

PACS numbers: 61.05.cp, 61.50.Ks, 61.66.Dk, 61.72.Bb, 61.72.Dd, 61.72.S-, 81.30.Kf

## Broadening of the Martensite X-Ray Diffraction Lines of Carbon Steels

V. A. Lobodyuk

*G. V. Kurdyumov Institute for Metal Physics, N.A.S. of Ukraine,  
36 Academician Vernadsky Blvd.,  
UA-03142 Kyiv, Ukraine*

The explanation of the broadening of the x-ray diffraction lines of martensite and appearance of the doublets of the diffraction lines is proposed and is based on the representation of the crystal structure of martensite in carbon steels as a system of the lattice blocks with the C atoms on the axes of the blocks.

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

На основі уявлень про кристалічну структуру мартенситу вуглецевих криць як систему блоків із кристалічних ґратниць із атомом С на осі блоків дано пояснення розширення рентгенівських дифракційних ліній мартенситу та появи дублетів дифракційних ліній.

**Ключові слова:** вуглецева криця, мартенсит, кристалічна структура, ґратниця, блок, ширина дифракційної лінії.

*(Received 12 March, 2024; in final version, 9 April, 2024)*

The angular width of the x-ray diffraction lines of the martensite phase in carbon steels reaches 10–12° [1, 2]. Such large broadening of the diffraction lines of martensite in steels has been explained as follows. During transformation of the parent f.c.c.  $\gamma$ -phase into the b.c.t. martensite  $\alpha'$ -phase, large (micro)stresses arise, and the coherent domains of 30–

---

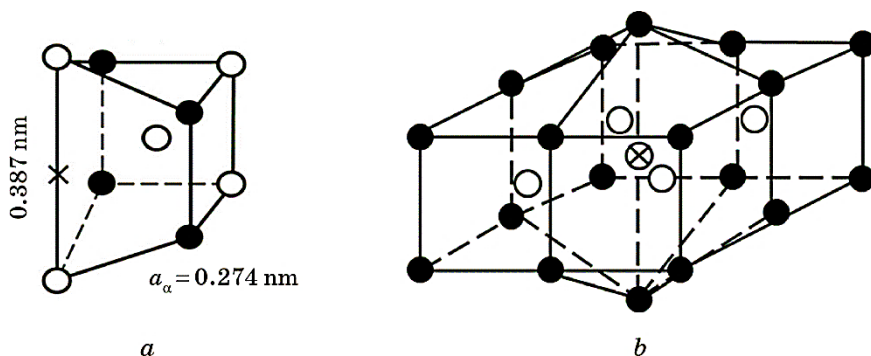
Corresponding author: Valentyn Andriyovych Lobodyuk  
E-mail: [lobodyuk@imp.kiev.ua](mailto:lobodyuk@imp.kiev.ua)

Citation: V. A. Lobodyuk, Broadening of the Martensite X-Ray Diffraction Lines of Carbon Steels, *Metallofiz. Noveishie Tekhnol.*, **46**, No. 6: 609–613 (2024). DOI: [10.15407/mfint.46.06.0609](https://doi.org/10.15407/mfint.46.06.0609)

150 nm in size appear. However, an x-ray study performed on the extracted martensite powders (1.0% wt. C steel) showed that, when an influence of the stresses is excluded, the diffraction lines still remain broad [3]. Thus, broadening of the x-ray lines may be caused by other reasons.

The crystalline structure of martensite in carbon steels has proposed to represent as system of the lattice blocks [4, 5]. Each block consists of four lattices with common edge (axis of the block), on which carbon atom is located (Fig. 1). Crystal lattices without C atoms are situated around the blocks. Within the blocks and around them, lattices have edges of the different dimensions and are distorted. The edge sizes depend on the distance to the axis of the block with the C atom. For example, the size of the edge  $c$  with carbon atom is  $c = d_{\text{Fe}} + d_{\text{C}} = 0.504$  nm, where  $d_{\text{Fe}}$  and  $d_{\text{C}}$  are the diameters of the iron and carbon atoms, respectively. The edge change decreases, when the distance to the axis of the block increases. The lattices with the dimensions of the edges of the b.c.c.  $\text{Fe}_\alpha$ -lattice have the smallest edge values.

