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Ab initio study of self-interstitials in hcp-Zr

F. Willaime *

Service de Recherches de Métallurgie Physique, CEA/Saclay, 91191 Gif-sur-Yvette cedex, France

Abstract

The formation energies of self-interstitials in hcp-zirconium have been obtained from first principles electronic structure calculations in the framework of the density functional theory in the local density approximation using a planewave pseudopotential approach with supercells containing 37 and 97 atoms. For the largest cell, five configurations are found to be nearly degenerate in energy. The most stable ones are the octahedral (O), split $\langle 0001 \rangle$ dumbbell (S), and basal octahedral (BO) configurations, with formation energies $E_f^i = 2.8$ eV, and the basal split (BS) with $E_f^i = 2.9$ eV. The crowdion (C) configuration is slightly less stable with $E_f^i = 3.1$ eV, while the basal crowdion (BC) is unstable and decays to BO. The effect of the exchange correlation functional is investigated by repeating the same calculations for 37 atom supercells within the generalized gradient approximation (GGA): the formation energies increase by almost 0.2 eV for the basal configurations and by more than 0.3 eV for the non-basal ones. From the analysis of the present results, the most stable configuration in hcp-Zr at low temperature is predicted to be BO, but BS and to a lesser extend O and S cannot be excluded.

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1. Introduction

Two types of defects, namely vacancies and self-interstitials, are formed in metals under irradiation. The evolution of defect population leads to significant changes in microstructure and causes a number of radiation-induced property changes. Self-interstitials in the anisotropic hcp-structure are particularly complex since they can adopt at least eight different configurations. Depending on which configuration is dominant, the resulting interstitial diffusion can range from one- or two-dimensional motion in the basal plane, to three-dimensional migration. This affects the diffusional anisotropy difference between vacancies and interstitials, which is believed to be at the origin of phenomena observed in hcp materials under irradiation, such as irradiation growth [1].

In hcp zirconium, which is particularly important in the nuclear industry, no clear conclusion on the relative stability of the various interstitial configurations has been drawn either from experiments, or from atomistic modelling based on empirical potentials. Huang diffuse scattering experiments performed at 6 K on Zr after electron irradiation [2], showed that the displacement field of interstitial atoms is rather isotropic, but no definite conclusion about the stable configuration was possible [3]. Internal friction measurements showed that, among the configurations that are sensitive to this experimental technique, one of them displays three-dimensional migration and is compatible with monoclinic symmetry, i.e. C type [4]. Since the review by Bacon on modelling of point defects in hcp metals by pair-potentials [5], self-interstitials in hcp-Zr have been studied with no less than eight non-pairwise empirical potentials, of the EAM or second-moment approximation type [6–13]. These calculations agree on a value of $E_f^i = 4.0 \pm 0.6$ eV, except in two extreme cases (2.5 eV in Ref. [12] and 7.7 eV in Ref. [8]), but the most stable configuration depends strongly on the potential: it is

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* Tel.: +33-1 6908 4349; fax: +33-1 6908 6867.
E-mail address: fwillaime@cea.fr (F. Willaime).

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indeed preferentially BC or BS [10–13], but it is O in one case [8], C in two cases [6,7], and BO in one case [9]. The tendency which emerges from these rather wide spread results is a BC or BS stable configuration with a formation energy around 4 eV, but predictive energetic models are clearly required.

Ab initio electronic structure calculations can, in principle, alleviate this uncertainty, but such calculations on interstitials are rather rare. The pioneer works on ab initio calculations on vacancies and interstitials in metals were performed in alkali metals [14,15] since these metals require smaller basis sets in a planewave formalism. They have been followed by a series of studies on vacancies in transition metals [16,17]. To perform similar calculations on interstitials requires considerable computational efforts since larger cells are needed to account for the accompanying large relaxation and long range elastic interactions. As a result this technique has been applied only very recently to interstitials in transition metals [18–20].

