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The effect of solutes on the precipitate/matrix interface properties in the Vanadium alloys: A first-principles study

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ABSTRACT

A correct description of the interaction between solutes and interface is the prerequisite for an understanding of the evolution and growth kinetics of precipitate. In this study, we use the first-principles calculations to characterize the solute (Cr, Ti, and Y) behaviors at the TiO-precipitate/V-matrix interface in Vanadium (V) alloys. After obtaining the equilibrium interface structure, the formation heat and segregation energies for solutes (Cr, Ti, and Y) are studied in detail to obtain the site preference and segregation behaviors for solutes in the interface region. We found that solute Ti prefer to the interface site and shows a segregation tendency at the interface. To the contrary, solute Cr and Y prefer to retain in the V matrix. However, from the standpoint of energy, the site preferences for all solutes are extremely weak when no vacancy is introduced to the interface. Considering the vacancy effect, the site preference of solute Y is changing and shows a segregation tendency at the interface. We also calculate the Griffith rupture work to uncover how the solutes influence the interfacial strength with or without the vacancy effect. Solute Cr is favorable for improving the interfacial rupture strength of the V alloys no matter where solute Cr is positioned. As for solute Ti and Y, when solutes are close to the interface, the interface-weakening effect is obvious. The improvement of solutes in interfacial strength is ascribed to the increased the hybridization behaviors between the solute atom and the Ti atoms in the precipitate.

1. Introduction

Vanadium-based alloys are considered as promising first wall materials due to their low activation characteristics, remarkable high temperature strength and void swelling resistance in the fusion environment [1–3]. High number density of tiny precipitates dispersed in the matrix present the pinning effect on the dislocations glide and climb, and therefore improve the mechanical strength of V alloys. These nanoscale precipitates in V-4Cr-4Ti alloys are Ti-rich and most likely to be Ti-(O, N, C) with the NaCl structure [4]. Recently, Impagnatiello et al. [5–7] used the high-resolution electron microscopy to characterize the TiO-type precipitate and identified the monolayer-thick TiO precipitate constitutes an early stage in the radiation-induced aging process of V-4Cr-4Ti at relatively low temperatures, and therefore possesses the capacity of absorbing additional light elements in fusion reactor operation conditions. Although a number of experimental works have shown the focus on the structure properties and evolution of the precipitate. However, there is no detailed understanding of the solute behaviors near the TiO-precipitate/V-matrix interface. Considering for V-4Cr-4Ti, Cr is added to the material as an effective solid-solution strengthener that increases the thermal creep and oxidation resistance, while Ti enhances the void swelling resistance of the alloy, both of solutes are the main composition element in V-4Cr-4Ti. Moreover, addition Y not only effectively reduces O content by Y_2O_3 slag-out on the melting ingot surface [8], but also increases the elevated temperature and strain hardening exponent of V alloys [9]. Therefore, a deeper insight into the solute behaviors near the TiO-precipitate/V-matrix interface is beneficial to control the evolution of precipitate and further design the new style V alloys.

First-principles calculations are ideal tools for the study of material properties at the atomistic and electronic levels, having been used previously to investigate the solute behaviors in the precipitate/matrix interface. Gong et al. [10] found that elements near the center of the *d* block of the periodic table are more favorable for improving the rupture strength of the Ni/Ni3Al interface in single crystal Ni-based superalloys. Marquis et al. [11] used first-principles calculations to study the Mg segregation and establish the equilibrium driving force for this interfacial segregation at Al/Al3Sc interface. Recently, Shin et al. [12] present an extensive first-principles database of the segregation behaviors of 34 elements to the Al/Al_2Cu interface and identify key

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descriptors that affect the solute segregation in Cu alloys. These results show that first-principles calculations can provide efficient and reliable strategies to predict solutes behaviors, including site preferences and segregation, as well as the solute effect on the interfacial strength.

In the present paper, we make a comprehensive investigation of the structure properties of the TiO-precipitate/V-matrix interface. Meanwhile, with or without the presence of a vacancy in the interface, the formation heat and segregation energies are studied in detail to obtain the site preference and segregation behaviors for solute (Cr, Ti, and Y) in the interface region. We also calculate the Griffith rupture work to uncover that how solute influence the interfacial strength. The origin of the solute effect on the interfacial strength is discussed from the viewpoints of electronic structures.

2. Methodology

All calculations are carried out using the Vienna Ab Initio Simulation Package (VASP) [13,14] with the projector augmented wave (PAW) method [15,16] and generalized gradient approximation Perdew-Burke-Ernzerhof functional (GGA-PBE) [17]. The computations were performed with a 68-atom periodic simulation cell to model the TiO-precipitate/V-matrix interface structure (shown in the Fig. 1) and studying the solute segregation. The interface of the precipitates with the matrix is characterized by an intergrowth of the bcc V and FCC TiO structures [7]. Therefore, the coherent TiO/V interface model with three monolayers TiO are constructed using the experimentally observed orientation relationship [6] between bcc V and TiO phases. As illustrated in Fig. 1, the supercell composes of eleven V layers, each containing four V atom, and three layers of TiO, each containing four Ti atoms and four O atoms. For the interface region, the V atoms are on top of O atoms. According to previous calculation studies [18], this metal-on-inorganics configuration had been confirmed to be the most likely atomic structure corresponding to the coherent interface. We also construct the different supercell with increasing the number of layers for V matrix to consider the rationality of supercell. The results shown that the supercell with eleven layers V matrix is sufficient for obtaining the rational interface structure. Therefore, we adopt this supercell (shown in Fig. 1) to study the solute behaviors at the interface. The calculations are obtained with 500 eV plane-wave cutoff and 3 × 3 × 1 k-point meshes for the 68-atom system. Once the Hellmann-Feynman force acting on atoms is less than 0.02 eV/Å, the atoms are regarded as being fully relaxed. The present equilibrium lattice constant a_V for bulk V is 2.99 Å, which is consistent with theoretical results [19,20] and the experimental value of 3.03 Å [21].

