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Molecular dynamics simulation of nano-indentation on Ti-V multilayered thin films

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ABSTRACT

We developed a second nearest-neighbor modified embedded-atom method potential for binary Ti-V system. The potential parameters were identified by fitting the lattice parameter, cohesive energy and elastic constants of CsCl-type TiV, and further validated by reproducing the fundamental physical and mechanical properties of Ti-V systems with other crystal structures. In addition, we also performed molecular dynamics simulations of nano-indentation processes of pure Ti film, pure V film, and two kinds of four-layer Ti-V films, V-Ti-V-Ti and Ti-V-Ti-V. We found that the indentation force-depth curve for the pure V film turns flat at an indentation depth of 2.8 nm, where a prismatic loop was observed. Such prismatic loop is not found in the V/Ti/V/Ti multilayer because the thickness of each layer is insufficient for the formation of such prismatic loops, which accounts for the increase of stress in the multilayer.

1. Introduction

Nano-multilayered metal films and transition metal nitride films have captured increasing attention because of the possible increase in hardness compared with their monolayers. It has been reported that strength and hardness of some nano-multilayered systems can increase remarkably when their modulation period decreases to a few nanometers [1–5]. Although some explanations have been given for such enhancement in hardness, such as Hall-Petch relationship [6], modulus difference induced hardening [3], coherent stress induced hardening [7], structural barrier [3], and solid solution induced hardening [8], the dominant mechanisms remain unclear. To clarify such enhancement mechanism, the investigation to the microstructures of nano-multilayered films and their evolutions during deformation is of primary importance.

There are several experimental reports on the enhancement in the hardness of Ti-V nano-multilayers. For instance, the hardness of a Ti-V multilayer can reach 16 GPa if its modulation period is reduced to 5.6 nm [4]. On the other hand, Sina et al. reported that the hardness of Al-Ti multilayer is maximized at a modulation period of 2.5 nm [9]. In addition, hardness can also be enhanced in the Ti-Ni multilayers [10]. However, it remains difficult to obtain sufficient information on microstructure of multilayers and its evolution, which are of ultimate significance for understanding the origin of the enhancement of hardness. Molecular dynamics (MD) simulation can serve as a powerful tool in gaining insights into the microstructures of the multilayers and their evolutions during deformation, particularly at nanometer scale. However, a proper potential function for the Ti-V systems is still lacking, despite the importance of potential function for MD simulations.

A second nearest-neighbor modified embedded atom method (2NN MEAM) potential is developed for the Ti-V binary system based on physical and mechanical properties obtained by first-principles calculations, with which MD simulations of the indentation on two kinds of Ti-V multilayers are conducted and the mechanisms for the hardness enhancement of the multilayers are clarified. For comparison, the MD simulations of the indentations on pure V and pure Ti specimens are also performed, and the microstructures and their evolutions during indentations are investigated.

2. Interatomic potential

2.1. 2NN MEAM potential for Ti-V system

The second nearest-neighbor modified embedded-atom method (2NN MEAM) potentials are adopted for the binary Ti-V system. The 2NN MEAM potentials for the Ti-Ti and V-V systems were provided by Kim et al. [11] and Lee et al. [12]. However, the 2NN MEAM potential

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Table 1
Parameters in the 2NN MEAM potential for Ti with a HCP structure and V with a BCC structure [11,12]. The E_c, r_e, α, A, β, t, C, and d represents the cohesive energy, the distance between nearest neighbor atom in equilibrium state, the exponential decay factor, the scaling factor for embedding energy, the exponential decay factor, the weight factor for the atomic density, the screening parameter, and the adjustable parameter, respectively.

	E_c (eV)	r_e (Å)	α	A	$\beta^{(0)}$	$\beta^{(1)}$	$\beta^{(2)}$	$\beta^{(3)}$	$t^{(0)}$	$t^{(1)}$	$t^{(2)}$	$t^{(3)}$	C_{min}	C_{max}	d
Ti	4.87	2.920	4.72	0.66	2.7	1.0	3.0	1.0	1.0	6.8	−2.0	−12.0	1.00	1.44	0.0
V	5.3	2.625	4.81	0.73	4.74	1.0	2.5	1.0	1.0	3.3	3.2	−2.0	0.49	2.80	0.0

Table 2
Parameters used in the 2NN MEAM potential for Ti-V.

E_c (eV)	R_e (Å)	B (GPa)	C_{min}				C_{max}				d	ρ_0^{Ti}/ρ_0^V
			Ti-Ti-V	V-V-Ti	Ti-V-V	Ti-V-Ti	Ti-Ti-V	V-V-Ti	Ti-V-V	Ti-V-Ti		
5.085	2.7	130	0.1	0.1	1.1	1.1	1.44	0.6	2.8	2.8	0	0.9

Table 3
Physical and mechanical properties of the TiV with a CsCl structure calculated with MD and FPC. The E_c, a, α, C_{ij}, and B represent the cohesive energy, the lattice constant exponential decay factor, the elastic constants, and the bulk modulus.

