Materials subjected to fast neutron irradiation/Matériaux soumis à irradiation par neutrons rapides

Helium and point defect accumulation: (ii) kinetic modelling

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Abstract

The main outstanding issues regarding modeling He diffusion and defect accumulation in α-iron are reviewed. During recent years, first principles calculations have provided a better understanding of defect stability and migration properties in pure α-iron, and accurate values of energetics of He migration and He-vacancy interactions. Such information has been used by several authors to study damage evolution under different irradiation conditions using both kinetic Monte Carlo and rate theory models. In this article a review of the main results is provided, in particular for He desorption. The influence of impurities such as carbon is discussed as well as the main challenges ahead for modeling. *To cite this article: M.J. Caturla et al., C. R. Physique 9 (2008).*
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Résumé

Accumulation d' hélium et de défauts ponctuels : (ii) modélisation cinétique. Les questions les plus importantes concernant la modélisation de la diffusion de l'hélium et de la formation de défauts dans le α-Fe sont passées en revue dans cet article. Pendant ces dernières années les calculs ab initio ont apporté une meilleure compréhension de la stabilité des défauts et de leur migration dans le fer pur, ainsi que des valeurs précises de l'énergie de migration de l'hélium et des interactions He-lacune. Ces données ont été utilisées par divers auteurs afin d'étudier l'évolution des défauts sous différentes conditions d'irradiation avec des modèles de type Monte Carlo et cinétique chimique. Dans cet article, nous discutons les principaux résultats obtenus, en particulier ceux sur la désorption de l'hélium. Nous discutons l'influence d'impuretés telles que le carbone ainsi que les plus importants défi pour la modélisation. *Pour citer cet article : M.J. Caturla et al., C. R. Physique 9 (2008).*
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1. Introduction

The importance of understanding how He affects the mechanical properties of irradiated materials has been recognized since the early 1950s [1]. This is particularly crucial for the development of radiation resistant materials for future fusion reactors [2]. In this case, the levels of He that will be produced from (n, α) reactions will greatly exceed those attained in fission reactors. It is well known that He stabilizes vacancy clusters into voids that can lead to

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swelling in certain metals and alloys [3]. Ferritic/martensitic steels, such as EUROFER, are particularly resistant to void swelling; however, it is not yet clear what the effects of He on the embrittlement of these materials are, specially at low temperatures [4]. For further information on this topic see also the article by Schaeublin, Henry and Dai in this issue [5]. The lack of experimental facilities that can provide the conditions expected in a fusion reactor demands the development of accurate, predictive theoretical models that can be applied to different conditions. As in most material science problems, there is not a single model capable of covering the broad range of time and length scales required to understand damage production and accumulation. A multiscale approach has been therefore developed in the last few years.

A large number of experimental studies exists related to He effects in metals, particularly for austenitic steels due to their propensity for swelling [3]. However, the number of experiments devoted to obtaining the basic, fundamental parameters of He diffusion and He-vacancy cluster nucleation is more reduced, at least for the case of ultra high purity Fe and Fe-based alloys. Thermal helium desorption spectroscopy (THDS) [6,7] has provided indirect information about effective activation barriers for migration of He and dissociation of He-vacancy clusters in α-Fe; however, the interpretation of such experiments is not straightforward. Thanks to the recent availability of computing power, new insights have been gained for He effects in α-Fe from first principles calculations [8,9]. These calculations have provided more accurate values for He migration and small He–V complex stabilities, and helped in the development of long term evolution models such as kinetic Monte Carlo (kMC) or rate theory (RT). These models, coupled to experiments designed for their validation, are starting to provide a more clear understanding of basic phenomena in irradiated materials.

This article is a review of the most recent results for the particular case of He in α-Fe. It does not, however, pretend to be a complete review of all existing data on He diffusion in metals. In the first section of the paper we review the basic mechanisms for He diffusion in α-Fe and stabilities of He-vacancy complexes based on ab initio calculations, as well as some of the results obtained with empirical potentials. We will focus on He effects since intrinsic defects have been described in the article by Fu and Willaime in this issue [10]. In the second part of the paper the results obtained with kinetic Monte Carlo and rate theory methods on He-vacancy cluster nucleation in α-Fe are reviewed, including the possible effects of impurities on these results. Finally, a discussion is presented on the existing knowledge and the need for further understanding of these effects.

