Ab initio study of H and He migrations in β-phase Sc, Y, and Er hydrides*

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(Received 1 November 2011; revised manuscript received 9 December 2011)

Ab initio calculations based on the density functional theory have been performed to investigate the migrations of hydrogen (H) and helium (He) atoms in β-phase scandium (Sc), yttrium (Y), and erbium (Er) hydrides with three different ratios of H to metal. The results show that the migration mechanisms of H and He atoms mainly depend on the crystal structures of hydrides, but their energy barriers are affected by the host-lattice in metal hydrides. The formation energies of octahedral-occupancy H (H_{oct}) and tetrahedral vacancy (V_{tet}) pairs are almost the same (about 1.2 eV). It is of interest to note that the migration barriers of H increase with increasing host-lattice atomic number. In addition, the results show that the favorable migration mechanism of He depends slightly on the V_{tet} in the Sc hydride, but strongly on that in the Y and Er hydrides, which may account for different behaviours of initial He release from ScT_2 and ErT_2.

Keywords: hydrogen, helium, metal hydride, *ab initio* calculation

PACS: 66.30.J–, 88.30.rd, 71.15.Mb **DOI:** 10.1088/1674-1056/21/5/056601

1. Introduction

Rare-earth metals can absorb a large number of hydrogen (H) atoms and its isotopes, forming corresponding metal hydrides, deuterides, and tritides. Because of their convenient availability, and the chemical and crystallographic similarities between metal hydrides and tritides, rare-earth hydrides have been studied for many years as reactor moderators and target materials in neutron generators.[1,2] Among rare-earth metals, scandium (Sc), yttrium (Y), and erbium (Er) are the most attractive ones due to their high-capacity H storage and different electronic structures. With H concentration increasing, a metal-H system undergoes different phases, transforming from an α-phase (hcp structure) to a hexagonal trihydride phase through a β-phase (CaF_2 structure). During the phase transformation, the pure β-phase of rare-earth metal hydrides is stable over a relatively small region of gas/metal ratio ranging from 1.85 to 2.15.[3,4] The H behaviours in metals and β-phase metal hydrides have been studied by a variety of experimental and theoretical methods.[2,5−10] The energetics and lattice contraction of a β-phase YH_2 have been studied by Sun *et al.* with the pseudopotential method.[5] Especially, Snow *et al.* calculated the mechanical properties of metal hydrides, including elastic constants, bulk modulus, Young's modulus, and shear modulus.[6] Wixom *et al.* investigated the site occupations and migrations of H, He, and O in a β-phase Er hydride by using the first-principles approach.[2] Their results suggested that the substantial H migration depends on nonideal stoichiometry and/or impurities that create octahedral H occupations.

It is also important to understand the helium (He) behaviour, because the ^{3}He accumulation in host metals occurs via a tritium (T) decay reaction $T \rightarrow {}^3He + \beta^- + \bar{\nu} + 18.582$ keV.[11] Experimen-

*Project supported by the National Natural Science Foundation of China (Grant No. 10976007), the Fundamental Research Funds for the Central Universities (Grant No. ZYGX2009J040), the Science and Technology Foundation of China Academy of Engineering Physics (Grant No. 2009A0301015), and the US Department of Energy, Office of Fusion Energy Science (under Contract DE-AC06-76RLO 1830).

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tal and computer-simulated results indicate that He atoms tend to be trapped at defects within crystal and precipitates, forming clusters or bubbles, which significantly degrades the mechanical properties of materials.[12−16]The He behaviours in rare-earth metal hydrides have also been widely investigated with different experimental methods.[12,13,17] Polycrystalline samples of ScT_x were measured over the past three years, showing that the He damage was governed by self-interstitial atoms and dislocation loops created by He clustering and bubble formation.[12] The evolution of lattice damage in Y–T–He systems was investigated by means of neutron scattering techniques.[13] Transmission electron microscopy has also been used to study the He release and microstructural changes of $Er(D, T)_{2-x}$.[17] In Ref. [6], Wixom *et al.* also found that if a connected network of vacant tetrahedral sites exists, He migration throughout the network can occur at room temperature.

