

Atomic scale modelling of diffusivity and melting point in iron and iron- chromium alloys using molecular dynamics simulation

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July, 2003

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Abstract

An EAM interatomic potential to be used for radiation effect simulations in Fe-Cr systems has been recently proposed. In the present work, this potential is used to calculate, by means of classical molecular dynamics (MD), the diffusivity of solute Cr atoms in an Fe-12%Cr random alloy. Fe self-diffusivity is calculated as well, both in the alloy and in the pure metal, for comparison. In addition, the melting point for both the pure metal and the alloy, as predicted by the potentials, has been determined and a comparison between the efficiency of vacancy and interstitial mechanisms for diffusion has been performed. This study allows the validity of the potential to be checked against experimental data outside its fitting range, while providing some insight into the description that this potential gives of irradiation effects. A correct prediction of the diffusivity of solute atoms at high temperature and the melting point are indeed an important pre-requisite for a correct prediction of ion mixing and point defect clustering within a displacement cascade during the thermal spike phase. The conclusion of the study is that the present potential is capable of reproducing with excellent accuracy both the diffusion coefficient and the melting point in Fe and in the Fe-Cr alloy. Atomic diffusion through interstitials is also seen to be a more efficient mechanism than through vacancies in the materials considered.

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1. INTRODUCTION

High-chromium ferritic steels have been long considered as potential first-wall and breeding-blanket structural materials in future fusion reactor systems [1]. More recently, they have also been chosen as candidate structural materials for accelerator-driven systems (ADS) [2]. Despite the excellent properties of these steels vis-à-vis nuclear applications, prolonged neutron irradiation effects are expected to be detrimental for the integrity of these materials. In this framework, the development of models capable of improving our understanding of the physical microscopic mechanisms leading to materials degradation under neutron irradiation is essential. The starting point to model at the atomic scale radiation effects in a high-chromium steel is clearly a valid empirical interatomic potential for the Fe-Cr system, which is the simplest model alloy that can be assimilated to the steel. An EAM interatomic potential to be used for radiation effect simulations in the Fe-Cr system has been recently proposed [3]. This potential is undergoing a thorough validation process, in order to determine up to what extent it can be relied upon for the study of radiation effects.

In the present work, this potential is used to calculate, by means of classical molecular dynamics (MD), the diffusivity of solute Cr atoms in a ferritic matrix containing 12% Cr. Iron self-diffusion has been studied as well, both in the pure metal and in the alloy. In addition, a melting point investigation in both materials is presented. Both magnitudes can be compared with experimental data. Checking how well an interatomic potential reproduces the diffusion coefficient of the atoms in the alloy is important for many reasons. Firstly, it gives an idea of the range of validity of the potential, up to high temperatures. Secondly, such a study can help identify mechanisms of diffusion of solute atoms in the solid under study (e.g. diffusivity via interstitial mechanisms). Both points are intimately connected with the correct reproduction of the behaviour of point defects in the material of interest. A correct description of the diffusivity is also an important prerequisite for a correct prediction of ion mixing and point defect clustering within a displacement cascade, particularly during the thermal spike. In addition, the capability of calculating diffusion coefficients in the alloy of interest is important in view of producing parameters describing point defect migration, of use for kinetic Monte Carlo simulations, as well as for rate theory approaches. This study will allow the validity of the potential for all these purposes to be checked against experimental data for diffusion coefficients and melting point.

2. COMPUTATIONAL METHOD

2.1 The interatomic potential

It is well known that pairwise potentials cannot provide a realistic description of point-defects and point defect interactions with solute atoms. To correctly describe equilibrium and dynamical properties of a solid, it is necessary to use a many body potential. In this study we used a many body empirical potential based on the EAM approach [4]. In this approach the total cohesive energy of a system of n atoms is given by the following expression:

$$E_{coh} = \sum_{i=1}^n E_i = \sum_{i=1}^n \left[\frac{1}{2} \sum_{j=1}^n \Phi(r_{ij}) + F(\rho_i) \right] \quad (1)$$

where $\Phi(r_{ij})$ is the pairwise (electrostatic) interaction between atom i and j ; the function $\rho = \sum_{j \neq i} \rho(r_{ij})$ represents the electron density of the host system with atom i removed (r_{ij} is a scalar distance between atom i and j) and $F(\rho_i)$ is a many body term representing the energy required to embed atom i into a homogeneous electron gas of density ρ_i . Details about the fitting procedure used to generate a potential of this type for the Fe-Cr system are given in [3]. The potential used for this work is denoted as PM-10, because it has been fitted to mixing enthalpy and bulk modulus for 10%Cr, using the mixing enthalpy value corresponding to the paramagnetic Fe-Cr alloy (above ~ 1000 K Fe-Cr alloys are paramagnetic), see ref. [5]. Some calculations have been repeated using the FM-10 potential, fitted on the "ferromagnetic" mixing enthalpy value for 10% Cr [5], obtaining results essentially coincident with those obtained using PM-10.

