Tetragonality and Real Crystal Structure of Martensite in the Carbon Steels

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The results of the previous investigations of martensite crystal structure in the carbon steels, in which, based on the doublet splitting of some XRD lines, the conclusion on tetragonality of martensite was made, is analysed. As proposed, the crystal structure of martensite in the carbon steels is considered as a system of the lattice blocks with C atoms at the block axes and the distorted lattices without carbon atoms around the blocks. Carbon concentration in the steel specifies quantity of the blocks. Edges of the lattices in the blocks and outside them have different sizes depending on the distance to the block axis with carbon atom. As defined, the martensite crystal structure in the carbon steels is pseudotetragonal or trigonal. New approach is proposed for an explanation of a great width value of the martensite XRD lines in the carbon steels.

Key words: carbon steel, martensite, crystal structure, lattice, tetragonality, lattice block, diffraction line width.

Проведено аналізу результатів попередніх досліджень кристалічної структури мартенситу вуглецевих криць, в яких на основі появи дублетного розщеплення ряду дифракційних ліній зроблено висновок про тетрагональність мартенситу. Запропоновано розглядати кристалічну структуру мартенситу у вуглецевих крицях як певну систему блоків із ґратниць з атомом C на центральній осі блоків і ґратниць без атомів C навколо блоків. Кількість блоків у кристалічній структурі мартенситу визначається концентрацією Карбону в криці. Ребра ґратниць мають різну величину, яка визначається відстанню до осі блоків з атомом C. Кристалічну структуру мартенситу в крицях можна визначити як псевдотетрагональну або

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тригональну. Запропоновано нове пояснення великої ширини дифрак-
ційних ліній мартенситу, що виникає у вуглецевих крицях.

Ключові слова: вуглецева криця, мартенсит, кристалічна структура, ґра-
тниця, тетрагональність, ґратницевий блок, ширина дифракційної лінії.

1. INTRODUCTION

Beginning from the time when the diffraction methods for the structur-
al investigations have appeared, much attention has always spared to
the study of the crystal structure. Especially a lot of the works have de-
voted to examining of the crystal structure of martensite in the carbon
(C) steels. Beginning from the first works on an investigation of the
crystal structure of martensite in the steels, it accepted that martensitic
lattice was body centred tetragonal (b.c.t.) [1−6]. This conclusion made
on an appearance of the doublet splitting of a number diffraction lines of
the martensitic phase in the steels. Value of the crystal lattice parame-
ters depends on the carbon concentration: a decreases a little and c in-
creases with C content growth in the steel [6]. However, the long-time
doublet splitting of the diffraction lines and tetragonality did not ob-
serve in (0.1−0.6) wt.% C steels and therefore they concluded that mar-
tensitic phase had the cubic lattice under these concentrations [4, 5].

Until recently, nobody explained how small quantity of the carbon
atoms (less than 7−8 at.% C) might change the body centred cubic lat-
tice (b.c.c.) of iron (Fe_α) to the tetragonal (b.c.t.) lattice. Really, C at-
oms are at one c edge only in some lattices and there are many lattices
without C atoms. In the recent years, some investigations have ful-
filled in which a new approach has proposed for describing the crystal
structure of martensite in the carbon steels [7, 8].

Changes in the Fe_α crystal structure under an introduction of the C
atoms and a manner of the description of the real crystal structure of
martensite in the carbon steels considered in this article. A new ap-
proach proposed also for an explanation of a great width of the diffrac-
tion lines of the martensitic phase in the carbon steels.

2. INVESTIGATIONS OF THE CRYSTAL STRUCTURE
OF MARTENSITE IN THE CARBON STEELS

Investigations of the crystal structure of martensite in the carbon
steels have begun in twenties of the previous century and proceed up to
now. The doublets of the diffraction lines (110)−(101) (011), (200)
(020)−(002), (211) (121)−(112) have observed in the x-ray diffraction
patterns of the martensitic phase [1−3, 6]. Authors of these investiga-

tions concluded that martensite in the steels, containing more than 0.6 wt.% C, has the tetragonal crystal lattice. The lattice parameter c, interdoublet distances and ratio of the lattice's parameters c/a increase with carbon content growth.

For a long time splitting of the diffraction lines of martensite did not observe in the steels with C concentration lesser 0.6 wt.% and it was concluded that martensite in these steels had the cubic lattice [4, 5]. Cubic structure explained by the fact that in the steels with the concentration C < 0.6 wt.% the martensitic point is above room temperature. During quenching partial decomposition of martensite occurs and, in the result, C concentration in martensite decreases [9, 10]. However, if decomposition delayed and temperature of the martensitic transformation decreased, splitting of the corresponding diffraction lines and doublets observed in the diffraction patterns [11].

Great discussion generated by a question whether martensite with the cubic lattice arose in the steels with large, more than 0.6 wt.% C, carbon concentration. First reports of the cubic martensitic structure (b.c.c.) in the steels with increased C concentration have appeared long time after [5, 11] but were questioned. However, a number of the works have published later, confirming a formation of martensite with the cubic lattice in the steels with high C concentration [12−16]. Explanation of the possible reasons of an appearance of the tetragonal or cubic martensite proposed in some works [17, 18]. The explanation founded on an assumption of ordering of the C atoms in the martensitic structure.

Next peculiarity of the x-ray diffraction patterns of martensite in the carbon steels needs note: the diffraction lines are very wide always. It suggested that broadening of the diffraction lines caused by an appearance of the micro stresses and small sizes of the coherent scattering domains [2]. However, the investigations, carried out on the extracted, to relieve the stress, martensitic powders of the steel with 0.98 wt.% C, showed broadening of the diffraction lines of martensite appeared in such powders [19]. Thus, not a whole broadening was due to an influence of the micro stresses and the coherent scattering domains. Possible reasons of broadening of the diffraction reflections will be discuss later.

Now let us consider the main results of the investigations of the martensitic crystal structure in the carbon steels.