Atomistic-level simulations of H and He migrations in Sc, Y, and Er hydrides are important to understand H and He behaviours in tritides, and can provide a significant insight into the behaviours of H and He in metal hydrides. Recently, we have investigated the migrations of H and He atoms in hcp-Sc by using *ab initio* calculations.[18] It is found that the migration energy barriers for H interstitials are quite different from those for He interstitials, but their migration mechanisms are similar. The He release properties and He bubble geometry in $ErT_{1.9}$, $ScT_{1.9}$, $TiT_{1.9}$, and $ZrT_{1.5}$ have been investigated by Snow *et al.*[6] They found that the release numbers of He are similar in the tritides that have similar crystal structures, and He bubble shape depends on the crystal structures of tritides. In the present work, the migration behaviours of H and He in Sc, Y, and Er hydrides is systematically investigated by using *ab initio* calculations based on the density functional theory (DFT). We focus on the effects of crystal structures of hydrides and metal properties on the migration mechanisms of H and He in metal hydrides, as well as the effects of He migration barriers on the early stage of He release from metal tritides.

2. Methodology

The present calculations were carried out by using the Vienna *ab initio* simulation package (VASP) code. The projector augmented wave method was used to determine the interaction between ions and electrons,[19,20] while exchange and correlation interactions were described by the generalized gradient approximation (GGA) proposed by Perdew and Wang.[21] Standard pseudopotentials of Sc, Y, Er, H, and He were obtained from the VASP library, which provides a good description of the properties of a perfect crystal. A 2×2×2 supercell of 96 atoms was used to represent the ground state of a β-phase MH_2 (M=Sc, Y, or Er) crystal, to which atoms were removed, added, or replaced to generate models with desired defects, such as H and He point defects. Periodic boundary conditions were imposed along three directions. Plane-wave basis sets with an energy cutoff of 500 eV were used in migration calculations, and a 4×4×4 Monkhorst–Pack grid was used to sample the Brillouin zone.

By using the chosen pseudopotentials, the computed equilibrium lattice constants for β-phase ScH_2, YH_2, and ErH_2 are 4.760, 5.210, and 5.122 Å, respectively, which are in good agreement with experimental values of 4.780, 5.205, and 5.123 Å.[5] Three independent elastic constants of β-phase ScH_2, YH_2, and ErH_2 were also calculated with three different cutoff energies, and the results are listed in Table 1. Other calculation results and experimental data are also presented for comparison. It is clear that the mechanical properties of ScH_2, YH_2, and ErH_2 converge at a cutoff energy of 500 eV. The bulk modulus, shear modulus, and Young's modulus agree well with the available experimental values. Therefore, the cutoff energy of 500 eV is used in the present study.

The climbing image nudged elastic band (CI-NEB) method[23] in the VASP code was used to investigate the migration mechanisms and energy barriers of H and He diffusions in β-phase Sc, Y, and Er hydrides at a supercell with a fixed volume condition. This method is used to find a saddle point and a minimum energy path between the initial and final states of a transition, which constructs a number of intermediate images along the energy path. A spring interaction between adjacent images is added to ensure continuity of the path. The transition state corresponding to the highest energy point along this path ascends. The migration energy barrier is the difference of the total energy between this transition state and the nearby local minima from the initial state to the final state of the path. The forces on all the atoms in each image of the CI-NEB chain converge to 0.01 eV.

Table 1. Calculated values (GPa) of elastic constants C_{ij} bulk modulus B, shear modulus G, and Young's modulus E in β-phase ScH_2, YH_2, and ErH_2, along with Snow *et al.*'s results[22] for comparison. The results are obtained from the second-order polynomial fit to the calculated energies for 13 values of the strain ranging from −1.8% to 1.8%. Brillouin zone samplings of 9×9×9 are used to get sufficient accuracy.

		Cutoff energy/eV	C_{11}	C_{12}	C_{44}	B	G	E
ScH_2	This work	400	168.9	64.9	80.9	99.6	67.8	165.7
		500	167.6	62.6	80.4	97.6	67.8	165.1
		600	165.4	62.6	79.4	96.9	68.2	162.8
	Snow *et al.*'s calculation[22]	–	166(5)	63(2)	80(1)	97.4	68	164
YH_2	This work	400	133.8	59.4	69.6	84.2	54.1	133.7
		500	132.4	58.0	69.1	82.8	53.9	132.8
		600	132.2	58.0	68.7	82.8	53.7	132.4
	Snow *et al.*'s calculation[22]	–	132(3)	58(2)	73(1)	82.8	50	124
	Snow *et al.*'s experiment[22]	–	–	–	–	90.±7	55.±10	135.±20
ErH_2	This work	400	142.3	64.1	75.0	90.1	57.8	142.8
		500	141.0	63.2	74.5	89.2	57.4	141.8
		600	140.9	63.0	74.3	89.0	57.3	141.6
	Snow *et al.*'s calculation[22]	–	140(4)	63(2)	78(1)	89.1	60	146
	Snow *et al.*'s experiment[22]	–	–	–	–	97±4	60±10	148±20