2.2 Calculation procedures

2.2.1 Diffusivity

Standard classical molecular dynamics simulations in the microcanonical statistical ensemble, with periodic boundary conditions, were used for these calculations (see ref. [6] for a complete treatise on MD). In order to calculate the diffusion coefficients, we used the same technique as described in [7]. According to the classical theory of diffusion [8] the diffusion coefficient of Cr as an impurity in α -Fe via vacancy jump can be written as:

$$D_{Cr} = c \cdot a_0^2 \cdot \Gamma_{Cr} \cdot f_{Cr} \quad (2)$$

where c is a constant coefficient that accounts for the geometry of the discrete jump direction in the lattice, a_0 is the lattice parameter of Fe, f_{Cr} is the impurity (Cr) correlation factor and Γ_{Cr} is a frequency, proportional to the probability that a neighbouring lattice site to a Cr atom is a vacancy and that the atom succeeds in jumping into it, that is:

$$\Gamma_{Cr} = v_{Cr} \cdot C_{V,eq}(T) \cdot e^{-\frac{G_m}{kT}} \quad (3)$$

where $C_{V,eq}$ is the vacancy concentration at equilibrium and v_{Cr} and G_m are, respectively, the attempt frequency of jump and the free energy barrier to be overcome, for a Cr atom in Fe jumping into the neighbouring vacancy. The vacancy concentration at equilibrium has also a Boltzmann expression:

$$C_{ve}(T) = e^{-\frac{G_{f,v}}{kT}} \quad (4)$$

Where $G_{f,v}$ is the free energy of formation of a vacancy in α -Fe. It is customary to express the diffusion coefficient by separating the temperature dependent factors from the others. This leads to the following expression:

$$D_{Cr}(T) = D_0 \cdot e^{-\frac{E_a}{kT}} \quad (5)$$

where $E_a = E_{f,v} + E_m$ is an activation energy given by the sum of the formation energy of the vacancy and the energy barrier for the Cr atom to jump into the neighbouring vacancy (note that, strictly speaking, these are not energies but enthalpies: the pV term of difference has been in this context neglected). The explicit expression for the prefactor is therefore:

$$D_0 = c \cdot a_0^2 \cdot f_{Cr} \cdot v_{Cr} \cdot e^{-\frac{S_{f,v} + S_m}{k}} \quad (6)$$

where $S_{f,v}$ is the vacancy formation entropy and S_m is the entropy associated to the Cr atom migration jump.

By MD, the Cr diffusivity in a virtual specimen of alloy, D^* , can be obtained using Einstein's random-walk law [9]:

$$D_{Cr}^*(T) = \frac{\langle R^2(t) \rangle (T)}{6t} \quad (7)$$

where t is the simulation time and $\langle R^2(t) \rangle (T)$ is the mean square displacement (MSD) of diffusing Cr atoms as a function of time, as calculated from the MD simulation after a long enough run at a certain temperature T . The vacancy concentration used in the simulation is inevitably much higher than the equilibrium concentration at T . Therefore, to obtain a coefficient diffusion comparable with experimental data the following correction has to be introduced:

$$D_{Cr}(T) = \frac{C_{v,eq}(T)}{C_v^*} D^*(T) \quad (8)$$

where $C_{v,eq}$ is calculated from equation (4) and C_v^* is known from the number of vacancies introduced in the simulation box. By repeating the same MSD calculation at different temperatures, the Arrhenius plot for the coefficient diffusion, $D_{Cr}(T)$, can therefore be produced, as a function of temperature. From this, we can directly evaluate the pre-exponential factor D_0 and the activation energy E_a , by fitting $D_{Cr}(T)$ to expression (5). The same formulation can be used to describe Fe self-diffusion.

