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# Atomic structures and electronic properties of interfaces between aluminum and carbides/nitrides: A first-principles study

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ABSTRACT

We perform a first-principles investigation of the atomic structures and electronic properties of interfaces between aluminum and four kinds of ceramics, TiC, TiN, VC and VN, under three orientations (001), (110) and (111). We find that the stable interfaces are those with bonding between Al atom and metalloid C (or N) atom, which is attributed to the overlap of *p* states of Al and *d* states of metalloid atoms at Femi level forming covalent components. Among the interfaces with the three orientations, the (111) interfaces are found to possess the largest adhesion energy in that the stacking of atoms follows intrinsic atomic distribution and this interfacial bonding is relatively strong. It is also found that the interfaces between Al and metal carbides (TiC and VC) are more stable than those between Al and metal nitrides (TiN and VN).

## 1. Introduction

Metal-ceramic multilayers have been receiving increasing research interests due to their excellent mechanical properties, high thermal stability and good electrical conductivity [1,2]. It is well known that metallic materials possess high ductility yet low strength, while ceramics often possess high strength and hardness yet low ductility. To date, it has been reported that a certain selective metal-ceramic multilayers are able to take full advantages of the two sorts of materials. For example, Bhattacharyya et al. [1] found that the nano-multilayered Al-TiN micropillars can possess remarkable hardness, high flow strength and high compressive deformability. In general, such plastic deformation in multilayers usually occurs in single layers between adjacent interfaces, and it is often accompanied by nucleation, glide, and transmission of dislocations, all of which rely strongly on structure and property of interfaces [2]. In addition, the interfaces can serve as barriers against movement of dislocations, resulting in strengthening and hardening of a material, and those with high diffusivity and low formation energy can reduce stress concentration, contributing to high plastic flow stability in multilayers [3–5].

First-principles calculation is thought as an effective mean to predict material properties, with which a lot of available results have been achieved. Siegel et al. [6–9] investigated the adhesive properties of specifically oriented interfaces between metals and carbides/nitrides, and revealed that the covalent Al-C/N bonds dominate mechanical properties of the interfaces. Liu et al. [10–12] investigated properties of the Al-TiN/TiC interface with a (001) orientation and showed that Ti-terminated interfaces are controlled by metallic and weak covalent bonds, whereas the N-terminated interfaces are mainly composed of polar covalent bonds. Sun et al. [13–15] investigated adhesive and mechanical properties of Al-TiC interfaces and the effects of Mg, Zn, Cu, Fe and Ti dopants, and showed that Fe and Ti can enhance the adhesive property of interfaces, while Mg and Zn show a negative impact in terms of adhesion. They also found that Mg, Fe and Ti can improve ductility of the interfaces. Yadav et al. [16] conducted first-principles calculation of the thermodynamic stability and the ideal tensile and shear strengths of Cu(111)/TiN(111) and Al(111)/TiN(111) interfaces, and showed that the Al/TiN interface have strong orientation preference determined by Al-N bonding at interface, yet such orientation preference has not been found for the Cu/TiN interface. Moreover, they found that both ideal tensile and shear strengths of Cu/TiN interfaces are lower than those of bulk Cu and TiN, suggesting that Cu/TiN interfaces are weaker than their bulk constituents, and thus highlighting the significance of interface in determining the mechanical properties of nanolayered structures.

However, in current researches the ceramics involved are usually metal oxides ($Al_2O_3$, $Y_2O_3$), metal nitrides (VN, TiN, ZrN, AlN), metal carbides (VC, TiC, SiC) and metal borides ($ZrB_2$, $AlB_2$) and the metals

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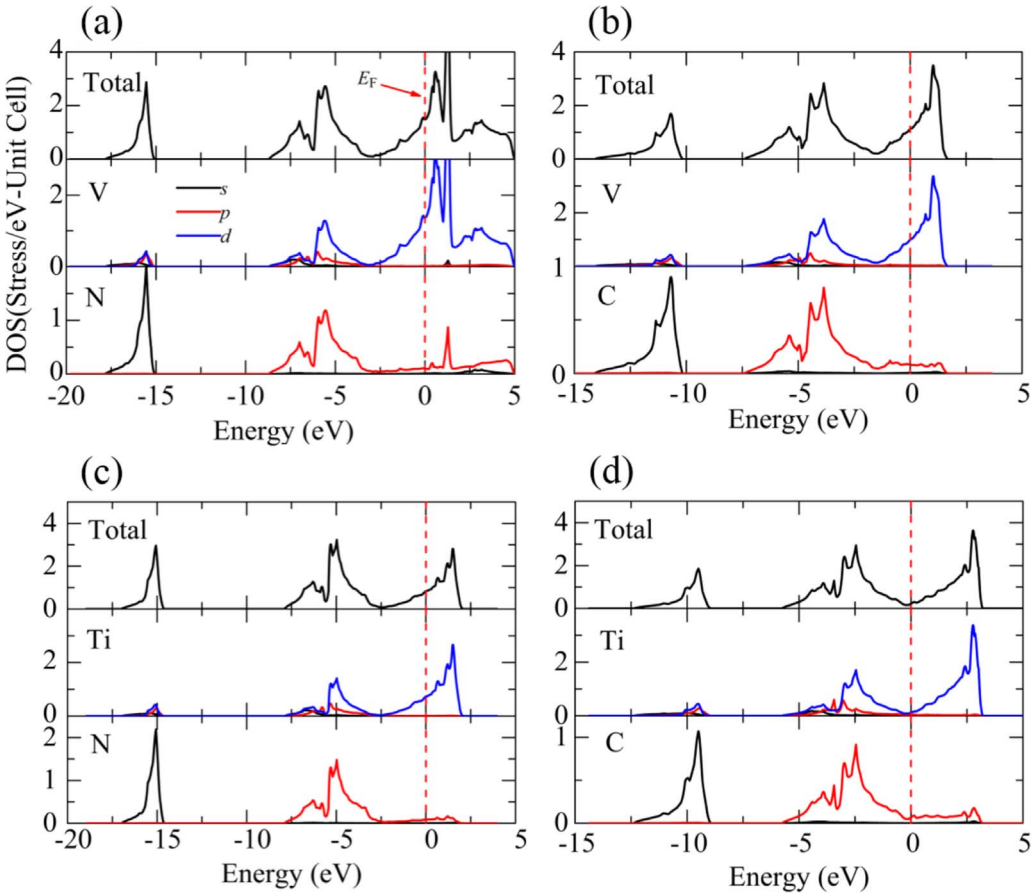


