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On tetragonality of the martensite crystal lattice in steels

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Abstract

The paper addresses the pseudo-tetragonal nature of the crystal lattice of martensite in carbon-containing steels. It is proposed that the periodic distortion of *c* cube edges by the presence of carbon atoms is better reflected in the root mean square distortions of martensite lattice, than by the value of doublet splitting of the corresponding X-ray reflections of the martensite crystal.

Keywords: martensite, carbon-containing steels, lattice structure, tetragonality

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1. Introduction

Based on nearly hundred years of research, it is well known that martensite is formed in steels on quenching, due to the diffusionless $\gamma \rightarrow \alpha'$ phase transformation. Since the late 1920s, when it was independently reported by Fink and Campbell [1] and Seljakow et al. [2] that the lattice structure of quenched carbon steels is body centered tetragonal (bct), the relationship between the carbon content and the lattice parameters received continued attention both in experimental and modeling research. The original evidence for martensite (α′ phase) lattice tetragonality came from the splitting of (002) and (200) peaks [1,2] on X-ray diffractograms. It was established that *a* lattice parameter of martensite (0.285 nm with accuracy of 0.0003nm) is always smaller than *a* lattice parameter (0.286 nm) of ferrite (α-phase, body centered cubic, bcc). On the other hand, with an increase in carbon (C) content in the steel from 0.8 to 1.2 wt. %, the *c* lattice parameter of martensite increased from 0.291nm to 0.302 nm, corresponding c/a ratio change***s*** from 1.024 to 1.058. Due to an inability to resolve the diffraction doublets of the tetragonal lattice in steels having C content < 0.6 wt. %, it was assumed that the c/a ratio in low carbon steels was 1. It was concluded [2] that the coordinates of C atom were $00\frac{1}{2}$ in bct lattice, i.e. located along the tetragonal axis (c-axis). The observed tetragonality of martensite lattice was explained by a statistical theory of the ordering of carbon in one preferred sub-lattice, out of the three possible sub-lattices of octahedral interstices [3,4]. Such ordering is the result of the Bain strain, which changes during homogeneous shear transformation the austenite lattice to martensite one and positions carbon atoms located in the octahedral interstices of austenite lattice only in one out of three sub-lattices of a new lattice [5], e.g. all C atoms are located on *c*-axis. Another explanation was given by Önman [6] proposing that two C atoms with the axes of C_2 group parallel to the tetragonal axis of the lattice replace some of the iron atoms. Zener [3] suggested that ordering of C atoms exists above (or below) a critical C concentration (or temperature) at a definite temperature (or concentration). The resulting reduction in elastic energy due to ordering dominates the decrease in entropy, thus leading to a decrease, instead of an increase, in free energy. However, while the C atoms are ordered immediately on completion of austenite to martensite transformation, above the critical temperature for a specific C concentration, C atoms having a sufficient mobility tend to randomize converting the bct lattice to bcc. Based on Zeners' findings, the cubic-to-tetragonal transition at room temperature takes place at approximately 0.6 wt. % C content in iron. Kurdjumov and Khachaturyan [4,7] also arrived at a similar conclusion using a self-consistent theory of the order-disorder transition with static concentration waves and microscopic elasticity theory. Revision of their calculations of the elastic interaction energy resulted in the critical C concentration at room temperature being 0.18 wt.% [8,9]. Later on, this value for the cubic-to-tetragonal transition of first-order nature was confirmed by Fan et al. [10] using a long-wavelength approximation for the stress-induced elastic interaction in the theory of microscopic elasticity theory formulated by Khachaturyan [11].