In this paper, we report an ab initio study of the self-interstitial formation energy in hcp-Zr for six different configurations (Fig. 1). The notation adopted by Johnson and Beeler is employed [21]. Site O has an octahedral coordination; S represents a ⟨0 0 0 1⟩ split dumbbell, i.e. two atoms sharing the same site in the *c* direction; the C site is midway between two nearest-neighbor atoms out of the basal plane, and can be viewed as a pseudo-crowdion. The three other configurations are in the basal plane: BO is below an O site; BC is midway between two nearest neighbors in the basal plane, and forms a crowdion in the dense *a* direction; and BS involves two atoms equidistant from a vacant lattice site. Two other configurations have been proposed: the tetrahedral (T), and basal tetrahedral sites (BT). They are not examined here since they are found to be higher in energy, or even unstable, with empirical potentials and by previous ab initio calculations in hcp-Zr [20].

The estimation of elastic constants is an important test for the validity of the present calculations. They indeed control the long-range elastic relaxation around the interstitial while the local rearrangement is dominated by the short-range repulsive part of the interatomic interaction. This is the reason why the first part of this paper is devoted to the study of elastic constants.

2. Method

The present first principles electronic calculations are performed in the framework of the density functional theory (DFT) with two different approximations for the exchange and correlation energy: the local density (LDA) and the generalized gradient approximations (GGA). For the latter we used the functional proposed by Perdew, Burke and Ernzerhof (PBE) [22]. The results reported here were obtained using the PWSCF planewave pseudopotential code [23].

The pseudopotentials for Zr are generated using the Vanderbilt ultrasoft pseudopotential package [24,25]. The atomic configuration is $4s^2 4p^6 5s^2 4d^2$ and the same value, $r_c = 2.1$ bohr (1 bohr = 0.529 Å), is taken for the three cutoff radii and two non-local projectors (i.e. two reference energies) are used per angular momentum component. The d-electron pseudopotential is used as the local component. Cutoff energies of 20 Ry for the wavefunctions and 100 Ry for the augmentation charges (1 Ry = 13.606 eV) are used to achieve convergence of

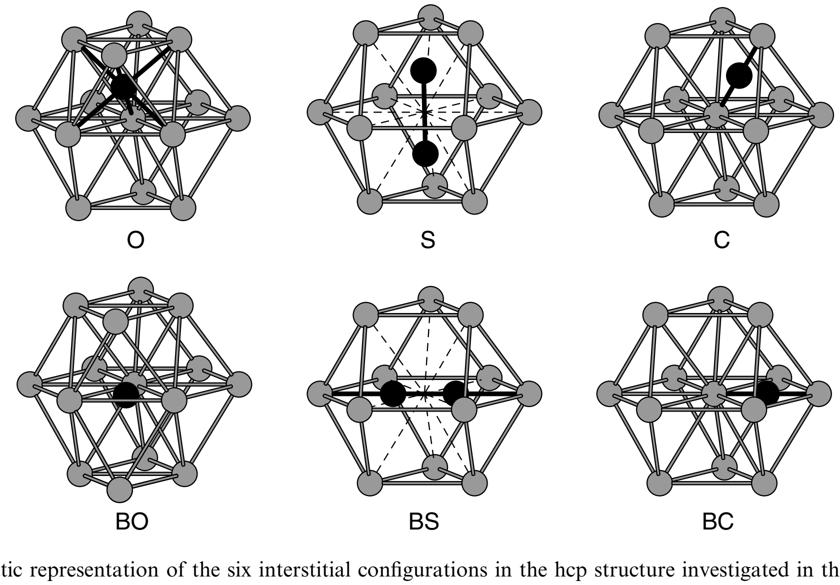

Fig. 1. Schematic representation of the six interstitial configurations in the hcp structure investigated in the present study.

the total energy to within 0.03 eV/atom. It was shown by several authors that at least the 4p states must be included as valence states in order to obtain correct bulk properties [26,27], and most pseudopotentials for Zr also include 4s valence states. As pointed out in Ref. [18], it is essential to use a pseudopotential with good transferability (i.e. including semi-core states and with small enough core radii) to correctly describe the very short distances between atoms around the interstitial. Bond lengths near an interstitial are indeed shorter than in the bulk by as much as 25%.

