# Effects of chromium on structure and mechanical properties of vanadium: A first-principles study*

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Stability and diffusion of chromium (Cr) in vanadium (V), the interaction of Cr with vacancies, and the ideal mechanical properties of V are investigated by first-principles calculations. A single Cr atom is energetically favored in the substitution site. Vacancy plays a key role in the trapping of Cr in V. A very strong binding exists between a single Cr atom and the vacancy with a binding energy of 5.03 eV. The first-principles computational tensile test (FPCTT) shows that the ideal tensile strength is 19.1 GPa at the strain of 18% along the [100] direction for the ideal V single crystal, while it decreases to 16.4 GPa at a strain of 12% when one impurity Cr atom is introduced in a 128-atom V supercell. For shear deformation along the most preferable $\{110\}\langle 111\rangle$ slip system in V, we found that one substitutional Cr atom can decrease the cleavage energy ($\gamma_{cl}$) and simultaneously increase the unstable stacking fault energy ($\gamma_{us}$) in comparison with the ideal V case. The reduced ratio of $\gamma_{cl}/\gamma_{us}$ in comparison with pure V suggests that the presence of Cr can decrease the ductility of V.

**Keywords:** vanadium, chromium, structure, mechanical properties, first-principles

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## 1. Introduction

At present, energy shortage is one of the most critical problems that mankind faces. Nuclear fusion energy, as a clean and infinite energy for future generations, has been regarded as a solution to the world's energy supply problem. Nowadays it is being developed internationally by the ITER (International Thermonuclear Experimental Reactor) Project. In the ITER project, a large magnetically confined thermonuclear fusion device, Tokamak, is being constructed. But formidable scientific and technological problems have to be solved. The choice of the structural material is considered one of the top challenges for state-of-the-art engineering. Vanadium (V) with a body-center cubic (bcc) structure and its alloys[1–3] have been identified as the most promising candidates for the structural materials in fusion reactors for their excellent performance at high temperature[4–6] and low activation property.[7–10] Also, their good compatibility with a lithium (Li) environment favors their use in reactors equipped with a liquid Li blanket.[11–13] Many efforts have been made on the critical issues of the V-alloys such as fabrication technology and material performance. The related research progress has been reviewed by Muroga *et al.*[14]

In a fusion reactor, V, as the structural material, will be irradiated by different energetic particles. Of special concern, high energy neutrons (14.2 MeV) will lead to the transmutation reaction of a V atom into chromium (Cr) in bulk V. For example, Sato *et al.* have reported that V atoms can transmute into Cr atoms under high energy neutron irradiation.[15] At the same time, Cr as an alloy element is a crucial factor in many metal materials. Moreover, the interaction between Cr and metal has great scientific and technological interest, which has a broad range of implications in the field of materials physics. For a high-concentration Cr solubility, it is easy to form V–Cr solid solution alloys, which are used to improve the performance of V metal. In the case of low-Cr solubility, a very small amount of Cr atoms might change the thermal and mechanical characteristics significantly due to the strong interaction between Cr and Loomis *et al.*[16] examined the swelling behaviors of bulk V by embedding Cr additions using a neutron irradiation method according to the immersion density of the unirradiated and irradiated materials. The results show that the addition of Cr can substantially increase the swelling of V. Subsequently in 1992, Loomis *et al.*[17] reviewed the influences of neutron irradiation on the tensile strength, ductility, creep, fatigue, ductile-brittle transition temperature, and swelling of vanadium-based alloys, as well as the compatibility of vanadium-based alloys with liquid lithium.

However, both the experimental and theoretical works

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mentioned above mostly focused on the cases of V–Cr alloys[11–14,18] with high Cr concentration in V. As mentioned above, impurity Cr atoms are produced by transmutation reactions in bulk V. Although the concentration of Cr is extremely low, it is believed to have strong effects on the electronic structure and mechanical properties of V such as the ideal (theoretical) tensile and shear behaviors. Consequently, exploring the interaction between Cr and V not only greatly helps us to understand the effects of Cr on the structure and properties of V, but also has a direct impact on the design and operation of fusion reactors.