We considered six different temperatures (from 1200 K up to 1700 K). The simulations covered, for each temperature, a span of 1 ns, the value of the MSD being calculated every 1 ps. The size of the box was equal in all cases: a cubic box with a $16a_0$ side, corresponding to 9000 atoms per box. The simulation was repeated for some temperatures using different vacancy concentrations and different box sizes, to make sure that these parameters did not influence the results after normalisation as in (8). In most cases, to be on the safe side, the concentration was 0.12% (1 vacancy in a 9000 atom box). This concentration of vacancies was chosen to avoid cluster formation. Indeed, vacancy clustering would make diffusion a more difficult process and we would not see a monotonous growth of the MSD in that case [6]. Whenever more than one vacancy was included in the box (0.12% concentration in boxes larger than 9000 atoms), we checked every 1 ps the coordinates of the vacancies and did not detect any cluster formation during the whole simulation time. For the simulations where the interstitial mechanism was studied, one interstitial, instead of one vacancy, was introduced in the system. For every temperature we estimated the equilibrium lattice constants before starting the simulation of diffusion.

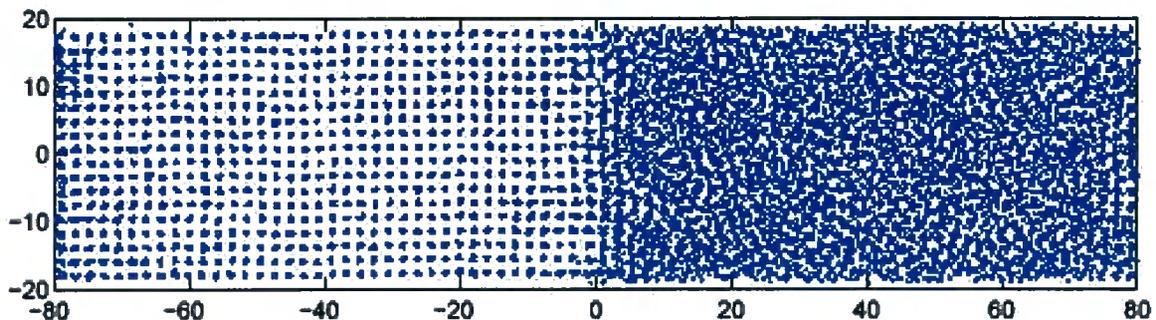


Figure 1. Simulation box for melting point investigation. Only the central part of the box, containing the interface, is shown.

2.2.2 Melting point

To determine the melting temperature predicted by the interatomic potential used in this work three different methods were employed. The variation of the pair correlation function (PCF) and the MSD versus temperature were analysed to identify the range in which the melting point was to be found. In particular, we calculated PCF and MSD from 1200 K up to 2200 K, every 100 K. For each temperature, we compared the PCF with the typical pair distribution for a liquid alloy (separately simulated). In the case of the MSD, we looked for a possible change of slope in the increase versus T , as a consequence of the enhanced diffusivity in the liquid phase. Within the range thereby identified, the more precise and computationally intensive two phase simulation method was used. This method consists in creating a solid-liquid interface, equilibrating it at a certain temperature and observing, for a long enough time (in our case 5 ns), in which direction the interface moves. If it moves towards the liquid, increasing the solid portion of the sample, then the temperature is below the melting point, while if it moves in the opposite direction the temperature is above the melting point. Around the melting point the interface is not expected to move. We considered temperature increments of 15 K and used a parallelepiped-like box, with the long side perpendicular to the solid-liquid interface (see figure 1). This allowed us to use periodic boundary conditions in the three directions, without any interference of boundary effects on the interface.

3. RESULTS AND DISCUSSION

3.1 Static calculation of migration energies in Fe-Cr

As a first check of the performance of the potential, we calculated statically the vacancy formation energy and the migration energy for Fe and Cr atoms in a bcc Fe matrix. In table 1 the results of these calculations are compared with experimental and *ab initio* data. As we can see, this potential gives reasonable results for basic microscopic energies bearing some relationship with diffusivity in FeCr. See ref. [5] for more details. Take into account that the experimental activation energy for Cr migration is measured in Fe-12%Cr, while the calculations were done with only one Cr atom in the system.

Table 1. Statically calculated microscopic energies of relevance for diffusion in Fe.