The five independent elastic constants of the hcp structure are calculated with the strain matrixes proposed in Ref. [28]: distortions preserving the hexagonal symmetry are used to calculate B, $C_{11}+C_{12}$, and C_{33}, while monoclinic and triclinic distortions are used respectively for $C_{11}-C_{12}$ $(=2C_{66})$ and C_{44}. The above elastic constants are obtained from a fourth order polynomial fit performed over the energies calculated for nine values of the strain ranging from −2% to +2%. The cutoff energy is increased to 28 Ry to reach sufficient accuracy. Since there are two atoms per unit cell in the hcp structure, it is important to account for possible internal relaxations [29,30]. For the above distortions, such displacements occur only in the $C_{11}-C_{12}$ case. It is taken into account by performing a careful structural relaxation at fixed strain. Note that a relaxation convergence threshold as low as 10^{-4} eV is necessary for the largest distortions and 10^{-5} eV for the smallest ones.

The recent ab initio calculations on interstitials in V, Mo, Fe and Zr [18–20] were performed using the supercell method under two conditions, namely at constant supercell volume or at constant pressure following the procedure used previously for vacancies. For interstitials, the constant supercell volume calculations tend to significantly overestimate the formation energies [18–20]. The constant pressure conditions are therefore much better than constant supercell volume conditions, but their drawback is that they require a higher accuracy in the calculation of stress tensors, and therefore larger values of the cutoff energy are needed. Slightly different conditions which overcome these difficulties are proposed here. The idea is to perform the calculations at constant volume per atom, i.e. such that the supercell volume divided by the number of atoms is the same with an interstitial as in the bulk. The size and shape of the supercell with an interstitial is simply obtained by isotropically scaling the bulk supercell, by a factor $[(N+1)/N]^{1/3}$ in each direction, where N is the number of atoms in the bulk supercell. These conditions mimic the constant-volume thermodynamic conditions. The formation energies calculated in constant volume ensembles and the formation enthalpies at constant pressure are known to converge to the same thermodynamic limit [31]. All components of the residual stress tensor – calculated as the difference with the bulk stress tensor – are found to be less than 5 kbar for all interstitial configurations in $N=97$ atom cells. This ensures that a similar accuracy on the formation energy is obtained as compared to constant pressure calculations, but with less computational effort.

The present calculations are performed on $3\times3\times2$ and $4\times4\times3$ supercells, i.e. with respectively $N=36(+1)$ and $N=96(+1)$ atoms. The Brillouin-zone (BZ) is sampled with special k-points taken on $6\times6\times6$ (respectively $4\times4\times4$) hexagonal grids, shifted along the z direction, containing 21 (respectively 8) irreducible k-points for the supercells with 36(+1) atoms (respectively 96(+1)) atoms. The equivalent grid for a two-atom cell has 222 (respectively 180) k-points. The integration over eigenvalues is performed by the smearing technique using the Hermite–Gauss function of order 1 and a smearing width $\sigma = 30$ mRy. [32] The relaxation is performed until a convergence of typically 0.02 eV in total energy is reached.

3. Results and discussion

3.1. Elastic constants

The values obtained for the lattice parameters and for the B, C_{11}, C_{33}, C_{44}, and C_{66} elastic constants are displayed in Table 1. As in previous LDA and GGA calculations [28,33], the agreement with experiments is very good [34], with an overall better performance of

Table 1
Bulk properties of hcp-Zr: lattice parameters (in Å), and elastic constants (in GPa)

	a	c/a	B	C_{11}	C_{33}	C_{44}	C_{66}
Experiment	3.23	1.593	97	155	173	36	44
LDA present work	3.15	1.615	105	135 (160)	181	21	24 (49)
LDA Ref. [33]	3.16	1.614	105	145	177	22	36
LDA Ref. [28]	3.19	1.585	103	(156)	182	25	(46)
GGA present work	3.23	1.600	94	146 (153)	156	28	42 (49)
GGA Ref. [33]	3.23	1.604	92	142	164	29	39

The experimental values for the elastic constants are taken at 4 K from Ref. [34]. The values in parenthesis for the elastic constants denote the results without internal relaxation.