In this paper, we thus investigate the structure, energetics, and diffusion properties of Cr in a V single crystal, as well as its effect on the theoretical mechanical properties of V, by using a first-principles method based on density functional theory. For the mechanical properties of V, we perform a first-principles computational tensile test (FPCTT) on a V single crystal with an alloy element Cr atom. Further, we have also applied a first-principles method to calculate the stacking fault energy and cleavage energy of the pure and Cr-doped V systems. Using the criteria of the ratio of "cleavage energy" and "stacking fault energy" we can investigate the ductile versus brittle character of the pure and Cr-doped systems. The results will provide a useful reference for V as a candidate structural material for fusion reactors.

## 2. Computational method

Our first-principles calculations were carried out using the Vienna *ab-initio* Simulation Package (VASP) code[19,20] based on density functional theory. The exchange–correlation between electrons is described using the generalized gradient approximation of Perdew and Wang[21] and the ion–electron interaction is defined by the projector augmented wave (PAW) potentials.[22] The plane wave energy cutoff is 350 eV, which is sufficient for the total energy and geometry of the 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.[23]

### 2.1. Energetic stability calculations

For the calculations of the solution energy and binding energy, we applied the 128-atom supercell containing $(4\times4\times4)$ 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 $(3\times3\times3)$ $\boldsymbol{k}$-points by the Monkhorst–Pack scheme[24] 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 Cr atom via a 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 Cr atom in bulk V can be written as

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

where $E_{\mathrm{V,Cr}}$ is the energy of the V supercell with one alloy element Cr atom, $E_{\mathrm{V}}$ is the energy of the ideal bulk V supercell, and $\mu_{\mathrm{Cr}}$ is the Cr chemical potential. The Cr chemical potential $\mu_{\mathrm{Cr}}$ is the energy per Cr atom, which is $-9.467$ eV according to the present calculation in a 128-atom Cr supercell with $(3\times3\times3)$ $\boldsymbol{k}$-points.

The solution energy of a substitutional Cr atom in bulk V can be written as

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

In order to describe the diffusion energy profile for a Cr atom when a vacancy is present in bcc V, we define the binding energy required to move a substitutional Cr atom from a lattice point to form an interstitial Cr atom and a V vacancy. Thus, the binding energy $E^{\mathrm{b}}_{\mathrm{Cr,Vac}}$ between the Cr atom and the vacancy is defined as

$$E^{\mathrm{b}}_{\mathrm{Cr,Vac}} = \left[E_{\mathrm{V,Cr(T-site)}} - E_{\mathrm{V}}\right] - \left[E_{(N-1)\mathrm{V,Cr}} - E_{\mathrm{Vac}}\right], \tag{3}$$

where the $E_{\mathrm{V,Cr(T-site)}}$ is the energy of the supercell with a Cr atom at the tetrahedral interstitial site (T-site). The $E_{(N-1)\mathrm{V,Cr}}$ and $E_{\mathrm{Vac}}$ are the energy of the supercell with and without a Cr atom positioned at one vacancy, respectively.

### 2.2. Tensile/shear calculations

Concerning the FPCTT, the [100] direction was chosen as the tensile direction because this direction is generally considered the weakest direction under tension in bcc metals. In the FPCTT, we employ a 128-atom supercell containing one Cr atom to determine the ideal tensile strengths. A uniaxial tensile strain is applied to the chosen crystalline directions. The corresponding tensile stress $\sigma_{\alpha,\beta}$ $(\alpha,\beta=1,2,3)$ is calculated from

$$\sigma_{\alpha,\beta} = \frac{1}{\Omega(\varepsilon)}\frac{\partial E}{\partial \varepsilon}, \tag{4}$$

where $E$ is the total energy and $\Omega(\varepsilon)$ is the volume at a given tensile strain of $\varepsilon$. The lattice vectors are incrementally added in the direction of the imposed strain. At each strain step, the structure is fully relaxed until all five of the other stress components vanish, leaving strain only 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 use the 288-atom supercell containing $(4\times6\times2)$ 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 is shown to yield

reliable total energies required for a single impurity Cr atom via a convergence test. The Brillouin zone was sampled with $(4 \times 2 \times 2)$ $\boldsymbol{k}$-points by the Monkhorst–Pack scheme. 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. The thickness of the vacuum layer is correspondingly set to 12.64 Å, which is half of the length of the $[\bar{1}10]$ direction in the supercell. The atoms are relaxed until the remaining forces are less than $10^{-3}$ eV·Å$^{-1}$. Moreover, we require numerical precision to compute the change of the cleavage energy on the scale of $10^{-6}$ eV/atom.