Based on the doublet splitting of a number of the x-ray diffraction lines it has concluded in the previous investigations that martensite with the tetragonal lattice appeared during quenching of carbon steels. The lattice parameters and c/a ratio determined using the doublet of the diffraction lines (110)−(101) (011) as the most intensive. The parameters of the martensitic lattice depend on the carbon concentration: c grows and a decrease a little with growth of C concentration, Fig. 1 [20].

Dependences of the tetragonality degree c/a on carbon concentra-
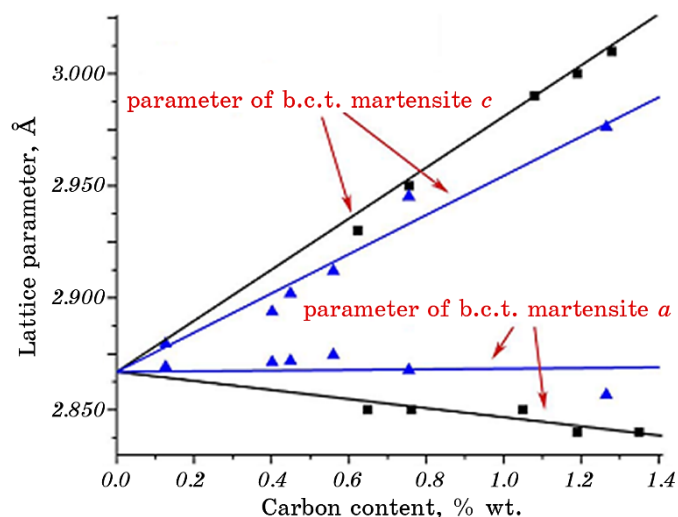
Fig. 1. Dependences of the lattice parameters of martensite on C content in quenched steels: ■—from [5], ▲—from [20].

tion in the steels, obtained in a number of the previous works, presented in **Fig. 2**.

Various slopes of c/a dependences on C concentration may be due to some differences in an accuracy of a determination of carbon concentration in steel and the methods used to measure the angles of the XRD lines.

Some distinguishing dependence of c/a ratio on carbon concentration received in [16]. There is $c/a = 1$ up to concentration 0.6 wt.% C, and only then, ratio c/a begins to grow with the C content increase (**Fig. 3**).

The empirical dependence has proposed to evaluate an influence of carbon concentration in steels on c/a ratio [6]:

$$c/a = 1 + 0.0467p, \tag{1}$$

where p is C concentration in wt.%.

Somewhat distinguishing dependence of c/a ratio and the lattices parameters c, a on C concentration has offered in [15]:

$$c/a = 1 + (0.0095 \pm 0.0001)x_C, \tag{2}$$

$$a = 0.28664 - (0.00027 \pm 0.00001)x_C \text{ [nm]},$$

$$c = 0.28664 + (0.00243 \pm 0.00003)x_C \text{ [nm]};$$

x_C is the number of C atoms per 100 Fe atoms and 0.28664 is the lattice parameter of b.c.c. Fe_α at 300 K.

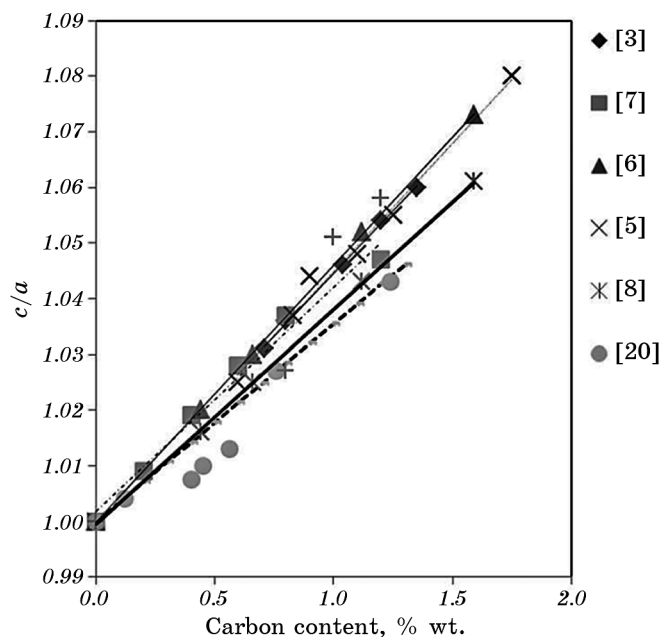The cubic structure of the martensitic phase in steels explains by

Fig. 2. Dependences of the c/a ratio on the carbon concentration, received in the different investigations.

disordered arrangement of C atoms in the octahedral interstices of the bcc lattice of α-iron [17, 18]. However, under certain conditions (corresponding quenching rate and temperature of the martensitic formation) C atoms are ordered and located only in the interstices along $[001]_M$ directions, that leads to an increase of c lattice parameter. In this case, the martensitic lattice of the carbon steel becomes tetragonal one, the doublets of some diffraction lines appear. Such explanation has proposed in many investigations.

The concept of carbon atoms ordering in martensite of steels have confirmed by the experimental results of a number of works [13, 14, 21, 22]. An influence of the cooling rate and holding at the different temperatures on the crystal structure of martensite in steels Fe–(3.0–6.3) wt.% Mn–(0.97–1.75) wt.% C investigated in [14]. X-ray diffraction study showed that after quenching and formation of martensite at temperature slightly lower $M_s = -58°$C well-separated doublet $(112)_M$–$(211)_M$ appeared (Fig. 4, a).