2. Basic mechanisms

In order to understand the long term evolution of defects under irradiation, the basic mechanisms for defect production, defect migration and the stabilities of defects must be known. The possible mechanisms for He migration have been proposed for decades and have been recently described by Trinkaus et al. in a review paper [11]. Fig. 1 shows schematically the elementary mechanisms for a substitutional He. We will use the notation HeV for a He at a substitutional site for consistency with the larger size clusters, which will be described as He_nV_m, where n is the number of He atoms and m the number of vacancies in the cluster. In the literature a He at a substitutional site is also denoted sometimes as He_s.

A He atom at an interstitial position can migrate quickly through the lattice until it finds a sink such as a vacant site, grain boundary, dislocation or the surface. A He at a substitutional site is able to migrate to different locations in the lattice by several mechanisms. Two of these mechanisms do not need the aid of another defect (Fig. 1: A and B). The He atom could exchange positions with a neighboring Fe atom, known as the exchange mechanism. However, the activation barrier for such migration is large, making this a very unlikely mechanism. On the other hand, a He at a substitutional site could jump into an interstitial site then migrate as an interstitial He, leaving a vacancy behind. This is the so-called dissociative mechanism, and has been considered as the main mechanism for migration of He in α-Fe, based on experimental measurements under specific irradiation conditions combined with rate theory analysis [6,12]. The dissociative mechanism could be described as:

$$HeV \rightarrow He + V$$
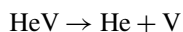
A substitutional He could also migrate with the aid of intrinsic defects, vacancies and self-interstitials, defects produced during irradiation (Fig. 1: C and D). Aided by a vacancy, it can migrate by exchanging places with a neighboring vacant site, known as the vacancy mechanism. Finally, aided by a self-interstitial the He atom could move from a sub-
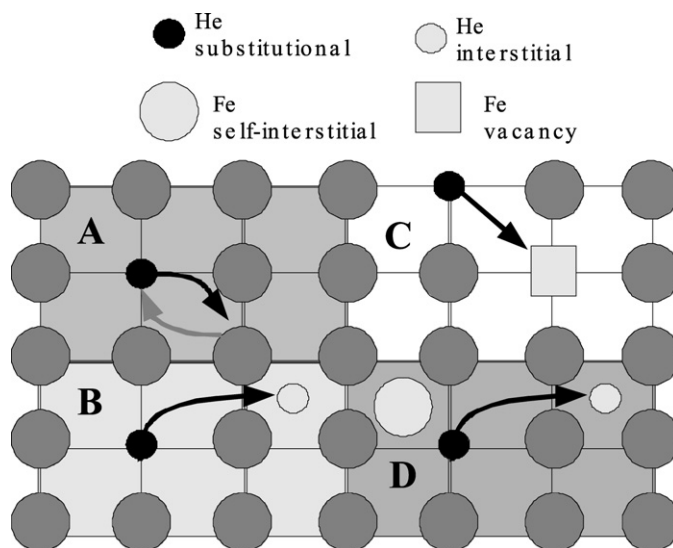
Fig. 1. Schematic view of the migration mechanisms for He from a substitutional site: A—exchange mechanism, B—Dissociative mechanism, C—Vacancy mechanism, D—Replacement mechanism.

Fig. 1. Vue schématique des mécanismes de migration de l'Hélium à partir d'un site substitutionnel : A—mécanisme d'échange, B—Mécanisme dissociatif, C—Mécanisme lacunaire, D—Mécanisme de kick-out.

stitutional site to an interstitial site by the replacement or kick-out mechanism [13] that can be described with the following reaction:

$$\text{HeV} + \text{I} \rightarrow \text{He}$$
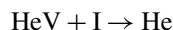
This mechanism has been studied by Ventelon et al. [14] with molecular dynamics simulations using empirical potentials and have shown that indeed a spontaneous recombination-replacement reaction occurs between a mobile self-interstitial atom and a substitutional He, ejecting the He atom into an interstitial position. The same authors have also studied the interaction of self-interstitial clusters and He, as will be explained below.

