



Ab initio approach to the effect of Fe on the diffusion in hcp Zr II: The energy barriers

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ARTICLE INFO

Article history:

Received 16 December 2008

Accepted 23 March 2009

PACS:

66.10.cg

66.30.-h

66.30.-j

82.20.Wt

ABSTRACT

Using density functional theory calculations together with the Monomer method for the search of saddle points (combined for the first time with an *ab initio* algorithm), we obtain the vacancy formation energies and the migration barriers for α -Zr self-diffusion and for the diffusion of interstitial impurities, including the ultra-fast diffuser Fe. Good agreement with measured diffusion coefficients is obtained, as a much lower energy barrier for the ultra-fast diffuser is found. We also suggest a possible mechanism for the increase in self-diffusion due to the Fe impurity, always present in the experimental samples.

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1. Introduction

Here we study by *ab initio* methods the atomic diffusion in the low temperature ($T < 1136$ K) hcp phase of Zirconium. This process is drastically affected by the presence of very small amounts of Fe, a fast diffuser unavoidably present in real samples. The interaction between Fe and Zr is involved in various processes that imply mass transport of high relevance to the nuclear industry, such as in the irradiation-induced deformation behavior of Zr–2.5% Nb [1] and in the phenomenon of breakaway growth in Zircaloy-2 [2]. It becomes clear then that the knowledge of the Fe–Zr interaction at the atomic level could be a key element for the understanding of all such phenomena.

Experimentally, an extremely fast diffusivity of Fe in α -Zr [3], coupled with very low solubility [4] are found. Tracer diffusion studies [3] have established that Fe diffusion is up to nine orders of magnitude faster than Zr self-diffusion, as shown in Fig. 1. Also an enhancement in the diffusion coefficient of substitutional impurities [5] and self-diffusion [6] was experimentally observed in most of the recent studies when Fe is added, Fig. 2, together with a downwards curvature in the Arrhenius plot (c.f. Fig. 1 for the self-diffusion).

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In the literature [7,8] the fact that Fe is a fast diffuser is associated with the self-diffusion enhancement but only in a qualitative way. Despite important efforts made to understand the effect of Fe on the diffusion of the IV-B group of elements [9], there are several questions left unanswered: (a) which are the stable positions of Fe in the Zr matrix, (b) if one is interstitial, why does it move much faster than other, standard, interstitial atoms such as Carbon, (c) what is the mechanism for fast diffusion, (d) what is the mechanism for the enhancement of self-diffusion, and finally (e) what is the origin of the curvature in the Arrhenius plot, found for all diffusers when the temperature range is wide enough.

The present paper is a continuation of our previous one [10], with the addition of a new type of calculation. Using an *ab initio* code as a subroutine for the Monomer method [11] we are able to calculate the migration energies for the different possible jumps leading to self and impurity diffusion. This allows us to answer the first four questions; the last one seems outside the reach of the present techniques, possibly requiring dynamic calculations involving temperature effects.

2. Calculation methods and results

As previously [10] two *ab initio*, density functional theory (DFT) codes, SIESTA [12,13], and WIEN2k [14] are used for the total energy calculations. The current super-cell of 48 Zr atoms, eventually including one Fe, is however somewhat larger than before. This represents a concentration of 2 at.% Fe, much larger than

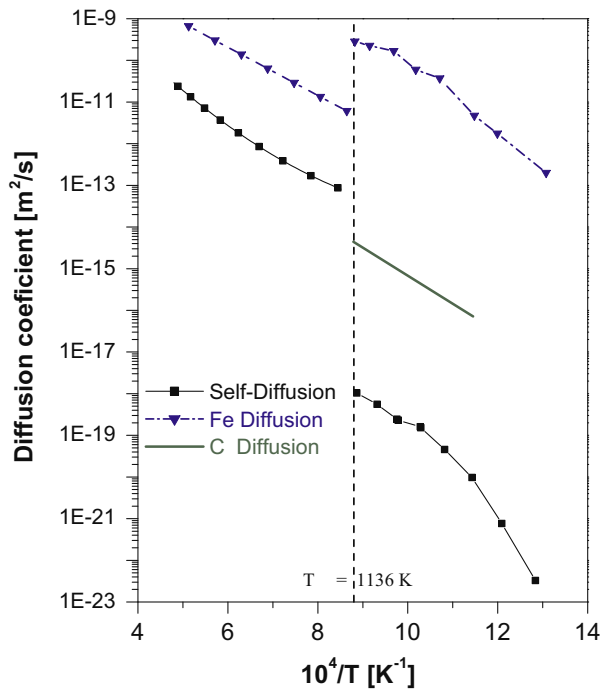


Fig. 1. Arrhenius plot for self-diffusion [24,25], C [22], and Fe [3] diffusion in Zr.