Recently, using Rietveld refinement to deconvolute overlapping martensite peaks in data obtained from a high resolution X-ray diffractometer, it was shown that martensite lattice is bct for a steel with 0.124 wt. %C [12].Tetragonality of martensite lattice due to C atoms ordering is manifested in appearance of martensite peaks splitting on X-ray diffraction (XRD) patterns. Experimental evidence of disorder-order transitions was obtained by Kritzkaya et al. [13,14] via subjecting a carbon steel (1 wt. % C) to neutron and electron radiation, which led to the disappearance of martensite peak splitting in XRD patterns with the martensite lattice being indexed as bcc. Subsequent prolonged holding at room temperature resulted in the reappearance of martensite doublet peaks corresponding to a bct lattice. Such disordering $\leftrightarrow$ ordering transition was observed to take place repeatedly during several tests in the temperature interval from 293 K (20°C) to 228K (– 45°C). Furthermore, the martensite lines appear much less sharp compared to the austenite lines on XRD patterns. This was explained by Selyakov et al. [2] by (i) formation of small martensite crystallites;(ii) inhomogeneity in carbon distribution and (iii) tetragonality of the martensite lattice. However, even after prolonged homogenization treatment of Fe – (0.19-0.57) C – (5.50-9.18) Mn – (1.62-5.5) Ni (wt. %) alloy for 36 h at 1473.15 K (1200°C), the martensite lines remained diffuse [15]. In order to eliminate the effect of residual strain arising during martensite transformation in bulk, X-ray diffraction was carried out on Fe powder with (0.8-1.5) wt. % C, but still showed diffuse martensite lines [16]. Thus, it could be suggested that the diffusiveness of martensite lines on XRD patterns is also related to the martensite lattice tetragonality.

Furthermore, it could be supposed that this diffusiveness is related to the variations in the *a* and *c* lattice parameters in neighboring unit cells, e.g. a set of *a* and *c* parameters exists in the crystal structure of martensite.

The XRD collects data from cube planes of different length, which manifests in the diffuse appearance of martensite lines. It is well known that due to the diffusionless austenite to martensite transformation, only one C atom is located in an octahedral interstice along the cube edge (c-axis) in the martensite lattice. However, C atoms are absent on the other three cube edges, which are parallel to the c-axis. Thus, these three cube edges change their length to a lesser extent; the degree of change depends on the distance of a particular cube edge to the one distorted by the presence of C atom. Thus, such deformed crystal lattice could not be described as tetragonal, but rather as *pseudo-tetragonal.* The diffuse appearance of martensite lines is also supported by the studies of static lattice distortions resulting from martensite transformation in carbon steels [16,17]. The root mean square (RMS) displacement of Fe atoms along c-axis $\langle \bar{u}_{st}^2 \rangle^{1/2}$ is twice as large compared to the two other axes, i.e. 0.0052 nm versus 0.0025 nm, respectively [17]. The displacement depends on the separation between Fe and C atoms, which is the smallest along c-axis. Such a lattice is not thermodynamically stable; it is metastable. The pseudo-tetragonality observed by XRD is caused by strong elastic strains arising from the presence of interstitial C atoms in Fe lattice.

However, until now, it is accepted in both experimental and modelling works that the martensite lattice in carbon steels is bct [12,19-24]. Thus, the aim of this paper is to clarify the nature of martensite lattice, as C concentrations of 0.2-1.5 wt.% in steels are insufficient to form a proper bct lattice, and find out how the local distortions in crystal structure result in a regular change of *c* lattice parameter manifested as pseudo-tetragonality.

2. Lattice distortions in bcc Fe due to the presence of interstitial C atoms

2.1. Dependence of martensite lattice parameters on C concentration in carbon steels

The original equation for a linear relationship between the lattice tetragonality and C content was formulated according to Eq. 1 [22,23]:

$$c/a = 1 + 0.045 \text{ wt. \% C} \quad (1)$$

Another empirical relationship was proposed [15]:

$$c/a = 1 + 0.0467 \text{ wt. \% C} \quad (2)$$

On another hand, Cheng et al. [24] using 0.28664 nm as the lattice parameter of pure bcc-iron at 300 K (26.85°C) established the linear dependences of lattice tetragonality ratio (Eq.3) for the bct iron-carbon martensite *a* and *c* parameters; the latter were determined as functions of the number of interstitials per 100 iron atoms, X_C:

$$c/a = 1 + (0.95 \pm 0.01)\, X_C \quad (3)$$

This relationship was further modified to Eq. 4 [12]:

$$c/a = 1 + 0.031 \text{ wt. \% C} \quad (4)$$

A summary of the literature data on the variation of c/a ratio as a function of carbon content is given in Fig. 1. It is seen, that all experimental data fits reasonably well to linear relationships. Some deviations, as well as differences between the linear relationships, are related to the accuracy of measurements of lattice peaks positions and concentration of C atoms. It is seen that earlier data was available only for martensite of $\geq$ 0.6 wt.% C [6,15,22] due to the techniques limitations, whereas more recent one also covers 0.128-0.6 wt. % C range [12, 25]. It should be also noted that data from Ref. [25] is the theoretical one.