Energies, eV	MD (our potential)	VASP [5,10]	Experiments
$E_{f,v}$ (formation, pure Fe)	1.54	1.95	1.5±2.0 [11]
$E_m(\text{Fe} \rightarrow \text{V})$ (migration)	0.73	0.65	0.55 [12]
$E_m(\text{Cr} \rightarrow \text{V})$ (migration)	0.71	0.58	0.63 [14]
$E_a(\text{Fe} \rightarrow \text{V})$ (activation)	2.27	2.60	2.60 [15]
$E_a(\text{Cr} \rightarrow \text{V})$ (activation)	2.20	2.50	2.39 [13]*

* For Fe-12%Cr

3.2 Cr and Fe diffusivity in α -Fe via vacancy mechanism

We evaluated the Cr diffusivity in a ferritic matrix containing 12% randomly distributed substitutional Cr atoms. The choice of this percentage was dictated by the availability of experimental results for this alloy [13], whose composition is reasonably close to the alloy to which the potential in use was fitted. This composition corresponds also to the smaller Cr concentration for which the diffusion coefficient of Cr in ferrite can be measured, as a consequence of the existence, in the Fe-Cr phase diagram, of a small enclave (~ 0 -12%Cr and ~ 1100 -1660 K) where only the γ phases is stable. More in detail, in the 1200-1400 K range the real Fe-12%Cr alloy crosses a region co-existence of γ and α phases. Since this phase transition is very unlikely to be reproduced by the interatomic potential, it has been ignored in the calculations, which were always performed in a bcc lattice, at all temperatures. The experimental data about Cr diffusivity in Fe-12%Cr were, on the contrary, obtained "skipping" the 1200-1400 K region [13]. The Fe self-diffusivity was also calculated in this alloy and in pure Fe using the same potential, for comparison.

As a prerequisite for the calculations, we determined the equilibrium lattice parameters for pure Fe and Fe-12%Cr in the range of studied temperatures, namely from 1200 K up to 1700 K: the results versus temperature are given in table 2. The difference between lattice parameters for pure Fe and the alloy is not big (on the order of 1%), in agreement with experimental results taken from [16].

Table 2. Lattice parameters and diffusivity data versus temperature in Fe-12%Cr, with $C_v^* = 0.0012$, as calculated by MD over runs of 1 ns ($t = 10^{-9}$ s).

T, K	$C_{v,eq}$ (per atom)	Lattice constant, Å	Cr - MSD, Å ²	Fe - MSD, Å ²	$D^*, 10^{-8}$ cm ² /sec		$D, 10^{-12}$ cm ² /sec	
					Cr	Fe	Cr	Fe
1200	3.424E-7	2.8902	1.22±0.05	1.05±0.02	2.03	1.75	5.76	4.99
1300	1.076E-6	2.8987	1.47±0.05	1.53±0.01	2.45	2.55	21.96	22.85
1400	2.871E-6	2.9060	2.34±0.05	2.07±0.01	3.90	3.45	93.29	82.52
1500	6.721E-6	2.9132	3.30±0.03	2.75±0.01	5.50	4.58	308.04	256.51
1600	1.415E-5	2.9278	3.47±0.02	3.35±0.01	5.78	5.58	681.49	657.91
1700	2.729E-5	2.9424	3.52±0.01	3.46±0.001	5.86	5.81	1332.55	1321.18

In figure 2 the MSD of the Cr solute atoms for all considered temperatures is shown. All curves have a monotonous growth character with time, as they are expected to have in the absence of disturbing phenomena, such as vacancy clustering or phase transition. The only diffusion mechanism operating in this system is the free migration of isolated single-vacancies. The MSD rises with rising temperature. The values of MSD for Cr and Fe were found to be always quite close to each other according to this potential. The diffusion parameters for Cr and Fe atoms calculated from the MSD using the random-walk law (7) are shown in table 2, before and after correction according to (8).

The correction from D^* to D in table 2 was made assuming $G_{f,v} \cong E_{f,v} = 1.54$ eV, as calculated using our potential. This choice seemed indeed to be the most consistent one, considering the large uncertainty about the actual value of the formation energy of a vacancy from experimental measurements. Strictly speaking, the formation energy of the vacancy in Fe-12%Cr should have been used, which has been assessed to be about 1.52 eV, according to this potential [5]. Yet, the small difference from pure Fe and the uncertainties in its calculation suggest that this effect is not so important and can be neglected. However, as will be discussed below, the effect of the entropy of formation of the vacancy, not considered in table 2, may have an important influence on the results.

The curves corresponding to the last two columns of data in table 2 are plotted in figures 3a and 3b for, respectively, Cr and Fe diffusivity. The absolute value of D at 0 K extrapolated from these curves gives the prefactor, D_0 , while the slope provides the activation energy, E_a , according to the interpolation of the data using the Arrhenius function (5). In the same figures, the corresponding experimental curves are also represented. The curve for Cr diffusivity in Fe-12%Cr was built using the actual prefactor and activation energy measured by Wolfe and Paxton, as reported in [13]. The prefactor and activation energy values to build the curve for Fe diffusivity were interpolated from experimental curves provided by Wolfe and Paxton in [13].

