential by Ko et al. [10] exhibit the better performance than EAM potential by Zhou et al. [9] for the simulation of NiTi alloys at the low temperature. Since the angle-dependent terms representing the direction of atomic bond are calculated implicitly, the MEAM potential by Ko et al. [10] can produce the highly accurate result.

3.2. Recrystallization of NiTi alloys
We performed the MD simulation of two-phase NiTi alloys by employing the standard EAM potential by Zhou et al. [9] and the MEAM potential by Ko et al. [10]. The purposes of using two-phase system is that the crystal structure in the lower site should induce the recrystallization process of the liquid structure in the upper side. The simulation temperature of $T = 1100 \text{ K}$ is below the melting point of NiTi alloys reported as $1583 \text{ K}$ [19].
Figure 3. Snapshot of the atomic configuration of two-phase NiTi alloy at 1100 K. (a) The result from EAM potential of Zhou et al. and (b) the result from MEAM potential of Ko et al. Blue and gray balls represent Ni and Ti atoms, respectively.

Figure 3 shows the snapshot of the atomic configuration of two-phase NiTi alloys after the equilibration for 50 ps at 1100 K. It can be seen clearly that the upper structure of the result from EAM potential of Zhou et al. [9] are more in order than the that from MEAM potential by Ko et al. [10]. Further, the more detail structural investigation is done by using atomic density analysis as shown in figure 4.

Figure 4. Average density profile of two-phase NiTi alloy at 1100 K. (a) The result from EAM potential of Zhou et al. and (b) the result from MEAM potential of Ko et al.
From figure 4, we also find from the density profile of NiTi alloy at 1100 K that the recrystallization of the system employing EAM potential by Zhou et al. [9] is almost complete. However, the irregular structure of NiTi alloy is still found in the system employing MEAM potential by Ko et al. [10], although the small parts of regular structure are found in the interface, i.e. at the $z$-position around 30 Å and 60 Å. From these results, we can say that the EAM potential by Zhou et al. [9] gives the rapid recrystallization of the NiTi alloys below the melting temperature. In this case, the comparison with quantum mechanical calculation is highly recommended in order to judge the results from these two different potentials.

4. Conclusion
We have performed the performance evaluation of standard EAM and MEAM potential for NiTi alloys developed by Zhou et al. and Ko et al., respectively. The result shows that the high accuracy of lattice constant of NiTi alloy can be achieved by using the MEAM potential of Ko et al. However, the rapid recrystallization process below the melting temperature is shown when the standard EAM potential by Zhou et al. are employed.

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