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Data Sets Formation on the Physical Properties of Oxide Scale Components for Theoretical Assessment of Efficiency Parameters of Laser Cleaning of Carbon Steels and Related Processes

O. G. Devoino[1)], **A. V. Gorbunov**[2)], **A. S. Lapkovsky**[1)], **N. I. Lutsko**[1)],
D. A. Shpackevitch[1)], **V. A. Gorbunova**[1)], **V. A. Koval**[1)]

[1)]Belarusian National Technical University (Minsk, Republic of Belarus),
[2)]Aeronautics Institute of Technology (Sao Jose dos Campos, Brazil)

Abstract. There is a need in machine-building industries nowadays to automate technologies, in particular, laser ones, to remove surface oxide layers – mill scale, rust – from steel products/pieces in order to improve the energy effectiveness of processing. Herewith, a theoretical assessment method for the intensity of heating of the oxide layer and the phase transition in it can be used to optimize laser cleaning (LC) of the steel surface. To realize this, it is possible to use some calculation and modeling procedures that require, as a first step, the data collection and verification on the temperature-dependent properties of iron-containing condensed phases, as possible components contained, in particular, in scale, which is typically widespread into various metal products. In this regard, the formation of database for characteristics of oxide scale components by the way of selection of information on thermophysical (including optical) properties of the components mentioned and of steel base, which are required for a reliable calculation of the thermal efficiency parameters of the technology for laser cleaning of carbon steels, as well as such actively developed related technologies as laser cutting, drilling, coating remelting, etc., was chosen as the task of our research. An analytical overview of published experimental data made it possible to systematize information on a number of transport and other physical properties of iron-containing components at ambient pressure, including thermal conductivity (κ) and diffusivity (a), density ρ, irradiation absorptance and integral emissivity in the temperature range from T ≈ 298 K to the melting temperatures of oxide and metal phases and above them. At the same time, a preliminary thermochemical estimation shows (on the calculated data) the existence of such thermodynamically stable forms of the condensed phase in the heating spot of scale layers during its LC at the melting point and above it, as Fe_3O_4, FeO, and Fe, which is consistent with known experimental data. Comparison of the values of a calculated by us (using the published values of κ, ρ and molar heat capacity and using extrapolation in the high-temperature region) for the types of scale components under consideration with a set of experimental values of this parameter in current literature revealed the presence of differences for both oxide and metal phases. These new values make it possible to fill in a gap in the temperature range T = 1600–1800 K that existed in the data on the thermal diffusivity. The value of $a = (0.83–0.92)\cdot 10^{-6}$ m^2/s was also calculated for liquid iron oxide for the $T \approx 1800$ K, which was not measured experimentally, that, obviously, prevented modeling of not only laser surface processing, melting and cleaning of steels, but also calculations in the field of metallurgical and other technologies, which are characterized by the presence of iron oxide melts during heating.

Keywords: laser processing, removal of surface oxide layers, mill scale, steel, iron(II) and iron(III) oxides, melting, evaporation, theoretical estimation, efficiency parameters, physical properties, thermal conductivity and diffusivity, absorptance, values comparison.

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Адрес для переписки
Горбунова Вера Алексеевна
Белорусский национальный технический университет
просп. Независимости, 67,
220013, г. Минск, Республика Беларусь
Тел.: +375 17 293-92-71
ecology@bntu.by

Address for correspondence
Gorbunova Vera A.
Belarusian National Technical University
67, Nezavisimosty Ave.,
220013, Minsk, Republic of Belarus
Tel.: +375 17 293-92-71
ecology@bntu.by

Формирование базы данных по физическим свойствам компонентов оксидной окалины для теоретической оценки эффективности лазерной очистки углеродистых сталей и родственных технологий

Докт. техн. наук, проф. О. Г. Девойно1), канд. техн. наук А. В. Горбунов2),
А. С. Лапковский1), Н. И. Луцко1), Д. А. Шпакевич1), канд. хим. наук, доц. В. А. Горбунова1),
канд. техн. наук, доц. В. А. Коваль1)

1)Белорусский национальный технический университет (Минск, Республика Беларусь),
2)Технологический институт аэронавтики (Сан-Жозе-дус-Кампус, Бразилия)