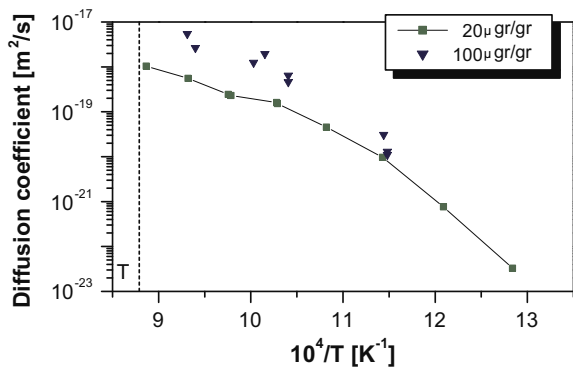


Fig. 2. Self-diffusion measured in Zr samples with different amounts of Fe [6].

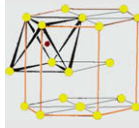
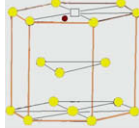
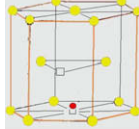
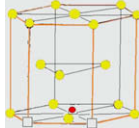
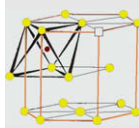
experimental values of about 100 ppm, though apparently the Fe atoms are already far enough in the periodical repetitions to make their interaction negligible.

SIESTA uses pseudopotentials and numerical atomic-like orbitals. The current calculations have been performed within the local density approximation (LDA) for exchange and correlation using the pseudopotentials and basis sets from the SIESTA home page. This method is very efficient at obtaining the equilibrium positions of the atoms by relaxing the structure via the conjugate gradients technique. The force convergence is chosen as 0.04 eV/Å. A spatial mesh cutoff of 450.0 Ry is used, with a smearing temperature of 0.15 eV, within a Fermi–Dirac scheme. Reciprocal space is partitioned in a $3 \times 3 \times 3$ Monkhorst–Pack grid. All calculations are atomically relaxed, though the cell boundary remains fixed.

WIEN2k is an implementation of the FPLAPW (full potential linear augmented plane waves) method. This is an all electron method, and therefore more demanding in computational resources than the above. Here, both LDA and the gradients correction (GGA) approximations have been employed for exchange and correlation, as the lattice parameters that minimize the crystal struc-

Table 1

Calculated total energy differences for cells with one Fe atom (eV). The total number of atoms in the cell is indicated in the first column, and to make energies comparable the energy of one Zr bulk atom was added or subtracted, as required. Calculations are performed within the LDA approach but for values within parenthesis which use GGA.

Configuration	SIESTA	WIEN2k
 Octahedral (48 + 1)	−0.36	−0.38 (−0.014)
 Off-site (47 + 1)	0	0
 Axial vacancy (46 + 1)	2.2	–
 Basal vacancy (46 + 1)	1.94	1.71
 OctaV (47 + 1)	1.91	1.44 (1.82)

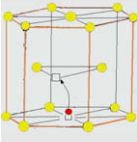
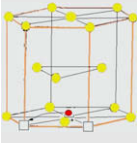
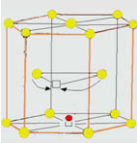
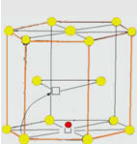
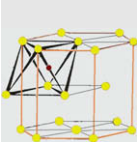
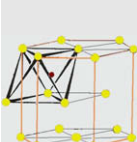
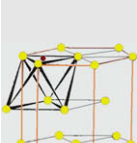
ture energy are different (LDA obtains $a = 5.94$ a.u. and $c/a = 1.62$ while GGA obtains $a = 6.11$ a.u. and $c/a = 1.59$). The number of plane waves used in the calculations is given by the parameter RKMax, which we set to seven, corresponding to an energy cutoff of 15 Ry. The calculation includes local orbitals for Fe-3p, Zr-4s and Zr-4p, and uses muffin tin radii of 2 a.u. for both Fe and Zr.