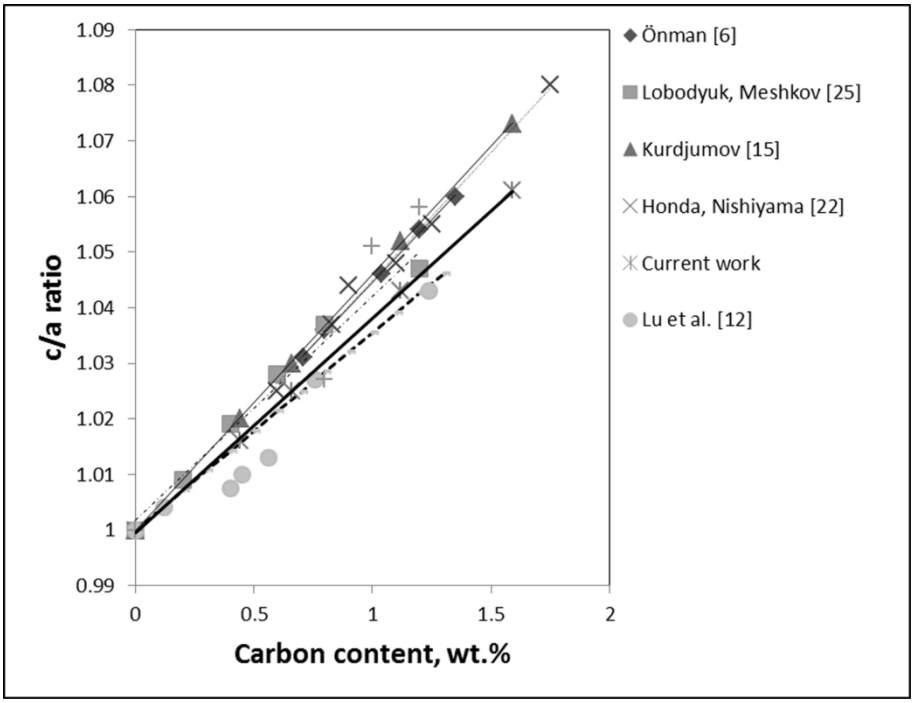

Fig. 1 Effect of carbon content in martensite on *c/a* ratio.

2.2. Distortion of bcc lattice in Fe due to interstitial C atoms

The high temperature phase of austenite contains C atoms in octahedral interstices located in the centre of face-centered cubic lattice. The lattice distortion of austenite is minimal in this case and a_γ lattice parameter increases as a function of C content in austenite according to Eq. 5 and Table 1 [25]:

$$\alpha_\gamma = 0.35586 + qp \quad (5)$$

where 0.35586 nm is austenite lattice parameter of pure Fe; p is the C content in austenite, wt. %, and q is a distortion of austenite lattice parameter due to addition of 1 wt. % C (Table 1): q = (0.0032 ± 0.0001) nm.

In two neighboring fcc lattices of austenite one body-centered tetragonal unit cell, bct, could also be identified as shown in Fig. 2a.

Thus, the lattice parameters of austenite could be expressed for both types of lattices as:

in fcc:

$$a_\gamma^c = b_\gamma^c = c_\gamma^c \quad (6)$$

and in bct*:*

$$c_\gamma^t = \sqrt{2}\, a_\gamma^t = \sqrt{2}\, b_\gamma^t \quad (7)$$

For pure Fe: $a_\gamma^c = b_\gamma^c = c_\gamma^c = 0.35586$ nm, whereas from Eq. 7 follows $a_\gamma^t = c_\gamma^t/\sqrt{2} = 0.2524$ nm.

