



First-principles calculations on interface structure and fracture characteristic of TiC/TiZrC nano-multilayer film based on virtual crystal approximation

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ABSTRACT

TiC (100)/TiC (100) interface and TiC (100)/TiZrC (100) interface were studied by first-principles calculation based on virtual crystal approximation for developing the novel TiC/TiZrC nano-multilayered film. Surface convergence calculation result demonstrates that both TiC slab and TiZrC slab with more than five atom-layers exhibit bulk-like interiors. Geometry models of TiC (100)/TiC (100) interface and TiC (100)/TiZrC (100) interface with different termination structures were constructed. The calculated interfacial work of adhesion and relaxed interfacial distance show that for both TiC (100)/TiC (100) interface and TiC (100)/TiZrC (100) interface, Ti-C termination structure is always more stable than C-C termination structure. The reason is that the Ti-C termination structure can maintain the alternating stacking of cations and anions at interface. Moreover, because that the covalent bonding strength and ionic bonding strength of TiC (100)/TiC (100) interface are larger than those of TiC (100)/TiZrC (100) interface, TiC (100)/TiC (100) interface shows the stronger interface stability. The tensile fracture process indicates that for TiC (100)/TiC (100) interface, the fracture occurs between the 2' and 1' layers in TiC (100) slab. While for TiC (100)/TiZrC (100) interface, the fracture occurs at the interface. Moreover, the sustainable imposed stress of TiC (100)/TiC (100) interface is much higher than that of TiC (100)/TiZrC (100) interface.

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1. Introduction

Nowadays, nano-multilayer film has been widely used in the fields of machining and aerospace because of the special superhardness effect [1]. In the early days, all the nano-multilayer films are composed of two or more kinds of nitrides [2–4]. With the development of the solid crystallization technology, various materials have been used as the modulation layers of nano-multilayer films [5,6], but the template layers are still mainly nitrides [7].

In recent years, the expansion of template layer material system is an important research direction for developing the novel nano-multilayer film. Some researchers have successfully expanded the template layer from nitrides to carbides. Li [8] prepared

TiC(template layer)/B₄C(modulation layer) nanomultilayer film, and indicated that when the thickness of B₄C layer is less than 0.5 nm, the film attains the highest hardness of 40.1 GPa. Fox-Rabinovich [9] investigated the microstructure and mechanical properties of TiC/TiN nanomultilayer film, and showed that the film has the highest microhardness when the crystallite structure is columnar. Dong [10] prepared TiC/VC nano-multilayer film, and indicated that TiC/VC superlattice can form an epitaxial structure when the modulation period is less than 5.2 nm, resulting the large hardness and elastic modulus.

On the basis of previous researches, our team prepared the novel TiC/TiZrC nano-multilayer film using magnetron sputtering technology. The results showed that when Zr/Ti atomic ratio in TiZrC is 13:87 (Ti_{0.87}Zr_{0.13}C), the TiC/TiZrC nano-multilayer film attains the highest hardness of 46.3 GPa. However, although the superhardness effect for this new nano-multilayer film is excellent, the bonding strength is weak. Therefore, it is crucial to investigate the interfacial properties of TiC/TiZrC interface for researching the

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essential reason of the obvious disadvantage.

First-principles calculations based on density functional theory (DFT) is an important method for micro-investigation at the atomic scale, which has been widely used in the research on interfacial properties. Yang [11] investigated the interfacial properties of NbC/NbN nano-multilayer films by first-principles calculations, and indicated that the interfacial properties are influenced by both termination structure and stacking sequence. Ivashchenko [12] employed first-principles calculations on researching the properties of TiN/SiN_x interfaces, and showed that the hardness of ≥ 100 GPa should be possible if the amount of impurity decreases to 100 ppm. Sakhraoui [13] studied the structural, electronic and magnetic properties of the new generation FeRh/MgO (001) magnetic film, and believed that both Fe-/Rh-terminations are stable.

In this work, TiC (100)/TiZrC (100) interface, which has the smallest mismatch and shows the strongest representative in TiC/TiZrC interface system, was investigated. Meanwhile, the TiC (100)/TiC (100) interface was set as the control group. Subsequently, the interfacial atomic structure, work of adhesion, charge distribution and tensile fracture process of the two interfaces were calculated and compared using first-principles calculations. The results can figure out the interfacial properties of TiC (100)/TiZrC (100) interface, and then provides the physical basis to remedy the disadvantage on bonding strength of the novel TiC/TiZrC nano-multilayer film.

2. Methodology and details

DFT (density functional theory) with ultrasoft pseudopotential is employed in the CASTEP (Cambridge Sequential Total Energy Package) mode, which utilizes plane-wave pseudopotential to perform first-principles quantum mechanics calculations [14,15]. GGA-PBE, GGA-WC, GGA-PBESOL, GGA-RPBE and GGA-PW91 functional were employed as exchange-correlation functional [16–19].

In order to check the validity of the computation method, as well as to estimate the necessary layer numbers of bulk-like slabs *N* used in subsequent interface systems, the bulk and surface properties of slabs were investigated and the results were compared with available experimental results [20,21].

