



First-principles calculation of possible carbon positions over cementite lattice

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The properties of iron-carbon alloys are largely determined by the formation of iron carbide. Therefore, knowledge about the structure of cementite plays an important role. The possible reason for changes in the nearest neighborhood of iron and carbon atoms in cementite during various heat treatments of steel could be the re-arrangement of carbon atoms over different interstitial sites of cementite iron sublattice. Crystal geometry analysis revealed four types of such sites: “normal” and “distorted” prismatic (NPS, DPS), and “normal” and “distorted” octahedral (NOS, DOS) sites. In this study, we tested this hypothesis using the density functional theory by full-potential method implemented in the WIEN2k program package. The simulated cementite supercells contained 16 and 32 atoms. We confirmed that carbon in NPS resulted in the system with the lowest energy and volume. Systems with all carbon atoms in DPS and one or all carbon atoms in DOS were mechanically unstable and transferred to conventional NPS structure during the system volume relaxation. In other cases, carbon atoms remained in NOS or DPS and yielded the increased structure total energy. The thermodynamic analysis showed that over 10% of carbon atoms might move from NPS to other sites.

Keywords: cementite, carbon positions, interstitial sites, first-principles calculation.

1. Introduction

The interaction between iron and carbon atoms leads to the formation of α - and γ -solid solutions and chemical compounds such as iron carbides. Cementite (iron carbide Fe_3C) is the most famous carbide, which is ferromagnetic with Curie temperature near 170°C [1]. The cementite has high strength and serves as the main hardening phase in carbide steels and white cast iron [1]. The properties of iron carbide have been studied for a long time. Initially, cementite was investigated as a component of steel, which significantly affects its mechanical properties. Also, researchers paid attention to cementite's magnetic properties due to the nondestructive testing of steel.

Cementite is one of the most frequent phases in commercial iron alloys. It has an orthorhombic lattice of the $Pnma$ space group. Unit cell with parameters $a = 4.524$, $b = 5.088$, $c = 6.741$ Å [2, 3] contains 12 iron and 4 carbon atoms. Iron atoms occupy two crystallographically inequivalent sites denoted in [4] as G (general):

$$\begin{aligned} & \pm[[x, y, z]]; \pm[[\frac{1}{2}-x, \frac{1}{2}+y, z]]; \\ & \pm[[x, y, \frac{1}{2}-z]]; \pm[[\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z]] \end{aligned} \quad (1a)$$

and S (special):

$$\pm[[u, v, \frac{1}{4}]]; \pm[[\frac{1}{2}-u, \frac{1}{2}+v, \frac{1}{4}]]; \quad (1b)$$

parameter values are $x = 0.333$, $y = 0.175$, $z = 0.065$, $u = -0.167$, $v = 0.040$ [2].

Positions of carbon atoms are a subject of discussion. The two variants described in the literature are the centers of octahedra [5]:

$$\begin{aligned} & [[0, 0, 0]]; [[\frac{1}{2}, \frac{1}{2}, 0]]; \\ & [[0, 0, \frac{1}{2}]]; [[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]] \end{aligned} \quad (2a)$$

and the centers of trigonal prisms

$$\pm[[r, s, \frac{1}{4}]]; \pm[[\frac{1}{2}-r, \frac{1}{2}+s, \frac{1}{4}]], \quad (2b)$$

the values of r and s parameters being $r = 0.43$, $s = -0.13$ [2].

Recent research has shown that both options are possible [6–10]. The opinion that carbon atoms occupy prismatic type positions (2b) has become predominant in the literature, though some authors supposed that both variants exist in different conditions [11].

But in our works [12–15] it was pointed out that the iron sublattice of cementite possesses four types of sites that may potentially serve at positions for carbon atoms. Extra sites were termed “distorted” prismatic (with centers described by formulae (2b) at $r = -0.449$, $s = 0.238$) and “distorted” octahedral sites with centers at

$$\begin{aligned} & [[\frac{1}{2}, 0, 0]]; [[0, \frac{1}{2}, 0]]; \\ & [[\frac{1}{2}, 0, \frac{1}{2}]]; [[0, \frac{1}{2}, \frac{1}{2}]]. \end{aligned} \quad (3)$$

Sites (2b) and (2a) were thus referred to as “normal” prismatic and “normal” octahedral ones. The viewpoint that carbon atoms may redistribute over iron sublattice of cementite was supported by some experimental works that

showed strong changes of short-range order during heat treatment or severe deformation of steel [16–26].