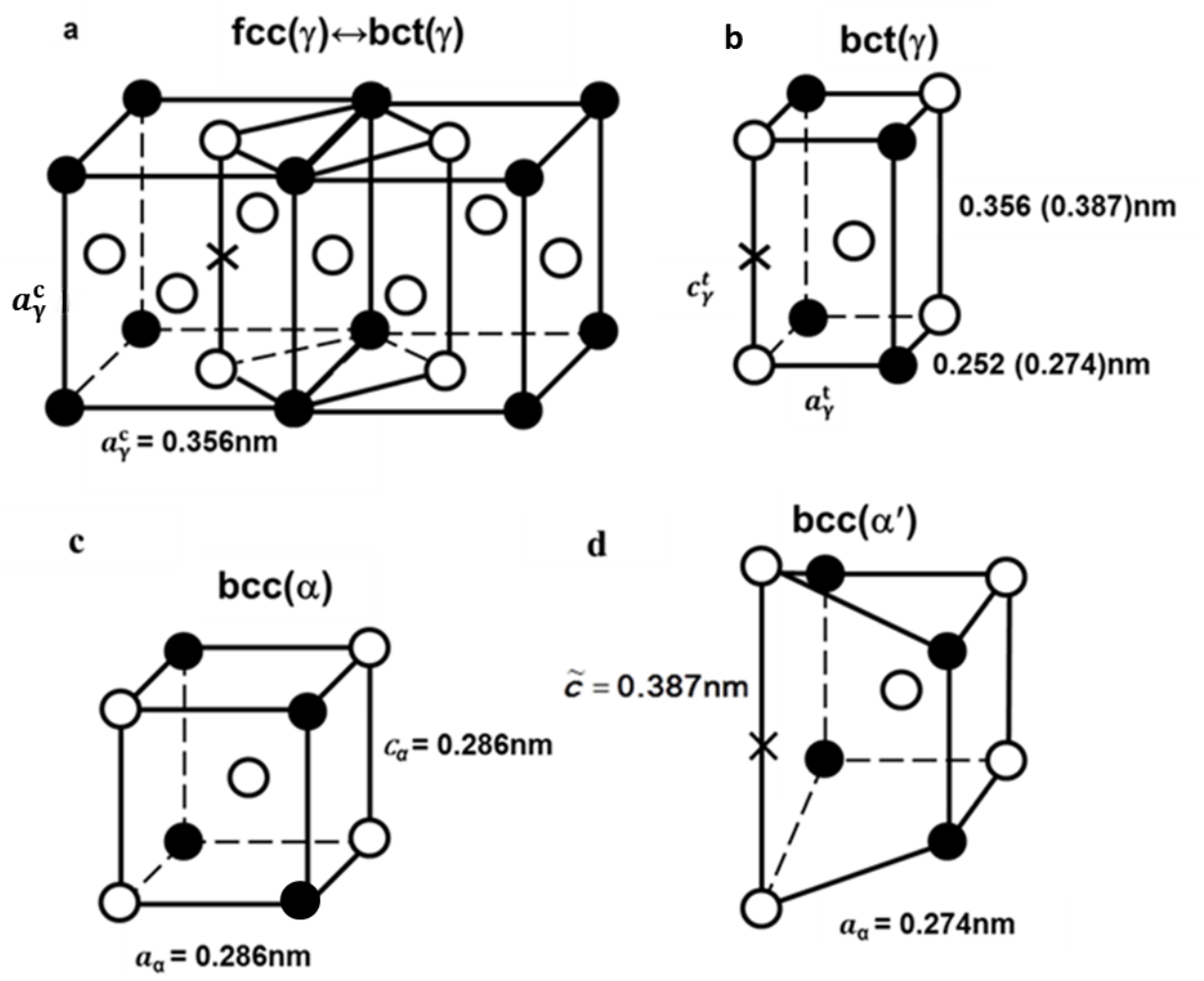

Fig. 2. Schematic representation of Fe crystal lattices*:*

a – The bct lattice of γ-Fe in two unit cells of fcc; ● – position of corner Fe atoms in fcc lattice; o – position of Fe atoms on the faces of fcc lattice; x – possible positions of C atoms.

b – The bct lattice of γ-Fe. Parameters are given for carbon-free Fe and in brackets for carbon-containing ones.

c – The bcc lattice of pure Fe after γ → α – transformation.

d – Distorted bcc Fe_α lattice, having *C* atom cube edge, $\tilde{c}$ (x – indicates the position of *C* atom).

