Calculation of Energy Characteristics of Point Defects in bcc Iron by Molecular Dynamic Technique

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The influence of the calculation procedure on the energy characteristics of vacancies and helium impurities in α-iron is considered. Calculations are performed with the help of long-range oscillating interatomic pair potentials found on the basis of a model pseudopotential approach. It is shown that for improving the convergence of the lattice sums one must introduce space windows. The best results were obtained with the Vashista-Singwi local-field correction and the modified window-modulation interatomic potential based on the Heine-Abarenkov pseudopotential with the Animalu formfactors.

Key words: Interatomic potentials, Pseudopotentials, Point defect, Helium, Binding energy.

1. Point Defects and Potentials

Numerical values of point defect characteristics are needed for comparisons with experimental data and tests of various theories describing the creation and transformation of defect structures originated by point defects. Presently the properties of point defects and their clusters are mainly obtained by computer simulations. Published data show that simulations made with different interatomic potentials can lead to different stable configurations and energy characteristics of the same point defects and their clusters [1]. This shows that a correct choice of the interatomic potential is essential.

Most of the earlier simulations of metals were made with empirical pair potentials whose constants are obtained from macroscopic properties of the metals [2]. These potentials have drawbacks, e.g. they neglect the energy part connected with the conduction electrons [3]. Fortunately there is an alternative way based on pseudopotentials. These can be divided into two groups: ab initio pseudopotentials and model pseudopotentials [4–7].

The ab initio pseudopotentials, first developed for simple metals, were later generalized for transition and noble metals [7, 8]. However, they are difficult to use in computer simulations because they usually can not be reduced to the form of interatomic potentials. Therefore the pseudopotential theory got real value for computer simulations only when model pseudopotentials were constructed [9–14]. These permitted to calculate the atomic properties of simple, transition, and noble metals and their alloys [15].

This success is due to a calibration procedure in which one uses the spectroscopic terms of positive ions as input data. For this purpose, the true one-electron atomic potential is replaced by a model one which gives the same phase shift. Since arising from electron wave scattering, the phase shifts are connected with the energy levels of electrons moving in an atomic potential. This approach takes into account details of the electronic structure and permits to reduce the model potential to an interatomic one.

On the basis of this approach, Animalu calculated and tabulated the model potential parameters for 30 transition metals [13]. Afterwards, considering more carefully the phase shift induced by resonant interaction of s- and d-electrons, Dagens et al. [16–21] calculated the model potential parameters for noble metals and nickel. Their final results are given in the form of an analytical expression which approximates the interatomic pair potential. During the last years the Heine-Abarenkov-Animalu model pseudopotentials and Dagens interatomic potentials were widely used for calculations of point defect characteristics by

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molecular dynamics simulations for transition metals and alloys, viz. Ni, α-Fe, Mo, Ti, Zr, Ni–W, α-Fe–He [1, 22–31].

It should be noted that recently some progress has been achieved in the development of physical models which go beyond the assumption of pair-wise interactions. These models consider the d-band bonding energy as thinning the tight binding approximation and are known under the names of effective medium, embedded atom, Finnis-Sinclair or glue model [32–36].

Here the total potential energy of a system is expressed as the sum of two parts: the first term is a two-body part, the second one, expressing the forces acting on an ion in terms of the positions of other ions, is a many-body term depending on the coordination number of the ion considered.

Many-body potentials derived from one of these models for some bcc transition metals have been used to study vacancy formation energy [37] and volume [38], surface energy and tension [39], vacancy, self-interstitial and stacking-fault properties [40], and small interstitial clusters [41]. However, these potentials do no permit to describe the differences between individual metals [41]. To our mind, this drawback is connected with the empirical and short-range nature of these potentials.