GGA. Both functionals tend to underestimate C_{44}. LDA also significantly underestimates the C_{66} shear elastic constant. Note that this discrepancy appears only if the relaxation contribution – which decreases the value of C_{66} by a factor of two – is taken into account. This effect has not been included in Ref. [28] and its amplitude is not reported in Ref. [33]. The perfect agreement with Ref. [28] on the unrelaxed value of C_{66} suggests that the discrepancy with experiment is due an insufficiency in the LDA method rather than in the present pseudopotential. Such large relaxation amplitudes have been reported with empirical potentials [29] and with tight-binding d band models [30]. The latter calculation also shows that for the Fermi level corresponding to Zr, the relaxation contribution is very sensitive to the d-band filling. The large LDA–GGA discrepancy on the relaxation contribution to C_{66} may therefore be related to the fact that it is very sensitive to small changes in the electronic structure. Apart from the value of the relaxation contribution within LDA which has yet to be confirmed by other calculations, the agreement with previous ab initio calculations is excellent.

3.2. Self-interstitials

Starting from atomic positions similar to the ones shown in Fig. 1, all configurations are found to be stable or metastable, except BC which decays to BO. The instability of the BC configurations was observed on 37 atom supercell LDA calculations, and was not investigated in further calculations. The stability of the other configurations with respect to small atomic displacements was not investigated either.

The positions obtained for the relaxed configurations within LDA in $N = 97$ atom cells are schematically represented in Fig. 2. The cages around the interstitials are significantly distorted with respect to Fig. 1. The shortest bond length is observed for the S configuration (2.37 Å between the two split atoms). Note that the BO site has a quite favorable coordination (with nine close neighbors) but it is also rather constrained with three very short bonds (2.45 Å).

The results obtained for E_f^i for the $N = 37$ (LDA and GGA) and $N = 97$ (LDA) cells for the five configurations that are stable or metastable in the calculation (O, S, C, BO, and BS) are summarized in Table 2. These energies are rather close, around 3 eV, and the relative stabilities of the various configurations will be discussed below as function of supercell size and the functional used. These formation energies are much smaller than the ones predicted by all empirical potentials except one [12]. This probably reflects the fact that the repulsive part of these potentials – which is usually the most empirical part – is too stiff and needs to be fitted to configurations with distances between atoms as short as the ones encountered in interstitials.

The comparison between $N = 37$ and $N = 97$ atom results shows that the interstitial formation energies change significantly between these two supercell sizes, decreasing by 0.15 eV on the average, but this decrease

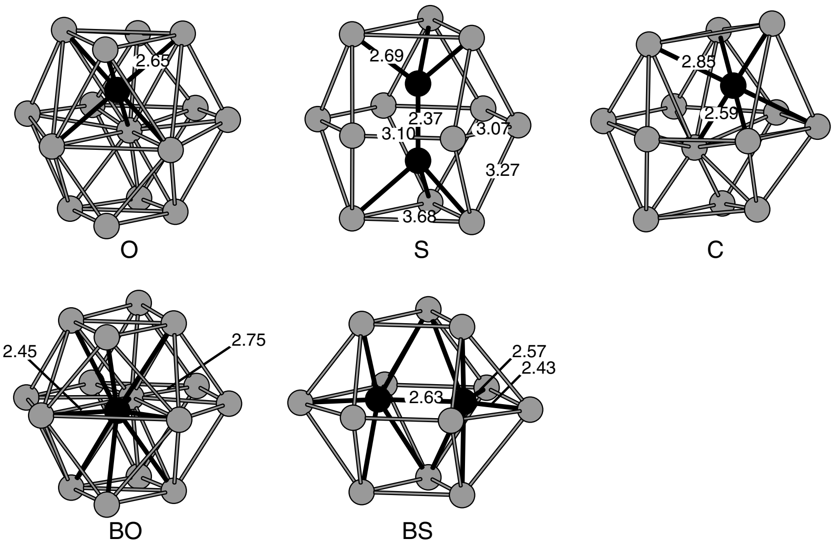

Fig. 2. Schematic representation of the relaxed interstitial configurations obtained from ab initio calculations in hcp-Zr. The positions correspond to LDA calculations for the $N = 97$ atom supercells. Only a few atoms around the interstitial or the split interstitial (black spheres) are represented. The bond lengths (in Å) are given for some bonds showing large distortions with respect to the bulk nearest-neighbor distance (3.14 Å).