Lastly, some authors starting from A. A. Baikov (1910) discussed the idea that cementite can change its chemical composition depending on the procedure of its treatment [27–31], i. e. that vacancies may form in carbon sublattice.

In recent years the question of the position of carbon atoms on cementite lattice was investigated by some authors using *ab initio* [32–36] and molecular dynamics [37] computer calculations. It was shown that the energy of formation of a carbon vacancy in cementite structure is 17.85 [33] or 0.68 eV [35] in ferromagnetic state and 0.28 [36] or about 0.3 eV [37] in paramagnetic state. The energy of cementite structure with all carbon atoms located on the “normal” octahedral interstitials was found to be 0.68 [33], 0.272 [34], or about 0.3 eV per C atom [37] higher than that of the same structure with all carbon atoms on “normal” prismatic sites. The values from the early work [32] are greater than others probably because no structural relaxation was performed.

The data for the cases of carbon atoms located on “distorted” prismatic and octahedral sites, as well as for only a part of carbon atoms shifted from “normal” prismatic sites to other ones are seemingly absent in the literature. Recently, the interest in cementite properties surged due to the new method of hardening steel by obtaining metastable compounds, one of which is the cementite phase. Moreover, lately, geophysicists suggest that cementite may be contained in the Earth’s core. Finally, ferromagnetic cementite nanoparticles could be used for targeted medicine delivery [1]. However, the experimental study of cementite is hindered by its metastability at atmospheric pressure. Also, usually, samples contain ferrite and a carbon phases. It leads to significant vitiation between different experimental studies. Therefore, theoretical investigations are needed to correctly interpret the empirical results. However, many problems in the theoretical description of cementite remain unsolved. For example, carbon atoms could redistribute among various interstitial sites of the iron sublattice in Fe_3C . In this work, we will discuss the results of our calculations in the framework of density functional theory.

2. Method of *ab initio* modelling

All calculations were performed in the software package WIEN2k [38] with a full-potential LAPW method using GGA-96 that provides high precision of results. Calculations were carried out with a Tornado complex of the Supercomputer center of the South Ural State University [39].

The method of modelling the structure of cementite where carbon atoms occupy “normal” prismatic interstitials is described in detail in [40]. The following parameters were used during modelling: $K_{\text{max}} = 5 \text{ a.u.}^{-1}$; muffin-tin sphere radii $R_{\text{mt}}(\text{Fe}) = 2.00 \text{ a.u.}$, $R_{\text{mt}}(\text{C}) = 1.45 \text{ a.u.}$; cut-off energy $E_{\text{cut}} = -7.0 \text{ Ry}$ (340 eV). Convergence criteria were a reproduction of full energy and the charge of every atom not greater than 10^{-4} Ry and $10^{-3} e^-$, respectively, and the strength force acting on every atom not greater than 1 mRy/a.u. (0.025 eV/\AA). It provided the accuracy of results below 0.01 eV . The structure optimization procedure is described in

detail in a previously published work [40]. Lattice parameters after structural relaxation were $a = 4.510$; $b = 5.063$; $c = 6.747 \text{ \AA}$ which differs from experimental values measured [8] at 4.2 K by less than 0.02%. Coordinates of iron atoms were those of Eqs. (1a,b) at $x = 0.329$; $y = 0.175$; $z = 0.068$; $u = -0.164$; $v = 0.036$, and of carbon atoms those of Eqs. (2b) at $r = 0.440$; $s = -0.124$.

In this work, we investigated a supercell, consisting of one or two unit cells of cementite with parameters $a = 4.510$; $b = 5.063$; $c = 6.747 \text{ \AA}$ (13.494 \AA for 32-atoms). The following structures were considered (Fig. 1):

1. 16-atom system where all 4 carbon atoms are in NOS (Fig. 1b);
2. 16-atom system where all 4 carbon atoms are in the DOS (Fig. 1c);
3. 16-atom system where all 4 carbon atoms are in DPS (Fig. 1d);
4. 16-atom system where 1 carbon atom is in the “normal” octahedral site (NOS) and 3 others in the “normal” prismatic sites (NPS) (Fig. 1e);
5. 32-atom system where 1 carbon atom is in NOS and 7 others in NPS (Fig. 1f);
6. 16-atom system where 1 carbon atom is in the “distorted” prismatic site (DPS) and 3 others in the NPS (Fig. 1g);
7. 32-atom system where 1 carbon atom is in DPS and 7 others in NPS (Fig. 1h);
8. 16-atom system where 1 carbon atom is in the “distorted” octahedral site (DOS) and 3 others in the NPS (Fig. 1i);
9. 32-atom system where 1 carbon atom is in NOS, 1 carbon atom in DPS (located 5.632 \AA from one another) and 6 others are in NPS (Fig. 1j).