Several efficient methods have been developed in recent years for finding activated states or, mathematically, saddle points [11,15–17]; here we employ the Monomer one, developed previously in our laboratory. In [11] it has been used in conjunction with a semi-empirical potential to study interstitials migration in hcp grain boundaries. Its coupling to an *ab initio* code is undertaken here for the first time, using SIESTA's facility to be interfaced as a subroutine ('SIESTA as a subroutine' feature). The Monomer computes the least local curvature of the potential energy surface using only the forces furnished by SIESTA. The force component along the corresponding eigenvector is then reversed (pointing 'up hill'), thus defining a pseudo force that drives the system towards saddles. Both, local curvature and configuration displacement stages are performed within independent conjugate gradients loops. The method is akin to the Dimer one from the literature [16], but roughly employs half the number of force evaluations.

Table 1 reports the calculated total energy differences per unit cell of cases containing one Fe atom, with and without vacancies. To be able to compare the results, the energy of one Zr atom in bulk Zr is added or subtracted, calculated with the same method, so that in all cases the number of atoms is the same (47 Zr and 1 Fe). The reference energy chosen is that of the off-site Fe position (to be discussed later) and all cases are non magnetic. WIEN2k calculations, LDA or GGA, use the lattice parameters that minimize the energy of

Table 2

Calculated activation energies for the different jumps (eV). Within parenthesis GGA calculations. Note 'Fe crowdion' is not a true saddle but a shallow energy minimum close to the actual 'oct–oct basal' jump.

Jump type	SIESTA	WIEN2k
 Fe off-off axial	0.82	–
 Fe off-off basal	1.16	–
 Basal Zr to axial vacancy	0.17	–
 Axial Zr to axial vacancy	0.12	–
 Fe crowdion	0.21	0.01 (0.27)
 Fe oct–oct basal	0.34	0.27 (0.49)
 Fe oct–oct axial	0.32	–

bulk Zr in each case. Table 2 reports the activation energy for the different possible jumps. The saddle points are obtained with the Monomer-SIESTA method, within the LDA approximation.

Unless otherwise stated, all energies reported in the following sections are obtained with SIESTA. However, some of the equilibrium and saddle configurations have been recalculated with WIEN2k, to confirm that the qualitative results do not depend on the calculation method or on the LDA or GGA approximations. In this context, all the calculations are estimated to be converged within 0.01 eV, though differences in energies obtained with different methods, SIESTA vs. WIEN2k, or LDA vs. GGA, may be expected to differ in 0.1–0.2 eV.

2.1. Stable positions of Fe atoms in the α -Zr lattice

The most stable position of the Fe impurity in the α -Zr lattice is an open question in the literature. Given its small atomic radius and fast mobility, it is a candidate to occupy an interstitial site. On the other hand the ultra-fast mobility of Fe, up to 10^9 times

the self-diffusion, is not observed in other interstitial elements, for instance Carbon, which moves only 3–4 orders of magnitude faster, as do other interstitial diffusers in metals. Also, Mössbauer measurements [18] show that at least two different configurations are present in the system, both non magnetic.

To clarify this subject several Fe positions in the α -Zr matrix are explored, with and without vacancies, and the more relevant ones are listed in Table 1. In all the calculations the octahedral position is lowest in energy. Yet, the so-called off-site configuration is competitive or even degenerate, depending on the method of calculation used. On the other hand, Fe in a substitutional position turns out to be magnetic, whereas in the octahedral and off-site configurations it is not. We exclude the substitutional position in what follows because it is not present in the experiments [18] and is also higher in energy.

In the off-site configuration the Fe atom is slightly displaced from the lattice node towards the octahedral position, whereas four nearest neighbor Zr atoms move closer to the Fe atom. The interatomic distances decrease to about 2.5 Å from the 3.13 Å nearest neighbor distance in the perfect Zr lattice. That distance is very similar to the interatomic distances in ZrFe intermetallic compounds, such as Zr_3Fe or Zr_2Fe [19]. On the other hand, in the octahedral position the equilibrium distance between Fe and a nearest neighbor Zr is 2.43 Å. For both configurations, off-site and octahedral, there is a strong interaction among the valence electrons of the involved species.

2.2. The mechanism of ultra-fast Fe diffusion

Now we try to assess the possible causes of the ultra-fast mobility of Fe in the α -Zr matrix. For such a purpose, the activation energies associated to the diffusive jumps for both Fe configurations, are calculated and compared with the vacancy jumps involved in self-diffusion. We notice that Fe in the off-site position can only diffuse via a vacancy mechanism (c.f. next section) as for self-diffusion, while Fe in the interstitial octahedral site may jump directly to a neighbor octahedral site.