Реферат. В настоящее время в машиностроительных производствах имеется потребность в автоматизации технологий, в частности лазерных, для удаления оксидных слоев – окалины, ржавчины – со стальных изделий с целью улучшения энергоэффективности обработки. При этом можно использовать теоретическую оценку интенсивности нагрева оксидного слоя и фазового перехода в нем для оптимизации лазерной очистки (ЛО) поверхности стали. Для нее требуются специальный сбор и верификация данных по зависящим от температуры свойствам железосодержащих конденсированных фаз как возможных компонентов, содержащихся, в частности, в окалине, распространенной в металлоизделиях. В связи с этим в качестве задачи данной работы было принято формирование базы данных по характеристикам компонентов оксидной окалины путем подбора сведений по физическим свойствам ее компонентов и стальной основы, требующихся для надежного оценивания теплотехнических параметров эффективности технологии лазерной очистки углеродистых сталей, а также активно внедряемых родственных технологий – лазерной резки, сверления, оплавления покрытий и др. Аналитический обзор опубликованных экспериментальных данных позволил систематизировать сведения по ряду переносных и других свойств железосодержащих компонентов при атмосферном давлении в области от 298 К до температур плавления металлических и оксидных фаз и выше них. При этом предварительная расчетная термохимическая оценка показала существование таких термодинамически стабильных конденсированных фаз в пятне нагрева окалины при ее ЛО в точке плавления и выше, как Fe_3O_4, FeO и Fe, что согласуется и с известными опытными данными. Сравнение определенных нами (по опубликованным значениям κ, ρ и теплоемкости и с применением экстраполяции в высокотемпературной области) значений a для рассматриваемых видов компонентов окалины с набором имеющихся в современной литературе опытных велечин этого параметра выявило наличие отличий как для оксидных, так и металлических фаз. Новые значения заполняют пробел в области температур 1600–1800 К, имевшийся к данному моменту по температуропроводности. Также нами получено значение $a = (0{,}83–0{,}92) \cdot 10^{-6}$ м^2/с для расплава оксида двухвалентного железа при температуре $T \approx 1800$ К, не определявшееся ранее экспериментально, что мешало проведению корректного численного моделирования как лазерных процессов поверхностной термообработки, плавления и очистки сталей, так и расчетам в области металлургических и иных технологий, для которых характерно наличие зон с железооксидными расплавами в ходе нагрева.

Ключевые слова: лазерная обработка, удаление оксидных слоев, окалина, сталь, оксиды железа, плавление, испарение, теоретическая оценка, физические свойства, коэффициенты теплопроводности и температуропроводности, коэффициент поглощения излучения

Для цитирования: Формирование базы данных по физическим свойствам компонентов оксидной окалины для теоретической оценки эффективности лазерной очистки углеродистых сталей и родственных технологий / О. Г. Девойно [и др.] // *Наука и техника.* 2024. Т. 23, № 3. С. 192–203. https://doi.org/10.21122/2227-1031-2024-23-3-192-203

Introduction and research objective

Laser removal of surface layers of rust and scale (i. e. descaling), as a potentially highly effective and environmentally friendly method to clean corroded metal surfaces, has been actively studied in the last decade and is gradually being commercialized in machinery industry, shipbuilding, mining and other industrial sectors [1–6]. It begins to compete with mechanical methods traditional for metalworking for removing surface rust and scale from metal, primarily steel, billets and parts/products, including obtained by hot rolling, forging, etc. However, so far the effectiveness of a group of laser cleaning (LC) technologies is considered as dependent on the empirical skills of laser equipment operators in recognizing changes in the conditions for removing oxide contaminants associated with unstable cleaning modes and thermal defects of surfaces [1]. At the same time, factors influencing the mechanism of removal of oxide layers and the quality of removal complicate the monitoring and control of the process in real time during LC operations, especially when they use modern pulsed lasers with a high pulse frequency and improved power [2]. In this regard, experts note that there is currently a noticeable need for automation of technologies for the treatment of billets and products made of steels, in particular carbon ones, from contaminating layers – scale and rust (which are oxide inhomogeneous structures with significant porosity) – to prevent excessive cleaning time, which can give the undesirable effect of partial melting of the steel surface substrate which was already cleaned of oxidic substance and, as a result, negatively affect the energy consumption of the metalworking technological process as a whole [1, 6].

To implement this, it is advisable to use preliminary theoretical assessment (including calculation and modeling) of the intensity of melting and ablation of the oxide layers during heating to find optimal LC regimes of inhomogeneous crystalline structures on surface of structural carbon steels (SCSs). In this case, it is necessary to preliminary form and verify databases/datasets on the properties of Fe-containing condensed phases, as possible components contained, in particular, in mill scale and other scales that are widespread in industrial metal products and parts. A feature of these properties is their variability with changes in temperature, pressure, wavelength of laser irradiation (LI) and some other parameters [1–6, 15–16, 22]. Taking into account the aforementioned, as objective for our study the formation of data sets on the characteristics of the components of oxide scale was chosen, with selecting and comparing available information on thermophysical properties, including transport and optical ones, for its components and steel substrate (at atmospheric pressure, as typical for modern laser processing technologies), required for theoretical assessment and calculation of thermal parameters of laser processes for carbon steels cleaning, as well as for calculations of such commercialized group of related technologies as laser cutting and drilling of steels, remelting of sprayed iron-containing coatings, etc. [1–6, 15–16].

