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The simulation of interface structure, energy and electronic properties of TaN/ReB_2 multilayers using first-principles

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ABSTRACT

Interface structure of TaN/ReB_2 multilayers was investigated using first-principles based on density functional theory (DFT). The hexagonal TaN and hexagonal ReB_2 were chosen in this paper, and nine different interfaces of TaN(100)/ReB_2(001) were chosen to calculate the interface energy, taking into account both N- and Ta-terminations. The interfacial electronic properties including charge density distribution, states of density (DOS) and Mulliken population were simulated to determine the nature of interface bonding. The results showed that B-N interface had the strongest bonding combined covalent bonding. The Re-N2 interface was the most stable interface. Meanwhile, Mulliken population and number of electrons of interface were calculated to predict the mechanical properties of monolithic TaN and ReB_2 coatings and TaN/ReB_2 multilayers.

1. Introduction

Superhard materials are of primary importance in modern science and technology. In recent years, there has been increasing interest in the deposition of nanocomposite and multilayers structure coatings with high hardness and elastic modulus [1–4]. Recently, hard and tough transition metal nitride and carbide alloy and interface systems have been investigated [5–9], such as WC/TiC interface [5], cubic TiWN [6], Superlattice supertoughness of TiN/MN [7], ultraincompressible tungsten carbides [8] and so on. Numerous investigations showed that Rhenium diboride (ReB_2) was considered to be one of the most promising superhard materials [10–15]. This ultra-incompressible superhard material was determined by two parameters: high valence electron density (Re has higher valence electron density) and bond covalence (short covalent B—B bond and strong Re—B bond) [11]. According to this principle, ReB_2 as the bulk superhard material was synthesized and the measurement average hardness is about of 48 GPa [14,15]. However, little studies about nanoscale multilayers based on ReB_2 were reported. According to the previous results, boride/nitride showed a really good prospect of superior mechanical properties such as exceptional hardness and lower residual stress [16,17]. Obviously, ReB_2 was considered to be one of the most promising superhard materials. Therefore, we chose ReB_2 as a basic material to constitute multilayer. At the same time, TaN was better at forming nano-crystalline characteristics in multilayers [18–20]. So, it is valuable to investigate the multilayers or nanocomposite coatings made up of ReB_2 and TaN.

For multilayers and nanocomposite films, the structure of the interfaces has a great effect on its properties. It is influenced by interface electronic and atomic reconstructions, moreover, by controlling the termination layer at the interface. At present, there have been many calculations about interfaces. For example, they have been used for mental/oxide interfaces [21–23], metal/ceramic interfaces, metal/metal carbides interfaces [24,25] and metal/metal nitrides interfaces [26,27]. So far, ceramic/ceramic interfaces have been few studied yet. The same hexagonal crystal structure of TaN and ReB_2 gives a good condition for epitaxial growth. Therefore, in order to forecast the properties of TaN/ReB_2 multilayers, we calculated the structure of TaN/ReB_2 system using density-functional theory (DFT) in this work.

We always deposit multilayers and nanocomposite coatings in Si(100) substrate, so in consideration of lattice matching, we chose TaN(100) as research subjects. According to previous studies of diboride/material interface, the diboride (001) was the most stable surface [28,29]. Besides, previous calculation of different surfaces of ReB_2 also showed the (001) was most stable [30]. In this work, we calculated the ideal adhesion energy (E_{ad}) and interface energy (γ) of several representative TaN(100)/ReB_2(001) interfaces, including three terminations of TaN by selecting the energetically preferred structure. We also investigated the nature of the interface bonds