However, splitting practically disappeared and the diffraction lines almost merged upon subsequent cooling to temperature $-196°$C and further martensitic transformation, Fig. 4, b. This explained by disordering of C atoms during cooling and proceeding of the martensitic transformation. The diffraction pattern changed again after heating to 20°C: doublet appeared, although not the same as at $-58°$C (Fig. 4,
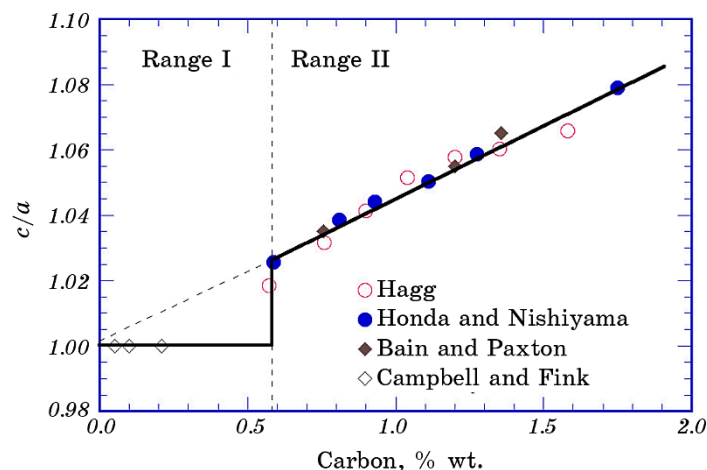
Fig. 3. Dependence of the *c/a* ratio on carbon concentration [16].

c), diffraction lines recovered partly.

Differences in the observed diffraction patterns explained as follows. When quenching and holding at −58°C carbon atoms are arranged orderly in the interstices situated along $[001]_M$ directions. This causes formation of the tetragonal lattice and an appearance of doublets. With rapid cooling to temperature −196°C, martensite forms, in which carbon ordering does not have time to occur. In the result, the diffraction lines do not split and doublets do not appear. Heating to 20°C leads again to the ordered arrangement of carbon atoms and an appearance of doublets (Fig. 4, *c*). Doublet appearance of a number of the lines in the diffractograms caused, on author opinion, by the formation of tetragonal martensite in a result of ordering of C atoms [14]. Author did not explain a great value, more than ten degrees, of the diffraction line widths of martensite.

Possibility of the reversible order−disorder transitions in martensite of carbon steels has confirmed by another experimental investigations. When ordered state in the samples of steel with 1 wt.% C was destroying by the irradiation of neutrons or fast electrons, doublets of the diffraction lines in the x-ray patterns were disappearing [21, 22]. However, holding at room temperature leads again to some ordering of the carbon atoms and an appearance of the diffraction doublets. Upon following cooling to −45°C ordered state disappeared but holding at 20°C restored ordering of the carbon atoms partially.

The concept of carbon atoms ordering in martensite of the steels explains formation of the cubic structure at any C concentration. In the case of chaotic distribution of the C atoms along any of three lattice edges *a*, *b*, *c*, they increase, accordingly. However, the diffraction lines of the tetragonal structure do not observe because the martensitic lat-
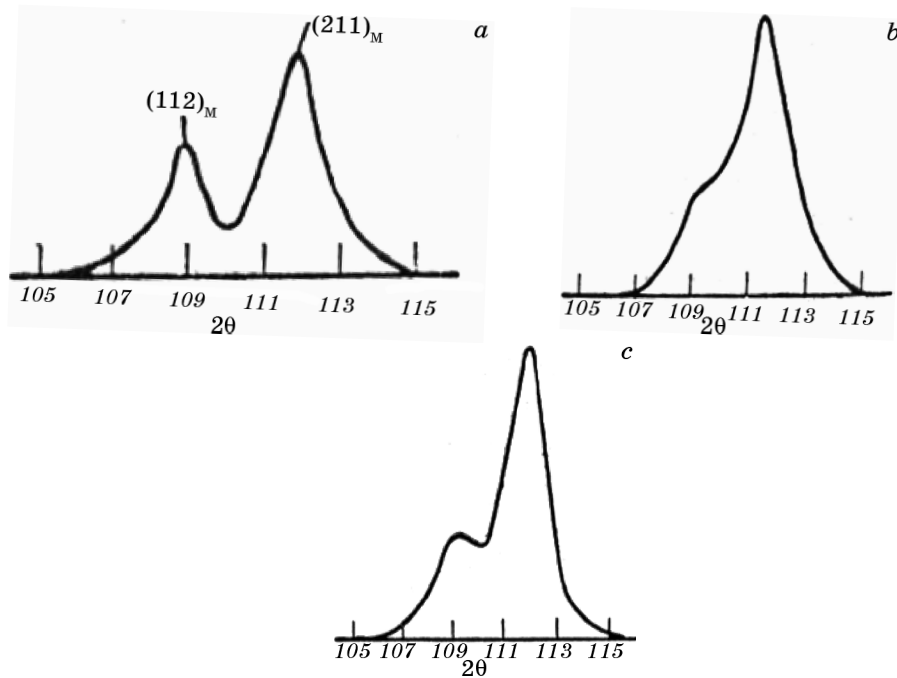
Fig. 4. Doublets of the diffraction lines $(211)_M$ and $(112)_M$ in steel Fe−0.97C− 6.3Mn (wt.%) that received at temperature −58°C (*a*), after cooling to −196°C (*b*), after heating to 20°C (*c*) [14].

tices remain b.c.c. 'in average'.

3. CRYSTAL STRUCTURE OF MARTENSITE IN CARBON STEELS

Conclusion about tetragonality of the crystal structure of the martensitic phase in carbon steels has made using observations of the doublet splitting of the number x-ray lines. However, this conclusion does not correspond to the real crystal structure of martensite for the following reasons.