Brief characteristics of the analyzed cleaning process for scale layers and some thermochemical properties of thermostable phases in the conditions of typical oxidic scale

When analyzing and modeling processes for removing (laser or other) layers of mill scale and other scales from steel surface, it is advisable to take into account the features of the layer microstructure. It is known that typical processing scale that occurs on carbon steels (for example, during industrial hot rolling of billets in contact with air) contains up to three oxide sublayers with a composition depending on the conditions of scale formation, i. e. temperature conditions during rolling, etc. [5, 7], and often oxide phases, as a result of thermal diffusion, penetrate each other with the formation of heterogeneous layers of complex composition. In a simplified manner, it is generally accepted that in the scale of a number of steels (including carbon steels with a total iron content not lower than 97 wt.%, for which the fraction of oxides of alloying elements can be neglected) a sublayer of wüstite (FeO, often with cation-deficit crystalline sublattice in the oxide phase, that allows its composition to be more precisely written as $Fe_{1-x}O$ ($x \leq 0.06$)) is in a direct contact with metal substrate surface. The next sublayer contains predominantly the spinel phase of Fe_3O_4 (including Fe(II) and Fe(III) cations). The scale may also contain a third – an outer sublayer based on the hematite Fe_2O_3 (with Fe^{+3} cations). As has been found, scale formed on steel under heating conditions at temperatures higher than 850 K consists, as a rule, of the three indicated oxide sublayers of varied thickness [7]. According to some published data, the elemental composition of typical oxidic scale on SCSs (which can be approximately considered as a simulator of heated material in the LC-zone on the surface of non-corrosion-resistant metal products/parts) can be taken to approximately correspond to the brutto-formula Fe_3O_4, although in its phase composition it can contain mixtures of Fe_2O_3, Fe_3O_4, FeO and Fe [5–6].

According to our preliminary thermochemical estimation (using the thermodynamic approach previously used for high-temperature reactive mixtures, including metal-containing ones [8, 9]), as the thermodynamically stable forms of the condensed phase under laser heating conditions of typical scale (with a stoichiometry close to Fe_3O_4 oxide) at melting temperatures and above them such substances were recognized as Fe_3O_4 (solid) and FeO (liquid) oxides and metallic iron (in solid and liquid forms). This is consistent with known experimental data [5–7, 18–19, 21]. Tab. 1 summarizes some data on the previously published thermochemical properties of condensed components of the scale, which are thermally stable (as the results of our above-mentioned estimation show) under the conditions of approximately calculated reactive mixtures (oxidative and non-oxidative types) based on the oxide scale when heated to the temperatures of melting and boiling points of the scale components.

Approximate energy balance and equations of oxide layer heating kinetics for theoretical assessment of cleaning regimes with varied laser irradiation power. Selection of data on the physical properties of condensed (solid and liquid) components of oxide scale, their comparison

Let us write the energy balance equation for the steady process of laser descaling of a metal surface, taking into account heat losses to secondary heating processes (into solid and gaseous media surrounding the heated layer of oxide material, which is the target layer from the point of view of processing) and using the expression for the resulting total energy consumption for the cleaning process under the influence of irradiation as E_w (in units of J per 1 kg of heated material, i. e. oxidic scale):

$$E_w = Q_w + E_w(1 - A) + Q_{hl-1} + Q_{hl-2} = \frac{Q_w + Q_{hl-1} + Q_{hl-2}}{A}. \qquad (1)$$

In the equation (1), A is radiation absorptance of LI by surface of the material, averaged over the full temperature range of the LC-process. Energy consumption Q_w (in J/kg) for heating of removed scale layer from the initial temperature (~298 K) to the final one (taken for technological reasons, e.g. as the temperature of the point of complete evaporation of the layer), i. e. energy consumption only to the target process of scale layer heating – can be approximately evaluated by expressions that use the thermal effects of phase transitions and the heat consumption for heating to the temperatures before these transitions.