When constructing an interatomic potential on the basis of any pseudopotential approach, it is necessary to choose an appropriate dielectric response function $\varepsilon(q)$ in order to describe the screening of the interatomic interaction by valence electrons. Taking into account exchange and correlation effects in an electron gas, one can write [4]

$$\varepsilon(q)=\frac{1-\varphi(q)(1-G(q))\,\chi(q)}{1+\varphi(q)\,G(q)\,\chi(q)}, \tag{1.1}$$

where $\varphi(q)$ is the Fourier transform of the Coulomb interaction, $\chi(q)$ the Lindhard function, $G(q)$ the local-field correction, and q the wave number. For the densities of metallic electron gases, the exact expression for $G(q)$ is unknown. The different approximations of $G(q)$ are considered in [4]. The most usable approximations were suggested by Geldart and Vosko (GV [42]), Geldart and Taylor (GT [43]), Singwi, Sjolander, Tosi and Land (SSTL [44]), and Vashista and Singwi (VS [45]). Although these approximations satisfy the limit relations for electron gas characteristics, it is very difficult to choose an appropriate local-field correction function because there is no definite criterion for such a choice. We suppose that by calculating the atomic properties of metals and comparing the results with experimental ones one can test the validity of the approximation chosen.

The interatomic pair potential calculated on the basis of a pseudopotential theory has a long-range oscillation. This causes difficulties when calculating lattice sums, in particular the crystal potential energy [46]. In this paper we consider the influence of local-field corrections on the correctness of long-range interatomic potentials which are used for calculating the properties of point defects in α-iron.

2. Calculation Procedure

We have used the Heine-Abarenkov type model pseudopotential [9] and the Animalu form factors [13]. The interatomic potential was found according to the formula [47]

$$\varphi(r)=\frac{(Z^*\cdot e)^2}{r}+\frac{\Omega_0}{\pi^2}\int_0^\infty w^2(q)\,\varepsilon(q)\,\chi(q)\,\frac{\sin(qr)}{r}\,q\,dq, \tag{2.1}$$

where Z^* is the effective ion valence, e the electron charge, Ω_0 the atomic volume, and $w(q)$ the form factor. In order to test the potential, we have chosen the following metal characteristics known from experiments: the vacancy formation energy E_v^f, the vacancy migration energy E_v^m and the elastic moduli C_{11} and C_{12}.

The vacancy migration energy was found in the dynamical way described in [27]. The elastic moduli were calculated according to the formulas [48]

$$C_{11}=\frac{1}{6\Omega_0}\sum_{l,\alpha}{}' x_\alpha^4(l)\left\{\frac{\varphi''(r)}{r^2}-\frac{\varphi'(r)}{r^3}\right\}_{r=r_l},$$
$$C_{12}=\frac{1}{6\Omega_0}\sum_{\substack{l\\ \alpha\neq\beta}}{}' x_\alpha^2(l)\,x_\beta^2(l)\left\{\frac{\varphi''(r)}{r^2}-\frac{\varphi'(r)}{r^3}\right\}_{r=r_l}, \tag{2.2}$$

where $\varphi'(r)$ and $\varphi''(r)$ are the first and second derivatives of the potential, respectively, r_l is the radius-vector modulus of the l-th atom, and $x_j(l)$, $(j=1, 2, 3)$ are the coordinates of the l-th atom. The vacancy formation energy was found as in [49]:

$$E_v^f=E_v^{f\,(un)}-E_v^R. \tag{2.3}$$

Here E_v^R is the crystal lattice relaxation energy referred to the vacancy formation. The static unrelaxed vacancy formation energy for the pair interatomic approxima-

Table 1. Vacancy relaxation energy.

	Number of mobile atoms	$R_c = 1.97\,a$						$R_c = 2.5\,a$		$R_c = 2.9\,a$	
		$\varphi(r)$			$\tilde{\varphi}(r)$			$\varphi(r)$	$\tilde{\varphi}(r)$	$\varphi(r)$	$\tilde{\varphi}(r)$
		SSTL	VS	GT	SSTL	VS	GT	SSTL			
E_v^R, eV	*a* 459	1.88	2.06	2.49	1.59	1.78	1.98	2.19	1.60	2.74	1.61
	b 1639	2.68	2.67	4.50	1.76	1.98	2.30				

tion is given by [49]

$$E_v^{f\,(un)} = -\frac{1}{2}\sum_i Z_i \left\{\varphi(r_i) + \frac{r_i}{3}\,\varphi'(r_i)\right\}, \tag{2.4}$$

where Z_i is the number of atoms in the i-th coordination sphere. The self-diffusion energy was found from the relation $Q^{SD} = E_v^m + E_v^f$; the self-diffusion was supposed to consist in monovacancy migration.