Property	MD	FPC	Other FPCs
E_c (eV)	5.085	–	–
a (Å)	3.08	3.08	3.280[a]
C_{11} (GPa)	168	169	169.6[a]
C_{12} (GPa)	108.9	120	122.3[a]
C_{44} (GPa)	38.1	22	33.6[a]
B (GPa)	128	138	–

[a] Ref. [22].

Table 4
Lattice constant a and cohesive energy E_c for the ZnS-, NaCl-type TiV, D03-type Ti_3V and the D03-type TiV_3.

Structure	Property	MD	FPC
NaCl	E_c (eV)	−6.614	−6.5997
	a (Å)	4.904	4.949
ZnS	E_c (eV)	−5.903	−4.9565
	a (Å)	4.900	5.188
Ti_3V	E_c (eV)	−6.742	−7.833
	a (Å)	3.032	3.273[a]
TiV_3	E_c (eV)	−6.742	−8.785
	a (Å)	3.032	3.306[a]

[a] Ref. [22].

for the binary Ti-V system are not available. In a 2NN MEAM potential, the total energy can be expressed as [13–17]:

$$E = \sum_i [F_i(\overline{\rho}_i) + \frac{1}{2}\sum_{j\neq i} S_{ij}\Phi_{ij}(R_{ij})] \quad (1)$$

where $F_i(\overline{\rho}_i)$ is the embedded function for the atom i embedded in a background electron density $\overline{\rho}_i$; S_{ij} and Φ_{ij} are respectively the screening function and the pair interaction between the atoms i and j separated by a distance of R_{ij}. A specific form of $F_i(\overline{\rho}_i)$ has been suggested by Lee et al. [14]. Φ_{ij} can be obtained with the following method.

For the Ti-V system, the stable B2 configuration is chosen as a reference structure, where the energy per atom (0.5 Ti atom+0.5 V atom) can be expressed as

$$E^U_{TiV}(R) = \frac{1}{2}F(\overline{\rho}_{Ti}) + \frac{1}{2}F(\overline{\rho}_V) + \frac{z_1}{2}\Phi_{TiV}(R) + \frac{z_2}{2}(\frac{1}{2}S_{Ti}\Phi_{TiTi}(aR) + \frac{1}{2}S_V\Phi_{VV}(aR)) \quad (2)$$

in which z_1=8 and z_2=6 are the number of the first and the second nearest neighbor atoms, respectively, and a is the ratio of the second nearest neighbor distance to the first one in the reference structure. The pair interaction between Ti and V atoms can be solved from Eq. (2) as

$$\Phi_{TiV}(R) = \frac{2}{z_1}E^U_{TiV}(R) - \frac{1}{z_1}F(\overline{\rho}_{Ti}) - \frac{1}{z_1}F(\overline{\rho}_V) - \frac{z_2}{z_1}(\frac{1}{2}S_{Ti}\Phi_{TiTi}(aR) + \frac{1}{2}S_V\Phi_{VV}(aR)) \quad (3)$$

where the embedded functions $F(\overline{\rho}_{Ti})$ and $F(\overline{\rho}_V)$ can be calculated, the pair functions $\Phi_{VV}(aR)$ and $\Phi_{TiTi}(aR)$ follow those of individual elements [11,12], $E^U(R)$ is the universal state equation and can be expressed with [18]

$$E^U(R) = -E_c(1 + a^* + da^{*3})e^{-a^*} \quad (4)$$

where

$$a^* = \alpha(\frac{R}{r_e} - 1) \quad (5)$$

$$\alpha = \sqrt{\frac{9B\Omega}{E_C}} \quad (6)$$

d is an adjustable parameter, and r_e, E_c, B and Ω are the equilibrium nearest neighbor distance, cohesive energy, bulk modulus and volume of the B2 Ti-V, respectively.

2.2. Identification of parameters in potentials

The parameters in the 2NN MEAM potential for both Ti and V are taken from the work by Kim et al. [11] and Lee et al. [12], respectively, as listed in Table 1. In Eq. (4), the E_c, B and Ω ccn be obtained from first-principles calculation, and the d could be determined by averaging those of the two pure materials (Table 1). In Table 1, there are two screening function parameters C_{max} and C_{min} for each of the two individual elements, which determine the screening extent of the atom k to the interaction between the two neighboring atoms i and j. For monoatomic materials, the three neighboring atoms have the same type (i-j-k=A-A-A or B-B-B). For a binary system composed of atom A and B, there are four sets of arrangements, i.e. i-j-k=A-B-A, B-A-B, A-A-B and A-B-B, indicating that eight screening parameters should be determined. These eight parameters can be determined in two stages, the global and the local stages [19,20]. The insensitive parameters, which less affect the physical and mechanical properties of the reference structures, can be determined in the global stage with conventional mix-rule [21], while the sensitive parameters should be identified in the local stage by fitting the physical and mechanical properties of the binary system. Another parameter that should be identified is the atomic electron density ρ_0 in the equilibrium reference