Table 1

Thermochemical properties of condensed components of scale (solid (s) and liquid (l)), which are thermodynamically stable in conditions of different reactive mixtures based on scale when heated to the points of complete melting T_m and boiling (evaporation) T_b of the components (with equilibrium composition); pressure P = 0.1 MPa

No	Parameter	Type of thermochemical system		
		Scale in oxidative medium	Scale in non-oxidative medium	Steel*
1	Composition on Fe-containing components (solid) near T_m, K	Fe_3O_4 (s)	Fe (s)	Fe (s) + Fe_3C (l) impurity
2	Composition on Fe-containing components (a priori liquid) near T_b, K	FeO (l) (or $Fe_{1-x}O$)	Fe (l)	Fe (l) + Fe_3C (l) impurity
3	T_m, K	1870	1809–1811	~1808 [5] (1500 for Fe_3C)
4	Theoretical enthalpy of melting (fusion) ΔH_m (†) [13], MJ/(kg of scale)	0.5843 (in MJ per kg of Fe_3O_4 – – 0.5960)	0.1754 (in MJ per kg of Fe – – 0.2473)	~0.1754 (and in MJ per kg of steel): ~0.2473 (SCS) [13] – 0.270 (◊) [74])
5	T_b, K (on published data)	3687	3133	3133
6	Theoretical enthalpy of vaporization ΔH_v (††)	3.24 MJ/kg of $Fe_{0.95}O$	6.34 – 6.367 MJ/kg of Fe	6.34 – 6.367 MJ/kg of Fe

* – unoxidized steel without scale; ‡ – in MJ per 1 kg of initial steel; ◊ – for structural carbon steel (SCS) of S235JR G2 grade (EU standard, it contains 0.063 % C, 0.41 % Mn, 0.13 % Si, 0.34 % Ni, 0.10 % Mo, 98.68 % Fe) [74]; † – for Fe-containing substance, which is thermodynamically stable under the given conditions at its melting point (per kg of initial scale (assuming its simplified composition)); †† – for Fe-containing substance, which is thermodynamically stable under given conditions at its boiling point according to the reference data on evaporation of iron and its oxide (wüstite) [59–61].

Conductive heat losses into the surrounding (quasi-cylindrical scale heating region) layers of materials – scale and steel substrate – are characterized by the following value:

$$Q_{hl\text{–}1} = f(a_{\mathrm{I}}, a_{\mathrm{II}}, T, t), \qquad (2)$$

and the heat losses into the "cold" gas area surrounding the scale heating zone via the convection-radiation mechanism is:

$$Q_{hl\text{–}2} = \mathrm{f}(\alpha, \varepsilon, T, t), \qquad (3)$$

where a_{I}, a_{II} are coefficients of thermal diffusivity of materials in the solid state (for the scale and for steel substrate, respectively); α – coefficient of convective heat transfer from the scale heated surface to the surrounding colder gas; ε – integral emissivity of the surface material, T – determining temperature of the heated surface, t – average heating time of the LI-spot area (i. e. the full exposure/duration of LI per the

The time spent for the heating, in particular, at the stage of phase transition (melting) t_m, can be determined from approximate expressions that were used, for example, in [15, 6] (this is kinetic dependence for the minimum time value and one more dependence, which includes theoretical enthalpy of melting ΔH_m). They contain such values as κ_{m}, a_m, A_m and ρ_{m} (i. e. is physical properties of the scale material at the melting temperature T_m): thermal conductivity, thermal diffusivity, LI absorptance and density, respectively.

A quite reliable engineering estimation for the intensity of heating under the conditions of laser processing technology can be carried out on the basis of simplified thermal model for regimes with varied irradiation power, by analogy with one previously used in calculations of systems for electron beam and laser melting of inorganic materials [11, 12], as well as the methodology, tested to model laser ablation of organic films [22]. In this case, a standard solution for the problem of heat diffusion in a semi-bounded body (i. e. in the scale in our case) with a second-type boundary condition (considered when modeling local heating of solids [10–12]) can be applied, using some revised thermophysical properties of iron oxides and steel substrate, given below (Tab. 2).

In many practical cases (including laser and electron beam processing of materials), the heat flux to the surface of a semi-bounded solid can be represented as a thin circular heat source with a uniform distribution of its intensity. In this case, we can consider a non-stationary axisymmetric problem of the influence of a continuous heat flow with constant intensity q, uniformly distributed within a circular region of radius R on the body surface. For a boundary-value problem (with mentioned boundary condition) to determine the temperature distribution $T(r, z, t)$ in a given type of half-space with an unsteady heat field, where the heating occurs from an external heat source constant in time, the following standard statement can be used [10, 11]:

$$a\Delta T = T_t(r \geq 0, z \geq 0, t > 0),$$

$$-\kappa T_z\,|_{z=0} = qH(t)\mathrm{H}(r - R),$$

$$T(r, z, 0) = T(\infty, z, t) = T(r, \infty, t) = T_r(0, z, t) = 0. \qquad (4)$$