For austenite with full occupancy of octachedral interstices by carbon (n_{at}= 33 *at*. %, *p* = 9.7 wt. %), these values according to Eq. 5 are: $a_\gamma^c = b_\gamma^c = c_\gamma^c = 0.3869$ nm; $c_\gamma^t = c_\gamma^c = 0.3869$ nm and $a_\gamma^t = c_\gamma^t/\sqrt{2} = 0.2744$ nm (see Fig. 2b).

When C atoms are located at the middle of cube edge of bct austenite lattice, the distance between the corresponding two Fe atoms increases, e.g. cube edge c_γ^t. In order to estimate this increase, the value of c_γ could be extrapolated using Eq. 5 for a such hypothetical C concentration in which one C atom is located at each one of four cube edges [25,26]. Calculations showed that in this case there are two Fe atoms and one C atom per bct unit cell; three atoms in total. The atomic concentration of carbon in such austenite is 1/3, which correlates to weight concentration *p* = 9.7 wt. % determined using the following Eq. 8:

$$p(\%) = \frac{12 n_{at}}{12\, n_{at} + 56(1 - n_{at})} \qquad (8)$$

where n_{at} is atomic concentration of carbon in steel, at. %.

At the same time, according to Eq. 5, c_γ^t = 0.38686 nm, e.g. the distance between two Fe atoms and C atom, inserted between them, should be ~0.387nm (Fig. 2d). During the $\gamma \rightarrow \alpha'$ transformation for a bct lattice to revert to a bcc lattice (Fig. 2c), the c axis is compressed and a and b axes are expanded uniformly as the result of Bain strain.

If one were to assume that following γ → α′ transformation during quenching the C atom remained in the same position relative to the Fe atoms, albeit in the distorted bct lattice of martensite (Fig.2d), then the c axis length would remain the same (c = 0.387nm). However, this cube edge containing C atom is extended compared to other three cube edges (in c-axis direction) which are free from carbon atom according to Eq. 9:

$$\frac{\tilde{c}}{a_\alpha} = \frac{0.387}{0.286} = 1.35 \quad (9)$$

Taking into account that the lattice parameter a_α in the martensite lattice decreases with increasing carbon concentration in steel [15], for the case when p = 9.7 wt. % and a_α = 0.274 nm the relative extension of edge cube $\tilde{c}$ (Eq. 9) would be ~ 1.41, which correlates to $\sqrt{2}$. Thus, the assumed maximum degree of tetragonality of the martensite lattice when carbon atoms are present on all cube edges parallel to c-axis is $\sqrt{2}$. However, as only one cube edge is occupied by a C atom, the experimentally determined martensite lattice tetragonality is well below $\sqrt{2}$. It also depends on the concentration of carbon, which determines the average number of cube edges containing C atoms. This dependence on the carbon content in steel can be modelled.

3. Model for calculation of the average value for the *c* parameter of martensite lattice.

Calculations were undertaken for a limited volume of martensite crystal having a square cross-section and one α'-phase lattice parameter thickness. This volume has the shape of compressed prism, for which the total number of Fe and C atoms always equals to 100 and where the Fe/C ratio changes according to the atomic concentration of carbon in the steel. Consequently, the number of unit lattices (and the number of cube edges c) decreases with an increase in the number of C atoms, as the number of Fe atoms forming the unit cell decreases. 100 Fe atoms form 50 unit lattices with one individual c cube edge each. However, in the Fe-33 at.% C alloy, there are 67 Fe atoms, which form only 33 unit lattices containing 33 cube edges of increased size $\tilde{c} = \sqrt{2}\,a$; the tetragonality of the lattice in such alloy is the maximum possible: $c/a = \sqrt{2}\,a$. In all alloys having an intermediate carbon content, the number m of increased cube edges $\tilde{c}$ will vary from 0 to 33 depending on carbon concentration (Table 2):

$$m = 100\,[1 - 0.5\,(1 - n_{at})] \quad (10)$$

where n_{at} is concentration C in at. %.

Depending on the carbon concentration in the martensite, the ratio of the fraction p of increased cube edges $\tilde{c}$ to the fraction s of regular cube edges with $c = a$, changes (Table 2). In the current model, the crystal of martensite is presented as a set of unit lattices of practically regular bcc lattice with lattice parameters $a = b \approx c$, among which a certain number of sets of four significantly distorted bcc lattices exists, which are combined in a single block with a common extended cube edge $c = \sqrt{2}\,a$ (Fig. 3b c.f. with 4 unit cells of ferrite shown in Fig. 3a).