Ab initio calculations in the framework of Density Functional Theory (DFT) have been used to study different He migration mechanisms and obtain the corresponding activation energies [8]. Details about these calculations are provided in [10] of this issue. Briefly, these simulations reveal that interstitial He can migrate with a barrier of 0.06 eV [8]. The barrier for the dissociative mechanism with a given vacancy concentration is 2.36 eV according to calculations with SIESTA code using localized basis functions [8]. This value is significantly lower than the one obtained by Morishita et al., 3.78 eV [15], using empirical potentials. A recently developed interatomic potential for He–Fe fitted partially to ab initio data predicts a value for the dissociative energy closer to the ab initio values, 2.44 eV [16]. Notice that the value that has been associated to the dissociative mechanism through experimental observations using THDS is still lower ∼1.4 eV [6]. The calculated value for the migration barrier through a vacancy mechanism is ∼1.1 eV [8]. Ab initio calculations have also been used to study the kick-out mechanism [17] showing that, in some cases, a small barrier for the recombination between the self-interstitial and the He substitutional can exist, of the order of 0.2 eV.

A full model for defect evolution will obviously require information about the behavior of intrinsic defects, vacancies and self-interstitials. These have also been studied using ab initio methods in α-Fe [18,19] but we will not go into the details since they are reviewed in [10]. We would like, however, to mention a key issue for our later discussion. Probably one of the most controversial points regarding defects in α-Fe is the nucleation and growth of self-interstitial clusters. Ab initio calculations have shown, in excellent agreement with experimental evidence, that the most stable configuration for a self-interstitial atom in α-Fe consists of a $\langle 110 \rangle$ dumbbell, and that the migration barrier for this defect is 0.3 eV [19]. Moreover, ab initio data also show that self-interstitial clusters with 5 defects preferentially have a $\langle 111 \rangle$ configuration [20]. These loops are considered to be highly mobile, with migration barriers of the order of 0.1 eV [21–23]. These values, however, have not been confirmed yet by ab initio calculations and only exist from simulations using empirical potentials. There is, on the other hand, information about self-interstitial clusters produced during irradiation obtained from transmission electron microscopy (TEM) measurements. Under TEM two types of

defects are observed in irradiated α-Fe, $\langle 111 \rangle$ and $\langle 100 \rangle$ loops [24]. The transition from the small loops that can be studied ab initio, to the experimentally observed loops is not yet fully resolved. If $\langle 111 \rangle$ loops are highly mobile as simulations suggest, there must be some type of trapping for these defects in order to be observed experimentally. The formation of $\langle 100 \rangle$ loops from either $\langle 111 \rangle$ or $\langle 110 \rangle$ is also not fully understood. Some calculations point towards a possible reaction between $\langle 111 \rangle$ loops to form $\langle 100 \rangle$ loops [25]. The direct transformation from one loop to another has also been suggested based on experimental observations [26]. There is, therefore, a lack of understanding in the behavior of self-interstitial clusters in α-Fe that, as will be shown below, limits the predictability of the existing and newly developed long term evolution models.

Besides information about mobilities of defects, the interaction of He atoms with vacancies has also been studied for different clusters sizes and He to vacancy content, using both ab initio and empirical potentials [8,15,16]. The simulations show that He stabilizes vacancy clusters by reducing the vacancy emission rates, which explains the formation of voids in the presence of He. Although this trend is obtained both in empirical potential calculations and ab initio simulations, the quantitative values obtained for the different binding energies of defects to clusters are significantly different between the two methods. For example, ab initio results show that the most stable $He_n V_m$ cluster corresponds to a ratio of $n/m \sim 1.3$ and a dissociation energy of $E^{\text{dis}} \sim 2.6$ eV, where the dissociation energy is defined as the sum of the binding energy of a defect to a cluster and the migration energy of that defect. The values obtained by Morishita et al. from empirical potential calculations are $n/m \sim 1.8$ and $E^{\text{dis}} \sim 3.6$ eV [15]. The empirical potential developed by Seletskaia and co workers [16] is in closer agreement with the ab initio results, except for the vacancy formation energy in α-Fe which is too low, since the Fe–Fe potential used was not modified from the original Finnis–Sinclair model of Ref. [27]. According to this interatomic potential, the dissociation energy of a He from a He_9V cluster is equal to 1.35 eV, which is closer to the experimental value of 1.4 eV proposed in Ref. [6]. However, this cluster may be unstable against the spontaneous emission of a self-interstitial atom due to its strong internal pressure.