It is well known that steels may contain 0.1−1.8 wt.% C, that in the atomic percent equal 0.5−8.1. In the previous investigations, it has assumed that when carbon implanted in γ-phase, C atoms located in the octahedral pores [1, 6]. In the result of $γ → α'$ transformation the martensitic lattice became tetragonal one. However, after the martensitic transformation carbon atoms from f.c.c. lattices of the parent phase remain only in some b.c.c. lattices of martensite. C atom settles down at one lattice edge only (for example, at *c* edge) and this new lattice becomes distorted. This lattice edge increases on the diameter of C atom and has size $c = d_{Fe} + d_C ≈ 0,504$ nm, where d_{Fe} and d_C are diameters of
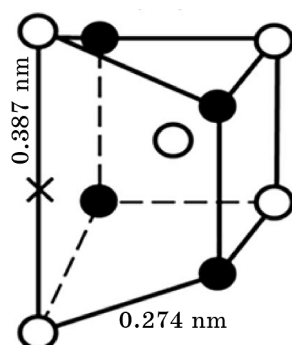
Fig. 5. Distorted martensitic lattice with C atom (×) at one *c* edge; ○ and ●— atoms Fe.

the atoms Fe and C. Other three *c* edges of the new lattice change essentially lesser (Fig. 5).

This distorted martensitic lattice with one C atom at one *c* edge is not tetragonal. Only two types of the tetragonal lattices (of Brave's type) known: simple tetragonal and body-centred tetragonal. Appearing during martensitic transformation in the carbon steels distorted lattices are neither tetragonal nor cubic because arising lattices have the different edges, do not have tetragonal symmetry and have only one C atom at only one edge of the lattice. It looks more like as triclinic: the sizes of the lattice edges are different and the angles at lattice tops differ from 90°. There are as many these distorted lattices as the number of the carbon atoms actually are in steel. Edges in the adjacent lattices also change.

New model of the martensitic crystal structure in carbon steels has proposed in [7, 8, 23]. The crystal structure of the martensitic phase
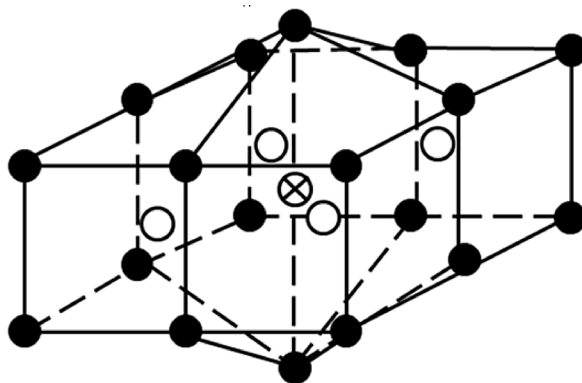
Fig. 6. Block of four lattices with common increased *c* edge (axis of the block) with C atom at axis (×—atom C, ○ and ●—atoms Fe [23].

presents as system of the blocks. Each block consists of four distorted b.c.c. lattices with C atom on the common edge—axis of the block (Fig. 6). Distorted b.c.c. lattices without carbon atoms are around each block. The carbon concentration in steel (number of C atoms) determines a quantity of the blocks.

The edge c with C atom (axis of the block) is the most increased, by the diameter of C atom. Other c edges of the lattices in the block change lesser.

By the estimations, the carbon content in this lattice block is 11.1 at.% (2.48 wt.%). The carbon concentration in steel defines the number of the blocks with C atoms in the crystal structure of martensite.

In the result of an influence of the C atoms in the blocks, nearest b.c.c. lattices have differently distorted c edges. The distortion value depends on the distance to the edge with C atom. The quantity relationship between the number of the blocks, the quantity of the distorted and undistorted b.c.c. lattices depend on the carbon concentration in steel. This relationship will influence the mean value of the interplanar distances in the martensitic phase, the peak position of the diffraction lines and the angle width of these lines.

It needs to carry out some changes and correction, presented in Fig. 6 model because before it has considered the change only one c edge at which C atom situated. However, increase of the c edge with C atom in the block results in some changes of the c edges in the neighbouring lattices. They increase also. These changes decrease with increase of the distance to the edge with C atom.

The graphical evaluation of the size of the c edges, adjacent to the c edges with C atoms, has fulfilled for the volume of the martensite containing 90 Fe atoms (45 b.c.c. lattices) and 5 C atoms (that is, for the concentration of 5.26 at.% C or 1.17 wt.%) [23]. The results of this evaluation showed in Table 1.

Evaluation for this selected volume showed that in the considered case average lattice parameter is 0.316 nm. Approximately the same c parameter ($c = 0.3155$ nm) determined for the steel Fe$-$1.63 wt.% C [24].

With an ordered arrangement of the carbon atoms, that is, under the formation of the lattices blocks with C atom only at one c edge, the

TABLE 1. Size and amount of the changed c edges under introduction of the C atom at one lattice edge c: c_1 is edge with C atom, c_2 are edges, closest to the axial edge with C atom in $[100]_M$ and $[010]_M$ directions and also in the lattices above and below of the block in $[001]_M$ direction, c_3 are edges along $[110]_M$ and $[010]_M$ directions, c_4 are edges at the distance $2a$ along directions $[100]_M$ and $[010]_M$.

Edge number	c_1	c_2	c_3	c_4
Edge size, nm	0.387	0.330	0.308	0.286
The number of edges	5	30	20	20

TABLE 2. Carbon concentration in steel at different number of the lattices without C atoms near one block.

Quantity of blocks (block—4 lattices, 1C atom)	Quantity of lattices without C atoms near block	Quantity of Fe atoms	Quantity of C atoms	Total quantity of atoms	C content, at.%	C content, wt.%
1	0	8	1	9	11.11	2.48
1	4 lattices in horizontal plane	16	1	17	5.9	1.31
1	8 lattices in horizontal plane	24	1	25	4,0	0.89
1	4 lattices above and 4 lattices below	24	1	25	4.0	0.89
1	8 lattices in horizontal plane + 4 lattices above and 4 lattices under	40	1	41	2.43	0.54
1	12 lattices in horizontal plane + 4 lattices above and 4 lattices under	48	1	49	2.04	0.46

doublets of the broadened lines have observed by the x-ray diffraction due to the 'collections' or the sets of the identical interplanar distances. In the case of the disordered arrangement of the C atoms over the crystal volume and arbitrary axis *a*, *b* or *c* of the blocks, x-ray diffraction pattern contains only wide unsplitted lines, that is, the diffraction lines of so-called 'cubic' or pseudocubic martensite. In this case, the blocks with one C atom at the common block axis situate in any direction [100], [010] or [001] and distribute arbitrarily over the whole volume of the steel. In the result, this leads only to the broadening of the x-ray lines in the diffraction patterns. The splitting of the x-ray lines and the doublets does not observe in this case.