Table 2
Ab initio values of the formation energies of various interstitial configurations in hcp-Zr (in eV)

		O	S	C	BO	BS
LDA present work	$N = 37$	2.73	2.95	3.18	2.97	3.23
	$N = 97$	2.79	2.80	3.07	2.78	2.90
GGA present work	$N = 37$	3.04	3.28	3.52	3.14	3.39
GGA Ref. [20]	$N = 37$	2.83	3.13	3.19	3.07	3.23
	$N = 97$	2.84	3.01	3.08	2.88	2.95

The present LDA and GGA results, obtained by constant volume per atom calculations, are compared with the constant pressure GGA results of Ref. [20] for two supercell sizes ($N = 37$ and $N = 97$).

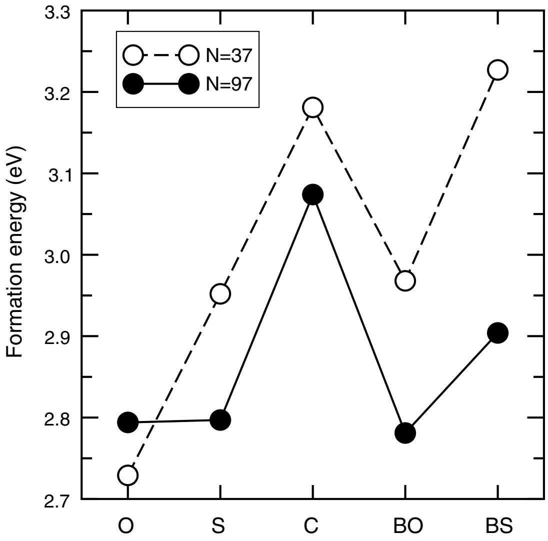

Fig. 3. Variation with supercell size of the interstitial formation energies in hcp-Zr for the O, S, C, BO, and BS configurations: comparison between ab initio results with 37-atom cells (open circles) and 97-atom cells (filled circles) obtained at constant volume per atom (see text) within LDA.

depends on the configuration (see Fig. 3): it is larger for basal configurations (up to −0.33 eV for BS) than for non-basal ones (E_f^i even tends to increase for O, as in Refs. [20,35]). The unexpected behavior for the O configuration – i.e. the increase of E_f^i with supercell size – is a quite robust result since it is not sensitive to changes in the energy cutoff or the k-point sampling. The same effect was reported for the ⟨1 1 1⟩ dumbbell in bcc V when going from 55 to 129 atom supercells [18]. As further discussed below, the number of atoms is a limitation in the present calculations, in particular for the basal configurations, but considerable computational effort is required to go to even larger cells. However E_f^i was shown to change only weakly beyond 100 atoms, i.e. by only 0.04 eV from 129 to 251 atoms for the ⟨1 1 1⟩ dumbbell in bcc V [18].

The GGA values of E_f^i are on the average nearly 0.3 eV larger than the LDA values. This effect of the functional is consistent with previous results in Si [36], and, as expected, opposite to the effect observed for vacancies [37,38]. However this effect is not the same for all configurations: the increase in E_f^i is 0.17 eV for the basal configurations (BO and BS) and twice more for the non-basal ones. This discrimination between basal and non-basal configurations can be seen as a consequence of the change in c/a ratio ($c/a = 1.600$ in GGA and 1.615 in LDA). Basal configurations are indeed favored by smaller values of c/a. When going from LDA to GGA, the increase of E_f^i due to the functional itself is partly compensated by the decrease due to smaller c/a ratio for basal configurations, while for non-basal configurations these two effects add up.

