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MECHANISMS OF CARBIDE FARMATION OF IRON AT THERMOCATALYTIC DISINTEGRATION OF CARBON MONOOXIDE

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A state of the-art review generalization and critically analysis of before accumulated research material by the mechanism of formation carbide at thermocatalytic in the thermal catalytic decomposition of carbon monoxide have been presented. It is established that as catalysts for thermal catalytic decomposition of carbon monoxide is necessary to use the oxides of metals for group of iron; recovery of iron should be performed at low temperatures in mixtures of CO-H_2; carburization process flow can take place simultaneously with the recovery process; the source and center of crystallization for free carbon in a certain temperature range are carbides metal catalyst, adsorption catalyst theory can explain some laws governing of the process, but it is not thorough.

Keywords: iron, monoxide carbon, catalyst, thermocatalytic decomposition, carbide

The reaction of thermocatalytic disintegration of carbon monooxide on metallic catalysts a long ago comes into the notice of researchers large possibility of receipt of wide nomenclature of cheap enough and necessary in an industrial plan production. However, taking into account the difficult mechanism of co-operation in the system *Fe-O-C-H*, she so not found the real use in a large-scale production.

In spite of plenty of experimental material, mechanism of formation of carbides of iron at thermocatalytic disintegration of carbonbearing gases yet finally not set.

The first clearly formed presentations about mechanism of carbon farmatiun of iron are expounded in-process B.A.Apaev [1], in which exposed to the analysis, both processes of vacation of carbon steels and co-operations of hydrocarbons with iron. The existent models of formation of carbides an author subdivided into three groups, at the number of the stages of forming for cementite. Offered approach allowed to generalize the charts of formation carbon only, mainly, at vacation of steels, however mechanisms, and, main, ratio of this difficult process yet were not studied enough.

L.N. Rudenko and S.T. Rostovtsev [2] pulled out the mechanism of direct co-operation of carbon monooxide and iron: disintegration carbon monooxide on a ferrous catalyst appears as two stages - activated adsorption of carbon monooxide on the surface of catalyst and moving away of oxygen of adsorption complex by other molecule of monooxide carbon.

Forming of structure of $Fe_{cryst}C_{cryst}$ type is one of maiden attempts to explain appearance of certain connection, which is such to carbide of unknown composition.

M.S. Kurchatov [3] offered other mechanism of disintegration monooxide carbon and formations of carbides. Chemosorption monooxide carbon on Fe_2O_3 passes on an adsorption-catalytic mechanism with formation of layer of type $Me = C = O$, which is similar to the structure of carbonyls for metals. Originally it is the activated adsorption, at which molecule monooxide carbon, inculcated in the crystalline grate of oxide, join to the knots of the extended grate that allows to provide forming of карбонильного complex, thus connection of ions of oxygen with a center near which a complex is formed weakens here.

Facts about kinetics of carburizing for iron authors [4] made attempt to explain from position of diffusive-kinetic theory of heterogeneous processes. The acceleration of process after the satiation of surface of sample marked in experiments confirms the leading role of carbides or iron, saturated by a carbon at the catalysis of reaction for disintegration of carbon monooxide.

Most full and in detail mechanism of thermocatalic disintegration for carbon mono-oxide and conditions of formation of carbides by V.V. Rukin and other [6] is generalized. At thermocatalytic disintegration of molecule monooxide carbon on the surface of iron the initial stage of process can be described by a chart:

$$CO_{gas} + Fe_{cryst} \Rightarrow Fe_{cryst}\left(CO\right)_{ads} \tag{1}$$

Subsequent stage of disintegration of monooxide carbon related with co-operating of gaseous molecule CO by oxygen of adsorption complex:

$$Fe_{cryst}\left(CO\right)_{ads} + CO \Rightarrow \left[Fe - C\right]_{sol} + CO_2 \ , \tag{2}$$

including also formation of solutions of ferrite the iron-carbon or austenite saturated by a carbon:

$$\left[Fe - C\right]_{sol} + C \Rightarrow \left[Fe - C\right]_{sol.sat\,C} \, . \tag{3}$$

The quantum-chemical analysis of co-operation in the system *Me-C-O-H* allowed to formulate in-process [8] single appropriate base, describing the processes of renewal and carburizing of metals for group of iron at their co-operating with the carbon monooxide.

To basis of the offered mechanism of co-operation in the system *FeO-CO* is fixed hypothesis of formation on the metallic (fresh reduced) surface of intermediate complexes as a result of co-operating of molecule of carbon monooxide with action of iron at credible participation of hydrogen.

At accordance with classification, resulted in-process [9], possibility of two ways of renewal of monooxide of iron by gas agents is assumed these:

– dissociative (fine) for high-spin complexes, formally flowing as oxidization of carbon monooxide;

– associative activated synchronous exchange of ligands by electronic pair through a coordinating center for lowspined complexes.

If the monooxide of carbon reacts with iron in the metallic (but not oxide) state, then because of his monogentallity trade-out by an electronic closeness much less intensive and obviously unsuffice for the break of carbon-oxygen connection, especially as in the real terms of adsorption on a metallic surface, especially fresh reduced, to formation of multiple connection with a molecule CO there are competitive, often more power advantageous variants.

Conclusions. From all offered charts only the adsorption-catalytic is in one or another measure able high-quality to explain some conformities to law of process, but also she is contradictory. Basic contradiction is caused by supposition about the considerable ratching of *C-O* at the chemosorption of molecule, that not confirmed by the results of the special researches.

Nevertheless, the got theoretical results help correctly to comprehend numerous kinetic facts and bases of mechanism co-operations, generalized both within the framework of the real work and present in the special literature, and in the end – to find the most rational methods and receptions of adjusting of processes of renewal and carburizing of iron, but however give the complete and final picture of mechanism of this difficult co-operation.

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