Summing the badly converging series (2.2) and (2.4), we followed the recommendations in [1] and multiplied the interatomic potential by the Tukey space window

$$\Pi_T(r) = \begin{cases} 1 & r \leqq R_1 \\ \dfrac{1}{2}\left(1 + \cos\left(\pi\,\dfrac{r - R_1}{R_N - R_1}\right)\right), & R_1 \leqq r \leqq R_N \\ 0 & r \geqq R_N\,, \end{cases} \tag{2.5}$$

where the radii R_1 and R_N were chosen to be those of the first and 80th coordination spheres, respectively.

The simulation cell has the form of a sphere with a bcc structure. Rigid boundary conditions were used for the outer atoms fixed in a spherical shell whose width is equal to the cut-off radius of the potential.

3. Test Results

As a rule, in order to spend minimal computing time for getting a result with a given accuracy, the cell dimensions were chosen such that the distance between the defect and the fixed shell is larger than the cut-off radius R_c. We have calculated the vacancy relaxation energy for cells which contain between 459 and 1639 mobile atoms (total number of atoms between 1471 and 4111, respectively). Figure 1, curve (1) shows the dependence of E_v^R on the number of mobile atoms for the SSTL approximation and $R_c = 1.97\,a$, where a is the lattice constant of α-iron. One can see that E_v^R becomes greater with increasing crystallite dimensions. This dependence is connected with the bad convergence of the lattice sums.

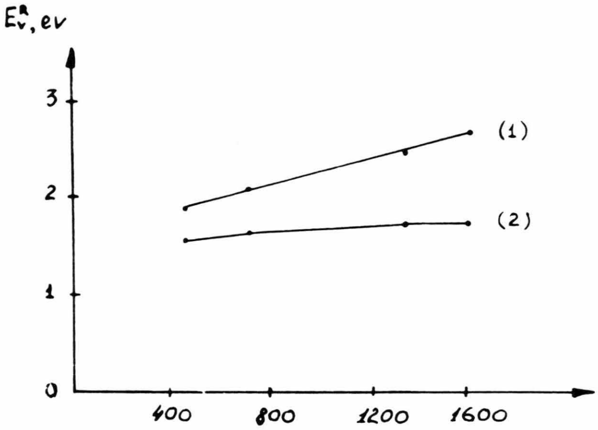

Fig. 1. Influence of the number of mobile atoms on the vacancy relaxation energy. (1): SSTL approximation, (2): with window-modulation.

In order to improve the convergence, we modified the interatomic potential by multiplying it by the Tukey space window

$$\tilde{\varphi}(r) = \varphi(r) \cdot \Pi_T(r)\,. \tag{3.1}$$

The calculation showed that the values of E_v^R obtained with the help of the modified potential are almost independent of the cell dimensions, Fig. 1, curve (2). Analogous results were obtained for the other approximations used (Table 1).

Table 1 gives also the values of E_v^R computed for the SSTL approximation with the help of $\varphi(r)$ and $\tilde{\varphi}(r)$ for three cut-off radii. The calculations were made according to the procedure suggested in [50], i.e., the crystal lattice relaxation was made with the cut-off radius $R_c = 1.97\,a$, but the relaxation energy was found for three cut-off radii $R_c = 1.97\,a$, $2.5\,a$, and $2.9\,a$. One can see that the vacancy relaxation energy is nearly

Table 2. Elastic moduli and vacancy characteristics of α-iron.

		Our results				[50]	[30]	Other calcu-lations	Experiment
		SSTL	VS	GT	GV				
$C_{11} \cdot 10^{-11}$, N/m		1.68	1.81	1.92	2.01	2.07	1.77	–	2.28 [51]
$C_{12} \cdot 10^{-11}$, N/m		1.07	1.14	1.13	1.20	1.89	1.57	–	1.32 [51]
E_v^f, eV	*a*	2.10	2.24	2.09	2.97	0.88	0.92	1.37 [58]	1.4 [52] 1.53 [53]; 1.6 p [54]
	b	1.93	2.06	1.77	2.72			1.39 [59]	1.79 p, 2.0 f [55]
E_v^m, eV		0.57	0.55	0.57	–	–	–	0.66 [2]; 0.68 [58]	1.24–1.5 [56]; 0.55 [57]
Q^{sd}, eV	*a*	2.67	2.79	2.66	–	–	–	2.05 [58]	2.36 p [55]
	b	2.50	2.61	2.34	–	–	–		2.36–2.75 f [55]

Meaning of *a* and *b* as in Table 1. $Q^{sd} = E_v^m + E_v^f$. – p: paramagnetic; f: ferromagnetic.