The interaction between self-interstitial atom (SIA) clusters and He has also been studied with empirical potentials [14]. These calculations reveal a strong interaction between SIA clusters and He either at interstitial or at substitutional positions, which could be a possible trapping mechanism for such mobile clusters. The main reaction between a substitutional He and a self-interstitial atom is the kick-out reaction. These results were compared to ab initio calculations for the particular case of a $\langle 110 \rangle$ self-interstitial atom and a He at an interstitial position, revealing also positive binding energies for some particular configurations, although lower than those obtained by the empirical potential calculations. Other ab initio calculations [17] also show a weak positive binding between a He interstitial at an octahedral position (the lowest energy configuration predicted by ab initio) and a $\langle 110 \rangle$ self-interstitial atom.

3. Long term defect evolution

The values mentioned above, and obtained either from ab initio calculations or from empirical potential simulations, have been used by several authors to study long term evolution of defects in α-Fe. In order to test the validity of the models, simulations are compared to existing experimental measurements or, in some cases, to experiments set up for that purpose. In particular, a kinetic Monte Carlo model based purely on ab initio calculations has reproduced the experimental resistivity recovery curves of electron irradiated α-Fe [19]. Kinetic Monte Carlo models using data from empirical potential calculations have been used to study damage accumulation in α-Fe under neutron irradiation [28–30]. Rate theory models have also been used to simulate electron irradiation experiments [31]. Some of these results will be reviewed in more detail in the article by Barbu [32] in this issue. Interestingly, all these different long term evolution models, although using different input parameters, have one point in common. They all need to introduce some assumptions to limit large self-interstitial cluster mobility. In some cases this is through the inclusion of immobile clusters for all sizes [31] or for clusters larger than a certain size [19,28,29], or they include trapping sites for self-interstitial clusters [30].

There is a smaller number of calculations devoted to study long term evolution of He in α-Fe based on ab initio or empirical potential calculations [15,33–37]. Simulations are compared, in most cases, with thermal helium desorption spectroscopy experiments, one among the few experiments from which information on He behaviour in iron can be obtained indirectly. Morishita et al. [15] have used the values obtained from empirical potential calculations on cluster dissociation energies to interpret their THDS experimental results. These same authors have also used these parameters for a kinetic Monte Carlo model to study long term evolution of He-vacancy clusters. The lifetime of clusters without

Table 1

Defect-defect binding energies from Refs. [8,19] and used both in the rate theory and kinetic Monte Carlo calculations of Figs. 2 and 3

Reaction	E_b (eV)	Reaction	E_b (eV)	Reaction	E_b (eV)
$V_2 \rightarrow V + V$	0.30	$He_3V \rightarrow He_3 + V$	4.59	$He_2V \rightarrow HeV + He$	1.84
$V_3 \rightarrow V_2 + V$	0.37	$He_3V_2 \rightarrow He_3V + V$	1.85	$He_2V_2 \rightarrow HeV_2 + He$	2.75
$V_4 \rightarrow V_3 + V$	0.62	$He_3V_3 \rightarrow He_3V_2 + V$	18	$He_2V_3 \rightarrow HeV_3 + He$	2.96
$I_2 \rightarrow I + I$	0.80	$He_3V_4 \rightarrow He_3V_3 + V$	1.57	$He_2V_4 \rightarrow HeV_4 + He$	3.12
$I_3 \rightarrow I_2 + I$	0.92	$He_4V \rightarrow He_4 + V$	5.52	$He_3V \rightarrow He_2V + He$	1.83
$I_4 \rightarrow I_3 + I$	1.64	$He_4V_2 \rightarrow He_4V + V$	2.3	$He_3V_2 \rightarrow He_2V_2 + He$	2.07
$HeV \rightarrow He + V$	2.3	$He_4V_3 \rightarrow He_4V_2 + V$	2.03	$He_3V_3 \rightarrow He_2V_3 + He$	2.91
$HeV_2 \rightarrow HeV + V$	0.78	$He_4V_4 \rightarrow He_4V_3 + V$	1.97	$He_3V_4 \rightarrow He_2V_4 + He$	3.16
$HeV_3 \rightarrow HeV_2 + V$	0.83	$He_2 \rightarrow He + He$	0.43	$He_4V \rightarrow He_3V + He$	1.91
$HeV_4 \rightarrow HeV_3 + V$	1.16	$He_3 \rightarrow He_2 + He$	0.95	$He_4V_2 \rightarrow He_3V_2 + He$	2.36
$He_2V \rightarrow He_2 + V$	3.71	$He_4 \rightarrow He_3 + He$	0.98	$He_4V_3 \rightarrow He_3V_3 + He$	2.57
$He_2V_2 \rightarrow He_2V + V$	1.61	$HeV_2 \rightarrow V_2 + He$	2.85	$He_4V_4 \rightarrow He_3V_4 + He$	3.05
$He_2V_3 \rightarrow He_2V_2 + V$	1.04	$HeV_3 \rightarrow V_3 + He$	3.3		
$He_2V_4 \rightarrow He_2V_3 + V$	1.32	$HeV_4 \rightarrow V_4 + He$	3.84		

