Computational Materials Science 77 (2013) 348–354

Contents lists available at SciVerse ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Behaviors of alloying element titanium in vanadium: From energetics to tensile/shear deformation

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ARTICLE INFO

Article history:
Received 10 January 2013
Received in revised form 27 April 2013
Accepted 29 April 2013
Available online 31 May 2013

Keywords:
Vanadium
Titanium
Mechanical properties
First-principles

ABSTRACT

Using first-principles simulation, we investigate the effect of alloying element titanium (Ti) on the mechanical properties of vanadium (V). The ideal tensile strengths of $Ti_{1.85}V_{98.15}$ and $Ti_{6.25}V_{93.75}$ alloys in the [100] direction are 18.6 GPa and 17.5 GPa, respectively. These values are, respectively, reduced by 2.6% and 8.4% in comparison with 19.1 GPa of pure V. This suggests that such alloying effect of Ti on the tensile strength of V appears to be relatively large. The generalized fault energies have been calculated including the unstable stacking energy (γ_{us}) and the cleavage energy (γ_{cl}) in a pure V and $Ti_{0.35}V_{99.65}$ alloy along the most preferable $\{110\}\langle 111\rangle$ slip system. Ti can decrease γ_{cl} from 1.705 J/m^2 to 1.704 J/m^2 and simultaneously increase γ_{us} from 0.308 J/m^2 to 0.311 J/m^2 in comparison with the pure V. The ratios of γ_{cl}/γ_{us} for the pure V and $Ti_{0.35}V_{99.65}$ alloy are 5.536 and 5.479, respectively. The value is decreased by 1.03%, meaning that the ductility of dilute $Ti_{0.35}V_{99.65}$ alloy can be slightly reduced in comparison with that of the pure V.

1. Introduction

Developing a credible structural material in the extreme conditions of fusion reactors is one of the most crucial task for realizing commercial fusion power reactors. Considerable efforts have been made to search a material, which should exhibit attractive characteristics such as low induced activation, good tolerance to high operating temperature and stress, long-term reliability under operating conditions. Vanadium (V) and its alloys have been recognized as the most promising candidates of the structural materials in fusion reactors. The excellent performance at high temperature [1–3] and intrinsic low activation property [4–7] of V meet the requirement for safety operation in the extreme conditions. Also, the high corrosion resistance in the reactor coolant lithium (Li) makes it possible to equip with liquid Li blankets in reactors [8]. So far, the theoretical and experimental data base of V and its alloys are limited, a lot of scientific and industrial attentions have been paid on these materials [9,10]. Many progress have been achieved on the critical issues for the V-alloys such as fabrication technology and materials performance [11].

Alloying of metals is a typical method to improve their performance in metallurgy. Alloy elements may bring wonderful properties that the host is lack of. Moreover, investigating the interaction between an alloy element and a metal on the microscopic level can help us to understand the macroscopic experimental evidences and determine the exact element ratio of components for alloys. Since V has been considered as an attractive candidate structural materials in fusion reactors, the properties of V and its interactions with different alloy elements are of great scientific and technological interest. Previous work showed that V possesses reasonable tensile properties and creep behaviors [12]. But in the harsh environment of fusion reactors, V has to be exposed to the high flux of heat and particles, especially the high energy neutrons (14.2 MeV). They will induce atomistic vacancy and interstitial defects, which may deteriorate the performance and lead to the failure of materials. The experimental evidences have attested that the harmful consequences of V under high energy neutrons irradiation are alleviated [11]. The swelling behaviors of intrinsic V and V-alloys after neutron irradiation have been investigated. The results revealed that the addition of titanium (Ti) in V can substantially suppress the swelling of crystal [13–15]. Loomis et al. have reviewed the influences of neutron irradiation on tensile strength, ductility, creep, fatigue, ductile–brittle transition temperature, and swelling of V-base alloys, as well as the compatibility of V-base alloys with liquid Li [16].

The experimental results have shown that Ti has strong effects on V mentioned above, however, the influences of alloying element Ti on the mechanical properties of V such as the tensile and shear behaviors received less attention. The ideal strength of a perfect

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http://dx.doi.org/10.1016/j.commatsci.2013.04.064

crystal can be determined by the maximum tensile stress at elastic instability when applying an increasing stress to an infinite, perfect crystal [17]. By virtue of the development of the density functional theory combined with the rapid progress of modern computers, it became possible to do a first-principles computational tensile or shear test (FPCTT/FPCST) to investigate the stress or energy as a function of strain and obtain the theoretical tensile or shear behaviors by deforming crystals to failure. So far, the ideal tensile or shear behaviors of single crystal such as W, Cu, Ir, Al, Ni, Mo, Nb, Fe, and NiAl have been published [18–27]. The tensile behaviors of the defective systems containing only one defect such as a point defect [28], an interface or a grain boundary have also been calculated [29–32].

In view of those aspects mentioned above, in this study, we first investigate the structure and energetics of Ti in V single crystal, further study the alloying effect of Ti on the theoretical mechanical properties of V. For the mechanical properties of V, we perform FPCTT on a pure V single crystal and a dilute $Ti_{1.85}V_{98.15}$ alloy, respectively. For comparison with $Ti_{1.85}V_{98.15}$ alloy, we also perform FPCTT on a $Ti_{6.25}V_{93.75}$ alloy. As to shear behaviors, We calculate the stacking fault energy and cleavage energy of a pure V and a dilute $Ti_{0.35}V_{99.65}$ alloy. Using the criteria of the ratio of "cleavage energy" and "stacking fault energy", we can obtain the ductile versus brittle character of the pure V and $Ti_{0.35}V_{99.65}$ alloy.