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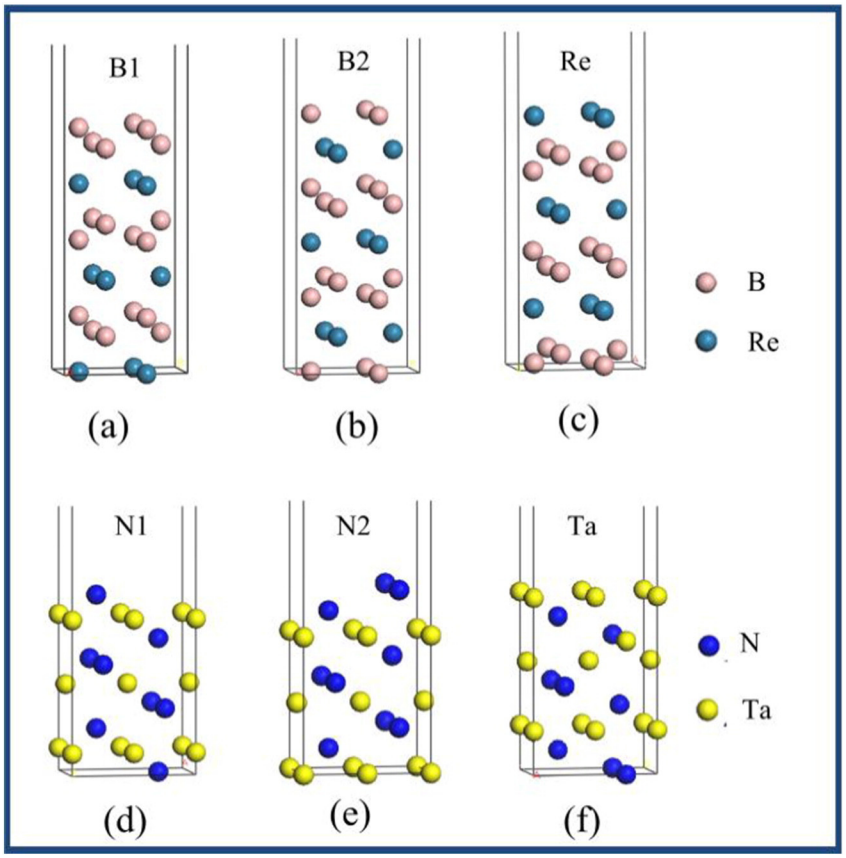

Fig. 1. Plots of ReB_2 (001) with 9 layers of atoms (a) B1-terminated, (b) B2-terminated structure and (c) Re-terminated structure and TiN(100) with 9 layers of atoms (d) N1-terminated structure , (e) N2-terminated structure and (f) Ta-terminated structure.

through the interfacial charge density, state of density (DOS), and Mulliken population using first-principles. The dipole corrections could be neglected in previous DFT calculations of polar transition metal nitride and carbide (111) surface properties [31,32] due to little effect of dipole corrections [33]. In this work, dipole corrections were also neglected.

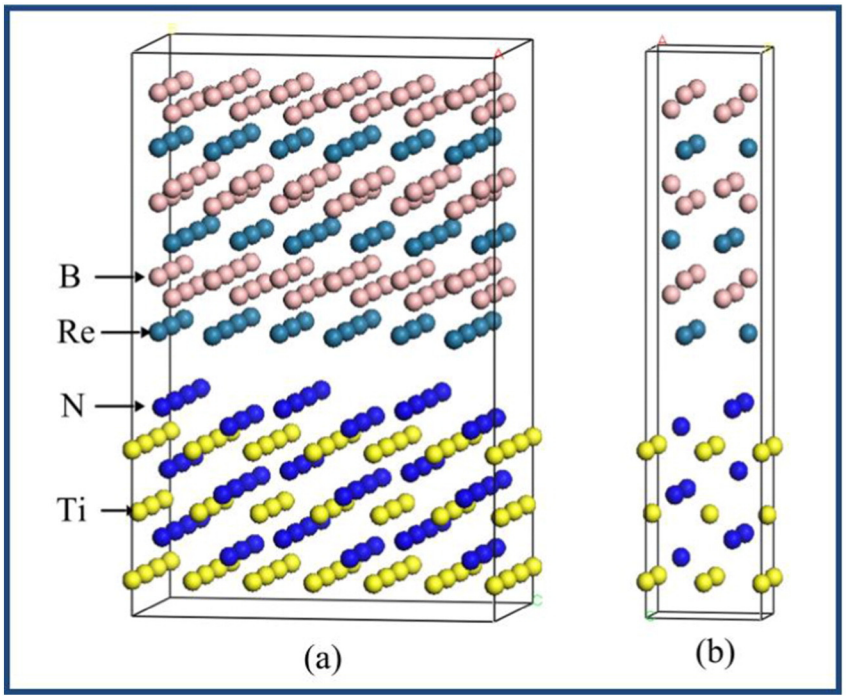

Fig. 2. Super cell (a) and unit cell (b) structure of Re-N2 interface.

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