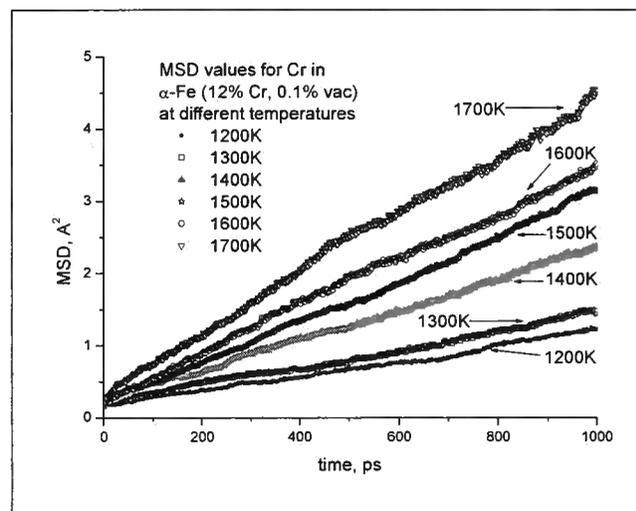


Fig. 2 - Cr atoms MSD at different temperatures in Fe-12%Cr. All simulations were performed with a vacancy concentration of 0.12%.

Calculated and experimentally measured values for prefactors and activation energies are compared in table 3, where also *ab initio* numbers for activation energies are indicated for comparison. It can be seen that the slope of the calculated curves, i.e. the activation energy, is quite close to the experimental slope, particularly for Cr atoms. The slight understimation is well contained within the standard deviation error bar related to the interpolation of data and, if we consider also the experimental uncertainties, the agreement can be said to be excellent. The same cannot be said, at first sight, for the prefactor, which appears to be underestimated in the calculation by slightly less than 2 orders of magnitudes. However, figures 3a and 3b show clearly that this gap is saved by taking into

account the effect of the vacancy formation entropy when applying the correction (8). This entropy contribution has been calculated for pure Fe, using the present potential, and found to equal $\sim 2.7k$, where k is the Boltzmann constant [17]. Introducing the formation entropy effect in the correction (8) is tantamount to multiply the diffusion parameters times a factor $\exp(2.7) \cong 15$. After this additional correction, also the values of the prefactors become comparable with the experimental ones. Of course, considering the uncertainties in the assessment of these values, this agreement is maybe partially fortuitous. Still, we can state that the potential proves satisfactorily capable of predicting the diffusivity of Cr and, though to a slightly lesser extent, also Fe in an Fe-Cr alloy via vacancy mechanism.

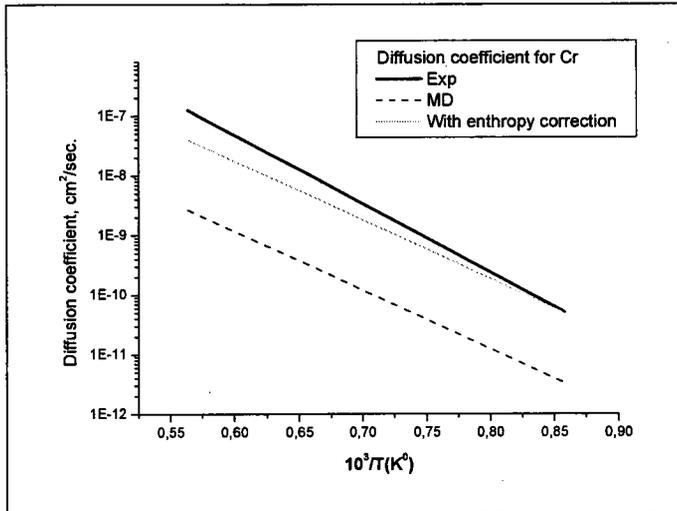


Fig. 3a Self diffusion of chromium in Fe-12%Cr alloy: experimental and calculated data.