3. Results

3.1. H migration

It is well-known that a perfect β-phase metal hydride forms a CaF_2 structure, where H atoms occupy all tetrahedral interstitial sites, while octahedral sites remain unoccupied[5] The total energies and corresponding equilibrium atomic configurations for β-phase Sc, Y, and Er hydrides have been calculated firstly, and then the CI-NEB method was used to determine the H migration mechanisms in the three metal hydrides. Three possible migration paths of an H atom in β-phase metal hydrides were considered and illustrated in Figs. 1, 2, and 3, respectively.

Calculated results show that a pair of octahedral-occupancy H (H_{oct}) and tetrahedral vacancy (V_{tet}) is stable when they are separated by the nearest neighbor distance at least in β-phase MH_2 (M=Sc, Y, or Er), which is similar to the results in Ref. [6]. Figure 1 shows the formation of the H_{oct}/V_{tet} pair in three metal hydrides, with a H/metal (H/M) ratio of 2.0 Figures 1(a) and 1(b) present the migration path and the migration energy paths, respectively. In an ideal MH_2, where the ratio H/M is 2.0, all the tetrahedral sites are filled, and an H atom may migrate along the path, forming an H_{oct}/V_{tet} pair, as shown in Fig. 1(a). In order to compare H migrations in the three metal hydrides, the energy barriers of H migrations in these hydrides are also listed in Table 2. From Fig. 1(b) and Table 2, it is clear that the formation barrier of an H_{oct}/V_{tet} pair in β-phase ScH_2 is the lowest among the three metal hydrides, i.e., the formation barrier in ScH_2, YH_2, and ErH_2 increase with increasing host-lattice atomic number. However, it is surprising to note that H_{oct}/V_{tet} pairs in the three hydrides have very similar formation energy. The formation energies of H_{oct}/V_{tet} pairs in β-phase MH_2 (M=Sc, Y, or Er) are 1.23, 1.20, and 1.20 eV, respectively, which suggests that the formation of H_{oct}/V_{tet} pairs is not correlated to metals in MH_2, but is only associated with the crystal structures of β-phase metal hydrides.

Figure 2 shows the migration of H_{oct} in metal hydride with H/M > 2.0. Figure 2(a) presents two possible migration paths and Fig. 2(b) presents low migration energy paths. When the ratio H/M is larger than 2.0, additional H atoms will occupy the octahedral positions to form H_{oct} because these positions are the most available for H. In this case, the migration of H_{oct} to another unoccupied octahedral site becomes a dominant mechanism of transporting H. Two possible migration paths were considered, one being a direct migration from an octahedral to its nearest octahedral (indicated by the solid line in Fig. 2(a)), the other being an indirect migration, i.e., a tetrahedral H migrates to the octahedral interstitial site and then the octahedral H synchronously jumps to the nearest tetrahedral site (indicated by the dotted lines in Fig. 2(a)). We found that the migration barrier of the direct migration is significantly higher than that of the indirect migration, i.e., the H_{oct} prefers to migrate through the tetrahedral site. The corresponding

migration energy barriers in β-phase MH_2 (M=Sc, Y and Er) are shown in Fig. 2(b). From Fig. 2 and Table 2, it can be found that the energy barrier of the H_{oct} migration in Sc hydride is the lowest, while that in Er hydride is the highest. However, the energy barrier differences between them are very small.