Such a theoretical block of 4 bcc unit cells of Fe is the minimum volume of martensite crystal, in which the averaged tetragonality of the lattice could be expressed if were distributed uniformly among all four cube edges the anomalous extension of one common cube edge with $\tilde{c}$ = 1.41a:

$$\frac{\bar{c}}{a} = \frac{1.4a + 3a}{4} = 1.1 \quad (11)$$

Despite using such a rough approximation and ignoring any possible effects of anomalous cube edge exhibiting a $\tilde{c}$ length extension of other cube edges of the same block structure, as could be seen below, this approach is a reasonable one for explaining the physical basis for the pseudo-tetragonality of martensite lattice in quenched carbon steels observed using XRD. If one were to imagine the condition where the entire martensite crystal is formed only by blocks comprising such four unit cells, then the observed by XRD tetragonality should be $\overline{c}/a$ = 1.10. This condition (1 C atom + 8 Fe atoms) corresponds to the Fe-C alloy containing 11 at. % C (2.5 wt. % C). Thus, according to Eq. 2, c/a ratio is 1.12. It could be assumed that $c/a \approx 1.1$ (Eq. 11) is the maximum possible value which could be obtained experimentally for martensite pseudo-tetragonality for quenched-in martensite of this composition.

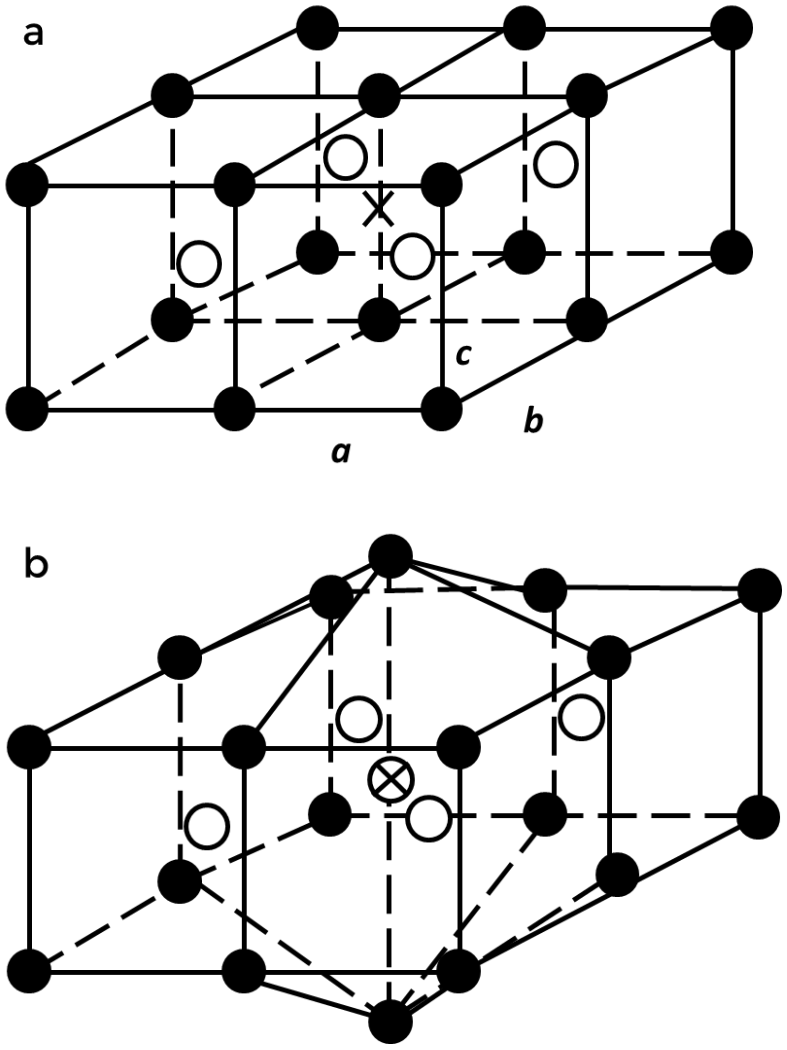

Fig. 3. Model of the block consisting of 4 lattice unit cells of:

a – α-phase, bcc, ferrite.

b –block containing one common extended cube edge $\tilde{c}$ due to the presence of C atom at the middle (average pseudo-tetragonality is $\overline{c}/a \approx 1.1$). x – indicates the position of C atom. ● – position of corner Fe atoms in *fcc* lattice; o – position of Fe atoms on the faces of *fcc* lattice; x – possible positions of C atoms.