Table 3. Optimal interatomic pair potential for α-iron.

r [nm]	φ [eV]	r [nm]	φ [eV]	r [nm]	φ [eV]
0.11482	30.03152	0.25277	0.34674	0.39072	−0.00372
0.11941	26.47485	0.25737	0.29724	0.39532	−0.00207
0.12401	23.30104	0.26196	0.25432	0.39992[3]	−0.00059
0.12861	20.47032	0.26656	0.21696	0.40451	0.00068
0.13321	17.94797	0.27116	0.18427	0.40911	0.00172
0.13781	15.70348	0.27576	0.15554	0.41371	0.00253
0.14241	13.70973	0.28036	0.13020	0.41831	0.00311
0.14700	11.94238	0.28496[2]	0.10777	0.42291	0.00348
0.15160	10.37941	0.28955	0.08791	0.42751	0.00366
0.15620	9.00074	0.29415	0.07033	0.43210	0.00367
0.16080	7.78798	0.29875	0.05481	0.43670	0.00353
0.16540	6.72420	0.30335	0.41118	0.44130	0.00327
0.17000	5.79382	0.30795	0.02932	0.44590	0.00292
0.17459	4.98248	0.31255	0.01909	0.45050	0.00252
0.17919	4.27698	0.31714	0.01038	0.45510	0.00209
0.18379	3.66524	0.32174	0.00311	0.45969	0.00165
0.18839	3.13625	0.32634	−0.00282	0.46429	0.00122
0.19299	2.68004	0.33094	−0.00751	0.46889	0.00082
0.19759	2.28763	0.33554	−0.01104	0.47349[4]	0.00047
0.20219	1.95098	0.34014	−0.01353	0.47809	0.00017
0.20678	1.66290	0.34474	−0.01507	0.48269	−0.00008
0.21138	1.41698	0.34933	−0.01579	0.48729	−0.00027
0.21598	1.20752	0.35393	−0.01580	0.49188	−0.00040
0.22058	1.02948	0.35853	−0.01522	0.49648[5]	−0.00048
0.22518	0.87836	0.36313	−0.01417	0.50108	−0.00052
0.22978	0.75020	0.36773	−0.01275	0.50568	−0.00052
0.23437	0.64151	0.37233	−0.01109	0.51028	−0.00049
0.23897	0.54928	0.37692	−0.00927	0.51488	−0.00044
0.24357	0.47088	0.38152	−0.00739	0.51947	−0.00038
0.24817[1]	0.40406	0.38612	−0.00552	0.52407	−0.00031

Upper numbers denote the number of the coordination sphere.

independent of the cut-off radius if the window-modulation interatomic potential is used.

For this reason we have made our further calculations with the modulated potential. The results got for four local-field corrections are given in Table 2. The experimental values of the elastic moduli C_{11} and C_{12}; the vacancy formation and migration energies and the theoretical results obtained by the other investigations are also given in this table. The comparison shows that the accuracy of the calculations is best for the GT and VS approximations. It should be noted that the analogous results for nickel (fcc lattice) are less sensitive to the choice of the approximation function [1]. The optimal modulated interatomic potential for α-iron obtained with the help of the VS correction is shown in Fig. 2 and given in Table 3.

4. Helium in Lattice

One of the central problems of solid state radiation physics is the influence of helium on the properties of materials. Helium and helium-vacancy complexes in metals were studied by molecular dynamics simulations with empirical interatomic metal-metal potentials [60]. However, as was mentioned above, interatomic potentials derived from pseudopotential theory lead to results differing qualitatively from those obtained with empirical potentials, e.g., the binding energy of two-dimensional vacancy clusters in transition fcc metals such as nickel was found to be higher than that of three-dimensional ones [24, 25], contrary to earlier results obtained with empirical interatomic potentials [25]. Therefore we expected a similar effect for helium and helium-vacancy clusters.