The binding energy of a reaction $C \rightarrow A + B$ is defined as $E_b = E_A^f + E_B^f - E_C^f$, where E_A^f, E_B^f and E_C^f are the formation energies of A, B and C, respectively. The inverse reactions, $A + B \rightarrow C$, occur when A and B are within the capture radius distance for that particular reaction.

He and with He are compared for a particular temperature in these calculations, as well as the migration of He–V clusters due to volume diffusion and surface diffusion [15,33]. A migration energy for diffusion of a $He_{20}V_{20}$ cluster of 0.89 eV was obtained.

The lifetimes and migration energies of He_nV_m clusters have also been studied by Borodin and co-workers using, in this case, input from ab initio calculations [36,37]. These authors show that vacancy clusters (without He) are mobile but at temperatures relevant for fusion conditions are unstable and dissociate, and, therefore, are not expected to contribute significantly to self-diffusion. However, the presence of He stabilizes these vacancy clusters that are also mobile. The authors argue that this diffusion can contribute significantly to He migration.

Ab initio data was used by Ortiz et al. [34] as input for a rate theory model of He in α-Fe. In particular it is considered that the migration barrier for single vacancies is 0.67 eV, for single self-interstitials 0.34 eV, for di-interstitials 0.42 eV and for He at an interstitial position 0.06 eV, values obtained by ab initio calculations [8,19]. Table 1 shows the values of binding energies of defects to different clusters used in the model, and also obtained from ab initio methods.

Simulations using these parameters were directly compared to THDS measurements performed by Vassen and co-workers [6] for different conditions of temperature, sample depth and He concentrations. A homogeneous distribution of He and Frenkel-pairs (FP) with a ratio of 200 FP per implanted He is considered as the initial defect distribution after implantation, values obtained from TRIM calculations [38]. After an initial equilibration at room temperature most of the He atoms are at substitutional positions and a few are forming He_2V clusters. Vacancies are mostly isolated, while self-interstitials have either recombined with the surfaces or with vacancies or are forming small self-interstitial clusters. Self-interstitial clusters with more than 2 defects are assumed immobile in this model. Considering this distribution of defects, He desorption during isothermal annealing is simulated for those temperatures used in the experiments [6]. Fig. 2(a) shows the fraction of He released as a function of time for three different conditions: (a) 559 K, 2.5 μm, 1.39 appm of He, (b) 577 K, 20.6 μm, 0.013 appm of He, and (c) 667 K, 2.6 μm, 0.109 appm of He. Solid lines are the results of the rate theory model while symbols are the experimental data from Ref. [6].

