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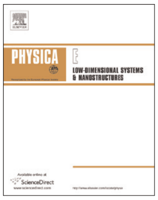

First-principles calculation and molecular dynamics simulation of fracture behavior of VN layers under uniaxial tension

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HIGHLIGHTS

- The 2NN MEAM potential of VN presented can reproduce fundamental physical properties of V–N system of other phases.
- MD simulation of the deformation and fracture of VN layers under tension showed that fracture occurs when broken bonds regions grow and coalesce to larger defects.
- Temperature may reduce the energy applied for deformation and failure of V–N systems.
- No dislocation and slip were detected in the VN layers during deformation.

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ABSTRACT

We develop the second nearest-neighbor modified embedded atom method (2NN MEAM) potential for vanadium nitride (VN) in terms of the individual vanadium and nitrogen. The potential parameters are determined by fitting the cohesive energy, lattice parameter, and elastic constants of the VN with the NaCl-type structure, which are obtained by first-principles calculations. We find that the developed potentials can be used to describe the fundamental physical properties of the V–N system with other lattice structures. The calculated tensile stress–strain curves of the VN layers by first principles agree with those obtained by molecular dynamic simulations, validating the use of the developed potential. The bond breaking and its growth and coalescence are found to play an important role in the formation of fracture. We also find that temperature influences markedly the breaking of bonds, which can be attributed to the deviation of atoms from their equilibrium positions due to the thermal activated vibration, or to the superposition of the thermal energy to the deformation energy. Moreover, no dislocations and slips are found throughout the deformation process.

1. Introduction

Transition metal nitrides, vanadium nitride (VN) and titanium nitride (TiN), have attracted a great deal of attention due to their excellent physical and mechanical properties, including high melting points, high hardness, high electrical conductivity, high resistance against corrosion and oxidation [1]. These excellent properties are suitable for a wide range of applications, such as the coatings for surface protection of cutting tools and thin films for electronic devices [2–4]. It has been found that TiN/VN nano-multilayered coatings, which are composed of alternatively arranged TiN and VN layers of nanometer thickness, possess a hardness of over 56 GPa, much higher than that of each respective nitride constituent [5]. However, the origin underneath the improvement of hardness for the TiN/VN nano-multilayered coatings remain not understood yet. To date, several explanations to the superhardness of the nano-multilayered coatings have been proposed such as the dislocation pile-up at the interface [6,7], the Hall–Petch effect [8], the strain mismatch effect at the interface [9], and the super-modulus effect [10]. Nevertheless, none of them has been confirmed.

To clarify the superhardness mechanism for nano-multilayered nitride coatings, it is requisite to understand the deformation and failure behavior of each respective transition metal nitride. This

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requires in-depth knowledge on microstructures of the nano-multilayered coatings, especially at the atomic scale. However, such microstructures are often difficult to obtain experimentally, yet can in principle be captured through theoretical calculations [11]. First-principles calculation represents a powerful tool to obtain accurate ground-state energies and fundamental physical and mechanical properties of materials at the atomic scale. It has already been used to investigate elastic properties (e.g. bulk modulus, elastic constants, and Young's modulus) [12–17], surface energy [18,19], phase stability [20–22], and electronic structures [23–26] of the V–N systems, as well as the bonding configuration and bond length change of nano-multilayer nitride coatings during deformation [27,28]. It has been realized that the strength and hardness testing can reveal inelastic deformation and failure behavior, thereby allowing us to gain insights into the structure–property interplay. For instance, the uniaxial tension tests along different crystallographic orientations have been simulated on the first-principles levels [23,29], but such simulations are usually performed using such a small sample that it may not possible to identify defects and their evolution during the simulation process. On the other hand, the temperature effect has to be considered.

Molecular dynamics (MD) simulations can also be applied to investigate behavior of materials, taking into account the effect of temperature. However, to the best of our knowledge, there is still no available interatomic potential for the binary V–N system, thus limiting the use of MD simulation. Here, we develop a second nearest-neighbor modified embedded atom (2NN MEAM) potential for the V–N system by fitting the results from the first-principles calculations. We apply both the first-principles calculations and MD simulations to clarify the deformation and failure mechanism of the VN thin layers subjected to a uniaxial tension at 0 K, 1 K and 293 K. The failure mechanism of the VN layers under uniaxial tension is discussed.

