МАТЕРИАЛОВЕДЕНИЕ И ТЕРМИЧЕСКАЯ ОБРАБОТКА МЕТАЛЛОВ

UDC 669.01 https://doi.org/10.18503/1995-2732-2019-17-2-49-54

TRANSFORMATIONS OF FINE STRUCTURE AND CARBON ATOMS DISTRIBUTION IN 100-M DIFFERENTIALLY HARDENED RAILS UNDER LONG TERM OPERATION

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Abstract. Using the methods of transmission electron microscopy, the authors of this paper show that the lamellar perlite grains, ferrite-perlite grains and structurally free ferrite grains constitute the main morphological components of category DT350 differentially hardened rails. The level of mechanical properties and the quality of steel rails comply with the Russian standard GOST R 51685-2013. The authors looked at the evolution of the carbide phase and the redistribution of carbon atoms in the surface layers of differentially hardened rails (the passed tonnage is 691.8 million tons) at the depth reaching 10 mm along the rail head centre line and the rail web. The authors found two complementary mechanisms of carbide phase transformation taking place in the surface layers when the rails are in operation: (1) cutting mechanism of cementite particles with the following departure in the bulk ferrite grains or plates (in the perlite structure); (2) cutting mechanism of cementite particles followed by their dissolution, transfer of carbon atoms onto dislocations (in Cottrell atmospheres and dislocation nuclei), transfer of carbon atoms by dislocations in the bulk ferrite grains (or plates) with the following repeated formation of nanosized cementite particles. The first mechanism stands for changing linear dimensions and morphology of carbide particles. The elemental composition of cementite does not see any significant changes. And the structural changes in the carbide can follow the second mechanism. The main cause of cementite dissolution is related to the energy of carbon atoms localized in dislocation nuclei and subgrains, which is higher compared with the cementite lattice. The binding energy 'carbon atom – dislocation' is 0.6 eV, and in cementite it can sometimes be 0.4 eV. It was found that the carbon atoms that stayed in the cementite lattice are located on the lattice defects, i.e. dislocations, grain and subgrain boundaries.
Keywords: Cementite, perlite, fraction, carbon atoms, rails, mechanisms, operation.

Introduction

The processes of formation and evolution of structural phase state and properties of rail surface layers under long service conditions represent a complicated complex of interrelated scientific and technical problems. The importance of information in this field is determined by the depth of understanding of fundamental problems of solid state physics, on the one hand, and the practical importance of the problem, on the other hand.

In the modern condition of high loads on axis and speeds of movement the rail surface layers undergo the severe plastic deformations under long service conditions resulting in the formation of structural phase states with atypically high microhardness and nanoscale grain sizes. In a relatively small number of papers [1–6] it is shown that already after the passed tonnage of 100–300 mln.t the cementite plates are either bent or fractured, and at the interphase boundaries the extremely high dislocation density is observed, cementite dissolution and austenite formation occur at the expense of the reverse $\gamma \rightarrow \alpha$ transformation [1–6]. These processes result in the redistribution of carbon and it is finally reflected on the level of mechanical properties [7–10].

As the mass production of 100m differentiatedly hardened rails began only 4 years ago in Russia, the determination of nature and evolution laws of carbide phase, fine structure and carbon atoms distribution in the head of these rails under long service conditions is of high priority and practical importance.

The majority of the used techniques of cementite phase evolution analysis lack the enough degree of locality. It does not permit to follow the evolution of the plate taken individually. Electron diffraction microscopy is the most developed method of aiming analysis of structural phase state of a material to date. This method enables to carry out simultaneously the complex analysis of the morphology and defect structure (the light field image method), phase composition (dark field method combined with imaging and indexing of electron-diffraction patterns) with the enough (for the problem being analyzed in the paper) degree of locality [11]. Carbon quantity in α- and γ – base solid solutions is usually estimated by the relative change in crystal lattice parameter of these phases [12]. The estimates of carbon quantity in carbide particles are made on the basis of the chemical composition of the carbide, the type of crystal lattice and the volume fraction of carbide phase particles in steel.

The purpose of the research is the determining and analyzing of the evolution mechanisms of carbide phase, fine structure and carbon atoms redistribution in rails under long service conditions by methods of layer-by-layer transmission electron diffraction microscopy [TEM] and X-ray phase analysis.

