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Alloying element's substitution in titanium alloy with improved oxidation resistance and enhanced magnetic properties

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ABSTRACT

First-principles method is used to characterize segregation and magnetic properties of alloyed Ti/TiO_2interface. We calculate the segregation energy of the doped Ti/TiO_2 interface to investigate alloying atom's distribution. The oxidation resistance of Ti/TiO_2 interface is enhanced by elements Fe and Ni but reduced by element Co. Magnetism could be produced by alloying elements such as Co, Fe and Ni in the bulk of titanium and the surface of Ti at Ti/TiO_2 interface. The presence of these alloying elements could transform the non-magnetic titanium alloys into magnetic systems. We have also calculated the temperature dependence of magnetic permeability for the doped and pure Ti/TiO_2 interfaces. Alloying effects on the Curie temperature of the Ti/TiO_2 interface have been elaborated.

1. Introduction and motivation

There are many achievements concerning the chemical doping effects on the magnetic properties of some alloys in recent years. It is reported that La doping could increase the Curie temperature of $Sr_{2-x}La_xFeMoO_6$, which is observed by means of photoemission spectroscopy [1]. Furthermore, it is found that this compound can transform into a three-dimensional antiferromagnetic metallic state through rich La doping [2]. Additionally, it is reported that substituting Nb for Mo could even enhance the extent of antisite disorder and decrease the Curie temperature [3].

In recent years, it has been observed that 3-d transition element can increase the magnetic moment of Ni-Mn based alloy. A larger magnetic moment appears if a fraction of Ni is replaced by Co [4–11]. What is more, it was observed that Ni–Fe–Mn–Sn alloys have the same phenomena [12]. From then on, the substitution of Ni in the Ni–Mn–Sn alloys with some transition elements, such as Cu, Cr and Mn, was attempted to improve the magnetic properties of Ni–Mn–Sn alloys [13–17]. The method proved to be effective. Theoretically, the alloying effect of 3-d transition element on magnetic properties in Ni–Mn–Sn alloys has also been investigated by using first-principles calculations [18]. Additionally, Gao et al. have carried out a first-principles research about the magnetic properties at TiPo(001) surface and TiPo/CdTe(001) interface. Calculated results showed that the surface atomic magnetic moments have obvious differences at Ti(Po)-terminated(001) surface compared to bulk values [19].

Alloying effects on the magnetic properties in titanium alloys have been neglected and this topic deserves investigating. In this paper, we perform a first-principles study about alloying effects on the properties of Ti/TiO_2 interface. The idea of alloying the Ti/TiO_2 interface arises from the following considerations: At first, the problem of high temperature oxidation resistance property in titanium alloys has been put forward. It is well known that alloying is an effective approach of enhancing the oxidation resistance property. Concurrently, the magnetism found in the titanium alloys may emerge as a result of the addition of some alloying elements, which should be further confirmed by theoretical and experimental methods. In this work, we have studied a possible existence of magnetism in the titanium alloys.

2. Methods

To construct the interface between titanium alloy and its oxide, (2×2) surface supercell expansions of each component are generated. The rutile TiO_2 slab is placed on top of the titanium alloy surface simply because the oxide grows on the alloy surface and must fit to the alloy. The initial starting interface structure is shown in Fig. 1.

Our calculations are mainly carried out by means of VIENNA AB INITIO SIMULATION PACKAGE [20], which describes the valence electronic states using periodic plane waves. We use Blochl's