To verify this hypothesis we conserved consciously the interatomic helium-iron potential in the same form as it was employed before [61], in order to comprehend the influence of the oscillating iron-iron poten-

Table 4. Interstitial helium characteristic for α-iron.

	Void		Split configuration			Number of atoms		Cut-off radius
	tetra	octa	⟨111⟩	⟨110⟩	⟨100⟩	mobile	all	
E^{f}_{He}, eV	5.04 5.53 [2]	5.18 5.36 [2]	5.05 6.16 [2]	5.12 6.28 [2]	5.18 –	749 –	2247 –	$2a$ [1] –

[1] a = Lattice constant. – [2] Data from [60, 61].

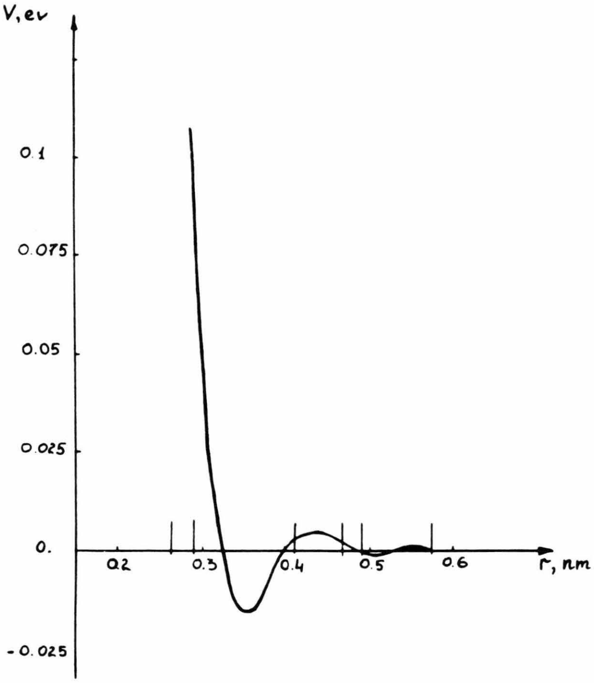

Fig. 2. Optimal interatomic pair potential for α-iron (vertical lines denote the coordination spheres).

tial in a pure manner. The interatomic helium-iron potential used has the form of a cubic polynomial with coefficients depending on the interatomic distance. This potential has an entirely repulsive character.

We have considered different configurations of interstitial helium in the bcc lattice of α-iron. The helium inclusion energy for these configurations was found as the difference between the energy of a crystal with and without helium. The results obtained are given in Table 4. The analogous data for an empirical iron-iron potential are also presented in this table. One can see that with the non-empirical oscillating long-range potential a tetrahedral configuration becomes energetically favourable, whereas with the empirical short-range potential it is an octahedral configuration.

Let us analyse the results obtained. It was mentioned that the total energy of a crystal with an impurity or defect consists of two parts: electronic and ionic. Consider the first part. The interaction of helium with transition metal atoms in the first approximation is defined by the repulsion between the closed electron shell of helium and the valence (s and d) electrons of a metal, so that helium atoms try to occupy the sites with the least electron density [60, 61]. The electron distribution in bcc iron is such that the density of d-electrons in the tetrahedral voids is smaller than in the octahedral ones [62]. Supposing a uniform distribution of s-electrons, we come to the following conclusion: in order to reduce the electron energy of bcc iron, helium must occupy preferentially tetrahedral positions.

The ionic part of the total energy can be approximated by the repulsion in a hard sphere model. For this model it was found that an octahedral interstitial configuration in a bcc lattice is stable if the interstitial radius is smaller than some definite value, which equals 0.09 nm for α-iron [63]. For large interstitial radii a tetrahedral site becomes more stable. According to [60, 64], the helium atomic radius is 0.143–0.148 nm. Consequently, from this view point helium will have a tendency to place itself in tetrahedral positions. Therefore our results are consistent with the least energy principle for both constituents of the total energy.

As for the relaxed split interstitial configurations of helium, their energy is near to the energy either of a tetrahedral or octahedral interstitial position.