The dimensions of the lattice edges were evaluated depending on the distance from the  $c$  edge with carbon atom for steel with 1.17% wt. C (5.26 at.% C) for martensite volume of 45 b.c.c. lattices, which includes 90 Fe atoms and 5 C atoms [5] (Table 1).



**Fig. 1.** Distorted b.c.c. lattice with C atom ( $\times$ ) at  $c$  edge (*a*); block of four distorted b.c.c. lattices with common enlarged edge (axis of the block), at which C atom is located ( $\otimes$  is C atom,  $\circ$ ,  $\bullet$  are Fe atoms) (*b*).

**TABLE 1.** Dimension and quantity of the lattice  $c$  edges after insertion of atom C at  $c$  edge.

Edge number	$c_1$	$c_2$	$c_3$	$c_4$
Edge size, nm	0.387	0.330	0.308	0.286
Quantity of the identical edges	5	30	20	20

Carbon concentration determines the number of the lattice blocks in steel. The maximal concentration of C in steel is of  $\cong 1.7\%$  wt. ( $\cong 8.16$  at.%), that is, for every 100 atoms, there are 92 iron atoms (which form 46 b.c.c. lattices) and 8 carbon atoms. Thus, carbon atom may be located only in every sixth lattice of the martensite-crystal structure and only at one lattice edge, in an octahedral pore.

Amount of the lattices without C atoms around one block depends on carbon concentration. This quantity changes from 46 to 6 and to 2 under carbon increase from 1 at.% (0.22% wt.) to 5 at.% (1.12% wt.) and to 8 at.% (1.79% wt.), accordingly [6]. It is necessary to note that the lattice with the C atom at one edge only is not tetragonal. It can be defined rather as distorted b.c.c. or distorted b.c.t. and, perhaps better, as trigonal, because the edges and angles at the lattice tops are different.

In the ordered state of the carbon atoms in steel, the axes of the lattice blocks are located mainly in one crystallographic direction  $[001]_M$ . Therefore, in the case of the crystalline structure with the blocks, the systems of the identical edges, which have the same interplanar distances  $d$ , appear. In this case, each widened reflection really consists of a set of separate overlapping reflections corresponding concrete edge size  $c$ .

Angular positions of the diffraction lines depend on the lattice parameter (interplanar distance  $d$ ). For example, the position of the  $(002)_M$  reflection for carbon steel changes from angle  $42^\circ 43'$  to angle  $32^\circ 26'$  in the interval of the lattice parameter  $c$  0.286–0.362 nm (Table 2). This corresponds really to changes of carbon concentration in steel from 0.2% wt. to 1.4% wt.

These values of the parameters  $c$  are closed to the lattice parameters  $c$  in the crystal structure of steel with the blocks (Table 1).

The general angular width of the  $(002)_M$  reflection for different  $c_M$  parameters may be about  $10^\circ$  (Table 2), and this value coincides with the width of the diffraction lines determined in many experimental studies.

**TABLE 2.** Angular position of the diffraction line  $(002)_M$  at different values of the lattice parameter  $c_M$  (radiation  $FeK_\alpha$ ,  $\lambda = 0.194$  nm).

$c_M$ , nm	$\sin \varphi$	$\varphi$	Note
0.362	0.5359	$32^\circ 26'$	$c_{max}$
0.342	0.567	$34^\circ 34'$	
0.322	0.602	$37^\circ 04'$	
0.302	0.642	$39^\circ 58'$	
0.292	0.664	$41^\circ 38'$	
0.286	0.678	$42^\circ 43'$	$c_{Fe\alpha'}$
0.319	0.633	$37^\circ 38'$	$c_{average}$

Therefore, for example, the angular width of the martensite line  $\{002\}_M$  in steel with 0.45% wt. C reaches  $12^\circ$  [2]; the width of the doublet line  $\{112\}_M$  in steel Fe-0.97 C-6.3 Mn (% wt.) is  $10^\circ$  [1]. Other examples of the great width of the martensite diffraction lines of steels can also be given.