Earlier we provided a preliminary calculation of energy characteristics for a small supercell of 16 atoms with 4 carbon atoms in the work [41].

Systems No. 2,3,8 (with all 4 carbon atoms in DPS or DOS and with 1 carbon atom in DOS) had very high energy due to small interatomic distances (see above) and were unstable, viz. during structural relaxation carbon atoms shifted spontaneously to NPS. So these three variants will not be considered in further treatment.

The formation energy E_f of cementite was estimated using the formula

$$E_f = E(\text{Fe}_k\text{C}_n) - kE(\text{Fe}) - nE(\text{C}), \quad (4)$$

where $E(\text{Fe}_k\text{C}_n)$ is the full energy of a cementite crystal containing k iron and n carbon atoms, $E(\text{Fe})$ is the energy of 1 Fe atom in bcc structure, and $E(\text{C})$ is the energy of 1 C atom in graphite structure.

3. Results and discussion

3.1. Various positions of carbon atoms

According to the technique presented in [40], similarly, for all cases of the arrangement of carbon atoms, the structure was optimized and the equilibrium internal coordinates and lattice parameters were found. These lattice parameters a , b and c as well as energy and magnetic characteristics of the

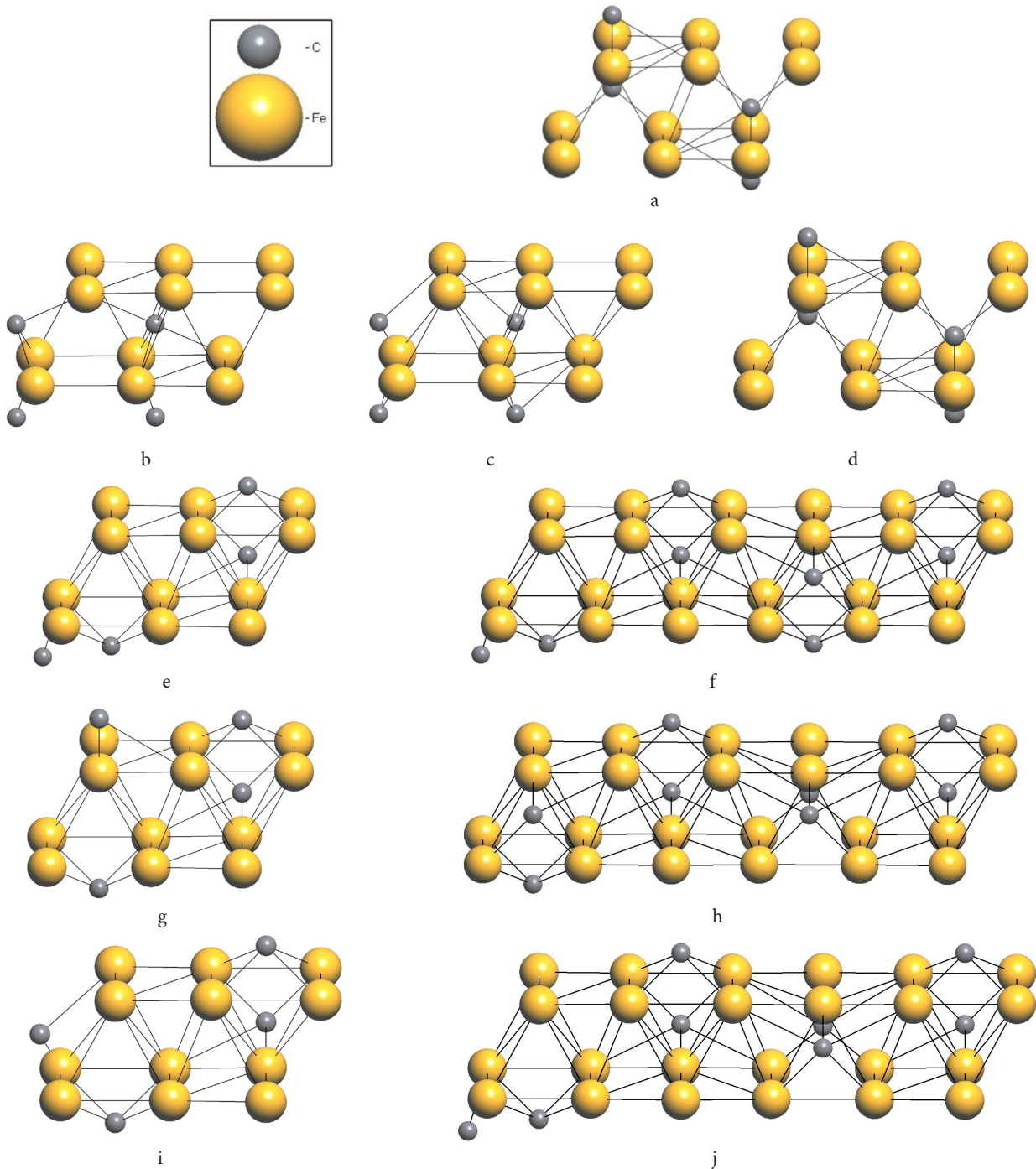


Fig. 1. (Color online) Structures of Fe_3C were considered 16 atom system with 4NPS (a), 16 atom system with 4NOS (b), 16 atom system with 4DOS (c), 16 atom system with 4DPS (d), 16 atom system with 1NOS (e), 32 atom system with 1NOS (f), 16 atom system with 1DPS (g), 32 atom system with 1DPS (h), 16 atom system with 1DOS (i) and 32 atom system with 1NOS, 1DPS and 6NPS (j).