Materials and methods of study

The samples of differentiatedly hardened rails DT 350 manufactured at the joint stock company «EVRAZ–WSMC» after the passed tonnage of 691.8 mln. t brutto at the experimental ring JSC «VNIIZhT» were used as the test material. According to the classification given in the paper [13] it corresponds to the severe plastic deformation. In the content of all chemical elements revealed as a result of the verifying analysis of chemical composition of rails metal it satisfies the requirements of Russian Standard R 51685–2013.

The study of phase composition and defect substructure of rails were performed by methods of electron diffraction microscopy [14–19]. The test foils were manufactured by methods of electrolytic thinning of plates cut out by electric spark method at the distance of 0.2 and 10mm from the tread surface along the central axis and along the fillet **(Fig.1)**. The study of crystal lattice state was realized by method of X-ray phase analysis.

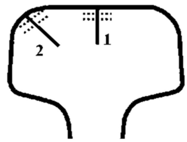

Fig.1 Diagram of rail sample preparation when studying its structure by methods of optical and electron diffraction microscopy. The solid lines designate the directions along the central axis (1) and the fillet (2); the dotted lines designate the sites of location of metal layers used for foils preparation (0,2 and 10mm from the surface)

Results and Discussion

The estimation of quality after long service conditions showed that by the level of mechanical properties **(Table 1)**, content by nonmetallic inclusions, macro- and microstructure the quality of metal satisfied the requirements of Russian Standard R 51685–2013 for rails of DT 350 category. The main morphological components of rail steel are the lamellar pearlite grains, the grains of ferrite-pearlite mixture and the grains of structurally – free ferrite.

The relative grain content of structurally – free ferrite amounted to 5% (note that the relative content of ferrite grains is practically independent of the distance to the tread surface) at 10 mm distance from tread surface; the grains of ferrite-carbide mixture – 5%; the balance - pearlite grains. At 2 mm distance from tread surface the relative content of grains of ferrite-carbide mixture increased by 10% in the surface layer (the layer adjacent to tread surface) it amounted to 35%. It is evident that these transformations of the structure were realized at the expense of fracture of lamellar pearlite grains. The studies of structural morphology of rails’ surface layer showed that the relative content of pearlite grains, where the lamellar structure retained, amounted to 25%; the balance – pearlite grains in which the cementite plates were cut into separately located particles by the sliding dislocations. These particles have the globular shape and their average sizes range within 30–50nm.

Two mechanisms of cementite plate fracture under deformation of pearlite structure steel are mainly discussed in scientific literature [20–28]. The first mechanism consists in the cutting of the plates by moving dislocations and carrying out the carbon atoms by them to ferrite to the field of stress dislocations. Estimations given in the research [20] show that in this case the maximum effect of cementite disintegration can not increase the tenth parts of a percent from the available quantity of cementite.

Table 1

Mechanical properties of rails after passed tonnage
of 691.8 mln.t

Material	Yield point, $\sigma_{0.2}$, N/mm^2	Ultimate strength, $\sigma_в$, N/mm^2	Elongation unit per length, δ, %	Contraction ratio, ψ, %	Impact toughness KCU at temperature +20^{o}C, J/cm^2
DT 350	820	1270	11.5	40	34
Requirements of Russian standard R 51685 – 2013 for DT 350 category rails not less	800	1180	9.0	25.0	15.0

The second mechanism consists in the pulling of carbon atoms by dislocations from the carbide phase lattice with the formation of Cottrell atmospheres due to the substantial difference of average energy of carbon atom bonds with dislocations (0.6eV) and atoms of iron in cementite lattice (0.4eV) in the plastic deformation process. The diffusion of carbon occurs in the stress field formed by dislocation substructure that is formed around cementite plates. In this case the degree of cementite disintegration must be determined by the value of dislocation density and the type of substructure. So, according to the author's opinion [20, 21] the model of cementite disintegration may be presented in the following way. The plastic deformation of pearlite steel causes the formation of cellular substructure with cell' boundaries located near the interphase boundary «cementite-ferrite». With the presence of thermodynamic stimulus (the bonding energy of carbon atoms with dislocations is higher than that with iron atoms in cementite) the carbon atoms, whose mobility is initiated by plastic deformation, are transferred from the cementite surface layers to the dislocations localized at the interphase boundary.