Thus, under block crystal structure of the martensite in steels, there are the sets of the identical  $c$  parameters in the martensite crystal structure at given carbon concentration in the ordered state of the C atoms. These sets of the identical  $c$  parameters in concrete steel arise as the result of the different lattice distortions and the change of the lattice edges, when C atoms are introduced at one edge in the martensite b.c.c. lattices and the lattice blocks are appear in the result.

In the disordered arrangement, carbon atoms can be located at any edge of the lattice  $a$ ,  $b$ , or  $c$ , and axes of the blocks are located arbitrarily along the  $[100]_M$ ,  $[010]_M$  or  $[001]_M$  directions. In this case, the lattice edges have different sizes too, but there is no preferable arrangement of the edges  $a$ ,  $b$  or  $c$  of the equal size. As the result, doublets of the diffraction lines do not appear; only broadening of the x-ray lines is observed.

Representation of the crystal structure of the martensite phase in carbon steels as system of the ordered lattice blocks with carbon atom on  $c$  axis and lattices without C atom around them well explains the appearance of the doublets of the diffraction lines of large width. In the structure with blocks, there are several identical 'sets' of the lattice edges with corresponding interplanar distances. This is a result of the fact that not every lattice contains the C atom, and the lattice edges are changed differently, depending on the distance to the block axis. However, at concrete C concentration, there are predominant 'sets' of the edges of the equal size and interplanar spacing, that results in the corresponding intensities of the reflection and its width. As the result, the systems of the overlapping reflections in the diffraction doublets appear that brings to widening of the diffraction lines.

Thus, proposed description well explains the x-ray patterns in the case of the lattice block structure with ordered arrangement of the C atoms in the crystal structure of martensite of steels, namely, widening of the diffraction lines and appearance of the x-ray doublets.

**Conclusion.** Representation of the crystal structure of martensite in carbon steels as system of the lattice blocks with the C atoms at the axes of the blocks permits to explain well the widening of the x-ray diffraction lines of martensite and appearance of the doublets of the diffraction lines. In the martensite crystal structure in the ordered state of the C atoms, there are sets of the identical lattice edges. Each set in concrete carbon steel corresponds to definite value of the lattice parameter  $c$  and the diffraction angle. Collections of the differently changed  $c$  edges determine the width of the diffraction lines of marten-

site of carbon steels observed experimentally.

Collection of the differently changed lattice edges may arise also in the crystal structures of the b.c.c. metals under alloying by the atoms with the diameter that distinguishes strongly from the basic atoms. In the result, a broadening of the x-ray diffraction line may arise also in the alloys with interstitial atoms.

## REFERENCES

1. Yu. L. Alshevskiy, *Fiz. Met. Metalloved.*, **27**, No. 4: 716 (1969) (in Russian).
2. Y. Lu, H. Yu, and R. D. Sisson Jr., *Mater. Sci. Eng. A*, **700**, Iss. 5: 592 (2017).
3. M. P. Arbuzov, *DAN USSR*, **74**, No. 6: 1085 (1950) (in Russian).
4. V. A. Lobodyuk, Yu. Ya. Meshkov, and E. V. Pereloma, *Metallurg. Mater. Trans.*, **50**, No. 1: 97 (2019).
5. V. A. Lobodyuk and Yu. Ya. Meshkov, *Metallofiz. Noveishie Tekhnol.*, **42**, No. 1: 123 (2020) (in Russian).
6. V. A. Lobodyuk and Yu. Ya. Meshkov, *Metallofiz. Noveishie Tekhnol.*, **43**, No. 8: 1031 (2021).