**Fig. 1.** Total and partial densities of states for the (a) VN, (b) VC, (c) TiN and (d) TiC bulks. Fermi level ($E_F$) is placed at zero and represented by vertical dashed lines.

**Table 1**
Surface energies ($W_{surf}$) for the slabs with different numbers of layers, $n$=3, 5, 7, 9, 11 and 13.

| Number of layers | 3 | 5 | 7 | 9 | 11 | 13 |
|---|---|---|---|---|---|---|
| $W_{surf}$ (J/m$^2$) | 1.557 | 1.513 | 1.507 | 1.502 | 1.502 | 1.501 |

involved are Al, Cu, Ti and Fe [6–25]. In addition, previous attention has mainly been paid to several particular orientation relationships at interfaces. Here, we perform a first-principles study of microstructures and electronic properties at the interfaces between aluminum and four ceramics, TiC, TiN, VC and VN, aimed at identify stable interfaces and the main factors that affect their mechanical properties. We select a reasonable relaxation model to calculate of deposition of Al atoms on (001), (110) and (111) surfaces of TiC, TiN, VC and VN substrates in order to reveal the formation mechanisms of interfaces. We also investigate the effects of shape and size of the cell used in the calculation, the stacking sequence of metallic and metalloid atoms at the interface, and the electronic properties of interfaces.

## 2. Calculation methods

Calculations were conducted with Vienna Ab-initio Simulation Package (VASP) within the framework of density function theory (DFT). The generalized gradient approximation by Perdew and Wang (GGA-PW91) [26] was used to address the exchange-correlation energy [27,28]. The pseudo-potentials based on the electronic configurations of $3d^24s^2$ for Ti, $3d^34s^2$ for V, $2s^22p^2$ for C, $2s^22p^3$ for N, and $3s^23p^1$ for Al were used to describe the electron-ion core interactions. Single-particle Kohn-Sham wave function was expanded using plane waves with a cut-off energy of 500 eV, and sampling of irreducible edge of

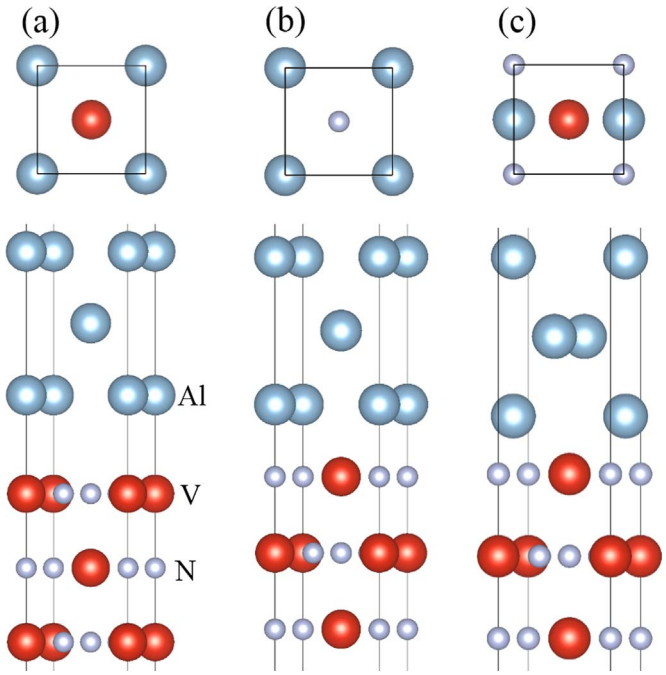


**Fig. 2.** Schematic plot of Al (001)-VN (001) interface: (a) V-site, (b) N-site and (c) Core-site. The upper figure shows top view.

Brillouin zone was performed with a regular Monkhorst-Pack scheme [29]. An 11×11×11 k-point mesh was used for bulk calculations and a 7×7×1 point mesh was used for surface and interface calculations. For the interface calculations, a 10 Å vacuum region was embedded into the