The first process occurring by the mechanism of carbide particles cutting and pulling their fragments apart is accompanied only by the change in their linear sizes and morphology **(Fig.2)**. The change in elemental composition of cementite in the process of fragmentation is minimal. During the occurrence of the second process (the action of the mechanism of dissolution «at the site») quite a different picture is observed. At the initial stage of transformation the cementite plates of pearlite colony are entangled by the sliding dislocations **(Fig.3)**. It is accompanied by breaking the cementite plates into separate weakly disoriented fragments. Then, with the increase in the degree of plastic deformation of the material the change in the carbide structure may occur due to the pulling of the carbon atoms out of cementite lattice.

The second transformation stage of cementite plates of pearlite colony being realized by the mechanism of dissolution at the site and consisting in the pulling the carbon atoms out the cementite crystal lattice is accompanied by the change in defect substructure of carbide that is caused by the penetration of sliding dislocations from the ferrite crystal lattice to the cementite crystal lattice **(Fig.4)**. Therefore, at this stage of cementite plates dissolution the interphase boundaries «α-phase / cementite» play a particular role. The coherent and half-coherent boundary [22] facilitate the penetration of dislocations from α-phase into cementite and inversely, and thereby it favours the fracture and dissolution of carbide. The large-angle incoherent interphase boundary stabilizes the carbide structure and leaves the possibility only for diffusion mass transfer. That is why the cementite plates in pearlite colony break down and the spherical particles of cementite retain at the boundaries of grains and subgrains.

The revealed quantitative regularities of change in the parameters of tread surface structure in the center of the head enabled us to analyze the carbon distribution in the structure of steel. The estimates concerning the content of carbon atoms on the structural elements of steel were made on the basic of the expressions generalized in **table 2**. The results of the estimates made are presented in **table 3**.

The estimates made showed that the operation of rail steel was accompanied by the essential redistribution of carbon atoms in the surface layer of rails. If in the initial state the main quantity of carbon atoms was concentrated in cementite particles then, after the operation of rails the site of carbon location, along with the cementite particles, was the crystal structure defects of steel (the dislocations, boundaries of grains and subgrains).

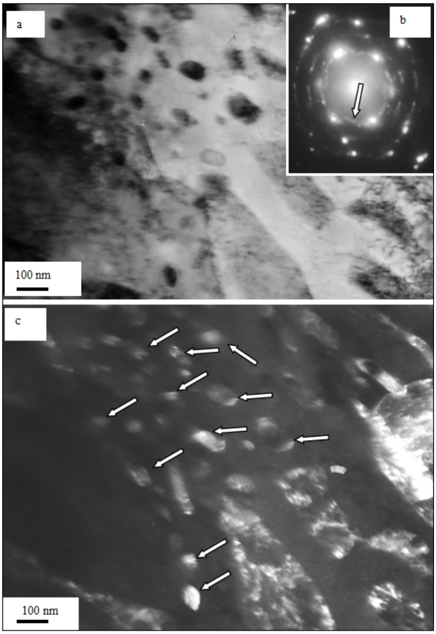

Fig.2 Electron microscopy image of tread surface structure
a – light field; b– microelectron of pattern; c – dark field obtained in reflection [012] Fe3C; in (b) the arrow designate the reflection of obtaining of dark field (c); in (c) cementite particles.

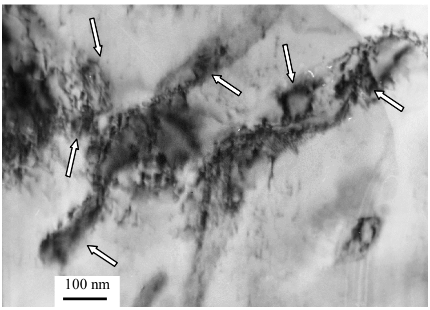

Fig.3 TEM image of pearlite colony structure being formed on dissolution of cementite plates by mechanism ‘at the site’; (the first stage of transformation process of cementite plates of pearlite colony). The arrows designate the frag-ments in cementite plates

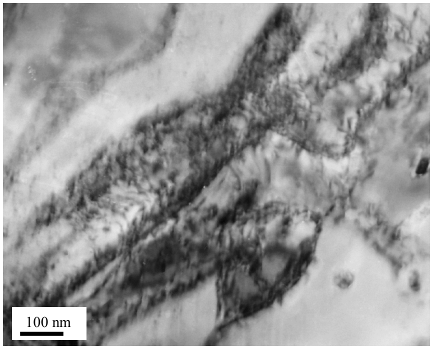

Fig.4 TEM image of the second stage of transformation process of cementite plates of pearlite colony being realized by mechanism ’at the site’