2. Computational method

Our first-principles calculations were carried out using the Vienna Ab initio Simulation Package (VASP) code [33,34] based on the density functional theory. The exchange–correlation between electrons is described using the generalized gradient approximation (GGA) [35] of Perdew and Wang (PW91) and the ion–electron interaction is defined by the projector augmented wave (PAW) potentials [36]. The 6*p*4*d*1*s* and 3*d*1*s* electrons were treated as valence electrons for metal V and Ti, respectively. The plane wave energy cutoff is 350 eV, which is sufficient for the total energy and geometry of V supercell. The calculated equilibrium lattice constant is 2.98 Å for bcc V, in good agreement with the corresponding experimental value of 3.03 Å [37].

2.1. Energetic stability calculations

For the calculations of the solution energy and binding energy, we applied the 128-atom supercell containing $(4 \times 4 \times 4)$ unit cells with the lengths of 11.92 Å in [100], [010], and [001] directions, respectively. The Brillouin zone of the supercell was sampled with $(3 \times 3 \times 3)$ ***k***-points by the Monkhorst–Pack scheme [38] and the Methfessel–Paxton smearing with a width of 0.20 eV. The size of this supercell was also shown to yield reliable total energies required for a single impurity Ti atom via convergence test. The supercell size, shape, and atomic positions were relaxed to equilibrium, and the energy relaxation iterates until the forces on all the atoms are less than 10^{-3} eV Å^{-1}.

The solution energy of an interstitial Ti atom in bulk V can be written as

$$E^{s}_{Ti} = E_{V,Ti} - E_V - \mu_{Ti}, \tag{1}$$

where $E_{V,Ti}$ is the energy of the V supercell with one alloy element Ti atom, E_V is the energy of ideal bulk V supercell, and μ_{Ti} is the Ti chemical potential. The Ti chemical potential μ_{Ti} is the energy per Ti atom, which is −7.740 eV according to the present calculation in a 128-atom Ti supercell with $(3 \times 3 \times 3)$ ***k***-points.

The solution energy of a substitutional Ti atom in bulk V is written as

$$E^{s}_{Ti} = E_{V,Ti} - (N-1) \times \frac{E_V}{N} - \mu_{Ti}, \tag{2}$$

2.2. Tensile/shear calculations

Concerning the FPCTT, The [100] direction was chosen as the tensile direction because this direction is generally considered as the weakest direction under tension in bcc metal according to prior work [39]. In the FPCTT, we employ the respective 54-atom supercell and 16-atom supercell containing one Ti atom (i.e., $Ti_{1.85}V_{98.15}$ alloy and $Ti_{6.25}V_{93.75}$ alloy) to determine the ideal tensile strengths. A uniaxial tensile strain has been applied to the chosen crystalline directions. Previously, symmetry is generally an important factor to determine the stress–strain relation in the FPCTT. Here, we do not consider the orthorhombic branching in the tensile process but employ the tetragonal path (Bain Path), i.e., the strained unit cell bcc → fcc structure transition, which is similar to our previous study [18]. The corresponding tensile stress σ is calculated from

$$\sigma(\varepsilon) = \frac{1}{\Omega(\varepsilon)} \frac{\partial E}{\partial \varepsilon} \tag{3}$$

where E is the total energy and $\Omega(\varepsilon)$ is the volume at given tensile strain of ε. The lattice vectors were incrementally added in the direction of the imposed strain. At each strain step, the structure was fully relaxed until all other five stress components vanished except that in the tensile direction. The tensile stress for each strain step can be calculated, and thus the stress–strain relationship and the theoretical tensile strength can be obtained.

As to the calculations of cleavage energies and generalized unstable stacking fault energies, we used the 288-atom supercell containing $(4 \times 6 \times 2)$ unit cells with the lengths of 10.32 Å, 25.28 Å, and 14.60 Å in [111], $[\bar{1}10]$, and $[11\bar{2}]$ directions, respectively. The size of the supercell was also shown to yield reliable total energies required for a single impurity Ti atom via convergence test. The Brillouin zone was sampled with $(4 \times 2 \times 2)$ ***k***-points by the Monkhorst–Pack scheme [37]. During the shear slip, the 288-atom supercell including the $\{110\}\langle 111\rangle$ slip system is divided into the upper and lower halves by the fault {110} plane. Thus, to calculate the cleavage energy, the slabs have to be formed by six atomic layers (i.e., 144 atoms) for (110) surface. While the thickness of the vacuum layer was correspondingly set to 12.64 Å, which is half of the length of the $[\bar{1}10]$ direction in the supercell. The atoms were relaxed until the remaining forces were less than 10^{-3} eV Å^{-1}. Moreover, we required numerical precision to compute the change of the cleavage energy on the scale of 10^{-6} eV/atom because $Ti_{0.35}V_{99.65}$ is a dilute binary alloy.

The cleavage energies (γ_{cl}) of the interface without and with Ti can be calculated by

$$\gamma_{cl} = \frac{E^{slab}_{up} + E^{slab}_{down} - E_{total}}{2A}, \tag{4}$$

and

$$\gamma_{cl(V-Ti)} = \frac{E^{slab}_{up} + E^{slab}_{down-Ti} - E_{total-Ti}}{2A}, \tag{5}$$

where E_{total} and $E_{total-Ti}$ are the total energies of the clean and Ti-doped system, E^{slab}_{up} is the total energy of the clean upper slab, E^{slab}_{down} and $E^{slab}_{down-Ti}$ are the total energies of the clean and Ti-doped down slab, respectively. A is the interface area of the system.

The generalized stacking fault energy (γ_{GSF}) can be defined as

$$\gamma_{GSF} = \frac{E(u) - E(0)}{2A}, \tag{6}$$

where ***u*** is the fault vector, $E(u)$ and $E(0)$ are the energies of the system with and without the stacking fault, respectively.