As reference, the vacancy formation and migration energies in pure Zr are calculated first. The SIESTA code, within the LDA approximation, gives a formation energy of 2.38 eV, while WIEN2k obtains 2 eV in our present calculations for both, LDA and GGA approximations, in good agreement with other calculations [20,21]. The difference is most likely due to a too short cut-off radius of SIESTA's numerical orbitals, and the result could be improved by placing so-called ghost orbitals in the vacant site. However, this would complicate the migration calculations and is therefore not considered. It will certainly not change the qualitative results, amounting essentially to an energy shift in every configuration including vacancies, thus leading to a virtual cancellation in the comparison. The migration jump is anisotropic, as was shown previously in Ref. [21]. In our calculations it requires 0.37 eV for the basal direction, and 0.51 eV for the axial one. Therefore, the activation energy for Zr self-diffusion predicted by SIESTA is 2.75/2.89 eV for the basal/axial direction. Recalculation of the barriers with WIEN2k within the LDA approximation, results in 2.37 and 2.43 eV, respectively.

Different configurations containing a vacancy are shown in Table 1, in all cases the vacancy formation energy is lower than in pure Zr, due to the presence of Fe. The case of a vacancy nearest neighbor to an octahedral Fe is not shown because it is unstable, decaying to an off-site Fe. A vacancy second nearest neighbor to the octahedral position is stable, and is named below as OctaV.

When a Fe atom is in the off-site configuration, there are essentially two non-equivalent forms to create a vacancy in a nearest neighbor position. As reported in Table 1, the formation energies are 1.94 eV for a vacancy in the same basal plane as Fe, and

2.2 eV for the axial position; this implies a binding energy between Fe and vacancy of 0.44 and 0.18 eV, respectively. Calculations of the off-site jumps are reported in Table 2. The lowest barrier for a Fe-vacancy exchange occurs in the axial direction and amounts to 0.82 eV. Therefore, the activation energy for off-site Fe diffusion via a vacancy mechanism is at least $(1.94 + 0.82) = 2.76$ eV, almost the same as for self-diffusion in pure Zr.

On the other hand, the jump of an octahedral Fe to a neighbor site in the same basal plane occurs through a saddle configuration, very close to the lattice crowdion position, with an energy cost of 0.34 eV, and about the same for the purely axial alternative. These are very small activation energy values, about one tenth that for self-diffusion, and thus compatible with an ultra-fast mechanism.

Above we have made reference to a standard interstitial species, namely Carbon. It is therefore interesting to compare the energy required to reach the saddle point, in an analogous calculation as the one performed for Fe. The saddle point close to the crowdion position entails an energy cost of about 1.7 eV, much higher than for Fe, and in good agreement with experimental values, 1.57 eV from [22] and 1.33 eV from [23]. On the other hand, the octahedral position for Carbon is preferred over the substitutional one by more than 10 eV, whereas the off-site configuration results unstable.

In synthesis, we obtain an average activation energy for self-diffusion in pure Zr of 2.8 eV and of 1.7 eV for Carbon, which diffuses between 3 and 4 orders of magnitude faster, as is usual for interstitial diffusers in metals. For interstitial Fe, which is an unusually ultra-fast diffuser, the activation energy obtained is only 0.34 eV. This is certainly related to the hybridization between the *d* orbitals of Fe and Zr that reduces the energy of the crowdion position, effect absent in the case of Carbon. Qualitatively, the *d*–*d* bonding between Fe and Zr is possibly more flexible than the *p*–*d* one between C and Zr, so that it does not feel as much the structure of the surroundings. This image is also consistent with C being more strongly bonded to Zr than Fe, as measured e.g. by the energy required to bring the foreign species from the host bulk to infinity.

Experimental values at the reference temperature of 1000 K for Carbon and Fe diffusion in α -Zr are $D = 2.5 \times 10^{-15}$ m²/s and $D = 10^{-10}$ m²/s, respectively as seen in Fig. 1. Using the measured pre-exponential factor for Carbon [22], $D_0 = 2 \times 10^{-7}$ m²/s, for both diffusers and the activation energies given by SIESTA, $Q_C = 1.7$ eV and $Q_{Fe} = 0.34$ eV, the calculated diffusion coefficients are $D = 5.4 \times 10^{-16}$ m²/s and $D = 4 \times 10^{-9}$ m²/s. Here, using the same D_0 value for both elements seems to be well justified, as both have the same migration mechanism. Therefore, the several orders of magnitude difference observed between the diffusion coefficients of these two interstitial diffusers in the same matrix, is rightly captured by the calculations. Let's point out that experiments could also be well fitted using, for example, $Q_C = 1.6$ eV and $Q_{Fe} = 0.6$ eV. The difference between these values and our calculated ones, is similar to the difference between the experimental measurements [22,23], thus showing that the agreement between experiments and calculations is very good.