The cleavage energies ($\gamma_{\rm cl}$) of the interface without and with Cr can be calculated by

$$\gamma_{\rm cl} = \frac{E_{\rm up}^{\rm slab} + E_{\rm down}^{\rm slab} - E_{\rm total}}{2A}, \tag{5}$$

and

$$\gamma_{\rm cl(V-Cr)} = \frac{E_{\rm up}^{\rm slab} + E_{\rm down-Cr}^{\rm slab} - E_{\rm total-Cr}}{2A}, \tag{6}$$

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

The generalized unstable stacking fault energy ($\gamma_{\rm GSF}$) can be defined as

$$\gamma_{\rm GSF} = \frac{E(\boldsymbol{u}) - E(0)}{2A}, \tag{7}$$

where $\boldsymbol{u}$ is the fault vector, $E(\boldsymbol{u})$ and $E(0)$ are the energies of the system with and without the stacking fault, respectively. $A$ is the fault plane area for a single stacking fault in the supercell.

## 3. Results and discussion

### 3.1. Energetic stability of Cr atom in V

We first analyzed the energetically-favorable site of the interstitial Cr atom in bulk V in terms of its solution energy using Eq. (1). It is important to point out that accurate calculations for randomly distributed interstitial Cr atoms in metals are not feasible. Here we only consider two high symmetry cases of the T-site and O-site, i.e., Cr atom stays at the center of the two interstitial sites, respectively. Figures 1(a) and 1(b) show the atomic structures of the tetrahedral interstitial site (T-site) and the octahedral interstitial site (O-site) for bcc V, respectively. The results show that a single Cr atom is energetically favored to occupy the T-site with a solution energy of 2.604 eV in comparison with 2.623 eV at the O-site. It can be seen that the solution energy for Cr at the T-site is only 0.019 eV lower than that at the O-site case. However, one can see that much higher solution energies exist for the Cr atom at both the T-site and O-site, suggesting the Cr atom is not favored to stay in the interstitial site. This is because the atomic radius of Cr (1.28 Å) is larger and the interstitial site does not have enough space to accommodate the Cr atom.

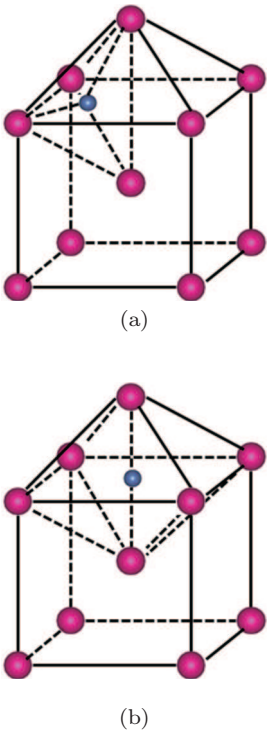


**Fig. 1.** (color online) (a) T-site and (b) O-site in bcc V. The larger red and smaller grey balls represent V atoms and Cr atoms, respectively.

Because the atomic radius of V is larger in comparison with some lighter elements such as hydrogen and helium, a relaxing expansion should be induced by the presence of Cr in the V lattice in comparison with the ideal V case. According to the present first-principles calculations, if the volume of the ideal V supercell is $\Omega$, the increased volume for the Cr atom at the T-site and at the O-site are $0.93\%\Omega$ and $0.95\%\Omega$, respectively. On the other hand, our calculations can fully confirm the reported experimental results by Loomis *et al.*,[16] who found the presence of swelling behaviors of the bulk V due to the embedding of Cr additions in the interstitial sites.

Apparently, both the T- and O-sites lead to much higher solution energy although the Cr atom is more stable at the T-site than at the O-site. Therefore, we further calculate the Cr solution energy using Eq. (2) when the Cr atom occupies substitutional site, corresponding to a Cr atom trapped by a monovacancy. The result demonstrates that the solution energy for Cr at this site is close to 0.147 eV, much lower than that at the T-site in intrinsic bulk V. At the same time, we found that the supercell will slightly compress when the Cr atom stays at the substitutional site and the corresponding volume change is close to $-0.12\%\Omega$. The main reason originates in that the atomic radius of Cr (1.28 Å) is smaller than that

of V (1.35 Å). Moreover, we can see that the volume change ($0.12\%\Omega$) is much smaller than those of the interstitial sites mentioned above. Thus, the larger space of the substitutional site makes it most preferable for the Cr atom in V.