Next estimations have carried out: 1. Carbon concentration in the steel in the dependence on the number of adjacent to the block lattices without C, Table 2; 2. The number of the blocks in the volume of 10^6 lattices at different C concentration, Table 3; 3. Angular distance between the reflection peaks $(200)_M$ and $(002)_M$, Table 4; 4. Angular position of the $(002)_M$ diffraction line at the different carbon concentrations, Table 5.

The results of an evaluation of general carbon concentration in steel in the case of the different number adjacent to the blocks lattices without C atoms, presented in Table 2. The concentration is 11.11 at.%

TABLE 3. The number of blocks at different carbon concentrations. Volume: 100×100×100 lattices = 1000000 lattices.

C concentration, at.%/wt.%	Quantity of C atoms per 100 Fe atoms	Real concentration, at.%/wt.%	Quantity of Fe/C atoms per 10^6 lattices	Quantity of blocks (lattices in blocks)	Quantity of lattices not in blocks	Quantity of lattices without C atoms around block
1.0/0.22	1	0.99/0.221	2000000/ 20000	20000 (80000)	920000	46
3.0/0.67	3	2.91/0.65	2000000/ 60000	60000 (240000)	760000	13
5.0/1.11	5	4.76/1.06	2000000/ 100000	100000 (400000)	600000	6
8.0/1.79	8	7.41/1.65	2000000/ 160000	160000 (640000)	3600000	2.25

(2.48 wt.%) for the block structure only and 2.43 at.% (0.46 wt.%) in the case of one block and twenty lattices without carbon atoms around. The first case (only blocks in the structure) is unrealistic since the carbon concentration in the steel (martensite) does not exceed 1.7–1.8 wt.%.

Thus, these evaluations confirm that the crystal structure of the steel for the real carbon concentrations may be represents as a system consisting of some quantity of the lattices blocks with C atoms on their

TABLE 4. Angular distance between diffraction peaks $(200)_M$ and $(002)_M$.

Reflection $(200)_M$, radiation FeK_α, $\lambda = 0.194$ nm					
C, wt.%	a, nm	d, nm	$\sin\varphi$	φ	$\Delta\varphi$ — angle distance between $(200)_M$ and $(002)_M$
0.2	0.2858	0.1429	0.6788	42°45′	0°30′
0.8	0.2849	0.1424	0.6809	42°55′	1°53′
1.4	0.2840	0.1420	0.6831	43°15′	3°22′
Reflection $(002)_M$, radiation FeK_α, $\lambda = 0.194$ nm					
C, wt.%	c, nm	d, nm	$\sin\varphi$	φ	$\Delta\varphi$ — angle distance between $(200)_M$ and $(002)_M$
0.2	0.2885	0.1442	0.6724	42°15′	0°30′
0.8	0.2955	0.1477	0.6565	41°02′	1°53′
1.4	0.3026	0.1513	0.6411	39°53′	3°22′

TABLE 5. Dependence of the martensitic lattice distortions magnitude in the steels on C concentration.

wt.% C	$(\overline{U_{\mathrm{d}}^2})^{1/2}$, nm	$(\overline{U_{\mathrm{st}}^2})^{1/2}$, nm	$\overline{c}/a$	c/a
0.08	0.0114	0.0046	1.016	1.005
0.10	0.0114	0.0057	1.020	1.005
0.35	0.0126	0.0059	1.020	1.016
0.84	0.0133	0.0085	1.030	1.040
1.0	0.0136	0.0100	1.035	1.047

axes and different number of the crystal lattices without C atoms around the blocks that depends on the carbon content.

It estimated also a quantity of the blocks and the number of the lattices without C atoms in the volume of the 10^6 lattices for the real carbon concentrations (0.22–1.79) in martensite of the steel, Table 3.

As seen, 46 lattices without carbon atoms locate around one block at the concentration 1 at.% C (0.22 wt.%). Only two (2.25) lattices without C atoms are adjacent to one block in the case 8 at.% C (1.79 wt.%). For the real C concentration 5 at.% (1.12 wt.%) there are six lattices without C atoms around one block with C atom. The edges in the lattices around the blocks also change, but significantly lesser than the edges in the block and significantly lesser than the central edge (axis) of the block.

Under ordering of the C atoms in steels, the periodic changes in the sizes of the c edges should observe in dependence on the distance to an axis of the block with carbon atom. Corresponding changes of the interplanar distances proceed also. Arising lattices may define as pseudotetragonal, pseudocubic or trigonal, as the lattice edges have different sizes and angles differ from 90°.

In the case of the disorder state of C atoms in martensite, the blocks axes with C atoms situate arbitrary along one of three directions $[100]_{\mathrm{M}}$, $[010]_{\mathrm{M}}$, $[001]_{\mathrm{M}}$ and one of the a, b or c lattice edge changes by the same value in dependence on location of C atom on the concrete edge. The changes of the other lattice edges depend on the distance to the edge with C atom. In this case, all three directions $[100]_{\mathrm{M}}$, $[010]_{\mathrm{M}}$, $[001]_{\mathrm{M}}$ are equivalent and in the result a, b, c parameters are averaged over the crystal. In this case, the lattices are distorted cubic (pseudocubic) however with changed parameters, which distinguish from the b.c.c. lattice parameter of α-iron. In the result, no line splitting observes in XRD patterns and the doublets do not appear, but the diffraction lines are broadening.