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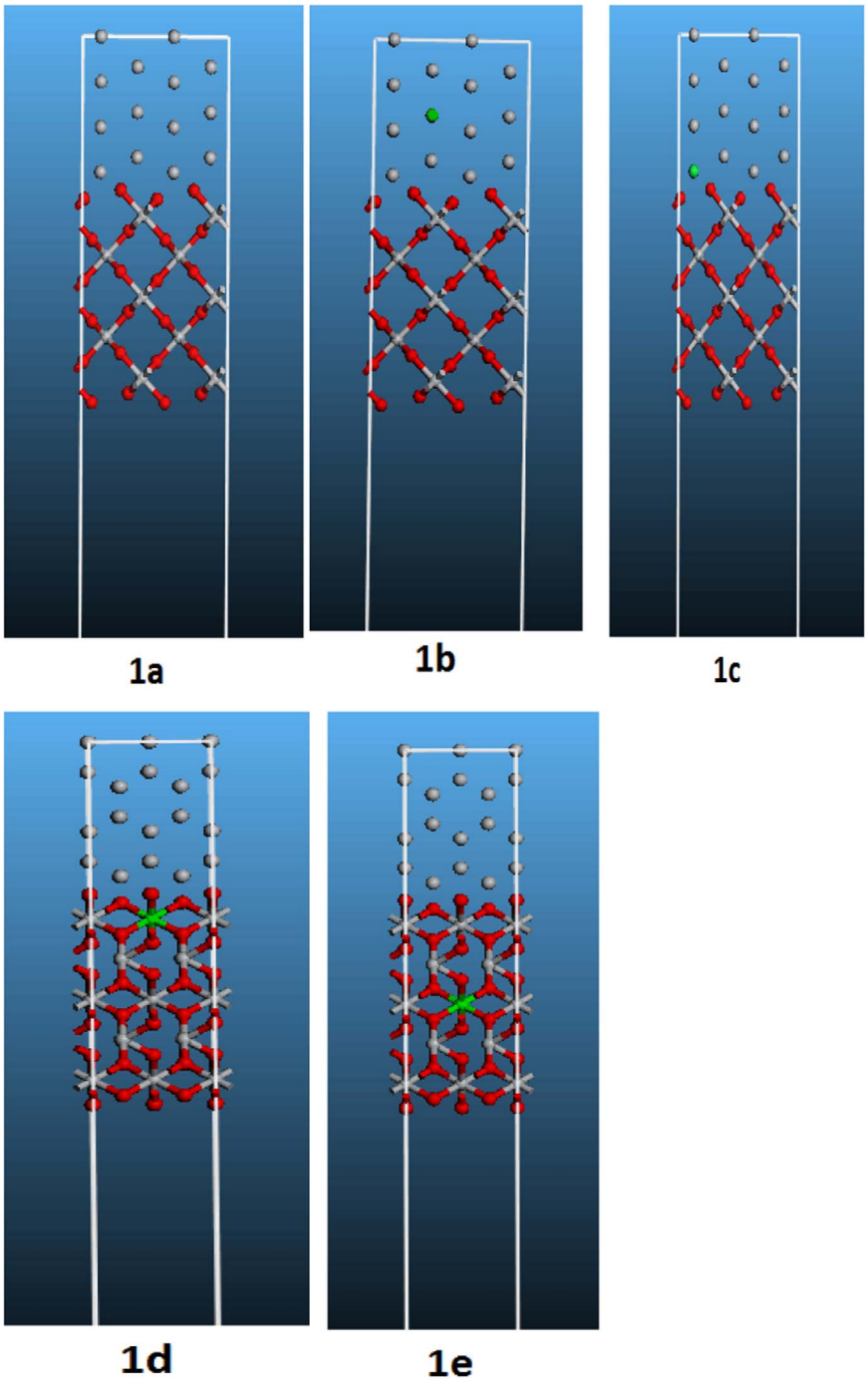

Fig. 1. A 2×2 supercell model of Ti$(10\bar{1}0)$/$TiO_2(100)$ interface (1a) and the alloyed Ti$(10\bar{1}0)$/$TiO_2(100)$ interface, with an alloying atom replacing a Ti atom in center of bulk Ti (b), the interface layer at Ti side(1c), the interface layer at TiO_2 side(1d) and in the center of bulk TiO_2(1e), respectively.

projector augmented wave (PAW) approach [21] to treat the core-valence interaction. This approach is based upon the well-known density-functional theory, in which the generalised gradient approximation to the exchange-correlation functional of Perdew-Burke-Ernzerhof (PBE) [22] is adopted. The calculations are spin polarized in order to exploit the magnetism of the investigated system.

The plane wave cut-off energy is set to be 450 eV and the convergence of the force on each atom is set to the default values in the VASP software. The vacuum space was set at 15 Å, which is sufficient enough to avoid the interactions between periodic images. The Monkhorst-Pack k-point sampling scheme [23] for the Brillouin zone is applied, in which k-point sampling chooses $(4 \times 3 \times 1)$ and $(4 \times 4 \times 1)$ for relaxation and static computation, respectively.

We have also implemented a calculation of magnetic permeability in this work. Accomplishment of such calculation has been carried out using the JMatPro programme [24].

3. Results and discussions

3.1. The analysis of segregation properties

To determine where the alloying atoms locate (in bulk Ti; bulk TiO_2; Ti side of the interface layer; or TiO_2 side of the interface