final structures are presented in Table 1 and Fig. 2. It should be noted that the results of modeling for the 16-atom supercell were previously presented by us in another work [41]. But to demonstrate the change in the cementite formation energy for fractions of C atoms shift from NPS to NOS or DPS, we were forced to present data for both a system with 16 atoms and a cell of 32 atoms. Thanks to a cell of 32 atoms, we were able to consider small concentrations of carbon and, as a result, to plot the changes in the energy of formation of cementite, the volume of the Voronoi polyhedron, and the magnetic moment from the fraction of carbon atoms.

Carbon fractions from 0 to 0.125 correspond to the 32 atom systems and from 0.25 to 1 for the 16 atom systems.

As noticed above, if all 4 carbon atoms in a 16-atom supercell are initially located on DPS, they all shift spontaneously to the NPS during structural relaxation. But if only one carbon atom is located on DPS atoms in a 16 and 32-atom supercell, it stays there, increasing the volume of the structure by 3.75% and 1.80% compared to the case of NPS, respectively. Thus, one can say that the Fe_3C structure with carbon atoms on DPS is stable if the fraction of occupied DPS is $x_{\text{C}}^{\text{DPS}} = 0.125$ or 0.25 and unstable if $x_{\text{C}}^{\text{DPS}} = 1.00$. It is

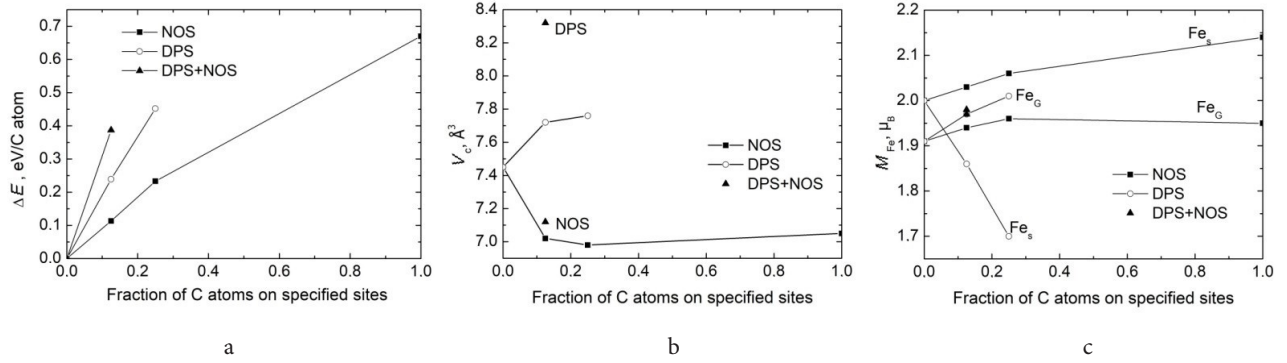


Fig. 2. Calculated values of the change of cementite energy when carbon atoms shift from NPS to NOS or DPS (ΔE) (a), Voronoi volume per one carbon atom V_c (b) and magnetic moments on iron atoms of two types [$M(Fe_G)$ and $M(Fe_S)$] (c) as a function of carbon atoms occupying NOS or DPS.