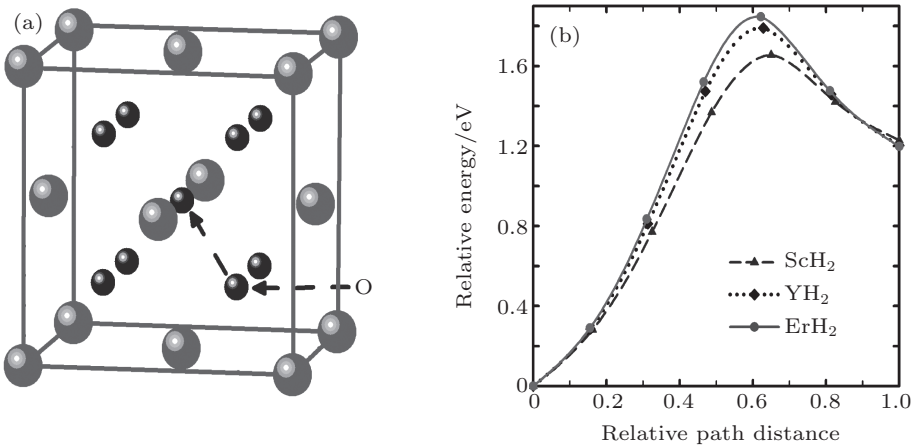


Fig. 1. Formation of an H_{oct}/V_{tet} pair in metal hydride with an H/M ratio of 2.0 (a) Migration path. The hollow sphere represents the initial position of an H that becomes a vacant in the final configuration, while the small spheres and the large spheres are H and metal atoms, respectively. The arrow indicates the pathway of H. (b) Migration energy paths. The dashed line represents the path in Sc hydride, and the dotted and solid lines indicate that in Y and Er hydrides, respectively.

Table 2. Energy barriers (eV) of H migration in β-phase Sc, Y, and Er hydrides.

	H_{oct}/V_{tet}pair formation	H_{oct} migration	V_{tet} migration
ScH_2	1.65	0.53	0.64
YH_2	1.79	0.54	0.85
ErH_2	1.84	0.56	0.92

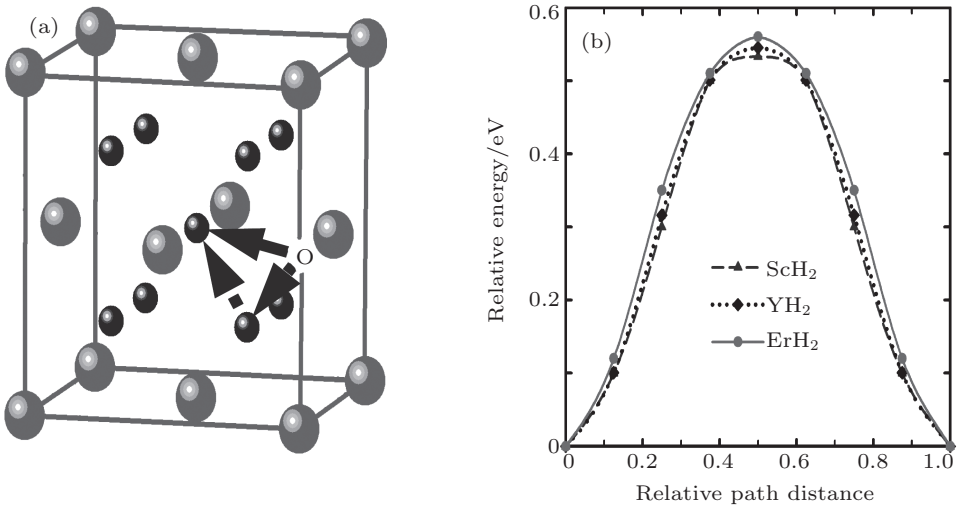


Fig. 2. Migration of H_{oct} in metal hydride with H/M > 2 (a) Migration path and (b) the corresponding migration energy paths. The symbol representations are the same as in Fig. 1.

When the H/M ratio is smaller than 2.0, there exist a number of unoccupied tetrahedral sites, forming tetrahedral vacancies. A possible migration mechanism of a V_{tet} in a metal hydride is shown in Fig. 3(a), where the symbol representations are the same as those in Figs. 1 and 2 and an H atom can directly migrate to a vacant site, which may be defined as a V_{tet} assisting migration mechanism. The correspond-

ing energy barriers of the V_{tet} migration in β-phase Sc, Y, and Er hydrides are shown in Fig. 3(b), which clearly demonstrates that the energy barrier of the V_{tet} migration in Sc hydride is significantly lower than that in Y and Er hydrides, but the energy barrier in Y hydride is similar to that in Er hydride.