Clearly there is a discrepancy between the model based on ab initio parameters obtained for pure α-Fe and the experimental measurements. This discrepancy is explained by the presence of impurities in the experimental sample that affect the mobility of vacancies in Fe. It is possible to obtain a very good agreement with the experimental data over several orders of magnitude and for all different conditions when some of the ab initio parameters are re-evaluated, as shown in Fig. 2(b). In this case, the vacancy migration energy was increased from the value obtained for pure α-Fe, from 0.67 eV to 0.83 eV. The binding energies of a vacancy to a He interstitial and to a He substitutional were decreased to 1.78 eV and 0.54 eV respectively. Interestingly, the value obtained for the vacancy migration for this fit is very close to that expected in the presence of Carbon from ab initio calculations [39–41]. Therefore, carbon is considered the most likely candidate for the impurity responsible of these effects. The values obtained from this fit
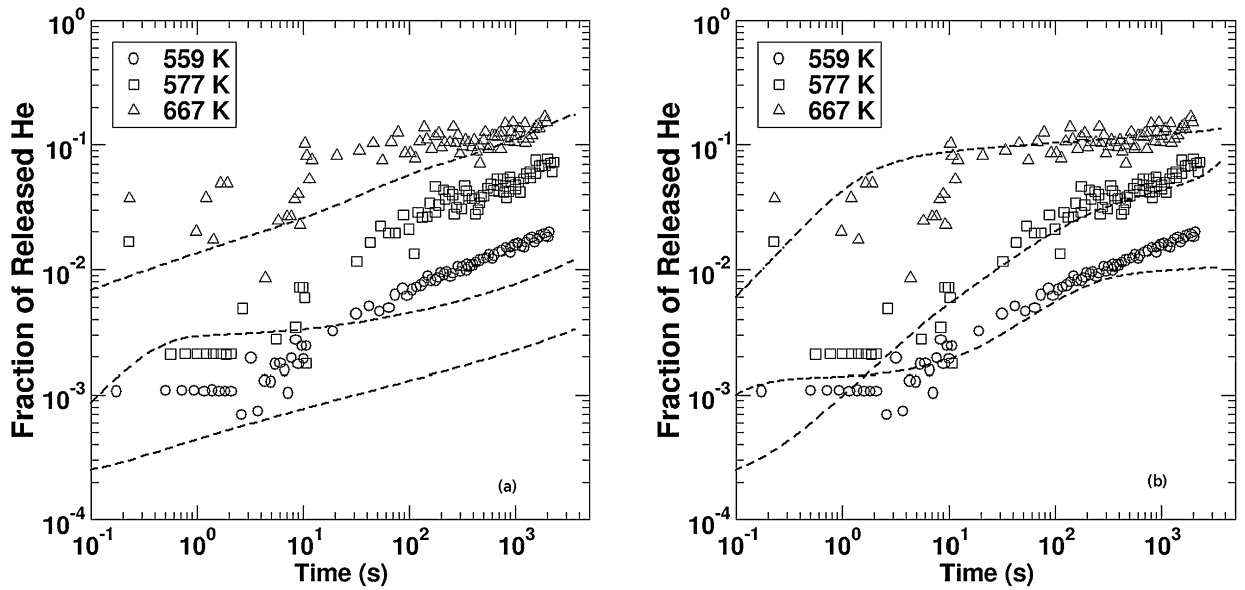
Fig. 2. Released fraction of He during isothermal annealing obtained from rate theory calculations (lines) and experiments (dots) from Ref. [6], for (a) simulations with ab intio input from pure α-Fe, and (b) fitted values of vacancy migration energy, V–He and V–HeV binding energies. For further details see Ref. [34].

Fig. 2. Fraction d'Hélium émise pendant un recuit isotherme obtenue à partir d'un modèle de diffusion (courbes) et expérimentalement (points, Réf. [6]), (a) avec des données calculées ab intio pour le fer pur, (b) avec des valeurs ajustées de l'énergie de migration de la lacune et des énergies de liaisons V–He et V–HeV. Pour plus de détails voir Réf. [34].

should then be interpreted as effective values for vacancy migration energy and dissociation energies of He–V clusters in the presence of impurities. These calculations also revealed that in the presence of defects produced by irradiation, several of the migration mechanisms for He explained earlier are active. In particular, the replacement or kick-out mechanism plays a significant role in the early stages of annealing.

As explained above, one assumption of most of the long term evolution models in α-Fe is the mobility of self-interstitial clusters. The effect of the mobility of these clusters on He desorption was studied using a kinetic Monte Carlo model [35]. These calculations revealed that if all self-interstitial clusters are considered mobile, the released fraction of He decreases considerably with respect to that measured experimentally. Fig. 3 shows the released fraction of He as a function of time for conditions (c) described above (667 K, 2.6 µm, 0.109 appm of He) and for three different assumptions regarding self-interstitial migration: (i) all self-interstitial clusters are considered immobile and only a single self-interstitial is mobile; (ii) all self-interstitial clusters of sizes larger than 3 are considered immobile; and (ii) all self-interstitial clusters are mobile. Values used for defect-defect binding energies were the same as those described above.