Similarly, the averaging of all cube edges *c* for the lattice containing 100 (Fe + C) atoms could be performed for all different atomic concentrations of carbon (Table 2) and the corresponding averaged length of cube edge $\bar{c}$ could be calculated. These calculations resulted in the following relationship for averaged lattice pseudo-tetragonality and the atomic carbon concentration (Eq.12) and presented as data for this work in Fig. 1:

$$\frac{\bar{c}}{a} = 1 + 0.41p \qquad (12)$$

These calculations differ from the experimentally observed relationships (linear for Ref. [15], Fig. 1) by angle coefficient γ = 0.0467 from Eq. 2 [15], a difference of only 12 %. These lower theoretical values compared to XRD data could be due to not taking into account the effect of the extended cube edge $\tilde{c}$ on the length of neighboring C-free cube edges. The proposed model for explanation of averaged tetragonality of martensite lattice is reasonable as the error for determination of parameter $\bar{c}$ is ± 0.002 nm and for determination of *c*/*a* ratio it is less than 0.6 % (for Fe-1wt. % C alloy). It should be also noted that calculated data using this model (Fig. 1) is located between the old data determined in the 1930-70s and the more recent, refined results of Lu et al. [12].

4. Discussion

Proposed model is only a rough approximation, as further refinement and a better correlation with experimental data could be achieved by incorporation of the precise length of C-free cube edges neighboring the extended $\tilde{c} = \sqrt{2}$ *a* one.

The main outcome of the proposed model lies not in the good fit with experimental data, but in the suggestion that the crystal α′-lattice of quenched steel does not exhibit tetragonality by nature, but presents a system of regular bcc unit lattices of α-Fe with inclusions of special blocks of four distorted bcc unit lattices (Fig. 2b), the main characteristics of which is the presence in the middle of the block of one extended cube edge with $\tilde{c} = \sqrt{2}\,a$ length. The latter is responsible for the specific biconvex 'tent-shape' of the block (Fig. 3b). The average value of cube edges *c* in such 'tent' is approximately $\bar{c}/a \approx 1.1$a, which could be considered as a manifestation of the pseudo-tetragonality of α′-lattice block with c/*a*≈1.1.

Depending on the C content, the density of blocks increases leading to the observation of doublets of {101}, {002} (and others). For the last 80 years this has been explained as the averaged tetragonality of martensite α′-lattice dependent on C content, but which physically, in reality, does not exist. The averaged parameter $\bar{c}$ manifests in the appearance of diffraction doublets, whereas the variations from *c*=*a* to c=$\tilde{c}$ are reflected in the degree of widening of corresponding diffraction lines.

The physical reason for the experimentally observed pseudo-tetragonality of martensite lattice is ordering of carbon atoms in the Fe-lattice at the midpoint of selected cube edges. This leads to the extension of these cube edges ($\tilde{c}$) compared to the regular carbon-free ones ($c_\alpha = a_\alpha$). Reduction in the degree of C atom ordering along cube edges c_α and C content in steel leads to the decrease in the lattice pseudo-tetragonality ratio *c*/*a* and finally *to* formation of bcc martensite.

The crystal structure of the martensite lattice containing interstitial C atoms in the lattice should therefore be described as pseudo-tetragonal one. Appearance of this pseudo-tetragonality phenomenon is due to the statistical averaging of displacement of Fe atoms in α′-lattice. Static lattice distortion measurement using XRD suggests that the RMS displacements of atoms from their lattice positions ($\langle \bar{u}_{st}^2 \rangle^{1/2}$ are related to the variations in the length of cube edges *c* in α′-phase. For example, according to Ref. [18], the value for this RMS distortion of α′-phase lattice for martensite with 1wt. % C is 0.01nm. In this case, the interstitial C atom displaces Fe atoms on both sides of cube edge and therefore the RMS extension of the *c* is 0.02 nm. The average length of the extended cube edge is:

$\bar{c}$ = 0.286 + 0.02 = 0.306 nm (13)

From Eq. 13 follows:

$$\frac{\bar{c}}{a} = \frac{0.306}{0.286} = 1.07 \quad (14)$$

The experimental value of *c/a* (Eq. 2) for the same Fe-C alloy is 1.05. There is little advantage in trying to improve the prediction of the $\bar{c}/a$ value based on the RMS lattice distortions of α′-phase in quenched steel, as the high density of dislocations [4] in martensite also contributes to this term. This explains a higher $\bar{c}/a$ value obtained in Ref. [13].