2. NN MEAM interatomic potential of VN

2.1. Potential formalism

In the MEAM, the total potential energy of a system can be expressed as [30–33],

$$E = \sum_i \left[F_i(\bar{\rho}_i) + \frac{1}{2} \sum_{j(\neq i)} S_{ij} \phi_{ij}(R_{ij}) \right], \tag{1}$$

where $F_i(\bar{\rho}_i)$ is the contribution from the atom i embedded in a background electron density $\bar{\rho}_i$, S_{ij} and $\phi_{ij}(R_{ij})$ are respectively the screening function and the pair-interaction between the atoms i and j distant by R_{ij}. The introduced S_{ij} differs from that in the conventional embedded-atom method (EAM). In the original MEAM [32], only the first nearest-neighbor (1NN) interactions are taken into account together with a strong multi-body screening function. The influence from the second and more distant atoms is neglected [34]. The details of the 2NN MEAM formalism can be found elsewhere [35].

A proper description for the interactions between different elementary atoms plays a key role in addressing a binary alloy system. For the binary V–N system, the NaCl-type structure is chosen and its total energy per atom (0.5 V atom+0.5 N atom) can be expressed as,

$$\begin{aligned} E^u_{VN}(R) &= \frac{1}{2}\Big[F_V(\bar{\rho}_V) + F_N(\bar{\rho}_N) + Z_1 \phi_{VN}(R) \\ &\quad + \frac{Z_2}{2}\big(S_V \phi_{VV}(aR) + S_N \phi_{NN}(aR) \big) \Big], \end{aligned} \tag{2}$$

where $Z_1=6$ and $Z_2=12$ are the numbers of the first and the second nearest-neighbors in NaCl-type VN, respectively, S_V and S_N are the screening functions for the second nearest-neighbor interactions between the V atoms and between the N atoms, respectively, and a is the ratio of the second nearest-neighbor distance to the first nearest-neighbor distance. The pair interactions between V and N atoms can be described by

$$\begin{aligned} \phi_{VN}(R) &= \frac{1}{Z_1}\Big[2E^u_{VN}(R) - F_V(\bar{\rho}_V) - F_N(\bar{\rho}_N) \\ &\quad - \frac{Z_2}{2}\big(S_V \phi_{VV}(aR) + S_N \phi_{NN}(aR) \big) \Big]. \end{aligned} \tag{3}$$

The embedding functions (F_V, F_N) and the pair interactions (ϕ_{VV}, ϕ_{NN}) can be computed with the potentials of the individual elements. In order to determine the $E^u_{VN}(R)$, the following universal equation of state [36] is considered for the NaCl-type VN,

$$E^u(R) = -E_c\left(1 + a^* + d a^{*3}\right) e^{-a^*}. \tag{4}$$

where the d is an adjustable parameter, and

$$a^* = \left(\frac{9B\Omega}{E_c}\right)^{1/2} \left(\frac{R}{r_e} - 1\right), \tag{5}$$

in which the B, Ω and r_e are the bulk modulus, the atomic volume and the equilibrium distance of the nearest-neighbor in the reference structure, respectively.

2.2. Identification of parameters in the potential for the V–N systems

Table 1 lists the parameters in the MEAM potential for pure V and N [32,37]. As described in the previous section, the determination of the pair interaction between different types of atoms is of crucial importance in applying the MEAM potential to an alloy system. The material parameters E_c, r_e, B and the adjustable parameter d are the main parameters in the MEAM potential for an alloy system. The E_c, r_e and B can be determined from the first-principles calculations, and the d can be obtained by taking an average of those of the two pure elements (Table 1). From Table 1, one can see that each element has its own screening function parameters of C_{min} and C_{max}, which determine the screening extent of the atom k to the interaction between two neighboring atoms i and j. The three atoms are of the same type (i–j–k=A–A–A or B–B–B). For a system with two different types of elementary

Table 1
Parameters in the MEAM potentials for the pure V with BCC structure and N with DIMER structure. The E_c(eV), r_e(Å), α, A, β, t, C, and d denote the cohesive energy, lattice parameter in equilibrium state, exponential decay factor, scaling factor for the embedding energy, exponential decay factor, weigh factor for the atomic densities, screening parameter, and 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
V	5.30	2.625	4.81	0.73	4.74	1.00	2.50	1.00	1.00	3.30	3.20	−2.00	0.49	2.80	0
N	4.88	1.100	5.96	1.80	2.75	4.00	4.00	4.00	1.00	0.05	1.00	0.00	2.00	2.80	0