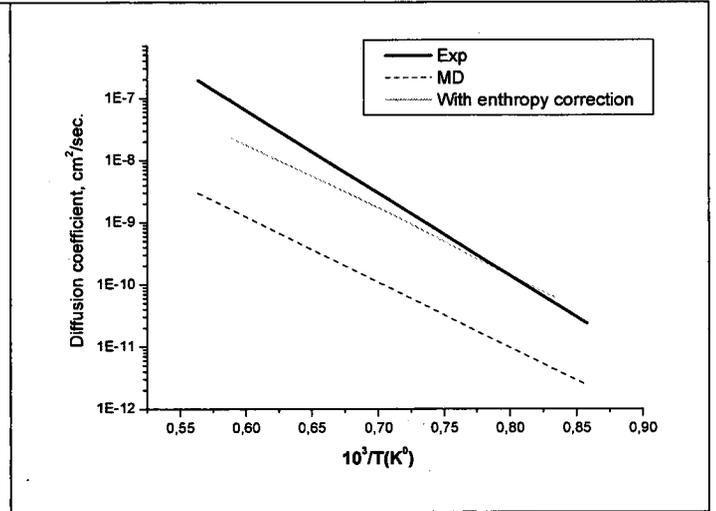


Fig. 3b Self diffusion of iron in Fe-12%Cr alloy: experimental and calculated data.

Table 3. Diffusion parameters for Cr and Fe atoms in an Fe-12%Cr alloy: calculated and measured values. In parenthesis deduced values.

Atom	Method	Log D_0	E_a (eV)	E_v^f (eV)	E_{mig} (eV)
Cr	MD simulation	0.0778	2.11±0.17	1.52 (Fe-12%Cr)[5]	(0.59±0.17)
	MD simulation (with entropy correction)	0.0912	Same as above		
	Experimental	0.1113 [13]	2.39 [13]	1.5 ÷ 2.0 (pure Fe) [11]	0.63 [14]
	VASP (1 Cr atom in Fe)	n.c.	(2.53)	1.95 [10]	0.58 [5]
Fe	MD simulation	0.0801	2.19±0.14	1.52 (Fe-12%Cr)[5]	(0.67±0.17)
	MD simulation (with entropy correction)	0.547	Same as above		
	Experimental [13]	(0.75) [13]	(2.54) [13]	1.5 ÷ 2.0 (pure Fe) [11]	
	VASP (pure Fe)	n.c.	(2.60)	1.95 [10]	0.65 [10]

3.3 Cr and Fe diffusivity in α -Fe via interstitial mechanism

Under irradiation interstitial atoms are created and diffusivity of both matrix and solute atoms is in principle possible through their movement. Another objective of this work was to assess the difference in efficiency of the diffusion via vacancy and interstitial mechanisms. We therefore made calculations of diffusivity in both pure α -iron and Fe-12%Cr by adding either one vacancy or one self-interstitial atom, in a box of the same size, and following the MSD of both atomic species (Cr and Fe) for 1 ns at different temperatures. The results of the MD calculations are shown in figures 4 and 5, after correction to the equilibrium concentration of vacancies (without entropy factor), according to (8). This correction is meaningless in the case of interstitials, for which no appreciable equilibrium concentration can be detected in real materials, not even at high temperatures, but in this way absolute values comparable with customary diffusion coefficient orders of magnitudes are obtained. The situation we have in mind is in any case that of a material under irradiation, where the concentration of vacancies and interstitials is comparable.

From figure 4 we can see that the interstitial mechanism is more efficient than the vacancy one, particularly for the transport of Cr atoms, as a consequence of a larger prefactor. Interstitials move, according to all EAM-type interatomic potentials [18], via $\langle 111 \rangle$ direction glide, by moving from a dumbbell to a crowdion configuration along that direction. This mechanism necessarily involves the effective displacement of about one atom to its first nearest neighbour position, in the bcc structure, every three jumps of the interstitial atom. In addition, it has been shown by *ab initio* calculations that the formation of mixed Fe-Cr dumbbells is favoured and is predicted by our potential [5]. These factors, together with the notoriously much higher mobility of interstitials compared to vacancies, clearly rationalise our result. On the other hand, the slope of all the curves in figure 4 is essentially the same, which means that the activation energy is more or less the same for diffusion via interstitials or vacancies in the Fe-Cr alloy. Figure 5 shows, in turn, that the diffusivity of Fe atoms via vacancy and interstitial mechanism in pure Fe is more effective than in the Fe-Cr alloy. This fact is easily explained by the interstitial "trapping" at Cr atoms mentioned above (formation of Fe-Cr dumbbells in Fe-Cr alloys), which is also indirectly proved by some experimental observations [19], and which is absent in pure Fe. The consequence is that interstitials move faster in pure Fe than in Fe-Cr. A quantification of how much faster is still lacking and is part of our future work.