### 3.2. Diffusion properties of Cr atoms in V

The kinetic diffusion properties are very important for us to understand the behaviors of Cr in V. The diffusion energy barrier, one of the fundamental parameters in metal, affects the feasibility of Cr migration. Therefore, we calculate the diffusion activation energy of Cr in V, based on first-principles. As to the diffusion of Cr atoms in bulk vanadium, we used the drag method, which was reported and explained by Willaime.[25] The Cr atoms' diffusion route can be easily determined using the drag method: the Cr atomic sites relative to the center of mass are constrained to relax in a hyperplane perpendicular to the vector from the initial to the final sites.[25,26] This method has been successfully applied in studies of the diffusion of impurity atoms in metal and metal-alloys.

Figure 2 plots the diffusion energy profile for Cr atom in bcc V. Here, we investigate a possible diffusion path in which Cr moves from one T-site to another T-site via a middle transition state O-site (T → O → T path). The energy barrier for this path is calculated to be 0.019 eV, which is just the difference between O-site and T-site. Further, with continuous migration, the interstitial Cr atom will be strongly trapped by a vacancy whenever it meets the vacancy. The binding energy ($E^{b}_{Cr,Vac}$) between Cr and the vacancy is calculated to be 5.03 eV (Fig. 2). Such strong trapping makes it very unlikely that the Cr atom will move from the vacancy. For the Cr atom to be released from the vacancy to become an interstitial Cr atom leaving an isolated vacancy behind, a quite large de-trapping energy of 5.03 eV must be expended.

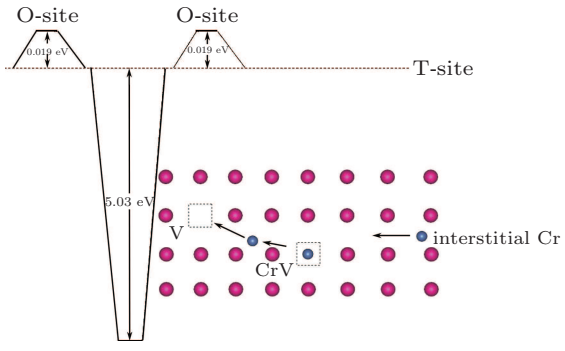



**Fig. 2.** (color online) Lattice structure at the (001) plane and diffusion energy profile for a Cr atom in bcc V. The larger red and smaller grey balls represent V atoms and Cr atoms, respectively.

### 3.3. FPCTT of V single crystal with Cr

After establishing the energetic stability of Cr in V, we finally examine the influence of Cr on the mechanical properties of V single crystal. Stress evolution with increasing strain in one certain direction shows straightforwardly the tensile strength change due to the presence of Cr. Figure 3 plots the stress curves as a function of tensile strain which are obtained with and without a Cr atom in V by the FPCTT in the [001] direction. For the ideal V single crystal, the stress increases with increasing strain until it reaches a stress maximum of 19.1 GPa at the strain of 18%; with greater strain the stress decreases. Therefore, we obtained the ideal tensile strength of 19.1 GPa in the [001] direction, which is the upper limit of the tensile strength of the ideal V single crystal. Nagasako *et al.* obtained a strength value of 17.8 GPa using PAW potentials.[27] One can see that our calculated value is slightly larger than that value mentioned above; however they are basically in agreement.

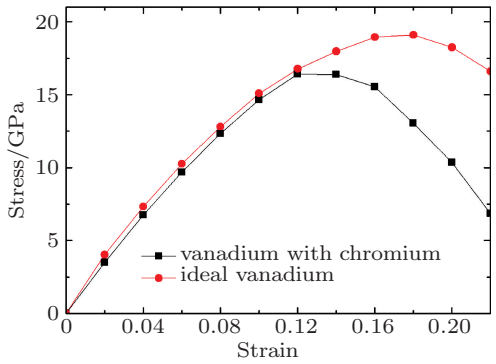



**Fig. 3.** (color online) Stress curves as a function of strain under tension in the [001] direction for V single crystal with and without an impurity Cr atom, respectively.

