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First-principles study of the binding preferences and diffusion behaviors of solutes in vanadium alloys

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ABSTRACT

In order to elucidate the role of solutes in vanadium alloys, the solute diffusions and the interactions of solute–solute and solute-vacancy have been investigated by means of the first-principles calculations. It is shown that large solutes are energetically favorable to combine with adjacent solute and to form the solute–solute nearest-neighbor pairs. In order to obtain qualitative understanding, the charge density differences for some special solute–solute binding are plotted to analyze the bonding interaction between solute atom and their nearest-neighbor host atoms. The solute–solute binding energies indicated that apart from the 3d transition metals, there is a clear trend of increasing binding energy with increasing solute volume. In particular, large solutes have larger binding energies for bonding with vacancies and can be considered as vacancy trappers in the crystal. As a comparison with solute diffusions, the self-diffusion coefficients of vanadium are determined. Activation energies for vacancy-mediated solute diffusion in vanadium are also determined. We conclude that the major contribution to the activation energy comes from the diffusion energy barrier, and both all follow the same trend. The noble metals have higher migration barriers than others, which means that these elements are inactive in the vanadium alloys. By contrast, the barriers for the large solutes almost cease to exist due to the formation of stable solute-centered divacancy.

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1. Introduction

Vanadium (V) alloys are considered as a candidate for blanket structural materials for fusion reactor systems due to their remarkable high-temperature mechanical and thermal properties in the fusion environment [1–3]. As is well known, the alloy composition and microstructure can be optimized by adding solute atoms in alloys design to improve their properties. In V–Cr–Ti alloys, Cr is known to increase the high-temperature strength and Ti can enhance the ductility by absorbing interstitial impurities, such as C, O, and N [4]. However, excess Cr or Ti also has been reported to result in loss of ductility [4]. Sakai et al. [5] reported that the ductile–brittle transition temperature of alloys increase with Cr concentrations, corresponding to the increase of flow stress due to solution-hardening by Cr. Hence, our understandings of the roles played by these alloying solutes are far from completed. In particular, the diffusion mechanisms of solutes in V alloys are not well known at all. Since the kinetic properties of solute diffusion lead to many microstructural and microchemical changes, understanding the diffusion mechanism of alloying elements can thus be essential for optimizing mechanical properties.

At low temperature, the diffusivity of solute in metal is usually governed by vacancy-mediated diffusion. Meanwhile, in metals, vacancy is the simplest and most common structural defect, and is apt to interact with solutes and impurities (such as C, N, and O) forming the nanoclusters and precipitates. Recently, vacancies were considered as an important factor in stabilizing the oxide nanoclusters in the oxide dispersion strengthened (ODS) steels [6,7]. Stepanov et al. [8] demonstrated that vacancies can be trapped by oversized solutes to suppress the radiation-induced segregation

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and void swelling. All these studies indicate that the interactions between vacancy and solutes in metals are the key to uncover the behaviors of solute diffusion and the growth of solute clusters. Even though there are many studies on this field [9–11], the effort is not enough, especially in the V alloys where their mechanical strength can be improved by high number density of tiny precipitates dispersed in the matrix [12,13].

The purpose of the present study is to investigate the systematic trends of the binding preferences and diffusion behaviors of solutes in V alloys. For this purpose we employ the first-principles electronic structure calculations to study the binding energies of solute–solute and solute-vacancy, as well as the solute migration barriers and activation energies; and then the calculated results are discussed.

2. Methodology

All the energies mentioned above are computed within the Vienna Ab Initio Simulation Package (VASP) [14,15] with the projector augmented wave (PAW) method [16,17] and generalized gradient approximation Perdew–Burke–Ernzerhof functional (GGA-PBE) [18]. The computations perform within a 54-atom periodic simulation cell. The binding energies and charge density difference are obtained with 400 eV plane-wave cutoff and 9 × 9 × 9 k-point meshes. Once the Hellmann–Feynman force acting on atoms is less than 0.01 eV/Å, the atoms are regard as being fully relaxed. The climbing-image nudged elastic band (CI-NEB) [19] method is used to estimate the migration barriers and determine the transition state. The required force convergence for all atoms on the CI-NEB technique is set to 0.03 eV/Å. The present equilibrium lattice constant for bulk V is 2.99 Å, which is consistent with theoretical results [20,21] and the experimental value of 3.03 Å [22].