Table 1. Characteristics of 16 and 32-atom cementite structures.

Characteristic	16 atoms				32 atoms		
	4NPS	1NOS+3NPS	4NOS	1DPS+3NPS	1NOS+7NPS	1DPS+7NPS	1NOS+1DPS+6NPS
Fractions of C atoms:							
x_C^{NPS}	1	0.75	0	0.75	0.875	0.875	0.75
x_C^{NOS}	0	0.25	1	0	0.125	0	0.125
x_C^{DPS}	0	0	0	0.25	0	0.125	0.125
Lattice parameters, Å:							
a	4.510	4.527	4.650	4.471	4.510	4.492	4.567
b	5.063	5.087	5.125	5.228	5.074	5.122	5.085
c	6.747	6.929	7.057	6.837	13.680	13.631	13.842
Unit cell volume, Å ³	154.04	159.57	168.21	159.81	313.07	313.64	321.47
Formation energy of cementite E_f , eV/f.u.	0.227	0.460	0.494	0.679	0.340	0.465	0.614
Magnetic moments on C atoms, μ_B	-0.11	-0.11	-0.13	-0.12	-0.11	-0.11	-0.10

necessary to note that the term “stable” means the stability of the position of the atoms after the structure optimization procedure. Atoms do not return to their original positions, but the energy of cementite formation increases.

As for the case of carbon atoms located in NOS, these structures are stable both at a small value $x_C^{NOS} = 0.125$, $x_C^{NOS} = 0.25$, and $x_C^{NOS} = 1.00$, but have a volume greater by 1.62, 3.59, and 9.19% compared to the case of NPS.

When considering the case when one carbon atom is in the NOS, one more carbon atom is in the DPS, and the remaining 6 are in the NPS, with the initial distance between them being 5.634 Å, it was found that this structure also remains stable. At the same time, the distance between these carbon atoms was decreased up to 5.354 Å and the volume of the entire structure increased by 4.35% compared to the NPS.

The obtained value of the formation energy of Fe_3C for the case of NPS (0.227 eV/f.u., i.e. 0.06 eV/atom) is in good correspondence with experimental data (0.05–0.08 eV/atom) [42,43] and results of previous theoretical assessments (0.22–0.26 eV/f.u.) [44,45]. The formation energy of Fe_3C is positive, which agrees with the metastable character of cementite and its rather easy decomposition with free carbon precipitated in the form of graphite. The formation energy of cementite is the highest if the carbon atom is located on DPS ($x_C^{DPS} = 0.25$). It should be noted that the formation energy of cementite with two different carbon positions (Fig. 1i) is

more favourable than when one of the four carbon atoms takes up a position in the DPS (Fig. 1f).

The energy of cementite in which one carbon atom located on NOS (Fig. 1g) is 0.233, and four ($x_C^{NOS} = 1.00$) by 0.267 eV/C atom higher than if carbon is in NPS, which corresponds well to the data reported [34] (0.272 eV/C atoms at $x_C^{NOS} = 1.00$). When one carbon atoms shifts from NPS to DPS ($x_C^{NOS} = 0.25$) the energy of the structure rises by 0.452 eV/C atom following the previous estimation of 0.42 eV/C atom [14]. With a smaller decrease fraction of carbon atoms from 0.25 to 0.125 in the NOS and DPS, the energy of cementite formation decreases to 0.340 and 0.465 eV/C atom, respectively (Table 1).

For clarity, the dependences of the value of the change in the energy of cementite during the transition of carbon atoms from NPS to NOS or DPS, the volume of the Voronoi polyhedron per one carbon atom, and magnetic moments on iron atoms of two types [$M(Fe_G)$ and $M(Fe_S)$] on the fraction of carbon atoms occupying positions different from NPS was present (Fig. 1b,c). From the presented data, it can be seen that the magnetic moments are characterized by a linear dependence, while the volume of the Voronov polyhedron and the change in the energy of formation of cementite have more complex behavior.