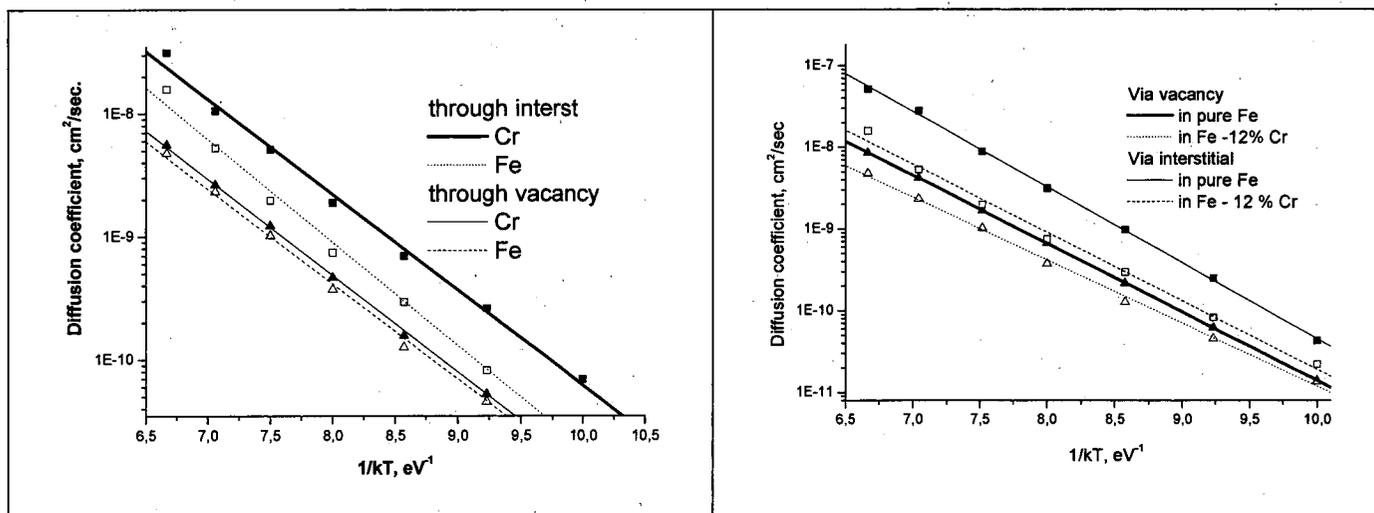


Fig. 4 Calculated diffusion coefficient of Fe and Cr atoms in Fe-12%Cr, via vacancy (triangle) and interstitial (square) mechanism.

Fig. 5 Calculated diffusion coefficient of Fe atoms in pure Fe and Fe-12%Cr, via vacancy (triangle) and interstitial (square) mechanism.

3.4 Melting point

The second part of this work is devoted to the estimation of the melting point in pure Fe and Fe-12%Cr. More precisely, in the case of the alloy what we intend to assess is the temperature of liquidus line, although in this specific case of Fe-Cr in the 12%Cr region, the solidus and the liquidus are so close to each other that, considering also the uncertainties of the calculation method and the fact that most likely the interatomic potential cannot reproduce all the details of the Fe-Cr phase diagram, it is roughly justified to talk about a melting point for the alloy too. PCF and MSD as a function of temperature are shown in figures 6 and 7. One can see that no unmistakable MSD slope change is observed anywhere in the studied temperature range, except maybe for Cr atoms (see figure 6), but the PCF analysis shows a transition between 1800 K and 1850 K (see figure 7). Therefore, the two phase method was applied in this region of temperatures, in order to find the melting point with reasonable accuracy. The results are shown in table 4, together with experimental data and the results of other calculations, with our potential and with a potential that has been widely used for the simulation of displacement cascades in Fe [20].

It is seen in table 4 that a really good agreement between experimental results and simulation results is achieved. Essentially, the calculation predict for pure Fe and Fe-Cr alloy the same melting point, around 1815 K, but both experimental values, which are very close as well, are contained in the uncertainty of the calculation.