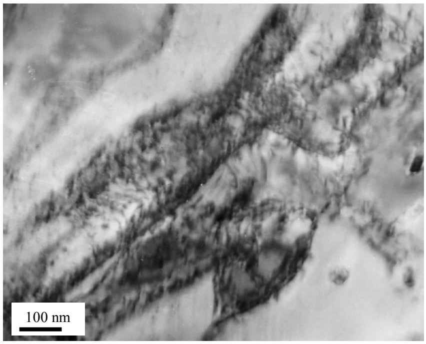

Fig.5 TEM image of the third stage of transformation process of cementite plates of pearlite colony being realized by mechanism of dissolution ’at the site’. The arrows designate the nanodimentional particles of carbide phase in the structure of cementite plates.

Table 2

Analysis method of carbon distribution in steel

Sites of carbon location	Estimate expressions	Literary source
α-iron base solid solution	$\Delta C_\alpha = \Delta V_\alpha \dfrac{a_\alpha - a_\alpha^0}{39 \pm 4} \cdot 10^3$ *	[32, 33, 34]
Particles of carbide phases	$\Delta C(Fe_3C) = 0{,}07 \cdot \Delta V_i$	[32, 14, 35]
Elements of defective structure	$\Delta C_d = C_0 - \Delta C_\alpha - \Delta C(Fe_3C)$	[32, 35]

*Here ΔV_α, ΔV_i – volume fraction α-Fe and carbide phases, respectively; a_α – present day parameter of α-phase lattice; a_α^0 = 0.28668 nm; a_α = 0.28782 nm; C_0 – average content of carbon in steel.

Table 3

Carbon distribution in rail steel structure after passed tonnage of 691.8 mln.t brutto

Structural elements	Carbon concentration, weight %		
	Surface	2 mm from the surface	10 mm from the surface
Cementite particles	0.33	0.71	0.75
α-Fe crystal lattice	0.0284	0.0	0.0
Defects of crystal structure	0.3816	0.03	0.0

Conclusion

By methods of modern physical material science the studies of structure, phase composition, defect substructure and redistribution of carbon atoms being formed at different distances along the central axis and the fillet in the head of 100-m differentiatedly hardened rails after long service were carried out and the fracture mechanisms of lamellar pearlite were analyzed. The structure of rail steel is presented by pearlite grains of lamellar morphology, and the grains of ferrite – carbide mixture and structurally free ferrite.

It is shown that the long service life of rails is accompanied by the occurrence of two processes of structural transformation and the phase composition of lamellar pearlite colonies simultaneously: (1) the cutting of cementite plates and (2) the dissolution of cementite plates. The first process being realized by the mechanism of carbide particles cutting and pulling of their fragments apart is accompanied only by the change in their linear sizes and morphology. The second process of cementite plates fracture of pearlite colonies is realized by the escape of carbon atoms from cementite crystal lattice to dislocations in consequence of which the phase transformation of rail metal is possible. It is noted that carbon atoms being leaved the cementite crystalline lattice are located at the defects of steel crystalline lattice (dislocations, grain and subgrain boundaries).