2.3. Self-diffusion enhancement: possible mechanisms

To relate the self-diffusion enhancement with the presence of Fe impurities, the first point to notice is that any experimentally detectable Fe content is most likely several orders of magnitude larger than the thermodynamic vacancy concentration C_V . In fact, for a vacancy formation energy of 2 eV and a reference temperature of 1000 K, $C_V = 8.4 \times 10^{-11}$, which is already about 4 orders of magnitude smaller than a 1 ppm of Fe for a very pure Zr sample. This suggests that if Fe atoms could induce their Zr neighbors to move along in an easy migration path, the assumed intrinsic va-

cancy mechanism for self-diffusion might have never been observed.

Given the two stable configurations previously reported, the fast diffusing octahedral Fe is unlikely to enhance self-diffusion, whereas the off-site Fe deserves consideration. Its presence produces both a decrease in the vacancy formation energy and a distortion of the lattice, with Zr atoms displaced from their lattice nodes towards the Fe site. In order to explain the diffusion enhancement one needs to find a mechanism involving the movement of the complex Fe-vacancy as a whole, with an energy cost lower than the single vacancy mechanism.

The off-site configuration can be thought of as the recombination product of an octahedral Fe and a first nearest neighbor vacancy, and it is also very close to a substitutional configuration. Our current SIESTA calculations predict off-site Fe to be 0.36 eV above the lowest energy octahedral (Table 1). For comparison purposes we shall consider only the activation energy Q , and take as reference the activation energy for the basal vacancy jump in bulk α -Zr, $Q_b = 2.75$ eV.

Mechanisms involving no vacancies are explored first, namely, ring exchanges comprising 2 or 3 atoms one of them being Fe. The computed activation energies are however always larger than 3 eV, which makes these mechanisms unlikely candidates to compete with the intrinsic one. Complexes including vacancies seem better candidates, and we concentrate in two structures of this kind. The first one is an off-site Fe with a nearby vacancy; in Table 2 it is seen that exchanges between Zr atoms and vacancies (both axial and basal) in the vicinity of Fe are easy, but what is needed for self-diffusion is the motion of the whole complex. The latter is controlled by the Fe jumps, therefore, as already found, a minimum $Q = 2.76$ eV results. However, there is still another factor to take into account, namely, off-site Fe is not the lowest energy configuration for Fe in Zr. Thus the above mentioned 0.36 eV must be added as part of the activation energy, raising Q to 3.12 eV. Again, this mechanism is not competitive with the intrinsic one.

In the second and more promising structure, here named OctaV, the off-site Fe dissociates into an octahedral Fe plus a second neighbor vacancy, as depicted in Fig. 3(a) and (b). Fig. 3(c) shows schematically how an effective three-dimensional Zr migration can result from the displacement of an off-site Fe into another off-site position, passing through an octahedral position with a second neighbor vacancy. The energy difference between the two structures is 1.9 eV and the energy barrier for the reverse process is only 0.1 eV (Fig. 3(d)), so that $Q \approx 2$ eV. As before, 0.36 eV should be added as activation, resulting in a final Q of 2.36 eV, i.e., almost 0.4 eV smaller than the reference intrinsic value. This proves our initial assumption, that mechanisms moving the whole Fe-vacancy complex may possess lower activation energy than the single vacancy mechanism.

As we saw in the previous section, differences in energy of this order can lead to orders of magnitude difference in the diffusion coefficient, but in this case there is a compensation factor due to the Fe concentration. The enhanced diffusion coefficient may be calculated as,

$$\frac{D^{\text{enh}}}{D_0} = (1 - C_{Fe})e^{-Q/kT} + C_{Fe}e^{-Q_{Fe}/kT} \approx e^{-Q/kT}(1 + C_{Fe}e^{\Delta/kT}), \quad (1)$$

where C_{Fe} is the total Fe concentration ($C_{Fe} \ll 1$), Q the vacancy activation energy, Q_{Fe} that for the proposed mechanism, and $\Delta \equiv Q - Q_{Fe} = 0.4$ eV. The experimentally measured enhancement [6] for a reference temperature of 1000 K and 160 at. ppm Fe ($C_{Fe} = 1.6 \times 10^{-4}$) is around 6. Thus, in order to match the experimental values, the quantity $C_{Fe}\exp(\Delta/kT)$ should be about 5, and this requires $\Delta \approx 0.9$ eV, a value larger than our calculation, though of the same order of magnitude. As a check, we have recalculated

