



# First-principles calculations of transition metal–solute interactions with point defects in tungsten

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## Abstract

The interactions of solute atoms with point defects can modify the microstructure of materials and affect microstructural evolution, ultimately leading to macroscopic changes in the mechanical properties of materials. In this paper, we performed a series of first-principles calculations to quantify the intrinsic properties of transition metal (TM) solutes and their interactions with point defects in W, including vacancies and  $\langle 111 \rangle$ -crowdions. This work provides good explanations for recent experimental results on the influence of solute on radiation response and might aid future material design regarding the choice of alloy composition. We find that the early TM elements do not segregate together while the late elements tend to accumulate to form small clusters in dilute W alloys. The solute–point defect interactions are mostly attractive with a few exceptions, and can be well understood in terms of the combination of, and competition between, electronic effects and strain-relief effects, which are characterized by the solute electronegativity and atomic size, respectively. Solute atoms with larger electronegativity more favorably bond to the vacancy and the smaller ones prefer to bind to the  $\langle 111 \rangle$ -crowdion, and vice versa. The present results, together with previous experimental results, suggest that Re might be a relatively suitable alloying element compared to other possible candidates, and Ta seems suitable for adding in W–Re alloy to adjust the concentration of Re and Os.

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## 1. Introduction

Tungsten (W) is a metal that possesses some attractive engineering properties, including high melting temperature, high-temperature strength, good thermal conductivity and low sputtering erosion. As a result, it is important for technological applications where components encounter high temperatures. Recently, W has received particular attention as the most promising candidate for various plasma-facing components, such as the divertor plate in the International

Thermonuclear Experimental Reactor (ITER), which will be exposed to high-energy, high-flux neutrons [1–3]. The high-energy neutron irradiation gives rise to a large number of point defects, such as vacancies and self-interstitial atoms, in the lattice. These point defects interact strongly with solute atoms, changing their migration and aggregation properties and ultimately leading to macroscopic changes in the material properties, such as hardening and embrittlement. A typical example is the non-equilibrium segregation process known as radiation-induced segregation [4], which occurs at point defect sinks during irradiation of an alloy. Under irradiation condition, quantities of point defects, far in excess of equilibrium concentrations,

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travel to low-energy sites such as surfaces, grain boundaries, dislocations, voids and other defect sinks [4]. Segregation takes place when a given alloying component has a preferential association with the defect flux. On the other hand, the solute atom also influences the diffusion of point defects, and further modifies the formation and growth of defect clusters, voids and loops. Both the enrichment/depletion of the solute element and the changes in point defect transportation and aggregation are controlled by the relative interaction between solute atoms and point defects. Thus, understanding the fundamental mechanisms of solute–point defect interactions not only helps to uncover the atomistic mechanisms of radiation-induced agglomeration, but also has an important role in developing predictive models of changes in the microstructure and mechanical properties of metals for engineering applications in fission and fusion reactors.

The solute–point defect interaction is quantitatively characterized by the magnitude of their binding energy, which can be accurately predicted by the first-principles density functional calculation [5]. Generally, there are two primary (and usually competing) factors governing the solute–point defect interaction, i.e. the electronic effect and the strain-relief effect. Sometimes one of these two factors plays a major role, and sometimes they combine or compete with each other. For example, for the case of non-transition-metal (non-TM) elements in Al- and Mg-based alloys [5–8], there is a correlation between the solute–vacancy binding energy and the solute size, with larger solute atoms binding more strongly with vacancies. In addition, solute–vacancy binding energies of the rare earth (RE) elements in Mg exhibit a strong linear correlation to the magnitude of the solute's displacement towards the vacancy. These correlations suggest that the strain-relief effect is a significant contribution to the interaction between the vacancy and the non-TM/RE solute atom. In contrast to the non-TM and RE solute elements, there is no correlation between the solute–vacancy binding and the solute size for 3d TM solutes in Al and Mg, suggesting that the strain-relief argument cannot explain this binding behavior, where the electronic structure band-filling effect is supposed to play a significant role. Recently, the interactions of TM solutes with point defects have attracted much attention in Fe-based alloys due to its application in fission and fusion reactors [9–12]. These systematic studies show that the interaction between TM solutes and point defects arises from the delicate balance between the electronic effect and the strain-relief effect.

Until now, the interaction of solute atoms with point defects in W has not been investigated to the same extent as for Fe. Few works have focused on the interaction between solute atoms and point defects in W, and published binding energies exist for only a few solute elements, e.g. C, Mo, Re, Ta and V [13–17]. Recently, Becquart and Domain presented data for the binding energies of the TM solute with vacancies at the first and second nearest neighbor positions without detailed discussion in their review

paper [18]. As pointed out in this review, comprehensive investigations are required to predict the behaviors of the solute and the point defect when they are close to each other. In this paper, we carry out a systematic first-principles calculation to predict the solute–point defect interaction in W. Here, the point defects include vacancies and self-interstitial atoms (SIAs). The TM elements are selected as representative solutes. Some of them are alloyed in W to tailor its properties or are introduced during transmutation reactions. For example, it has been proposed to add Re, along with Ta, Ti and V, to W in order to improve the material ductility [19]. Re and Os are also the primary neutron-induced transmutation products of W, and Hf is a transmutation product of W isotopes [20]. Some TM elements, such as Mo, Fe, Cu, Mn, Cr and Ni, are impurities in W [21]. Other TM elements are chosen to construct an extensive first-principles database of predicted solute–point defect binding and gain insight into fundamental and general trends in solute–point defect binding.

## 2. Computation method

The present calculations are performed within density functional theory (DFT) as implemented in the Vienna Ab initio Simulation Package (VASP) [22,23]. The interactions between ions and electrons are described by the projector augmented wave potential (PAW) method [24]. Exchange and correlation functions are taken in a form proposed by Perdew and Wang within the generalized gradient approximation (GGA) [25].  $4 \times 4 \times 4$  and  $5 \times 5 \times 5$  supercells are used to investigate the interaction of the solute atom with vacancies and SIAs, respectively. The relaxations of atomic position and optimizations of the shape and size of the supercell are performed. The plane wave cutoff and  $k$ -point density are both checked for convergence for each system to be within 0.001 eV per atom. Following a series of test calculations, a plane wave cutoff of 500 eV is used and a  $k$ -point grid density of  $3 \times 3 \times 3$  is employed. The structural optimization is truncated when the forces converge to less than  $0.01 \text{ eV \AA}^{-1}$ .

The properties of the point defect are first calculated to verify the accuracy of our calculations. The calculated values are compared in Table 1 with experimental data and other DFT calculation results. Our results for vacancy and SIA formation energy are within the range of scatter of the experimental data and are slightly larger or smaller than other DFT results [26–30]. Note that in this paper the SIA denotes the  $\langle 111 \rangle$ -crowdion if it is not mentioned specifically. The  $\langle 111 \rangle$  dumbbell configuration spontaneously relaxes to the  $\langle 111 \rangle$  crowdion configuration; the study by Nguyen-Manh et al. [27] shows that the formation energy of the  $\langle 111 \rangle$  dumbbell (9.548 eV, two atoms share a lattice site) is very similar to that of the  $\langle 111 \rangle$  crowdion configuration (9.551 eV, four atoms share three lattice sites). These slight differences between our results and other calculations are probably due to the difference in computation methods. For example, the GGA in Perdew and Wang

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