We further investigate the effect of Cr on the ideal tensile strength of V single crystal. Here we choose the most stable substitutional Cr case for tension in the [001] direction. Similar to the tension of the ideal V single crystal, the strain increase leads to a continuous stress increase. The stress differs slightly with that of the ideal V at the beginning until the strain of 12%. However, when the strain is beyond 12%, the stress drops suddenly to 16.0 GPa at the strain of 14% in contrast with the ideal V (17.9 GPa). With further increased strain, the stress decreases substantially and then drops to 10.4 GPa from 18.2 GPa at the strain of 20%. Thus, the ideal tensile strength of V single crystal with Cr is about 16.4 GPa at the strain of 12%. In comparison with the ideal V case, the ideal tensile strength is reduced by 14% in the [001] direction due to the presence of the Cr impurity. This demonstrates that a Cr atom, to some extent, will degrade the tensile strength of V single crystal. Harrod *et al.* investigated the tensile properties of V with increasing addition of Cr at room temperature in an earlier experiment.[28] They found that the tensile strength reduces by 15% for the concentration at the 0.78% Cr alloyed with V (i.e., one substitutional Cr in 128-atom supercell). We note that this value is in good agreement with the results calculated in this work. To give a physical picture to understand such an effect of Cr impurity in V, we now turn to

the electronic-structure analyses of pure V and Cr–V system, respectively. In Fig. 4, we draw the valence charge density distribution maps. Note that the charge density in the [001] direction between the Cr atom and the 1NN V atoms decreases more slightly in the Cr–V system than that of V–V atoms in pure V, suggesting that the Cr–V bonding is weaker than that of the V–V bonding. Such weaker bonding behavior might be directly responsible for the decrease of tensile strength of the Cr–V system in the [001] direction.

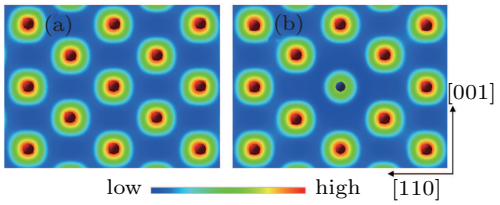



**Fig. 4.** (color online) Valence charge density distribution maps: (a) Pure V, (b) Cr–V system. The larger red balls and the smaller blue ball represent V atoms and Cr atom, respectively.

### 3.4. Effects of Cr on the ductile versus brittle character of the V system

A crystal can be divided into two semi-infinite slabs along the (*hkl*) crystallographic plane, which is called the fault plane. When a crystal is subjected to shear stress, the two slabs will separate from each other along this plane or fracture through a crack propagation. So we can connect the macroscopic brittle versus ductile behavior of a solid material with a microscopic model of two competing processes, (i) the opening of a crack and (ii) the emission of dislocations at the crack tip.[29,30] The cleavage energy ($\gamma_{\rm cl}$) is defined as the energy required per unit area to divide the solid into two semi-infinite halves along the fault plane, ignoring diffusional and plastic degrees of freedom. It is a direct measure of the interface bond strength, which can be described by process (i). In a cleavage experiment it sets the lower bound to the actual energy cost.[31] On the other hand, we can also define the generalized stacking fault energy ($\gamma_{\rm GSF}$) as the energy cost per unit area when the two halves are displaced with respect to each other by a certain vector $\boldsymbol{u}$.[32,33] For $\boldsymbol{u}=0$ case, it corresponds to the ideal crystal without any slide. The value of $\gamma_{\rm GSF}$ varies periodically with the slip vector $\boldsymbol{u}$ on the (*hkl*) plane for the atomic arrangement of the system with the same period. When $\boldsymbol{u}$ is equal to the half of the slip vector, the generalized stacking fault energy will reach its maximum, which is named as the unstable generalized stacking fault energy ($\gamma_{\rm us}$). The $\gamma_{\rm us}$ represents the energy barrier for dislocations to overcome from the crack tip when shearing along the slide direction on the fault plane, as described by process (ii) above. The ratio of cleavage energy and unstable stacking fault energy ($\gamma_{\rm cl}/\gamma_{\rm us}$) demonstrates a capability of a crack extension,[34–36] which is relevant to the ductile/brittle character. A material is said to be ductile if the emission of a dislocation is energetically favorable over cleavage at the crack tip with an increasing $\gamma_{\rm cl}/\gamma_{\rm us}$.[31]

Now we turn our attention to calculating the $\gamma_{\rm cl}$ and $\gamma_{\rm us}$ of the V crystal with and without the Cr atom in the $\{110\}\langle111\rangle$ slip system as shown in Fig. 5, and further use the criteria of $\gamma_{\rm cl}/\gamma_{\rm us}$ to investigate the effects of the Cr atom on the ductility of V crystal. Our choice of the $\{110\}\langle111\rangle$ slip system as a model system is partly because it is the most preferable slip system in bcc metals.