The analytical solution of a two-dimensional parabolic problem for a non-stationary temperature field in heated half-space (with boundary condition of the second kind), suitable to simulate some solid materials [10], has the following form:

$$Q(\rho,\ x,\ \tau) = 0.5\int_0^{\infty}(J1(\lambda))\Big[\big(\exp(-\lambda x)\big)\mathrm{erfc}\times$$
$$\times\left(\frac{x}{2\tau^{0.5}} - \lambda\tau^{0.5}\right) - \big(\exp(-\lambda x)\big)\mathrm{erfc}\left(\frac{x}{2\tau^{0.5}} + \lambda\tau^{0.5}\right)\Big]\frac{d\lambda}{\lambda}. \qquad (5)$$

This equation contains the following nomenclature: J_0 and J_1 are Bessel functions (of the real argument) of zero and first order; erfc – complementary error function; λ – dummy variable [10]; thermal Fourier number for heat diffusion process $\mathrm{Fo} = \tau = (a{\cdot}t/R^2)$ [11]; a – coefficient of thermal diffusivity of the material (oxide scale in our case); t – time; R – radius of the heating zone (i. e., the LI-spot on the heated surface); dimensionless simplexes for the axial and radial coordinates (i. e., depth z and radius r coordinates of the laser beam spot on the surface) of the cylindrical heating region in the material: $x = z/R$ and $\rho = r/R$.

When solving an equation (5), one can find the values of several basic values that characterize the LC-process, including Fourier number for heat diffusion τ* and the corresponding heating time t^* required to melt the scale layer in the cylindrical zone (under the LI-spot) to complete depth of the layer, and the heat flux q^* required for the melting.

As mentioned above, to perform this kind of kinetic heating calculations, which make it possible to find the efficiency parameters of LC-process, data set on the properties of scale in various forms, depending on temperature and other factors, used in (4), (5) equations, is needed. We carried out a special review of published data on the thermophysical properties (including some transport and optical characteristics) of the phases, which exist in the layers of the metal oxide scale under consideration and at the boundary with them, that necessary both for calculations in laser cleaning technology and in related ones (e.g. cutting, drilling etc.). The results of the review are presented in Table 2.

A comparison of the values of the thermal diffusivity coefficient a calculated by us (based on the published values of κ, ρ and c_p, using extrapolation to the high-temperature region) for the seven types of scale components under consideration with the experimental values of this parameter available in modern literature (see rows 8 and 9 in the Tab. 2) shows the presence of certain differences for both oxidic and metallic phases, reaching for the solid phases such level as 50% and even higher. This extrapolation procedure allows us to fill the gap in the region T = 1600–1800 K, which currently exists in array of published data on the thermal diffusivity a of iron-containing phases. In addition, such new calculated range of a as $0.83 \cdot 10^{-6}$ to $0.92 \cdot 10^{-6}$ m^2/s was obtained for liquid FeO at ~1800 K (i. e. averaged value $a = (0.875 \pm 0.045) \cdot 10^{-6}$), which was absent in the literature, and this made it difficult until now to carry out correct modeling not only for laser-thermal processes, but for related metallurgical ones in devices with zones of fused FeO_x formation. It should be noted that, as we showed above, according to a preliminary thermochemical estimation, the thermodynamically stable forms of condensed phase under laser heating conditions of typical oxidic scale (with a stoichiometry close in Fe : O ratio to the Fe_3O_4 oxide) on carbon steels at melting temperatures and above them include only two oxides (Fe_3O_4, FeO) and metallic iron, which is consistent with known experimental data on the Fe-O-system chemistry [7, 18–19, 21, 46, 48].

Table 2

Thermophysical properties of iron-containing components for calculation of heating kinetics and efficiency parameters for laser cleaning of scale layers on carbon steel surface, given according to the published data [5, 13–58, 62–79] and on our extrapolation of these data to high temperatures; pressure P = 0.1 MPa