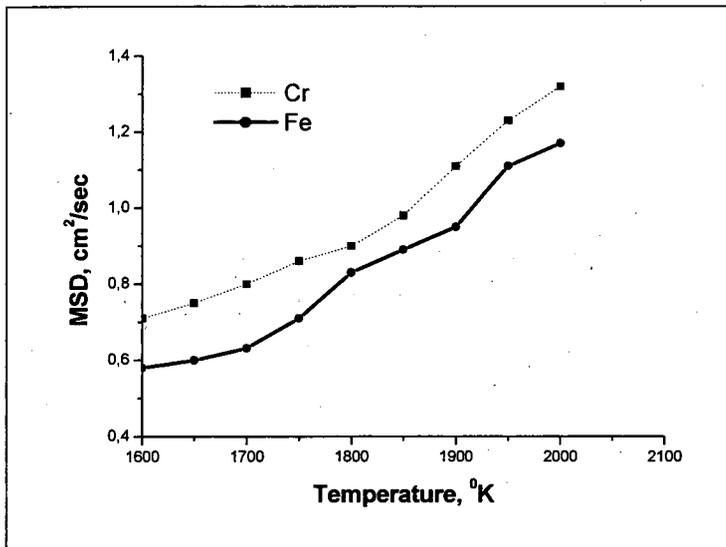


Figure 6. MSD dependence on temperature for Cr and Fe atoms in Fe-12%Cr

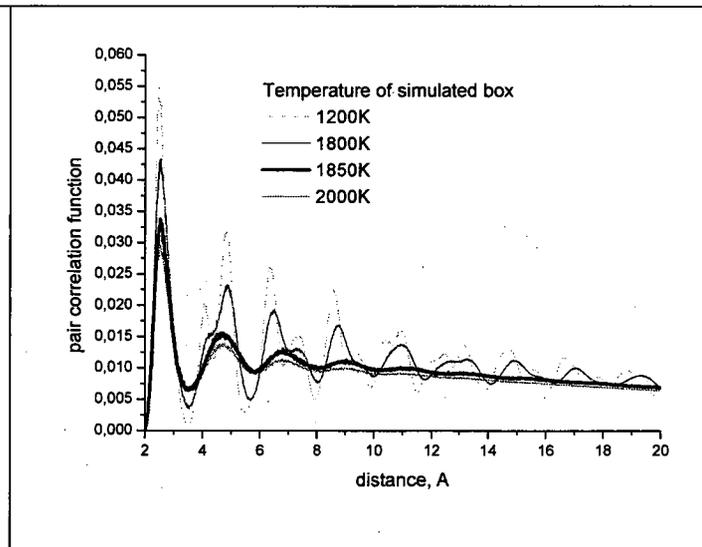


Figure 7. Pair correlation functions for Cr and Fe atoms in Fe-12%Cr at different temperatures

Table 4. Melting point temperatures: simulation results and experimental data.

Results	Fe – 12% Cr	Pure Fe
Our calculation	1815 ± 15 K	1815 ± 15 K
Experimental	1806 K	1811 K
Other calculations		1840 ± 5 K (this potential, [17]) 2200 ± 200 K (Finnis-Sinclair potential [20])

4. SUMMARY AND CONCLUSION

In summary, the diffusion coefficients as a function of temperature for Cr solute atoms and Fe atoms in Fe-12%Cr and pure Fe have been determined by computer simulation, using a standard molecular dynamics code and using a new embedded atom method potential for the Fe-Cr system. The diffusion via vacancy and interstitial mechanism was also studied. The potential used predicts diffusion coefficients for Cr and Fe atoms in Fe and Fe-Cr alloys in good agreement with available experimental data, provided that the results of the calculations are corrected to take into account the real vacancy concentration at equilibrium, at the different temperatures, and that the vacancy formation entropy contribution is included in the correction. The activation energy for Cr solute atom diffusion has been calculated to be 2.11 ± 0.17 eV, in excellent agreement with both the experimental and the *ab initio* values, considering that the latter were not obtained in an Fe-12%Cr alloy, and quite close to the sum of vacancy formation and migration energies obtained using the same potential from static calculations. In a comparison of diffusivity via vacancy and interstitial mechanism, the latter is seen to be more effective than the former, particularly in the case of Cr atoms. The diffusivity of Fe atoms via vacancy and interstitial mechanism in pure Fe is seen to be higher than in FeCr. These results can be easily rationalised by considering the mechanism of interstitial glide predicted by all EAM-like potentials in Fe alloys and the existence of a "trapping" effect of interstitials at Cr atoms (Fe-Cr dumbbell formation), which has been predicted by *ab initio* calculations and seems to agree with experimental observations. In the second part of this work the present Fe-Cr potential was shown to correctly predict the melting point for both pure Fe and Fe-12% Cr.

In conclusion, the present potential seems promising from the point of view of its use for the prediction of primary damage state generation in displacement cascade MD simulations.

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