We estimated also the helium migration energy in the following way. There are two routes for helium migration (Fig. 3) through the sites tetra-octa-tetra and tetra-⟨110⟩ split-tetra. In the first case the energy barrier equals 0.14 eV, in the second one 0.08 eV. The earlier estimates obtained with the help of empiric potentials gave [60, 61, 65] 0.1, 0.13, 0.17, and 0.3 eV.

Now consider the binding energy of helium with a vacancy. We have taken as this energy the difference

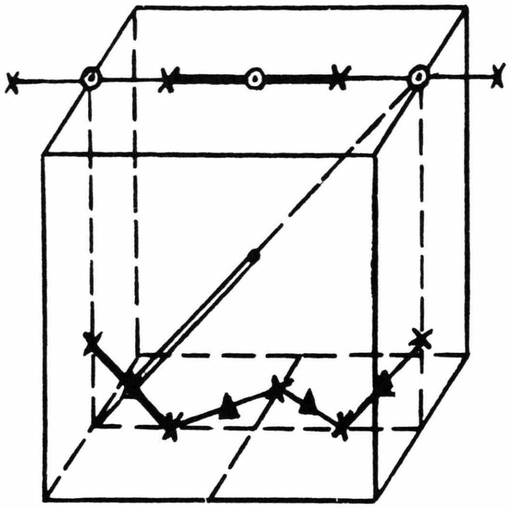

Fig. 3. Migration paths of helium in a bcc lattice: ⊙ octahedral position; × tetrahedral position; ▲ helium position in mixed split ⟨110⟩ interstitial.

for the following cases: a crystal with a vacancy and helium in a tetrahedral site, and the same crystal with helium occupying the vacancy. It could be noted that the distance between the vacancy and the interstitial helium in the first case must be such that these defects do not interact. We got a binding energy 3.84 eV, whereas the previous estimates [60, 61, 65] gave 3.75 eV. The reason of discrepancy is mainly due to the helium formation energy which was already discussed.

5. Conclusion

We have investigated the influence of different ways of calculation on the vacancy and helium characteristics and elastic moduli for α-iron. The calculation showed that the results depend considerably on the calculation procedure used. However, it is not difficult to improve the convergence of the lattice sums by introducing some kind of space window; e.g. the Tukey space window permits to get minibiased values. As for the local-field corrections, the best results were obtained with the Geldart-Taylor and Vashista-Singwi approximations.

Appendix: Tukey Space Window

We consider the justification of using space windows for the calculation of some characteristics via oscillating interatomic potentials. Let us take, for example, the vacancy formation energy E_v^f. The first part of the sum (2.4) describes the potentials at the given site of a crystal lattice produced by all the other atoms, the second one is the virial part which characterizes the lattice compression due to defect formation. Both parts give the unrelaxed vacancy formation energy $E_v^{f\,(un)}$.

It is known that this sum converges badly; also the energy oscillates with the number of the coordination sphere. Therefore, if one chooses the cutoff radius of a potential in an arbitrary way, one can get, in principle, any value of E_v^f [66]. To avoid this mistake, one uses methods which, in fact, are modifications of the Evald and Evjen methods [67]. For example, the potential can be multiplied by the Gauss damping multiplier. However, in this case it is necessary to find and select the optimal values of the potential cut-off radius and damping decrement [50].

In terms of the probability theory and mathematical statistics [68], this problem is equivalent to the search of a sample estimate for a value whose variance does not depend on the sample volume. In this problem, introducing a damping factor means a transition to a smoothed sample estimate. In fact, Ewald's method and its modifications are equivalent to looking at a potential through the Gauss space window. Obviously, one can construct any other space windows [68, 69].

In order to diminish the variance of E_v^f we acted as follows. The smoothed interatomic potential was obtained by multiplying the potential $\varphi(r)$ by the Tukey space window, which was chosen in the form (2.5). The first term on the right side of (2.3) was calculated by summing as far as $k = 80$. The second term, i.e. E_v^R, was obtained by the molecular dynamics technique with artificial dissipation of the crystallite kinetic energy. Here the potential cut-off radius was restricted to the N-th coordination sphere and N was changed in the interval 6 to 13; that was enough to guarantee the convergence within the error limits ± 0.01 eV. Such a way of smoothing does not distort the maximum contribution of the first sphere to the vacancy formation energy and also provides fast convergence and minibiased sample estimate of this value.

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