No	Properties	Crystalline solids					Liquid substances
		Iron (Fe)	Steel	Hematite Fe_2O_3	Magnetite Fe_3O_4	Wüstite $Fe_{1-x}O$ ($x \leq 0,06$)	FeO melt / iron melt
1	2	3	4	5	6	7	8
1	Melting point T_m, K (on published data)	1809 [14, 44], 1811 [13]	1808 [5] (Q345 SCS ♯)	1812 [13] – 1838 [5]	1870 [5, 13]	1642 [17]; 1644 [18, 19]	←
2	Boiling point T_b, K (on published data)	3133 [14]	3023 [5] (Q345)	2973 [5]	2896 [13], 3273 [5]	3687 [20–21]	←
3	Boiling point $T_{b\text{-}c}$, K (on calculated thermodynamic data for systems with different gases)	2460÷ 3300	–	–	–	3200÷3400	←
4	Thermal conductivity κ, W/(m·K)	78.48 [22] and 78.0 [24] (at 293 K); 35.0 (our extrapolation (extr.) of [24] data to the $T_m \approx 1810$ K); 8.0 (for Fe_3C) [55, 56]	~52.0 [5] (Q345), 49.8 [15, 16] (AISI 1095), 56.0 [80] (for low-carbon steels); 30.24 (for SCS at 1623 K) [70]; 27.3 (at the range of 1073–1473 K) and 37.5 (at $T \leq 1073$ K) for SCS [29]	4.0 [5], 0.58 [58]; 3.3 (our extr. of [24] data to the $T_m \approx$ ≈ 1810 K)	Decrease from 3.5 to 1.7 (in the range of 300÷676 K) [51], 2.0 [5]; 3.0 (our extr. of [24] data to the $T_m \approx$ ≈ 1870 K)	Rise from 1.8 to 2.5 (in the range of 300÷1164 K) [41] (FeO); 4.3 (our extr. of [24] data to the $T_m \approx$ ≈1640 K)	4.0 (it is extrapolation of author of [27] to the T = =1823 K) / 33.3÷34.4 (at T = = 1818–1868 K) [49] and 37.0–38.0 (at ~1830 K) [81], 39.1±2.5 (at T = = 1794–2050 K) [79], from 40.0 to 60.0 (calculation for the range of T from 2250 to ~3700 K) [83]; 36.5 (for SCS) [74, 75]

Continuation of the Table 2

1	2	3	4	5	6	7	8
5	Density ρ, kg/m^3	7874 (at 293 K) [13]; 7500 (estimation for δ-Fe for the range 1644 K < T < < 1809 K) [46]	7860 (at 300 K) [5] (for Q345 SCS) and [57] (for SCS with the carbon fraction of 0.08÷0.17 %)	4900 [57] and 5260 [58] (at 300 K); 4950 (our extr. of [23] data to the $T_m \approx 1810$ K)	5190 [51] и 5000 [57] (при 300 K); 4850 (our extr. of [23] data to the $T_m \approx$ ≈1870 K); for Fe_3O_4 melt – 4380÷3715 (at T from 1870 to 2900 K) [71]	5850÷ 6050 [41] (300 K, FeO); 5300 (our extr. of [23] data to the $T_m \approx$ ≈ 1640 K); 5587 (for FeO at T < 1644 K) [48]	~4600 (extrapolation to 1773 K) [28]; ~5079 (estimation of [46]); 4520÷ 3390 (at T from 1650 to 3400 K) [71] / 7015 (estimation for T > 1809 K) [46]; 7030 ($T \approx 1810$ K) and ~5974 ($T \approx 3000$ K) [63]; 7023÷6208 (for the range T = = 1810 ÷ 3133 K) [71]
6	Molar heat capacity c_p, J/(mol·K)	25.1 (for the α–δ-phase [13–14]) and 26.5 (for the γ-phase [14]) (at 300 K); 42.6 and 39.0 (at 1800 K for the α–δ-phase and γ-phase) [14]	440÷760 J/(kg·K) (for the range of 293÷873 K) and 650 J/(kg·K) at 1473 K [29]; ~920 J/ (kg·K) (at ~1800 K for Q345 SCS) [5]	104.2 (at 300 K); 145.8 (at 1800 K) [14]	147.7 (at 300 K); 200.8 (at 1800 K) [14]	49.97 (at T = 300 K); 64.03 (at T = 1600 K) [14]	68.20 (at T = = 1650–5000 K) for FeO [14] / 46.02 (at T = = 1809–3100 K) [14]; 45.4±3.2 (at T = 1848–1992 K) [79] and 45.1±3 (at $T_m \approx 1810$ K) [82]
7	Molar mass μ (on [14]), kg/mol	0.055845	~0.055	0.159688	0.231533	0.071844 (FeO); 0.06889 ($Fe_{0.947}O$ [42, 24])	0.071844 (FeO); 0.068886 ($Fe_{0.947}O$ [42]) / 0.055845
8	Thermal diffusivety a (♦), m^2/s (*10^6)	23.0 (at 300 K) [43], 22.06 (at 293 K) [22]	at 300 K – 19.0 (AISI 1010 SCS with 0.1 % C) [45] and 14,9÷15,1 (SCS with 0.17 % carbon fraction) [57]; at 300 K: 12.2, and at 1676 K: 6.02 (SCS with 0.135 % carbon fraction) [50]	at 293 K ~0.70 and at 1273 K – ~0.20 (sintered samples with 20 % porosity) [54, 57]	Decrease from 1.1 to 0.41 (for the range of 300÷676 K) [51]; at 293 K ~0.3÷0.42 and at 1273 K – ~0.40 (sintered samples with 30 % porosity) [54]	~0,3 – 1.4 (at ~300–500 K) [53–54] (at porosity of 42 % [54])); the rise from 0.37 to 0.58 (in the range of 300–1164 K) [41] (FeO); ~0.3 (1023 K) [51]; ~0.48 (300–870 K) – $Fe_{0.91}O$ [68]	– / 6.0÷6.5 (at 1818–1900 K) [49]
9	Calculated (by us) thermal diffusivity a (♦), m^2/s (·10^6), based on the given (in this Table) values of κ, ρ and c_p, presented in the references	at T = 300 K: 21.0–22.1; ~6.12 (at ~1800 K on the extrapolation data)	~7.19 (at ~1800 K for Q345 SCS)	~0.73 (at 1800 K – on the extrapolation data)	1.06 (at 300 K; ~0.713 (at 1800 K – on the extrapolation data)	0.42 (at 300 K; ~0.873 (at 1600 K on the extrapolation data)	0.92÷0.83 (at ~1800 K for FeO(l)) / ~5.76 (at ~1810 K) ÷ ~6.9 (at ~(1850–2000 K), with use of values of κ and c_p from [79])