Thus, ordered and disordered states of the carbon atoms in the martensitic structure of the steels and, accordingly, so-called 'tetragonal' or 'cubic' martensite, have only one difference. In the 'tetragonal' marten-

site the blocks with C atoms at the axes (*c* edges) are located mainly along directions $[001]_M$. In the 'cubic' martensite C atoms may situate at one of the lattice edges *a*, *b*, *c* and the axes of the blocks locate along one of the directions $[100]_M$, $[010]_M$ or $[001]_M$ arbitrarily. This leads to an averaging of all lattice parameters *a*, *b*, *c* to some average parameter a_{av}.

Position of two lines $(200)_M$ and $(002)_M$ calculated and angular distance between the peaks of these lines determined for the carbon concentrations in steel 0.2, 0.8 and 1.4 wt.%. It turned out that for the steel with 1.4 wt.% C this distance is 3°22′ only (Table 4).

4. STATIC DISTORTIONS IN THE MARTENSITIC PHASE

Assignment of the crystal structure of martensite in the carbon steels as system of the lattices blocks with C atom at the blocks axes and the distorted lattices without C atoms around them gives a good possibility to understand the reasons of an appearance of the significant dynamic and static distortions during martensitic transformation. Their evaluation based on the measuring and analysing of an intensity of the x-ray diffraction reflections during changes of temperature and carbon concentration in the steel [25−27].

Investigations have shown that a value of the decrease in an intensity of the reflections grows with an increase of the dynamic distortions, caused by the thermal oscillations of the atoms. Dynamic distortions characterize by the value $(U_d^2)^{1/2}$, where U_d is the size of the displacement of the atom from a position of the equilibrium in the lattice. For the steels with 0.08−1.0 wt.% C, the dynamic distortions change next manner: at temperature 23°C from 0.0114 to 0.0136 nm and at temperature −185°C from 0.0076 to 0.0086 nm, respectively.

In addition to the dynamic distortions, the static distortions also arise in the solid solutions. Their appearance occurs in the result of the displacement of the atoms from the ideal positions in the lattices. Static distortions remain constant over time at low temperatures and in the absence of the diffusion. Such distortions characterized by the value of the root-mean-square deviation from the ideal position of the atoms in the lattice $(U_{st}^2)^{1/2}$. The magnitude of the static distortions depends on the number, distribution and arrangement of the atoms of another kind in the crystal structure of the material, the number of the displaced atoms and a value of the displacement.

Method of the determination of the static distortions bases on a comparison of the changes in the intensity of the x-ray doublets [25]. Since the static displacements do not depend on the temperature, method allows one to evaluate the average displacements of the atoms in any direction (for example, along directions $[100]_M$, $[010]_M$, $[001]_M$). The evaluation of the static distortions in $[001]_M$ direction showed that for steel with 1.3 wt.% C $(U_{st}^2)^{1/2} = 0.015$ nm [25] and for steel with

1.57 wt.% C $(\overline{U_{\text{st}}^2})^{1/2} = 0.018$ nm [27].

Magnitude of the static distortions in steel depends on the carbon concentration and increases with its rise [25]. If for the steel with 0.1 wt.% C value of distortion is $\approx 4 \cdot 10^{-3}$ nm, then at the concentration 1.0 wt.% C the distortion is in 2.5 times higher, $10 \cdot 10^{-3}$ nm. However, proposed method gives a possibility to estimate only some volume-averaged displacements of the atoms.

Magnitude of the root-mean-square displacements $(\overline{U_{\text{st}}^2})^{1/2}$ of the atoms from the ideal positions in the martensitic lattice of the carbon steels reflects the statistically averaged over the entire volume a value of the deviation (in nm) of the iron atoms from the ideal positions which directly affects the average value of the c edges with the carbon atoms. The changes of the edges a, b in the case of ordering of the C atoms in the martensite of the carbon steels are significantly smaller.

Dependence of the average size of the lattice edge $\overline{c}$ on the value of the root-mean-square displacements of the atoms $(\overline{U_{\text{st}}^2})^{1/2}$ presents as:

$$\overline{c} = c + (\overline{U_{\text{st}}^2})^{1/2}. \tag{3}$$

Relative values of the root-mean-square magnitude of the edges $\overline{c}$ distorted by the located on them carbon atoms determine by the following relationship:

$$\overline{c} / a = 1 + (\overline{U_{\text{st}}^2})^{1/2} / a. \tag{4}$$

Calculated magnitudes presented in Table 3. The value $\overline{c} / a$ corresponds to the degree of the tetragonality c/a, which depends on the carbon concentration in the martensite of the steel. This allows comparing these parameters at different C concentrations in steel, Table 5.

Two dependences of c/a (according to [2]) and $\overline{c} / a$ (calculated using formula 4) presented in Fig. 7.

The dependence c/a on the carbon concentration correlates quite satisfactorily with the experimental dependence of the relative value $\overline{c} / a$, calculated taking into account the static distortions in martensite of the steels with different carbon contents in the range up to 1 wt.% C. Such correspondence is natural enough since it entirely corresponds to the physics of the phenomenon under discussion, namely, to the displacement of the Fe atoms from the equilibrium positions in the lattice due to the presence of C atoms on some edges of the martensitic lattices. This is the physical reason for the diffraction fixation of the interplanar distances d of the different magnitudes, which leads to a broadening of the x-ray lines.