The first case represents the assumption used by Hardouin-Dupart et al. [31] in their rate theory model to reproduce electron irradiation experiments. The second case is an effective way of considering that either all ⟨111⟩ loops react to form ⟨100⟩ immobile loops, or that they interact with impurities that trap these loops. The last case would be equivalent to not including any form of trapping for self-interstitials of any size or type. For this last case, the mobilities used are the ab initio values of [19] for sizes 1, 2 and 3 and the values obtained by Soneda [23] for clusters larger than 3. It is clear from this figure that the mobility of self-interstitial clusters plays a very significant role in He desorption. He is released at very short times when all self-interstitial clusters are considered immobile. Including mobile self-interstitial clusters delays the release of He by orders of magnitude, since the kick-out mechanism for He migration is effectively suppressed. These calculations again reveal that in order to reproduce the experimental observations it is necessary to assume that at least some self-interstitial clusters are immobile, which is in agreement with the results of other authors [28–31] using models to simulate completely different conditions and experiments as those reported here.
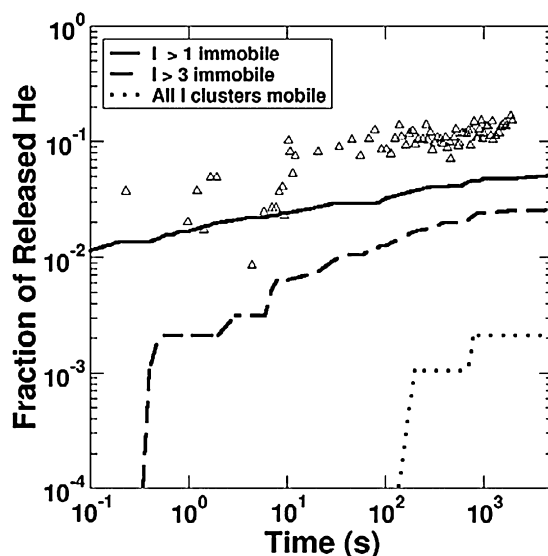
Fig. 3. Released fraction of He during isothermal annealing obtained from kinetic Monte Carlo calculations (lines) and experiments from Ref. [6], for simulations with input from pure α-Fe, and different assumptions for self-interstitial cluster mobility.

Fig. 3. Fraction d'Hélium émise pendant un recuit isotherme obtenue à partir d'un modèle kinetic Monte Carlo (courbes) et expérimentalement (points, Réf. [6]), avec des données calculées pour le fer pur et suivant différentes hypothèses sur la mobilité des clusters d'interstitiel.

4. Conclusions

Ab initio DFT calculations have provided valuable information about basic mechanisms of He diffusion and He–defect interactions in α-Fe that have been used in the development of long term evolution of these defects under irradiation conditions. These kinetic models have been applied to interpret experimental measurements, mostly THDS experiments. Ab initio calculations predict a value for the dissociation of a He substitutional into a vacant site and a He interstitial that is higher than the value that was originally assigned to this mechanism from experimental observations. This discrepancy has been explained by the presence of impurities in the experimental measurements that affect the mobility of vacancies and the stability of some clusters [34]. The most likely impurity to produce this effect is considered to be carbon. Other authors [16] using empirical potential calculations fitted partially to ab initio data, interpret this experimental observation as the result of the dissociation of larger $He_n V_m$ clusters, in particular a He–V cluster containing 9 He atoms and one vacant site. There is also still some controversy about the dominant mechanism for He migration under irradiation conditions. According to some calculations [34,35] the migration through the vacancy mechanism for conditions with low ratios of FP per He atom is negligible. Other authors, however, consider this as the only mechanism responsible for He migration [36,37].

New experiments, with controlled conditions of temperature, He content, impurity content and sample depth will help solving some of these issues and controversies. Some of these experiments are already being undertaken by different groups [15,42]. The selection of the proper conditions for the experimental measurements should be guided by simulations in order to test their validity.

Acknowledgements

References

[1] G.W. Greenwood, A.J.E. Foreman, E.A. Rimmer, J. Nucl. Mater. 4 (1959) 305.
[2] R. Andreani, E. Diegele, R. Laesser, B. van der Schaaf, J. Nucl. Mater. 329 (2004) 20.