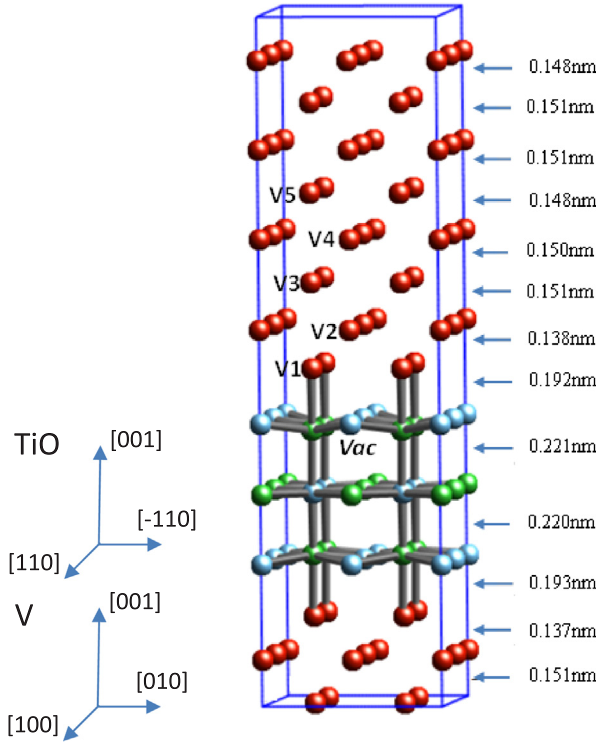

Fig. 1. Atomic structure used in the present first-principles calculations for coherent interface between the V matrix and TiO precipitate after a complete relaxation of all degrees of freedom. Red, blue, and green spheres represent V, Ti, and O atoms, respectively. The numbers in the figure from V1 to V5 represent the different locations for introduced solutes (Cr, Ti, and Y). The numbers on the image right represent the interlayer distances. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

The site preference of solute elements (M = Cr, Ti, or Y) at TiO/V interface can be predicted by calculating the formation heat H_f when a matrix atom is substituted by solute atom at specific site at the interface. The formation heat H_f can be described as [22,23]:

$$H_f = [E(V_i Ti_j O_k M_l) - i\cdot E_c(V) - j\cdot E_c(Ti) - k\cdot E_c(O) - l\cdot E_c(M)]/(i+j+k+l) \tag{1}$$

where $E(V_i Ti_j O_k M_l)$ is the total energy of the TiO/V interface supercell with i, j, k, and l atoms of V, Ti, O, and solute atom M. $E_c(V)$, $E_c(Ti)$, and $E_c(M)$ are the energies per atom in bcc-V, hcp-Ti, and bcc-Cr/hcp-Y unit cell, respectively. $E_c(O)$ is half of the total energy of the oxygen molecule.

Solute segregation to the matrix/precipitate interface can facilitate lowering the interfacial free energy, which can lead to mitigation of the coarsening of precipitate. The solute segregation energy can be described by comparing the total energies as shown in [12]:

$$\Delta E_{seg} = E_{Vx}(V_i Ti_j O_k M_l) - E_{V5}(V_i Ti_j O_k M_l) \tag{2}$$

where E_{Vx} represents the total energy when the solutes are positioned at different sites (V1–V4) from the TiO/V interface, the E_{V5} is assumed to be sufficiently far away from the interface to be considered as V bulk position. A more negative segregation energy represents that the solutes segregate more strongly to the position.The Griffith work of rupture can be used to qualitatively evaluate the tensile cleavage strength of the bulk or interface structure. Herein, we also calculate the Griffith rupture work G_w and considering the effects of alloying elements on the TiO/V interface. The G_w can be written and calculated by the following expression [10]:

$$Gw = (-1/2S)\cdot[E(V_i Ti_j O_k M_l) - E_V^{surface} - E_{TiO}^{surface}] \tag{3}$$

where $E_V^{surface}$ and $E_{TiO}^{surface}$ are the total energies of V matrix surface and TiO surface, respectively. S is the area of the coherent plane of TiO/V interface. A more positive Griffith rupture work indicates that a larger force or energy is required to cleave the coherent region.

3. Result and discussion

3.1. The TiO-precipitate/matrix interface structure

Using the High-resolution electron microscopy, recent works on the low temperature behavior of V-4Cr-4Ti reveal the structure characteristic of mono-layer thick TiO-precipitate induced by proton irradiation [6]. This uniform precipitate presents a NaCl-type FCC structure and contains a number of vacancies. According to the phase diagram [24], γ-TiO is the high-temperature phase with a NaCl-type (Rocksalt-type, B1) cubic structure, which can be seen as an FCC Ti sublattice where every interstitial octahedral site is occupied by an O atom. Using the first-principles calculations, we obtain the equilibrium lattice parameter a_{TiO} for NaCl-type perfect bulk TiO is 4.29 Å, which is also consistent with other computation data [25,26] and the experimental value of 4.184 Å. At early stage in the radiation-induced aging process, precipitate seems to be composed of only one atomic layer [6] and is

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