Starting from LDA positions in reduced coordinates, relaxation within GGA decreases the energy by 0.03–0.12 eV in 37 atom cells. This attests that the relaxed interstitial geometries are very similar, but this further relaxation is not negligible in order to predict reliable E_f^i differences.

The size dependence of the present LDA constant volume per atom calculations, and the GGA constant pressure calculations of Refs. [20,35] are very similar. As a first approximation, one can therefore extrapolate the present GGA results performed only on 37 atom cells, to 97 atoms by adding the energy correction found either within LDA or within the GGA constant pressure calculations of Refs. [20,35]. Preliminary results with 97 atom cells indicate that these extrapolations are accurate enough to predict formation energies to within 0.1 eV, but the full calculation needs to be performed to obtain the correct relative stabilities.

The following analysis can be made on the $N = 97$ LDA results, and the GGA results extrapolated to 97 atoms for E_f^i (see Fig. 4). Four configurations (O, S, BO and BS) are found to be within 0.2 eV, while C is nearly 0.2 eV or more higher in energy. In LDA, O, S and BO are perfectly degenerate, while in GGA BO is the most stable configuration.

As compared to the present GGA results on 37 atom cells, the values of E_f^i of Refs. [20,35] are on the average smaller by almost 0.2 eV (see Table 2). The relative stabilities are also significantly different, with a discrepancy

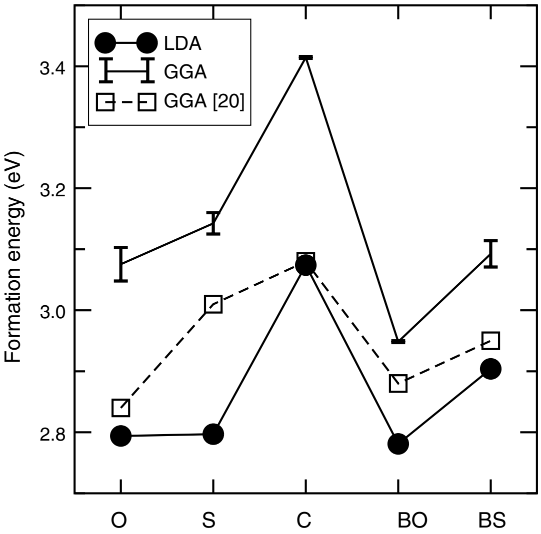

Fig. 4. Self-interstitial formation energies for three sets of ab initio calculations in hcp-Zr. The present results (solid lines), within LDA (filled circles) and GGA (error bars), are compared with the GGA results of Refs. [20,35] (open squares and dashed line). All results correspond to $N = 97$ atom supercells; the present GGA results are estimations obtained from two types of extrapolations from $N = 37$ atom calculations (see text).

of up to 0.3 eV for the C–BO relative stability. These discrepancies can be attributed to one or several differences in the set-ups of these two quite similar calculations. Among these differences note that in Refs. [20,35] constant pressure conditions and the Perdew-Wang 91 GGA functional are used. But the main difference comes from the pseudopotential. In Refs. [20,35] the 3s states are not included in the valence states, and most of all the core radii are larger, namely up to 1.6 Å [26] instead of 1.1 Å here. Note that with the present pseudopotentials there is no overlap between the ionic cores for all the interstitial configurations (the shortest distance between atoms is 2.4 Å), and this ensures in principle a better transferability.