For the ideal slip plane, i.e., there is no Cr atom on the slip plane, the $\gamma_{\rm cl}$ is calculated to be 1.705 J/m$^2$ with the aid of Eq. (5). This value will decrease to 1.704 J/m$^2$ when a Cr atom substitutes a V atom on the plane, according to Eq. (6). This suggests that the impurity Cr atom can, to some extent, weaken the strength of the slip plane slightly. The underlying physical mechanism could be understood as follows. Similar to the case of tension above, it can be seen that the charge density in the [110] direction between Cr atom and 1NN V atoms decreases more slightly in Cr–V system than that of V–V atoms in pure V as shown in Fig. 4. This demonstrates that the bonding property of Cr–V is weaker than that of V–V, and this difference might be directly responsible for the decrease of cleavage energy of the Cr–V system with a Cr atom embedded into the [110] plane.

To study the $\gamma_{\rm us}$ of the V crystal, it can be separated into two halves by the (110) plane with the upper half displaced relative to the lower one by the vector $\boldsymbol{u}$. The calculation of $\gamma_{\rm GSF}$ is based on Eq. (7), and only those atomic relaxations that are perpendicular to the (110) slip plane are allowed. The $\boldsymbol{u}/\boldsymbol{b}$ changes periodically from 0 to 1 because the atomic structure returns to the original configuration after one complete period

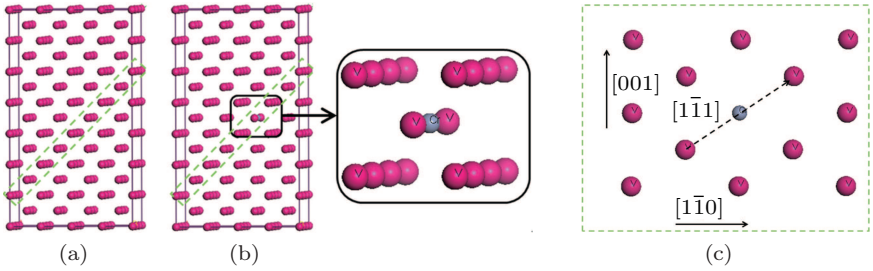



**Fig. 5.** (color online) Supercell with $\{110\}\langle111\rangle$ slip system. (a) Pure V system. (b) Cr-doped system with one Cr atom at the substitutional site. (c) Slip direction $[1\bar{1}1]$ on the slip plane (110). Larger red balls and smaller grey balls represent V atoms and Cr atoms. The green square represents the slip plane.

(Note that $\boldsymbol{b}$ is also the slip vector and represents half of the total length along the [111] direction, i.e., $\boldsymbol{b} = [111]/2$). At first the atoms of the upper slab move along the slip direction from their equilibrium positions to their 1NNs on the lower slab. As shown in Fig. 6, the $\gamma_{\rm GSF}$ begins to increase because the distances between the atoms on the interface smaller than the equilibrium distances induce a mutual repulsion between the two atomic layers. When $\boldsymbol{u}/\boldsymbol{b} = 1/2$, $\gamma_{\rm GSF}$ reaches its maximum, reflecting that the interatomic distance between the two atomic layers at the slip plane is the smallest during the shear deformation period. The maximum $\gamma_{\rm GSF}$ at $\boldsymbol{u} = 1/2\boldsymbol{b}$ is defined as the corresponding unstable stacking fault energy $\gamma_{\rm us}$. With the atoms moving to the next equilibrium positions, the $\gamma_{\rm GSF}$ further declines as shown in Fig. 6. When $\boldsymbol{u}/\boldsymbol{b} = 1$, the $\gamma_{\rm GSF}$ reaches minimum. This means the atoms reach other equilibrium positions and the relative distance between the upper and lower layers at the interface returns to the equilibrium distance. As shown in Fig. 6, the $\gamma_{\rm us}$ of pure V crystal is calculated to be 0.308 J/m$^2$. While the $\gamma_{\rm us}$ of the Cr-doped system is 0.313 J/m$^2$, which is 0.005 J/m$^2$ higher than that of the pure V system. This indicates that the shear deformation along the $\{110\}\ \langle 111\rangle$ slip system for the pure V system is easier than that of the Cr-doped case.