Significant anisotropy of the static distortions noted in [19]. As shown by the studies on the martensitic powders of the steel with 0.98 wt.% C, the static distortions along $[001]_M$ direction are by two times
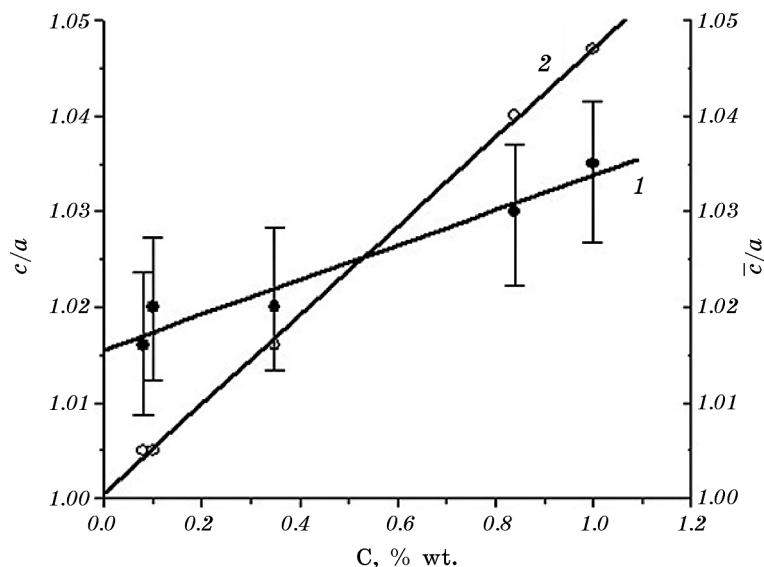
Fig. 7. The dependences of c/a (*1*) and $\bar{c}/a$ (*2*) on the carbon concentration in martensite of the carbon steels.

greater than along $[100]_M$: 0.0052 and 0.0025 nm, respectively. Author of this work concluded also that carbon in the steel leads to a broadening of the x-ray lines of martensite.

5. BROADENING OF THE MARTENSITIC DIFFRACTION LINES IN THE CARBON STEELS

The diffraction lines of the martensitic phase in the carbon steels are very wide always. Angular width of these lines runs up to 10–12°. Various explanations of this great broadening have proposed.

To present time the broadening of the martensitic x-ray line in the steels has explained in the following way: during transformation of the parent f.c.c. γ-phase into b.c.t. martensitic phase the stresses arise and the scattering coherent domains (crystal blocks) 30–70 nm in sizes appear in the martensitic phase. However, carried out on the extracted powders of martensite in the steel (1.0 wt.% C) x-ray investigation showed that, when an influence of the stress excluded, the diffraction lines remained widened nevertheless [19]. Thus, not the whole x-ray line broadening caused by the coherent domains and stresses. Some other reasons may exist.

The crystal structure of martensite in the carbon steels can present as system of the lattice blocks [7, 8]. All lattices, both in the blocks and around them, have edges with the sizes that depend on the distance to the

axis of the blocks with C atom (that is, there are different c sizes of the lattices). Lattice edges changes decrease with grow of the distance to the axis of the block and the sets of the equally changed c edges appear. In the result, the definite systems of the interplanar distances for concrete type of the reflections (for example, $(002)_M$) arise that leads to an appearance of the wide x-ray diffraction lines. These broadened lines consist of a number of the overlapping diffraction reflections corresponding to the definite set of the identical interplanar distances with equal c parameters.

The angular positions of the $(002)_M$ diffraction line vary with change of the c parameters. For example, position $(002)_M$ changes from $42°43'$ to $32°26'$ in the interval of c parameter 0.286–0.362 nm (Table 6).

These changes of the parameter c correspond really to variation of the C concentration in steel from 0.2 wt.% to more than 1.4 wt.%.

Thus, for these values of the c_M parameters (Table 6) angular width for $(002)_M$ reflection is about $10°$ that practically coincides with the diffraction line width determined in many experimental investigations. For example, the angular width of the $(200)_M$–$(002)_M$ martensitic line in the steel with 0.45 wt.% C reaches $12°$ [2], the doublet width of the $(211)_M$–$(112)_M$ line in the Fe–0.97C–6.3Mn steel is $10°$ [14]. There are other examples of the large width of the martensitic diffraction lines in the steels.

Thus, really there are sets of the c parameters in the martensitic crystal structure at the ordered state of the steels at given carbon concentration. Differences of the c parameters in the concrete steel are the result of the edge changes and distortions of the lattices because of installation of one C atom at one edge in some b.c.c. lattice and appearance of the blocks.

Value of the concrete c parameters depends on the number of the lattices blocks and the number of the lattices without C atoms for given carbon concentration in the steel. In the result, an intensity of the diffraction line of the given 'set' of the c edges depends on the number of the equally changed lattice edges and corresponding interplanar dis-

TABLE 6. Angular position of the diffraction line $(002)_M$ at different C concentration in steel, radiation $FeK\alpha$, $\lambda = 0.194$ nm.

c_M, nm	$\sin\varphi$	φ	$\Delta\varphi$	Note
0.362	0.5359	$32°26'$	$5°12'$	c_{max}
0.342	0.5673	$34°34'$		
0.322	0.6025	$37°04'$		
0.302	0.6424	$39°58'$		
0.292	0.6644	$41°38'$		
0.286	0.6783	$42°43'$	$5°5'$	$Fe_{\alpha'}$
0.319	0.6335	$37°38'$		$c_{average}$

tances; position of the concrete diffraction is determined by the interplanar spacing.

Agreement of the calculated and experimental diffraction line widths confirms proposed model of the crystal structure of martensite in the carbon steels as system of the lattice blocks with C atom on axes of the blocks and the lattices without carbon atoms around the blocks.

Thus, the martensitic lattice of the carbon steels cannot be tetragonal because arising during transformation lattice has different size of the edges and top angles not equal 90°. It may be determined as distorted tetragonal, pseudotetragonal or trigonal, and so-called degree of the tetragonality c/a is some mean value that does not characterizes the crystal structure of the martensitic phase in the carbon steels.

6. DISCUSSION

A number of the questions arises when consider the previously received results of the crystal structure investigations of the martensitic phase in the carbon steels. The first is to what extent the doublets of the diffraction lines, appearing on the x-ray diffraction patterns of the martensitic phase in the carbon steels, reflect tetragonality of the martensitic crystal structure. The second is what really stipulate large, 10−14°, diffraction lines width of the martensitic phase in the steels. In addition, the main question is next: how 3−8 at.% carbon (for example, in 50 b.c.c. lattice is 3−8 atoms C and 97−92 atoms Fe), placed in some octahedral pores of the bcc lattices (at the c edges) of the martensitic phase, can change these lattices to body-centred tetragonal?