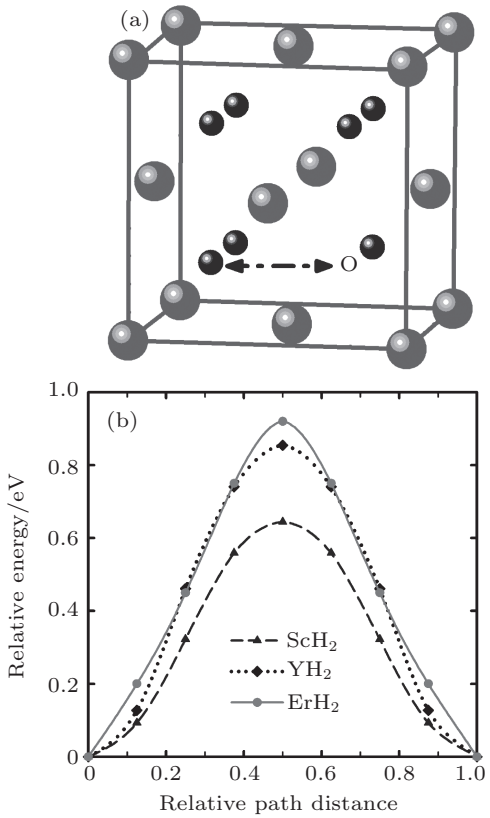


Fig. 3. Migration of V_{tet} in metal hydride with $H/M < 2.0$. (a) Migration path and (b) the corresponding migration energy paths. The symbol representations are the same as those in Fig. 1.

Furthermore, from Figs. 1, 2, and 3, as well as Table 2, it is of interest to note that the three migration mechanisms of H follow a similar trend in the three metal hydrides, i.e., the formation energy barrier of an H_{oct}/V_{tet} pair is the highest, which suggests that it is almost impossible to thermally form H_{oct}/V_{tet} pairs at room temperature. These results obtained above suggest that migration mechanisms of H mainly depend on crystal structures of β-phase metal hydrides, but the energy barrier of H migration increases with increasing host-lattice atomic number.

3.2. He migration

As described above, He atoms can be accumulated in metal tritides due to tritium decays. Although most He atoms are firstly retained in lattices, they can be released approximately at their generation rate from the tritide. Much effort in experiments has been devoted to explaining why He is retained at low-level concentrations, but no longer retained at some critical concentrations.[24] These phenomena may be correlated to the migration behaviour of He atoms, and thus it is of interest to systematically study the migration mechanisms of He in metal tritides.

In metal hydrides containing He generated from the tritium decay, a He atom may move to a V_{tet} site, forming a He tetrahedral interstitial (He_{tet}). The present calculations clearly demonstrate that a He atom prefers to occupy a tetrahedral site (He_{tet}), rather than a neighbouring octahedral site (He_{oct}) in the three metal hydrides, which is similar to the He occupation in ErH_2 studied in Ref. [6]. The relative stability of a He_{tet} is determined by using the binding energy (E_b) of a He atom to a V_{tet}, which can be calculated using the following equation:

$$E_b(\mathrm{He}) = E_{tot}(\mathrm{V}) + E_{tot}(\mathrm{He_{oct}}) - E_{tot}(\mathrm{He_{tet}}) - E_{per}, \quad (1)$$

where $E_{tot}(V)$, $E_{tot}(He_{oct})$, and $E_{tot}(He_{tet})$ are the total energies of the computational cells containing a V_{tet}, a He_{oct}, and a He_{tet}, respectively. E_{per} is the total energy of a perfect computational cell. The calculated binding energies of a He atom to a tetrahedral vacancy are 0.83, 0.57, and 0.57 eV for Sc, Y, and Er hydrides, respectively. It is clear that the He_{tet} in Sc hydride is the most stable, and the He_{tet} in Y and Er hydrides is of similar stability. It is worth noting that the dissociation of a He atom from a V_{tet} depends not only on the binding energy, but also the migration energy.[25]

The CI–NEB method embedded in VASP code was used to investigate He migration mechanisms in β-phase Sc, Y, and Er hydrides. Three possible mechanisms and their corresponding migration energy paths are illustrated in Figs. 4, 5, and 6, respectively. The energy barriers are also provided in Table 3.

If a He presents an ideal hydride, where tetrahedral sites are all occupied by H, it prefers an empty octahedral site or displaces an H, forming a He_{tet}. However, the energy required to displace an H is 0.55, 0.76, and 0.77 eV in Sc, Y, and Er hydrides, respectively, which suggests that a He atom tends to stay at an octahedral site in these ideal hydrides. The He atom may migrate from an octahedral site to another one in hydrides, as long as it gains enough energy. Figure 4(a) shows a possible path for a He_{oct} migrating to its neighbouring octahedral site (O–O), where the medium sphere represents He atom and the hollow sphere the initial position of the He, while the small spheres and the large spheres represent H and metal

atoms, respectively. The arrow indicates the migration path of He. The corresponding energy paths are shown in Fig. 4(b). From Fig. 4(b) and Table 3, it is clear that the differences of energy barriers are relatively small for the three hydrides. However, the variation of energy barriers does not follow that of H migration in these hydrides, i.e., the migration energy does not increase with increasing host-lattice atomic number.