5. Conclusions

1. It is reasonable to consider crystal structure of the martensite in carbon-containing steels as pseudo-tetragonal.

2. It is suggested that origin of the pseudo-tetragonality is result of the periodic distortion of *c* cube edges. This distortion is best represented by the RMS of the static distortions of the martensite lattice ($\langle \bar{u}_{st}^2 \rangle^{1/2}$) rather than by the value of doublet splitting of the corresponding X-ray reflections of the martensite crystal.

3. The small difference between the values obtained using both approaches is not important, as in both cases the assumed value of pseudo-tetragonality *c/a* does not reflect the real crystalline nature of martensite lattice and is simply an accepted term for lattice description.

4. The atomic-crystalline structure of martensite of carbon steel is best referred to as pseudo-tetragonal one (or "tetragonal-like") and distortions of the α′-lattice describe the average distortions, rather than represent a true tetragonality.

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Figure captions.

Fig. 1 Effect of carbon content in martensite on *c/a* ratio.

Fig. 2 Schematic representation of Fe crystal lattices*:*

a – The bct lattice of γ-Fe in two unit cells of fcc; ● – position of corner Fe atoms in fcc lattice; o – position of Fe atoms on the faces of fcc lattice; x – possible positions of C atoms.

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● – position of corner Fe atoms in *fcc* lattice; o – position of Fe atoms on the faces of *fcc* lattice; x – possible positions of C atoms.

Table 1. Effect of carbon content on lattice parameters in Fe-C alloys [25].

Phase	Carbon content, wt.%	Average number of atoms in the unit cell	Lattice parameters *a* and *c*, nm	Tetragonality, *c/a*
Ferrite, bcc	0	2.000	0.2861	1.00
Austenite, fcc	0	4.000	3.5586	
	0.2	4.037	3.5650	
	0.4	4.089	3.5714	
	0.6	4.156	3.5778	1.00
	0.8	4.224	3.5842	
	1.0	4.291	3.5906	
	1.4	4.427	3.6034	
Martensite	0	2.000	*a*= 0.2861	1.000
	0.2	2.018	*c* =0. 2861	1.009
	0.4	2.036	*a*= 0.2858	1.019
	0.6	2.056	*c* = 0.2885	1.028
	0.8	2.075	*a*= 0.2855	1.037
	1.2	2.094	*c*= 0.2908	1.047
	1.4	2.132	*a* =0.2852	1.065
			c = 0.2932	
			a=0. 2849	
			c= 0.2955	
			a= 0.2846	
			c=0.2979	
			a= 0.2840	
			c =0. 3026	

330 Table 2. Parameters for calculations of average value $\overline{c}_{\alpha'}$ for cube edge distorted by carbon atoms in martensite
331 lattice as a function of carbon content (per 100 atoms of Fe-C alloy)

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at.% C	wt.% *C*	Number of C atoms per 100 Fe-C atoms	Number of Fe atoms per 100 Fe-C atoms	Number of unit cells α-Fe	Total number of individual *c*-edges	Number of distorted edges $\tilde{c}$	Number of regular, non-distorted *c*- edges, s	Mean relative length of c-edge, $\overline{c}_{\alpha'}/a$	Tetragonality, Eq. 2 [15]
0	0	0	100	50	50	0	50	1.000	1.000
2	0.44	2	98	49	49	2	47	1.016	1.020
3	0.66	3	97	48	48	3	45	1.025	1.030
5	1.12	5	95	47	47	5	42	1.043	1.052
7	1.59	7	93	46	46	7	39	1.061	1.073
10	2.33	10	90	45	45	10	35	1.090	1.107
20	5.10	20	80	40	40	20	20	1.200	1.230
33	9.70	33	67	33	33	33	33	1.400	1.450

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