According to these three sets of calculations four configurations (O, S, BC and BO) are likely to be either the most stable configuration in hcp-Zr or less than 0.2 eV above it in energy; while the C configuration appears to be slightly less stable (see Fig. 4). Making further predictions is quite delicate, since the energy differences which are involved are comparable to the change in energy due to supercell size (from $N = 37$ to $N = 97$), or due to the functional or the pseudopotential. Further calculations are therefore clearly needed in order to draw more firm conclusions: the effect of pseudopotential needs to be clarified, and the dependence on supercell size requires more investigation. Concerning the functional, since GGA performs much better than LDA for bulk properties believed to be important for interstitials (c/a ratio and elastic constants), a stronger weight should be put on the GGA results. The present pseudopotentials are also believed to be more transferable to interstitial calculations since they have smaller core radii. The main limitation of the present calculation comes from the supercell size. Interstitials indeed induce long-range stress fields, and the effect of the elastic interaction of an interstitial with its periodically repeated images needs to be investigated over larger supercells to make more quantitative predictions. The comparison between $N = 37$ and $N = 97$ results, suggests that when going to even larger cells, the decrease of E_f^i should be most important for BS, then for BO, and then for S and C, while the value of E_f^i for O is likely to be already nearly converged. Going to larger sizes should therefore clearly favor the BS and BO configurations with respect to the other configurations. The fact that the experimental value of the c/a ratio is slightly lower than the GGA calculated one, should also favor the BO and BS basal configurations. For these reasons, the tentative predictions that can be made from the analysis of the present results is that BO should be the most stable configuration, immediately followed by BS, but O and S cannot be completely excluded. The energy differences between these four configurations are so small that two or more configurations may coexist in hcp-Zr and that their relative concentrations may also change with temperature because of differences in vibrational and/or electronic formation entropy.

The fact that five configurations are very close in energy shows that the energy landscape seen by the interstitial is quite flat, and it suggests a quite low value of the migration energy. In particular, the migration from a BO site to another BO site was proposed to occur via a BS configuration [5]. Neglecting the barrier to escape from the BS configuration, the energy difference between these two configurations (0.12 eV) can be taken as a first estimate for the in-plane migration energy of the BO configuration. The off-plane interstitial migration energy may also be rather low. A value of 0.15 eV was indeed reported in a molecular dynamics study performed with an empirical potential giving a stable basal configuration (BS) [39].

Another unexpected consequence of the present calculations, is that the activation energy for self-diffusion by the self-interstitial mechanism, i.e. the sum of the interstitial formation and migration energies (3.1 eV according to the above estimate), is found to be comparable to the experimental value of the activation energy for self-diffusion in Fe-free hcp-Zr samples, i.e. 3.17 eV [40]. It can therefore not be excluded that self-interstitials contribute to self-diffusion in hcp-Zr. This point also requires further investigation since an even lower value of the activation energy was proposed for the vacancy mechanism by ab initio calculations [20].

4. Conclusion

An ab initio study of the elastic constants and self-interstitial formation in hcp-Zr has been performed both in the LDA and GGA approaches. The calculated values of the elastic constants are in good agreement with experiments, with an overall better performance of GGA. A large value of the internal relaxation contribution is found within LDA.

As in previous ab initio calculations rather low values are found for the interstitial formation energies ($E_f^i \simeq 3$ eV). This result is at variance with seven empirical potentials for Zr, which yield $E_f^i = 4.0 \pm 0.6$ eV, or even more in one case. Only one empirical potential gives a similar value ($E_f^i = 2.5$ eV).

Six configurations of the interstitial have been examined. The BC configuration is unstable and decays to BO and the O, S, C, BO and BS configurations are found to be quite close in energy. The effect of supercell size has been studied within LDA on 37 and 97 atom cells. This effect is rather large, in particular for the basal configurations. The effect of functional, tested on 37 atom cells, is not negligible: the GGA values of E_f^i are almost 0.2 eV larger than in LDA for basal configurations, and more than 0.3 eV larger for non-basal configurations. This discrimination between basal and non-basal configurations is suggested to be related to the change in c/a ratio ($c/a = 1.600$ in GGA and 1.615 in LDA).

Within LDA, four configurations are found to be nearly degenerate in energy in 97 atom cell calculations: O, S, and BO ($E_f^i = 2.8$ eV), followed by BS ($E_f^i = 2.9$ eV); the C configuration is slightly less stable ($E_f^i = 3.1$ eV). Going to larger cells is expected to decrease the formation energies of the basal configurations more than the others. The GGA functional, which appears to perform better than LDA for elastic constants, lattice parameter and c/a ratio, favors basal configurations with respect to non-basal ones, compared to LDA. For these reasons, the most stable configuration in hcp-Zr is predicted to be BO or BS but O and S cannot be excluded. Further calculations, in particular GGA studies on larger cells, are required to draw more firm conclusions.

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