Continuation of the Table 2

1	2	3	4	5	6	7	8
10	Absorptance (§) A at wavelength of LI $\lambda = 1064$ nm (or 1053 nm [30] (at $T \approx 300$ K))	0.36–0.363 [22]; 0.31–0.38 ($T \approx 300$ K) nd ~0.32 ($T \approx 1800$ K) [65]; 0.39 (for $T \approx 1800$ K) [63]	0.35 (◊) [5], 0.46 [15–16] (AISI 1095 †), 0.52 [30] (CR4 ‡) and 0.30 [34] (AISI 1006 ††); 0.30–0.36 ($T \approx 300$ K) and 0.31–0.32 ($T \approx 1270$ K) for steel of 35NCD16 grade (⁑) [65]; 0.35–0.38 (at $T \approx 1809$––3000 K) for SCS [64]	0.60 (◊) [5]; 0.69 [30, 32]	0.53 (◊) [5]; 0.80–0.83 [30, 33]	0.81 [30, 31]	For the oxide melt – from 0.56÷0.64 (at $T =$ = 1840–1900 K) to 0.66÷0.71 (at $T =$ 2100–2300 K) (and the drop of A in the range of $T > 2300$ K) [76] / 0.31 [62]; ~0.45÷0.49 [63]
11	Absorptance (§) A at wavelength of LI $\lambda = 527$ nm [30] (at $T \approx 300$ K)	~0.42 ($T \approx 300$ K) and ~0.44 ($T \approx$ ≈ 1800 K) [65]	0.67 [30] (CR4 steel)	0.97 [30, 32]	0.83 [30, 33]	0.80 [30, 31]	– / 0.48 [62]
12	Reflectance (§) R at wavelength of LI $\lambda = 1064$ nm (or 1053 nm [30] (at $T \approx 300$ K))	0.637–0.64 [22]; 0.69–0.62 ($T \approx 300$ K) and ~0.68 (at $T \approx$ ≈1800 K) [65]; 0.61 (at $T \approx$ ≈1800 K) [63]	0.65 [5], 0.54 [15, 16] (AISI 1095), 0.48 [30] (CR4) and 0.70 [34] (AISI 1006); 0.64–0.70 ($T \approx 300$ K) and 0.68–0.69 ($T \approx 1270$ K) for the 35NCD16 steel [65]; 0.65–0.62 ($T \approx 1809$–3000 K) for the SCS [64]	0.31 [30, 32]	0.17–0,20 [30, 33]	0.19 [30, 31]	for the oxide melt – from 0.36÷0.44 (at 1840–1900 K) to 0.29÷0.43 (at 2100–2300 K) [76] / ~0.69 [62]; ~0.51÷0.55 [63]
13	Reflectance (§) R at wavelength of LI $\lambda = 527$ nm [30] (at $T \approx 300$ K)	~0.58 ($T \approx$ ≈ 300 K) and ~0.56 ($T \approx 1800$ K) [65]	0.33 [30] (CR4)	0.03 [30, 52]	0.17 [30, 33]	0.20 [30, 31]	– / 0.52 [62]
14	Integral emissivity (IE) ε	0.35-0.36 (at $T =$ = 1672–1811 K) [52] (for the $\lambda = 650$ nm); 0.61 (at 1050 K) [37, 38]; ~0.35 (at ~300 K) [78]	0.35, 0.60 and 0.62 (at the values of $T = 348$ K, 1773 K and 3133 K, respectively) [34] (for AISI 1006); 0.61 (at 1050 K) [38]; ~0.45 (at $T \geq 1270$ K for $\lambda =$ = 1000–1500 nm for the SCS) [74]	0.626 (at 300 K) [69]; 0.75–0.85 (at 850–1300 K) [37, 39]; rise from 0.57 to 0.74 (for the range of 1100–1400 K for powder samples) [59]; 0.75–0.87 (at 740 K) and 0.64–0.83 (1220 K) – for	~0.61 (at 1050 K) [37, 38]; 0.85–0.89 (at 773÷1473 K for ~(Fe_3O_4 + + FeO)) [36, 67]	~0.61 (at 1050 K) [37, 38], 0.70 (at $T \geq 1000$ K) [35]	IE at $\lambda =$ = 600–1064 nm for the oxide melt: ~0.70 (at $T > 2000$ K) [73, 77], / 0.35 (at 1810 K) [37, 40] and 0.314 (at $T_m \approx 1810$ K) [82]; normal spectral emissivety – 0.3–0.44 (at 1810–1970 K) [47] (for the $\lambda = 650$ nm), 0.362 (at 1811 K