References

1. Ivanisenko Yu., Fecht H.J. Microstructure modification in the Surface Layers of Railway Rails and Wheels. Steel tech, 2008. Vol. 3, No. 1, pp. 19–23.
2. Ivanisenko Yu., Maclaren I., Sauvage X., Valiev R.Z., Fecht H.J. Shear-induced α→ γ transformation in nanoscale Fe–C composite. Acta Materialia. Vol. 54, pp. 1689–1669.
3. Ning Jiang-li, Courtois-Manara E., Kurmanaeva L., Ganeev A. V., Valiev R.Z., Kubel C., Ivanisenko Yu. Tensile properties and work hardening behaviors of ultrafine grained carbon steel and pure iron processed by warm high pressure torsion. Materials Science and Engineering A, 2013. Vol. 581, pp. 81–89.
4. Gavrilyuk V.G. Decomposition of cementite in pearlite steel due to plastic deformation. Materials Science and Engineering A, 2003. Vol. 345, pp. 81–89.
5. Li Y.J., Chai P., Bochers C., Westerkamp S., Goto S., Raabe D., Kirchheim R. Atomic-scale mechanisms of deformation-induced cementite decomposition in pearlite. Acta Materialia, 2011. Vol. 59, pp. 3965–3977.
6. Gavrilyuk V.G. Effect of interlamellar spacing on cementite dissolution during wire drawing of pearlitic steel wires. Scripta Materialia, 2001. Vol. 45, pp. 1469–1472.
7. Ivanisenko Yu., Fecht H.J. Microstructure modification in the Surface Layers of Railway Rails and Wheels. Steel tech, 2008. vol. 3, no. 1, pp.19–23.
8. Ivanisenko Yu., Maclaren I., Souvage X., Valiev R.Z., Fecht H.J. Shear-induced α→γ transformation in nanoscale Fe-C composite. Acta Materialia, 2006. Vol. 54, pp. 1659–1669.
9. Gavrilyuk V.G. Effect of interlamellar spacing on cementite dissolution during wire drawing of pearlitic steel wires. Scripta Materialia, 2001. Vol. 45, pp. 1469–1472.
10. Gromov V.E., Yuriev A.B., Morozov K.V., Ivanov Yu.F. Microstructure of quenched rails. Cambridge: CISP Ltd, 2016, 156 p.
11. Gromov V.E, Kozlov E.V, Bazaikin V.I. et al. Physics and mechanics of drawing and die forging. Moscow: Nedra, 1997, 293 p.
12. Lakhtin Yu.M. Physical metallurgy and thermal treatment of metals. Moscow: Metallurgiya, 1977, 407 p.
13. Glezer A.M. On the nature of ultrahigh plastic (megaplastic) strain. Bulletin of the Russian Academy of Sciences. Physics, 2007, vol. 71, no. 12, pp. 1722–1730.
14. Thomas G, Gorindge M.J. Transmission electron microscopy of materials. Moscow: Intekst, 1983, 320 p.
15. Hirsh P, Hovy A, Nicolson P. Electron microscopy of thin crystals. Moscow: Mir, 1968, 574 p.
16. Utevskii L.M. Deffraction electron microscopy in material science. Moscow: Metallurgiya, 1973, 584 p.
17. Ray F. Egerton Physical Principles of Electron Microscopy. An Introduction to TEM, SEM, and AEM. Berlin: Springer Science+Business Media, Inc, 2005, 211 p.
18. Kumar C.S.S.R. (Ed.) Transmission Electron Microscopy Characterization of Nanomaterials - New York: Springer, 2014, 717 p.
19. Barry Carter C., David B. Transmission Electron Microscopy. Berlin: Springer International Publishing, 2016, 518 p.
20. Gavrilyuk V.G., Gertsriken D.S., Polushkin Yu.A., Falchenko V.M. Mechanism of decomposition of cementite in the plastic deformation of steel. Fizika, 1981, vol. 51, no. 1, pp. 147–152.
21. Gridnev V.N, Gavrilyuk V.G. Cementite decomposition under plastic deformation of steel. Metallophizika, 1922, vol. 4, no. 3, pp. 74–87.
22. Male R.F, Hagel U.K. Austenite – pearlite transformation. *Uspehi fiziki metallov, V.3*. Moscow: Metallurgiya, 1960, pp. 88–156.
23. Belous Kh.V, Cherepin V.T. Changes in carbide phase of steel under the effect of cold plastic deformation. F.M.M., 1962, Vol. 14, No. 1, pp. 48–54.
24. Gavrilyuk V.G. Distribution of carbon in steel. Kiev: Naukova Dumka, 1987, 207 p.
25. Smirnov O.M, Lazarev V.A. Diffusion and redistribution of carbon in iron and its alloys in the process of deformation. FMM, 1983, Vol. 56, No. 1, pp.115–119.
26. Gromov V.E., Yuriev A.A., Ivanov Y.F., Glezer A.M., Konovalov S.V., Semin A.P., & Sundeev, R.V. Defect substructure change in 100-m differentially hardened rails in long-term operation. Materials Letters, 2017. Vol. 209, pp. 224–227.