[3] F.A. Garner, Materials Science and Technology, vol. 10A, VCH, Germany, 1994 (Chapter 6).
[4] N. Baluc, et al., Nucl. Fusion 44 (2004) 56–61.
[5] K. Nordlund, S. Dudarev, C. R. Physique 9 (3–4) (2008) 343.
[6] R. Vassen, H. Trinkaus, P. Jung, Phys. Rev. B 44 (1991) 4206.
[7] K. Morishita, R. Sugano, B.D. Wirth, J. Nucl. Mater. 323 (2003) 243.
[8] C.C. Fu, F. Willaime, Phys. Rev. B 72 (2005) 064117.
[9] T. Seletskaia, Y.N. Osetsky, R.E. Stoller, Phys. Rev. Lett. 94 (2005) 046403.
[10] C.C. Fu, F. Willaime, C.R. Physique 9 (3–4) (2008) 335.
[11] H. Trinkaus, B.N. Singh, J. Nucl. Mater. 323 (2003) 229.
[12] H. Ullmaier, Numerical data and functional relationships in science and technology, Landolt–Börnstein New Series, vol. III/25, 1991, p. 381.
[13] L.K. Mansur, E.H. Lee, P.J. Maziasz, A.P. Rowcliffe, J. Nucl. Mater. 141–143 (1986) 633.
[14] L. Ventelon, B.D. Wirth, C. Domain, J. Nucl. Mater. 351 (2006) 119.
[15] R. Sugano, K. Morishita, H. Iwakiri, N. Yoshida, J. Nucl. Mater. 307–311 (2003) 941.
[16] T. Seletskaia, Yu.N. Osetsky, R.E. Stoller, G.M. Stocks, J. Nucl. Mater. 351 (2006) 109.
[17] C.C. Fu, F. Willaime, J. Nucl. Mater. 367 (2007) 244.
[18] C. Domain, C.S. Becquart, J. Foct, Phys. Rev. B 69 (2004) 144112.
[19] C.C. Fu, J. Dalla Torre, F. Willaime, J.-L. Bocquet, A. Barbu, Nature Mat. 4 (2004) 68–74.
[20] F. Willaime, C.C. Fu, M.C. Marinica, J. Dalla Torre, Nucl. Instrum. Meth. B 228 (2005) 92.
[21] D.J. Bacon, F. Gao, Y.N. Osetsky, J. Nucl. Mater. 276 (2000) 1.
[22] B.D. Wirth, G.R. Odette, D. Maroudas, G.E. Lucas, J. Nucl. Mater. 276 (2000) 33.
[23] N. Soneda, T. Diaz de la Rubia, Phil. Mag. A 81 (2001) 331.
[24] A.E. Ward, S.B. Fisher, J. Nucl. Mater. 166 (1989) 227.
[25] J. Marian, B.D. Wirth, J.M. Perlado, Phys. Rev. Lett. 88 (2002) 255507.
[26] K. Arakawa, M. Hatanaka, E. Kuramoto, K. Ono, H. Mori, Phys. Rev. Lett. 96 (2006) 125506.
[27] M.W. Finnis, J.E. Sinclair, Phil. Mag. A 50 (1984) 45.
[28] M.J. Caturla, N. Soneda, E. Alonso, B.D. Wirth, T. Diaz de la Rubia, J.M. Perlado, J. Nucl. Mater. 276 (2000) 13.
[29] N. Soneda, S. Ishino, A. Takahashi, K. Dohi, J. Nucl. Mater. 323 (2003) 169.
[30] C. Domain, C. Becquart, Phys. Rev. B 65 (2001) 024103.
[31] A. Hardouin Duparc, C. Moingeon, N. Smetniansky-de-Grande, A. Barbu, J. Nucl. Mater. 302 (2002) 143.
[32] A. Barbu, C. R. Physique 9 (3–4) (2008) 353.
[33] K. Morishita, R. Sugano, Nucl. Instrum. Meth. B 255 (2007) 52.
[34] C.J. Ortiz, M.J. Caturla, C.C. Fu, F. Willaime, Phys. Rev. B 75 (2007) 100102.
[35] M.J. Caturla, C.J. Ortiz, J. Nucl. Mater. 362 (2007) 141.
[36] V.A. Borodin, P.V. Vladimirov, J. Nucl. Mater. 362 (2007) 161–166.
[37] V.A. Borodin, P.V. Vladimirov, A. Moslang, J. Nucl. Mater. 367 (2007) 286.
[38] J.F. Ziegler, J.P. Biersack, U. Littmark, The Stopping and Range of Ions in Solids, in: J.F. Ziegler (Ed.), The Stopping and Range of Ions in Matter, vol. 1, Pergamon, New York, 1985, p. 25ff.
[39] C. Domain, C.S. Becquart, J. Foct, Phys. Rev. B 69 (2004) 144112.
[40] L. Joly, C.C. Fu, J.L. Bocquet, F. Willaime, A. Barbu, in preparation.
[41] C.J. Först, J. Slycke, K.J. Van Vliet, S. Yip, Phys. Rev. Lett. 96 (2006) 175501.
[42] Group of Prof. B.D. Wirth, U.C. Berkeley.