Results obtained for magnetic moments on iron atoms in the Fe_3C structure with carbon in NPS (1.91 and 2.00 μ_B on G and S type atoms, respectively) are in good correspondence

with both previous calculations [44, 45] and with the average experimental value of $1.78 \mu_B$ [46]. There is a small induced magnetic moment of $-0.11 \mu_B$ on carbon atoms. The change of the position of carbon atoms may result in either an increase of magnetic moments on iron atoms (NOS) or a decrease of them (DPS for Fe_s). For the case where carbon is located in the NOS position, the volume of the Voronoi polyhedron decreases, and the magnetic moments on the iron atoms increase. For the DPS case, V_C increases, while the magnetic moment for Fe_s decreases, but for Fe_G , on the contrary, it increases. Moreover, if one atom is in NOS and the other is in DPS, then the magnetic moments for Fe_s and Fe_G are almost equal.

In a number of works [47–49], it was assumed that carbon can easily leave the cementite lattice. Therefore, we simulated the formation of a vacancy in cementite. As a model, we used a supercell containing 96 iron atoms and 32 carbon atoms, i.e. 8 elementary cells. The energy of formation of a carbon vacancy was 0.50 eV, which is in reasonable agreement with other data (0.68 eV [35]). The energy of formation of an iron vacancy is 2.5–3 times higher (1.34 eV for Fe_G and 1.60 eV for Fe_s). This indicates that the previously voiced assumption is correct, carbon can indeed easily leave the cementite lattice.

3.2. Thermodynamic assessment

The obtained results can be used to refine the estimates of equilibrium fraction of carbon atoms in different sites of the Fe_3C structure made in [14]. Given the total number of carbon atoms unchanged, the sum

$$x_C^{DPS} + x_C^{DPS} + x_C^{DPS} = 1, \quad (5)$$

the minimum free energy of the system is achieved at

$$x_C^{NPS} = \frac{1}{1 + \sqrt{B_{NOS} + B_{DPS}}}, \quad (6a)$$

$$x_C^{NOS} = \frac{B_{NOS}}{B_{NOS} + \sqrt{B_{NOS} + B_{DPS}}}, \quad (6b)$$

$$x_C^{DPS} = \frac{B_{DPS}}{B_{DPS} + \sqrt{B_{NOS} + B_{DPS}}}. \quad (6c)$$

where $B_i = \exp(-\Delta E_i/kT)$. Results of calculations using Eqs. (6) from [19] with the values of $\Delta E_{NOS} = 0.113$ and $\Delta E_{DPS} = 0.239$ eV/atom (see Fig. 2 (a) at $x = 0.125$) show that in carbon steels even at temperatures below the A_{c1} point (1000 K) the fraction of carbon atoms at DPS may reach several percent, and at NOS it may be even greater than 0.1. Of course, the values of ΔE obtained in this paper refer to the ground state of cementite, which is ferromagnetic, and may change significantly above the Curie point. However, the results from [50] show that the carbon dissolution energy for ordered two-layer antiferromagnetic and paramagnetic states of gamma iron changes by no more than 30%. Thus, even these approximate estimates support the idea proposed in [17] that redistribution of carbon over the interstitial sublattice of cementite is possible. It may serve as an explanation of strong changes of short-range order of atoms in cementite during heat treatment of steels observed experimentally by different methods in [21–31].

4. Conclusions

Using *ab initio* calculations, we showed that the transition of all carbon atoms from “normal” prismatic positions to “normal” octahedral positions in the cementite structure led to the system’s total energy increase. At the same time, structures with all carbon atoms in “distorted” prismatic or octahedral positions or one carbon atom in a “distorted” octahedral site were mechanically unstable and transferred to NPS.

We found that structure with one carbon atom in NOS, another carbon atom in DPS, and the remaining 6 carbon atoms are in NPS was also stable. In this case, the carbon-carbon distance and the cementite formation energy were less than the corresponding values for the DPS system at coordinat $x = 0.25$. Thus, the lower the concentration of carbon atoms in positions other than NPS, the structure is the more energetically favorable.

The formation energy of a vacancy in cementite indicated that carbon could relatively easily leave the lattice.

Thermodynamic analysis showed that even at temperatures lower than 1000 K over 10% of carbon atoms may shift from “normal” prismatic positions to other types of sites.

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