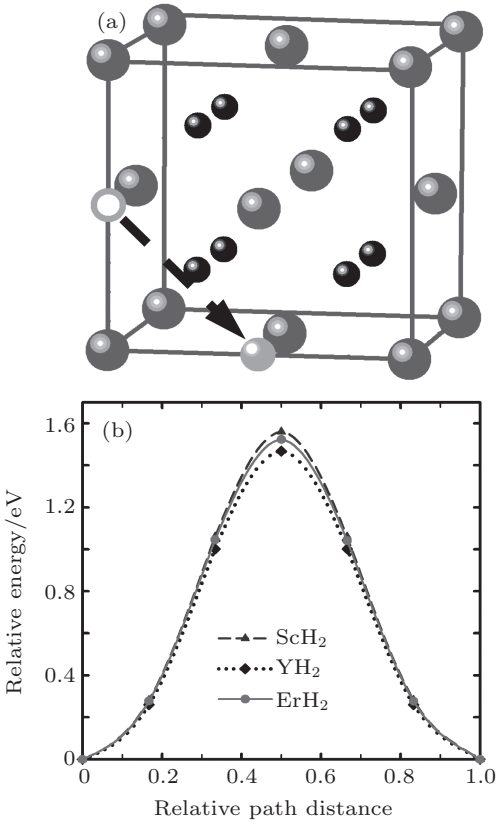


Fig. 4. He migration from an octahedral to its neighbouring octahedral site (O–O). (a) Migration path. The medium spheres represent He atoms, the hollow sphere represents the initial position of He and the small spheres and the large spheres represent hydrogen and metal atoms, respectively. The arrow indicates the migration path of He. (b) Migration energy paths. The symbol representations are the same as in Fig. 1(b).

Table 3. Energy barriers (eV) of He migration in β-phase Sc, Y, and Er hydrides.

	O–O	O–T*–O	O–V_{tet}–O
ScH_2	1.56	0.71	0.70
YH_2	1.47	0.83	0.53
ErH_2	1.52	0.90	0.51

Another possible migration path of H_{oct} is shown in Fig. 5(a), where He migrates from an octahedral site to another one through an intermediate filled tetrahedral site T* (O–T*–O). The corresponding migration energy paths, as well as the initial, middle, and final configurations (I, II, III), are shown in Fig. 5(b), where the symbol representations are the same as in Fig. 4. In this migration path, a He atom pushes one of its nearest tetrahedral H atoms to the nearest octahedral interstitial site and synchronously jumps to a tetrahedral site T* (middle configuration II in Fig. 5(b)). Then, the He atom migrates to the nearest empty octahedral site, with the H atom jumping back to T* (final configuration III in Fig. 5(b)). It is clear that

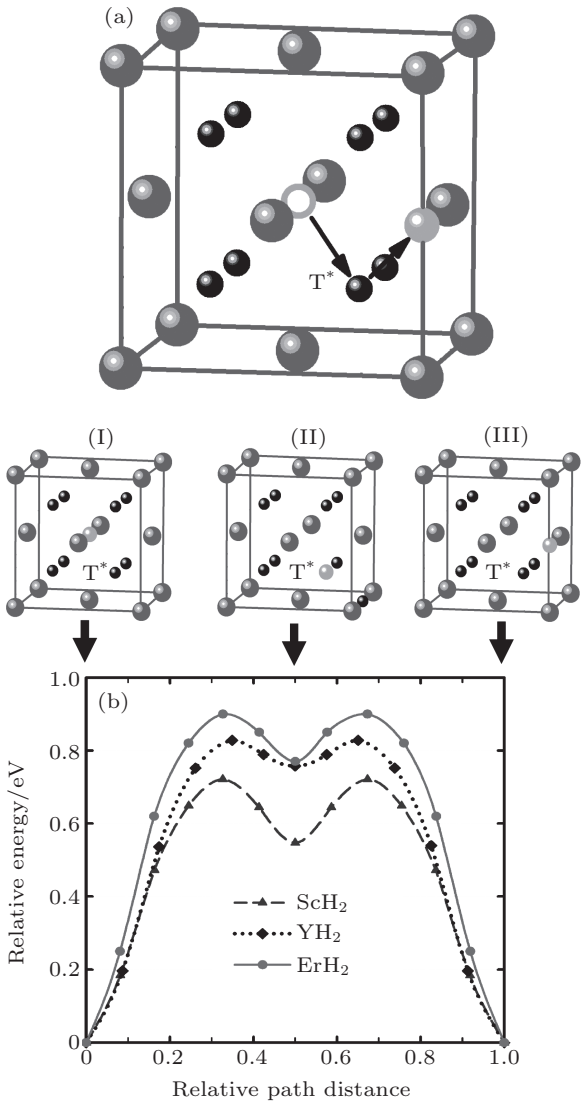


Fig. 5. He migration from an octahedral to another octahedral site to another one through an intermediate filled tetrahedral site T* (O–T*–O). (a) Migration path and (b) the corresponding migration energy paths. (I), (II), and (III) are the initial, middle, and final configurations, respectively. The symbol representations are the same as in Fig. 4.

the energy barrier increases in the order of Sc, Y, and Er hydrides, which is similar to that of H migrations in these metal hydrides.