The binding energy E_{bind}^{A-B} between two point defects (A, B) in the supercell is calculated by Ref. [23]:

$$E_{bind}^{A-B} = E_{tot}^{A} + E_{tot}^{B} - E_{tot}^{A+B} - E_{tot}^{bulk} \tag{1}$$

where E_{tot}^{A}, E_{tot}^{B}, and E_{tot}^{A+B} stand for the total energies of the supercell contained defect A, B, and two defects with the first nearest-neighbor (1NN) or second nearest-neighbor (2NN) site distance, respectively. E_{tot}^{bulk} is the total energy of perfect V bulk. In Eq. (1), B can represent the solute atom or the vacancy. If the former, the E_{bind}^{A-B} indicates the solute–solute binding energy; if the latter, the E_{bind}^{A-B} means solute-vacancy binding energy. All computations of the defect energies in present work are obtained under the fixed periodicity vectors condition, while the results usually overestimate the defect energies due to the interaction of defects with its periodic images [24,25]. However, the focal point for this work is the changing tendency of the binding preferences and diffusion behaviors of solutes in vanadium. Meanwhile, the convergences of the computations with respect to k point grids and supercell size have been investigated in previous work in our research group [21]. Therefore, our results not consider the effect from the elastic image interaction.

The solute volume V_{sol} is also calculated using the following expression to determine the atomic size of each solute impurity [9]:

$$V_{sol} = V_{cont-sol} - V_{tot} \tag{2}$$

where $V_{cont-sol}$ and V_{tot} are the volume of the supercell with and without a single solute atom, respectively.

3. Result and discussion

3.1. Binding preferences of solutes in V

In our previous work, the solution energies of 3d, 4d, and 5d solute atoms in V have been evaluated by first-principles calculations [26]. The results showed that the solution energies initially decrease and then increase with increasing atomic number in the periodic table, suggesting that the solution energy is strongly related to the atomic size of solute. For more details, the reader is referred to Ref. [26]. In addition to solution energies, we further calculate the solute–solute binding energies (by Eq. (1)) that can be used to elucidate the clustering trend of solutes in the superalloys [27]. Fig. 1 shows the calculated binding energies of the 1NN and 2NN solute pair as a function of the solute impurity volume, given by Eq. (2). The results revealed that in the 1NN distance, the solute–solute binding energies E_b^{s-s} are almost all negative, except for the large atomic sizes of solutes (such as Sc, Y, Zr, La, and Hf). From a thermodynamic perspective, a negative binding energy indicates a repulsive interaction and a positive energy denotes an attractive interaction. Thus, we conclude that large solutes are energetically favorable to combine with adjacent solute to form the solute–solute NN pairs, others are on the contrary. This phenomenon can be explained by the strain model [10]: when big-sized solutes are introduced to crystal, local stress field are created. Larger-sized solutes will close to each other so as to relax the local distortion in

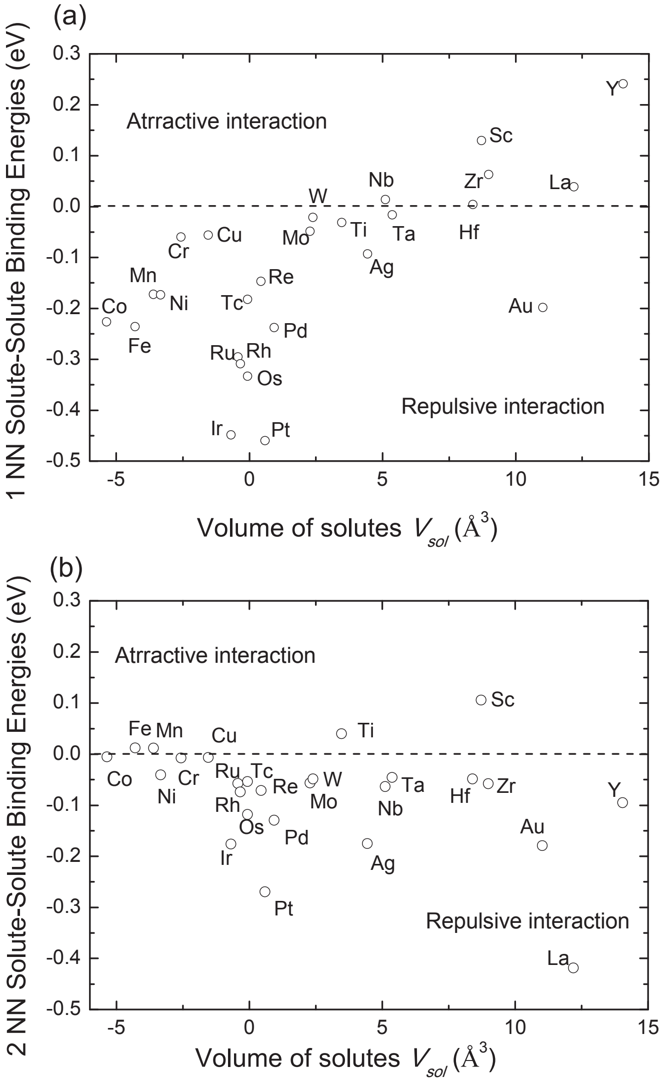

Fig. 1. First-principles calculated the 1NN (a) and 2NN (b) nearest-neighbor solute–solute binding energies as a function of the solute impurity volume for 3d, 4d, and 5d solutes.

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