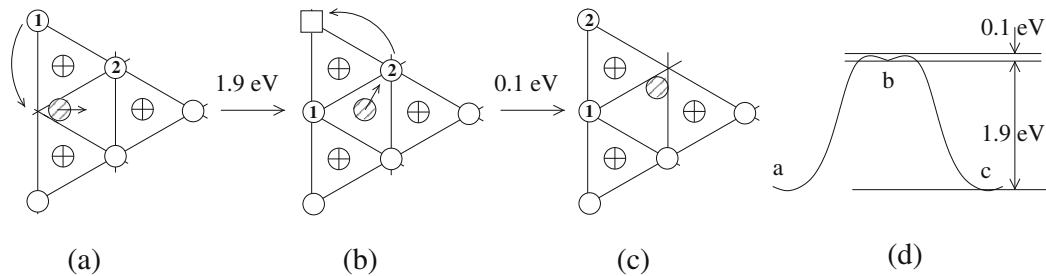


Fig. 3. Diffusion jump through the OctaV configuration; two basal planes of the Zr lattice are shown by crossed and empty circles. (a) Initial off-site Fe; Fe rests about on the plane of the empty circles; 1 and 2 mark Zr atoms taking place in the overall cooperative motion whose first stage is suggested by the arrows. (b) OctaV configuration; Fe rests close to an octahedral position. (c) Final off-site Fe. (d) Energy barriers involved in the complete sequence.

the involved structures energy with WIEN2k, using both LDA and GGA approximations, obtaining a value of $\Delta \approx 0.45$ eV, in good agreement with SIESTA predictions.

On the other hand, the pre-exponential factor D_0 is given by,

$$D_0 = va^2f \exp\left(-\frac{\Delta S^f + \Delta S^m}{k}\right), \quad (2)$$

where v is the attempt frequency, a the jump distance, f the correlation factor and $\Delta S^f, \Delta S^m$ are the entropy of formation and migration, respectively, of the jumping defect. Therefore, it seems a rough approximation to use the same D_0 as for the intrinsic vacancy mechanism, which involves the jump of only one atom, while the proposed mechanism through OctaV implies the coupled movement of several atoms. Certainly, the attempt frequency and the entropy factors should be different, providing an additional correction to the enhanced coefficient, though not evaluated in the present work.

Finally, we should notice that for a jumping Fe atom in the OctaV configuration, two different paths are almost equally probable. One is the Fe atom going to another off-site configuration, the other is a jump to an octahedral position away from the vacancy. Both require similar activation energies, of a few tenths of eV. In the latter case, the Fe atom initially in an off-site configuration dissociates into an octahedral Fe plus a free vacancy. The octahedral Fe will later migrate in an ultra-fast fashion until a second far away vacancy is found. This could be interpreted as ultra-fast vacancy migration, not contributing directly to modify the activation energy, but impacting on the dynamics of the process (e.g. correlation factors), and thus deserves further study.

3. Conclusions

Ab initio calculations show that Fe atoms co-exist in two stable non magnetic positions in the hcp Zr matrix, the octahedral and a the so-called off-site, where Fe is slightly displaced from the lattice node towards the octahedral position, and four nearest neighbor Zr move closer to it, resembling the Zr_3Fe intermetallic structure.

The octahedral Fe atoms are the ultra-fast diffusers. A very low energy, only a few tenths of an eV, is required for the jump from one interstitial position to the next. This is the main cause for such ultra-fast movement, when compared with other interstitial diffusers, such as Carbon, with activation energies above 1 eV. This effect is ascribed to the hybridization between the d orbitals of Fe and Zr.

Fe atoms in the octahedral and off-site positions are interchangeable through the OctaV configuration. The off-site configuration dissociates into an octahedral Fe plus a second neighbor vacancy with an energy cost lower than the vacancy formation energy in pure α -Zr. A diffusion mechanism for Zr atoms involving the OctaV configuration, with activation energy lower than a simple vacancy mechanism, is proposed in order to explain the experimentally measured enhancement of the self-diffusion coefficients due to the presence of Fe.

Acknowledgement

The work was partially supported by ANPCyT PICT-20479, and by CONICET PIP 5322/04 and PICT 5062.

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