If there is a V_{tet} near the He_{oct} interstitial, it is

expected that the He can easily migrate from an octahedral site to another one through the vacant tetrahedral site V_{tet} (O–V_{tet}–O), as shown in Fig. 6(a). This may be also defined as a vacancy assisting migration mechanism of the He_{oct} interstitial, which is different from the two above-discussed He migration mechanisms, and the corresponding energy paths are shown in Fig. 6(b). For this migration mechanism, the He atom spontaneously falls into the vacant tetrahedral site (O–V_{tet}) without an energy barrier, which indicates that the He atom can be easily trapped by the tetrahedral vacancy, forming a He_{tet}. However, the migration energy of an interstitial He from a tetrahedral to another one through its neighbouring octahedral site is 0.70, 0.53, and 0.51 eV for Sc, Y, and Er hydrides, respectively, which is the energy difference between the formation energies of octahedral and tetrahedral interstitial He atoms.

From Figs. 4 (b), 5(b) and 6(b), as well as Table 3, it is clear that the energy barrier for the O–O migration of He is 1.56 eV, whereas that for the O–T^*–O migration is only 0.71 eV in a perfect ScH_2. Thus, it is expected that the O–T^*–O migration will be a dominant mechanism for He diffusion in a perfect ScH_2. However, vacant tetrahedral sites, V_{tet}, in a metal tritide may be created for several reasons, such as the decay of tritium into He or initial underloaded H. Furthermore, the energy barrier for a V_{tet} migration in Sc hydride is above 0.64 eV, and thus it is possible that a V_{tet} diffuses to a nearby position of an octahedral He generated in thermally activated processes, which assists He atoms in migrating from one octahedral site to another one through a vacant tetrahedral site V_{tet} (O–V_{tet}–O). It is of interest to find that the energy barriers of He migration for O–T^*–O and O–V_{tet}–O mechanisms are almost the same in Sc hydride, as shown in Figs. 5(b) and 6(b) and Table 3, which implies that the He migration is independent on the presence of V_{tet}.

Figures 4, 5, and 6 show that the He migration behaviour in Y and Er hydrides is similar to that in Sc hydride. The energy barriers of the O–O jumps are the highest, but He prefers to migrate through O–T^*–O jumps in Y and Er hydrides when the V_{tet} is absent, which is the same for the He migration in Sc hydride. However, Figs. 5(b) and 6(b) and Table 3 clearly indicate that the energy barrier for the O–V_{tet}–O jump of He is lower than that for the O–T^*–O jump in Y and Er hydrides, which suggests that the He migration strongly depends on the existing vacant tetrahedral site. Therefore, He atoms can be easily trapped by the vacant tetrahedral sites in Y and Er hydrides, and only 0.53 and 0.51 eV are required for He atoms to migrate from a tetrahedral site to another one through its neighbouring octahedral site, respectively. It is expected that the O–V_{tet}–O jump is a dominated mechanism in Y and Er hydrides. It should be noted that this result is different from the He migration in Sc tritide, which may account for different behaviours of He release observed in Sc and Er tritides.[23] The Sc tritide exhibits a rapid release mode at a low He-to-metal ratio (He/Sc≈0.2) in a $ScT_{1.9}$ film, but it is not clear if Sc tritide samples have any initial stable low ^{3}He emission stage. However, Er tritide films initially release about 0.3% of He atoms, and then He atoms