End of Table 2

1	2	3	4	5	6	7	8
				powder samples [66]			for the λ = = 684 nm) and 0.38 (2300 K for the λ = = 684 nm) [52]; IE for λ = = 650–850 nm for the melt of S235 SCS (⁝) 0.35÷ 0.095 (at the range of 1810÷2100 K) [72]

§ – as a rule, in the direction of irradiation normal to the surface; ♦ – values are given for materials assuming their near-zero porosity; ◊ – values of *A*-parameter in [5] are taken for the conditions of LI-absorption with a wavelength λ = 1064 nm [26]; † – structural carbon steel (SCS) of AISI 1095 – composed of 98.4–98.8 % Fe, 0.3–0.5 % Mn and 0.9–1.03 % C (analogues in the Russian Federation (RF) and CIS – У8 and У10 steels); †† – AISI 1006 SCS – composed of 99.4–99.7 % Fe, 0.25–0.4 % Mn and 0.08 % C (analogue in the RF – 05кп steel); ‡ – CR4 SCS – composed of 99 % Fe, 0.6 % Mn and 0.1% C (analogue in the RF – 08Ю steel); ♯ – Q345 SCS (standard of China, it contains 0.21 % C, 0.96 % Mn, 0.12 % Si and up to 98.5 % Fe) – analogues in the RF – 09Г2, 09Г2С, 10Г2Б; ⁑ – low-alloyed structural steel of 35NCD16 grade (French standard, it contains up to 0.4 % C, up to 0.6 % Mn, up to 0.4% Si, up to 2.0 % Cr, up to 4.2 % Ni, up to 0.6 % Mo) – analogue in the RF – 40Х2Н4МА grade; ⁝ – S235 SCS (EU standard, it contains up to 0.20 % C, up to 1.40 % Mn and up to 98 % Fe; analogue in the RF is the steel of Ст3сп grade).

CONCLUSIONS

1. In order to form the data sets on a number of industrially significant characteristics of oxide scale components, a detailed review and selection of published experimental information were carried out on the group of physical properties (including transport and optical) of iron oxides and steel base (at a pressure of 0.1 MPa), required for theoretical assessment of thermal technical parameters of the efficiency of laser cleaning technology for carbon steels, as well as related technologies, using calculation methods. Information on the properties of iron-containing components, including density, coefficients of thermal conductivity and thermal diffusivity (a), optical absorptance and emissivity in the temperature range from $T = 298$ K to the melting points of oxide and metal phases and above them, was systematized. According to a preliminary estimation, Fe_3O_4, FeO, and metallic iron belong to the thermodynamically stable condensed phases under conditions of laser heating of a typical mill scale (with integral stoichiometry close to Fe_3O_4 oxide) at melting temperatures and above them, which is consistent with empirical data.

2. Comparison of the values of the coefficient a for thermodynamically stable scale components, which were calculated using currently known values values of κ, ρ and heat capacity and using additional extrapolation of properties to the high-temperature range, with a set of experimental values of this a parameter available in the literature showed certain differences for both oxide and metallic phases. These values make it possible to fill in the existing gap in the $T = 1600–1800$ K region in the data set on thermal diffusivity of the phases. A calculated value $a = (0.83–0.92)\cdot10^{-6}$ m^2/s was obtained for Fe(II) oxide for temperature above the melting boundary $T \approx 1800$ K, which was not measured before, which limited the opportunities not only for modeling surface laser heat treatment and cleaning of steels, but also made it difficult to calculate the kinetic data in the field of metallurgical and related processes and apparatuses in which some zones exist with iron oxide melts during the heating of steel, cast iron and their partial oxidation products.

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