The kinetic cutoff energy *E_c* and *k*-point were increased until the calculated energy converges within the required tolerance. *E_c* determines number of plane waves and *k*-point does the sampling of the irreducible wedge of the Brillouin zone [22,23]. In this work, *E_c* was set to 340 eV consistently, while *k*-point was set to $7 \times 7 \times 7$ for bulk, and $7 \times 7 \times 1$ for surface and interface. Meanwhile, the atoms were relaxed to achieve the minimum total energy of the system to fulfill the geometry optimization, the convergence tolerances were set as energy for 1.0×10^{-5} eV/atom, maximum force for 0.03 eV/Å, and maximum displacement for 1.0×10^{-3} Å.

3. Bulk and surface calculations

3.1. Bulk properties

The crystal structure of TiC is shown in Fig. 1. From Fig. 1, TiC shows face-centered cube crystal structure with FM-3M space group, and each TiC cell contains eight atoms. In order to assess the accuracy of the computation method in this work, in particular of the pseudopotentials used, a series of calculations on the bulk properties of TiC were performed by GGA-PRBE, GGA-WC, GGA-PBESOL, GGA-PW91 and GGA-PBE. The results were compared with published experimental results.

The calculated bulk properties including lattice constant '*a*', bulk modulus '*B₀*' and formation energy '*E_{for}*'. The lattice constant '*a*' and

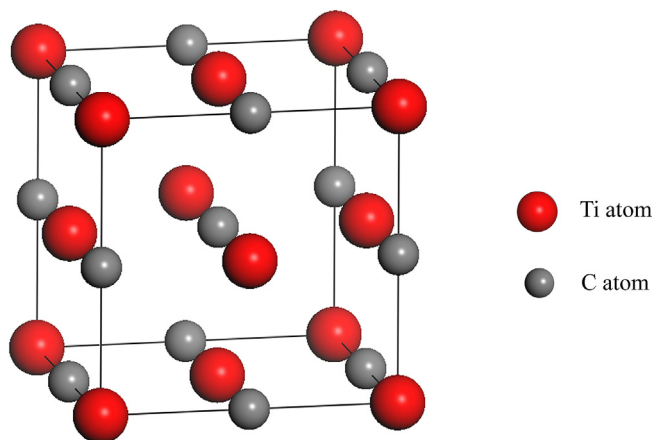


Fig. 1. Crystal structure of TiC.

bulk modulus '*B₀*' can be obtained directly, and the formation energy '*E_{for}*' can be calculated by Eq (1) [24]:

$$E_{for}^{TiC} = \frac{1}{m+n} (E_{TiC}^{bulk} - mE_{Ti}^{bulk} - nE_C^{bulk}) \quad (1)$$

in which, E_{TiC}^{bulk} is the bulk energy of TiC, E_{Ti}^{bulk} and E_C^{bulk} are the energies of the constituent elements, with all substances in their standard states at 1 atm: bulk Ti and bulk C; *m* and *n* are the numbers of Ti atom and C atom in a TiC unit cell.

The calculated lattice constant '*a*', bulk modulus '*B₀*' and formation energy '*E_{for}*' of TiC by different functional within the GGA approach are listed in Table 1. From Table 1, the calculated '*a*', '*B₀*' and '*E_{for}*' of TiC by GGA-RPBE are 4.291 Å, 251 GPa and −0.83 eV/atom. While from experimental results [25–27], '*a*', '*B₀*' and '*E_{for}*' are 4.328 Å, 267 GPa and −0.88 eV/atom. Therefore, GGA-RPBE results show the errors of 0.85%, 6.0% and 5.68%, respectively. Moreover, the errors of GGA-WC results are 1.34%, 6.74% and 4.55%, and those of GGA-PBESOL results are 0.53%, 6.0% and 7.95%.

It's worth noting that GGA-PW91 results and GGA-PBE results are closest to the experimental results. The errors of GGA-PW91 results on '*a*', '*B₀*' and '*E_{for}*' are 0.34%, 1.87% and 3.47%, while those of GGA-PBE results are 0.21%, 3.37% and 2.27%, respectively. It is obvious that GGA-PW91 method shows the greater accuracy than GGA-PBE method in calculating elasticity modulus, while GGA-PBE method has an advantage in optimizing structure and calculating energy. Considering that this work only involves the interface structure and energy without elastic modulus calculation, GGA-PBE was selected as the exchange-correlation functional in the further calculations.

3.2. Virtual-crystal approximation

As above mentioned, Zr/Ti atomic ratio in TiZrC is only 13:87, so

Table 1

Calculated lattice constants '*a*', Bulk modulus '*B₀*' and formation energies '*E_{for}*' of TiC compared with published experimental (Expt.) results.

	<i>a</i> (Å)	<i>B₀</i> (GPa)	<i>E_{for}</i> (eV/atom)
GGA-RPBE	4.291	251	−0.83
GGA-WC	4.386	249	−0.84
GGA-PBESOL	4.351	251	−0.81
GGA-PW91	4.343	262	−0.91
GGA-PBE	4.337	258	−0.86
Expt.	4.328 [25]	267 [26]	−0.88 [27]

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