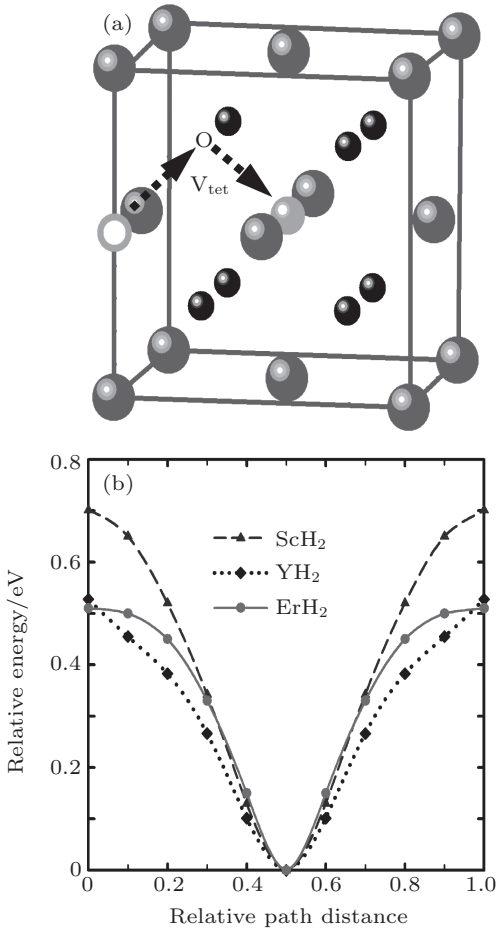


Fig. 6. He migration from an octahedral site to another one through a vacant tetrahedral site V_{tet} (O–V_{tet}–O): (a) Migration path and (b) the corresponding migration energy paths, where the small hollow represents the vacant tetrahedral site, other symbol representations are the same as those in Fig. 4.

are released at approximately their generation rate at a higher He-to-metal ratio (He/Er = 0.31 for $ErT_{1.9}$ films).[23] With a continuous tritium decay in metal hydrides, it is possible that a large extended network of V_{tet} forms.[2] Such a network can greatly enhance the He mobility, which leads to the He release at approximately its generation rate from the tritide.

In order to gain more indepth insight in the diffusion mechanism, we made a comparison between the diffusion barriers of H and He in Sc hydride and those in hcp-Sc. The relative stabilities and migrations of H and He defects in hcp-Sc have been investigated by using *ab initio* calculations based on DFT.[18] There are four well-known interstitial sites for the H atom located in hcp metals, including tetrahedral (Tet), octahedral, basal tetrahedral (BT), and basal octahedral (BO). Both H and He atoms prefer to occupy the Tet sites in hcp-Sc. The migration energy barriers of the Tet-Tet jump perpendicular to the basal plane and Tet–O–Tet jump for H interstitials are 0.10 and 0.51 eV, respectively. Both of them are lower than that of H migrations in Sc hydride. The interstitial He in hcp-Sc can directly jump from one Tet site to another perpendicular to the basal plane with a low migration energy of about 0.03 eV. Furthermore, the energy barriers of the Tet–BO–Tet and Tet–O–Tet jumps for He interstitials are about 0.31 and 0.35 eV, respectively, while the lowest energy barrier of He migration in Sc hydride is 0.70 eV. We also find that the diffusion barriers of H and He in the three metals are similar. These results suggest that the migrations of H and He in metal hydrides are more difficult than those in simple metals.

4. Conclusion

The migration mechanisms of H and He in Sc, Y, and Er hydrides are investigated by using CI-NEB. Three possible migration mechanisms of H are considered with three different H/M ratios, and the results show that migration behaviours of H are similar in the three hydrides. Formation energies of H_{oct}/V_{tet} pairs are about 1.2 eV in the hydrides. In ideal stoichiometric hydrides with a H/M ratio of 2.0, H_{oct}/V_{tet} pairs are difficult to be thermally generated due to their high formation energies. The H diffusion will be dominated by the H_{oct} mechanism with a H/M ratio > 2.0, while the V_{tet} mechanism with a H/M ratio < 2.0 is more favorable. It is of interest to note that energy barriers of the H_{oct}/V_{tet} pair formation as well as energy barriers of the V_{tet} and H_{oct} migrations increase with increasing host-lattice atomic number.

For He migration, three migration mechanisms were also considered in Sc, Y, and Er hydrides. The results show that the favorable migration mechanism of He slightly depends on tetrahedral vacancies in Sc hydride, but is strongly correlated to the V_{tet} in Y and Er hydrides. In Y and Er hydrides with a V_{tet}, the He migration between two tetrahedral sites (unoccupied by H) becomes dominated. Without a V_{tet}, He prefers to migrate from an octahedral site to another one through a filled intermediate tetrahedral site, which is much more favorable than the mechanism of direct octahedral transition in Sc, Y, and Er hydrides. Also, it is of interest to note that energy barriers of the H and He migrations are strongly associated with the host-lattice atoms in metal hydrides, and are different for the same migration mechanism in β-phase Sc, Y, and Er hydrides.

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