27. Gromov V.E., Yuriev A.B., Morozov K.V., Ivanov Yu.F. Microstructure of quenched rails. Cambridge CISP Ltd, 2016, 157 p.
28. Ivanov Yu.F., Gromov V.E., Yuriev A.A. Metal structure and properties gradients of surface layers of differentially quenched rails after long term operation. Fundamental problems of modern material science, 2017, vol. 14, no. 3, pp. 297–305.
29. Ivanov Yu.F., Kornet E.V., Kozlov E.V., Gromov V.E. Hardened structural steel: structure and mechanisms of hardening. Novokuznetsk: SibSIU, 2010, 174 p.
30. Kalich D., Roberts E.M. On the distribution of carbon in martensite. Met. Trans, 1971, vol. 2, no. 10, pp. 2783–2790.
31. Fasiska E.J., Wagenblat H. Dilatation of alpha-iron by carbon. Transactions of the Metallurgical Society of AIME, 1967, vol. 239, no. 11, pp. 1818–1820.
32. Ivanov Yu.F., Popova N.A., Gladyshev S.A., Kozlov E.V. Interaction of carbon with defects and carbo-formation processes in structural steels. Collection of papers “Interaction of defects of crystal lattice and properties”. Tula: TulPI, 1986, pp. 100–105.

Received 07/11/18
Accepted 10/12/18

ИНФОРМАЦИЯ О СТАТЬЕ НА РУССКОМ

УДК 669.01 https://doi.org/10.18503/1995-2732-2019-17-2-49-54

ПРЕОБРАЗОВАНИЯ ТОНКОЙ СТРУКТУРЫ И РАСПРЕДЕЛЕНИЯ АТОМОВ УГЛЕРОДА В 100-М ДИФФЕРЕНЦИРОВАННО ЗАКАЛЕННЫХ РЕЛЬСАХ ПРИ ДЛИТЕЛЬНОЙ ЭКСПЛУАТАЦИИ

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Аннотация. Используя методы просвечивающей электронной микроскопии, показано, что зерна пластинчатого перлита, зерна феррито-перлитной смеси и зерна свободного феррита являются основными морфологическими составляющими дифференцированно закаленных рельсов категории ДТ350. Уровень механических свойств и качество стальных рельсов удовлетворяет требованиям ГОСТ Р 51685-2013. Изучена эволюция карбидной фазы и перераспределение атомов углерода в поверхностных слоях дифференцированно закаленных рельсов (пропущенный тоннаж 691,8 млн т) на глубине до 10 мм вдоль центральной оси и шейки головки рельса. Установлено действие двух взаимодополняющих механизмов трансформации карбидной фазы в поверхностных слоях стали при работе при эксплуатации рельсов: (1) режущий механизм частиц цементита с последующим перемещением в объем ферритных зерен или пластин (в структуре перлита); (2) режущий механизм и последующее растворение частиц цементита, перенос атомов углерода на дислокации (в атмосферах Коттрелла и дислокационных ядрах), перемещение дислокациями атомов углерода в объем ферритных зерен (или пластин) с последующим повторным образованием наноразмерных частиц цементита. Первый механизм сопровождается изменением линейных размеров и морфологии частиц карбида. Изменение элементного состава цементита не является существенным. Изменение структуры карбида может происходить по второму механизму. Основной причиной растворения цементита является энергетическое преимущество локализации атомов углерода в ядрах дислокаций и субзернах по сравнению с решеткой цементита. Энергия связи «атом углерода - дислокация» составляет 0,6 эВ, а в некоторых случаях в цементите она составляет 0,4 эВ. Установлено, что атомы углерода, оставшиеся в кристаллической решетке цементита, расположены на дефектах кристаллической решетки стали (дислокации, границы зерен и субзерен).

Ключевые слова: цементит, перлит, фракция, атомы углерода, рельсы, механизмы, эксплуатация.

Поступила 07.11.18
Принята в печать 10.12.18

For citation

Yuriev A.A., Gromov V.E., Grishunin V.A., Ivanov Yu.F., Qin R., Tang G., Konovalov S.V., Semin A.P. Transformations of fine structure and carbon atoms distribution in 100-m differentially hardened rails under long term operation. *Vestnik Magnitogorskogo Gosudarstvennogo Tekhnicheskogo Universiteta im. G.I. Nosova* [Vestnik of Nosov Magnitogorsk State Technical University]. 2019, vol. 17, no. 2, pp. 49–54. https://doi.org/10.18503/1995-2732-2019-17-2-49-54

Образец для цитирования

Yuriev A.A., Gromov V.E., Grishunin V.A., Ivanov Yu.F., Qin R., Tang G., Konovalov S.V., Semin A.P. Transformations of fine structure and carbon atoms distribution in 100-m differentially hardened rails under long term operation // Вестник Магнитогорского государственного технического университета им. Г.И. Носова. 2019. Т.17. №2. С. 49–54. https://doi.org/10.18503/1995-2732-2019-17-2-49-54