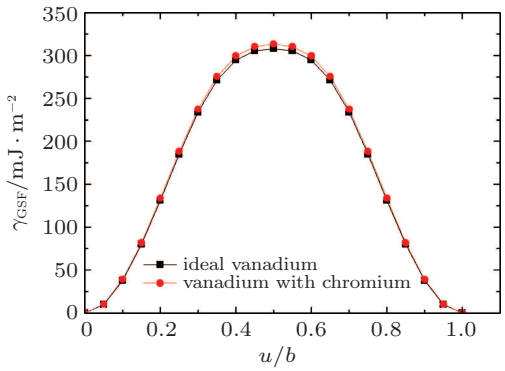



**Fig. 6.** (color online) The generalized stacking fault energies vary as functions of slip in the $\{110\}\ \langle 111\rangle$ slip systems for pure V crystal and Cr-doped case.

Finally, we use the criteria of the ratio of $\gamma_{\rm cl}/\gamma_{\rm us}$ to investigate the ductile versus brittle character of the pure V and the Cr-doped systems. As calculated above, it is clear to note that the presence of the Cr atom decreases the cleavage energy $\gamma_{\rm cl}$ from 1.705 J/m$^2$ to 1.704 J/m$^2$ and simultaneously increases the unstable stacking fault energy $\gamma_{\rm us}$ from 0.308 J/m$^2$ to 0.313 J/m$^2$. Correspondingly, the ratios of $\gamma_{\rm cl}/\gamma_{\rm us}$ for pure and Cr-doped systems are 5.536 and 5.441, respectively. The ratio is decreased by 1.71%, which can thus suggest that the ductility of V crystal is slightly decreased for the presence of Cr. Recently, Loomis *et al.*[37] investigated the ductile properties at low temperature with increasing addition of Cr in V alloy. They found that ductility decreases with the embedding of Cr. Thus, our theoretical calculation results are supported by the corresponding experimental investigations. This can provide quite a useful reference for further study of the dilute $Cr_xV_y$ binary alloy.

## 4. Conclusions

Using first-principles calculations, we have investigated structure, stability, and diffusion of Cr, as well as the Cr-vacancy interaction, in V single crystal. For an interstitial Cr atom in V, the tetrahedral interstitial site is more energetically favorable than the octahedral interstitial site by about 0.019 eV. With low diffusion barriers, a vacancy can easily trap a Cr atom. We found that the binding energy between a single Cr atom and a vacancy is very strong, at 5.03 eV. The first-principles computational tensile test (FPCTT) shows that the ideal tensile strength is 19.1 GPa at the strain of 18% along the [100] direction for the ideal V single crystal, while it decreases to 16.4 GPa at the strain of 12% when one Cr atom occupies a substitutional site. The ideal tensile strength is reduced by 14% in the [100] direction due to the presence of Cr. This suggests that the Cr atom, to some extent, degrades the ideal tensile strength and plastic property of V single crystal. For shear deformation along the most preferable $\{110\}\ \langle 111\rangle$ slip system in V single crystal, we find that one substitutional Cr atom can decrease the cleavage energy ($\gamma_{\rm cl}$) from 1.705 J/m$^2$ to 1.704 J/m$^2$ and simultaneously increases the unstable stacking fault energy ($\gamma_{\rm us}$) from 0.308 J/m$^2$ to 0.313 J/m$^2$ in comparison with the ideal V case. Further, the ratios of $\gamma_{\rm cl}/\gamma_{\rm us}$ for pure and Cr-doped systems are 5.536 and 5.441, respectively. The presence of Cr can cause the ratio to decrease by 1.71%, suggesting that Cr can slightly decrease the ductility of V crystal. All the theoretical calculation results are supported by the corresponding experiments.

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