However, beginning from the first investigations, the martensitic crystal structure of the carbon steels has accepted as tetragonal one and doubts about martensitic structure did not even arise although investigations of this structure have begun in the twenties of the last century and continue to date with different intensity.

Conclusion about tetragonality of the martensitic structure in the steels based on the result of an appearance of the doublets some diffraction lines in the x-ray patterns. However, it is known that during martensitic f.c.c. → b.c.c. transition carbon atoms locate at one edge only of some b.c.c. lattices and change these edges to the value $d_{Fe} + d_C = 0.5036$ nm (d_{Fe} and d_C are diameters of the iron and carbon atoms). Under real C concentration in steel quantity of the carbon atoms is not sufficient for situate in the whole lattices of the martensitic phase. Edges in the lattices without C atoms also change, but differently in dependence on the distance to the edge with C atom. In the result, the distorted lattices with different size edges and changed corner angles arise. It is not possible to call these distorted lattices as tetragonal lattice.

It has proposed to present the martensitic crystal structure of the carbon steels as system of the blocks, each consisting of four lattices

with carbon atom on common c edge, and distorted b.c.c. lattices near them, that did not contain C atoms [7, 8, 23]. This representation describes the real crystal structure of the martensite and diffraction observations quite well. In such lattice block common c edge with C atom has the largest size and is an axis of the block. This representation well explains also an appearance of the doublets of a number of the x-ray diffraction lines and great width of these lines.

The number of the blocks in the martensitic structure depends on the carbon concentration in steel. Under change of the C content from 0.22 to 0.6, 1.06 or 1.65 wt.%, the number of the carbon-free lattices around the block with C atom varies from 46 to 13, 6 or 2 lattices, respectively. In the lattices without carbon, c edges have different sizes and the greater the distance is from the edge with C atom the lesser these edges changed.

Conception of the carbon atoms ordering gives the possibility of better understanding of the martensitic crystal structure in the carbon steels [17, 18]. Experimental investigations confirm that C ordering really occurs and, depending on heat treatment and cooling rate, ordering of the carbon atoms in martensite of the steels or disordered state may occur [13, 21, 22]. Only under ordered arrangement of the C atoms, axes of the lattice's blocks are located in one direction $[001]_M$ and state arises that must be called pseudotetragonal (or trigonal). In the case of the disordered state of the C atoms, the axes of the blocks are situated randomly along all three directions [100], [010] or [001] of the b.c.c. lattice. In the result, pseudocubic structure of the martensitic phase observes.

Imaging of the crystal structure of the martensitic phase in the carbon steels as a system of the ordered lattices blocks and carbon-free lattices around them gives also good explanation of an appearance of the diffraction line doublets with large width ($12-14°$). In the structure with the blocks, there are some 'sets' of the lattice edges and corresponding interplanar distances. It is the result that not every lattice contains C atom and the lattice edges change differently in the dependence on the distance to the block axis. However, at each C concentration predominant 'sets' of the c edges with identical size and corresponding interplanar spacing arise that brings to maximum reflection intensity at the corresponding angles. In the result, the systems of the overlapping reflections appear. It brings to the broad diffraction lines. This description explains well x-ray patterns in the case of the ordering of the C atoms in martensite of the steels.

Some other process takes place under disordered arrangement of the C atoms in martensite. In this case, the axes of the lattice blocks situate arbitrary. Lattice edges have also different sizes, as in the case of the ordered state, but no predominant locations of the identical edges a, b or c observe. Edges situated arbitrary over a volume of the crystal. In this case, doublets of the diffraction lines do not appear and only line broadening observes.

In the case of the simultaneous presence of the lattice edges with $c_M = 0.362$ nm and $c_M = 0.286$ nm (and other intermediate c_M values) width of the diffraction line $(002)_M$ is $10°17'$ (Table 6). This value is in good coincidence with experimentally observed width $(10-12°)$ of this reflection.

Thus, imagine of the crystal structure of the martensitic phase as system of the blocks with C atom at their axes and distorted b.c.c. lattices without C atoms around the blocks allows well describe the real crystal structure of the martensitic phase in the carbon steels. This representation gives also a good possibility to explain an appearance of the diffraction doublets of some lines, great width of the diffraction lines and so-called cubic martensite in the steels.

7. CONCLUSIONS

1. Crystalline structure of martensite in the carbon steels at the real carbon concentration $0.1-1.7$ wt.% needs to present as a system of the lattices blocks with C atom on their axes surrounded by the lattices without C atoms. Carbon content in the steel determines the quantity of the blocks, spaces between them and the number of the lattices without C atoms around the blocks: the higher C concentration, the greater number of these blocks and the smaller amount of the lattices without C atoms. Crystal structure of the martensitic phase in the carbon steel may be determined as pseudotetragonal in the case of C atom ordering or as pseudocubic in the disordered state of the C atoms.
2. The magnitude of the c parameter in the case of the distorted lattice state is determined by the distance to the axes of the blocks with carbon atoms. The number of the equally changed c edges and value of the interplanar distances determine intensity of the corresponding diffraction lines.
3. Parameters of the crystal lattice of the martensitic phase in the carbon steels, using position of the diffraction maximums, are some averaged values and do not correspond to the parameters of the real crystal structure of martensite in the steels.
4. Block crystal structure of martensite in the carbon steels explains well an appearance of the static distortions during transformation.
5. The number of the lattices with changed c edges determines experimentally observed diffraction lines width of martensite in the carbon steels. Since martensitic lattice is not tetragonal, c/a ratio does not characterize the crystal structure of the martensitic phase. This ratio can use for an evaluation of the C concentration in the steels.

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