

DOI 10.26886/2414-634X.3(22)2018.4

UDC 691.327

SYSTEMIC, STRUCTURAL ORGANIZATION OF FUNCTIONS OF CEMENT – ENERGY CARRIER

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The electronic structure and build of atoms determine the electronic structure and build of all minerals and grains of cement. The main property of an atom is the value of the charge of its nucleus. It determines the charge of the grains and, in total, the energy capacity of cement. An indicator of the cement capacity is given. Cement is presented as an accumulator of the energy of charges, and a transmitter of it. Knowledge of the electrical and thermodynamic properties of the main atoms and minerals of cement will allow to regulate its capacity and the given electronic structure and formation of concrete.

Key words: system organization, atom, mineral, grain, cement, concrete, properties

Resource and energy intensity in the cement industry causes an urgent need to find ways to reduce it by changing the technological cycles of cement production.

In order to reduce the prime cost of cement, due to the reduction in its clinker content and its provision with the necessary building and technical properties, multicomponent cements are increasingly used, which are obtained by grinding portlandcement clinker and mineral additives of various types.

The main minerals and grains of cement consist of a sum of atoms, different in their nature, activity, mass and significance in ensuring the quality of the final product.

The way of solving the main chemical and physical problems, in the interaction of atoms and in the creation of concrete with given properties, which appears to be effective – the evaluation and accounting of the energy capacity of cement. Selecting an appropriate atomic composition will determine the technology and longevity of products and structures. This is all the more necessary because the atomic and mineralogical compositions of cement are not the best. In cement formations, the total number of oxygen and hydrogen atoms is 76-83% and only 17-25% are represented by metal atoms [1]: whose chemical bonding energy (for example, Ca = O is 1076 kJ/mol) is several times greater than the energy of hydrogen and oxygen bonding atoms (for example, O-O only 192 kJ/mol).

Cement energy is formed by selecting raw materials with atoms of increased charges. For example, the effective charge of atoms that are not part of cement, sulfur 5.2, chromium 5.8, bromine 8.0, compared to the charge of calcium - 2.8, of which cement contains more than 60%.

The interaction between charges of different signs creates a new substance with new thermodynamic characteristics. Thus, while being roasted at about 1450°C, the liquid phase (high-temperature cement) upon cooling goes into a vitreous phase, cementing the refractory components (fillers) forming a clinker with the grain size from 20 to 60 mm, i.e. micro cement in the form of large granules. Their specific surface is low. Therefore, it becomes an electrically neutral, almost inactive, semi-finished product.

According to the theory of S. Zhurkov, a solid body is destroyed under the action of an external load, which causes the disruption of interatomic

bonds and the appearance of local and then severe disruptions. The process of destruction of clinker grain after its cleavage along the boundaries of defects occurs at the contact of the interphase surface, mainly calcium silicates with an intermediate substance; a crack is formed, the development of which contributes to further destruction. Depending on the grinding conditions, some of the dislocations that have appeared are the embryos of the resulting cracks, which are subsequently revealed [2].

Clinker milling is the breaking of chemical interatomic bonds, the formation of fracture surfaces, when on one half of the surface there remains a positive charge, and on the other – a negative one. It seems erroneous to consider that a chemical bond with a plus and a minus breaks into two halves, one of which is positive, and the second chemical bond is negative. Our experience with magnets suggests that, however small we crush it, the + or – of the particles of a magnet are impossible to destroy. Obviously, nature has determined that when a single chemical bond breaks, two new chemical bonds are formed, each of which is always full value: it has both + and -.

And yet two new chemical bonds are qualitatively different from the broken one. In new chemical bonds on the surface of the cement grain, bared by the milling, one pole of the charge is pinched, constrained, valently connected in a dense body of the grain, and the other opposite pole is free, calm, located in the surrounding air environment. Because of this, at the surface of the divide, the effective charge of the new chemical bond is in a constrained, valence state, while the opposite charge, in the ambient air, is in a free state. Between the poles of the same chemical bond a difference of potentials is formed.

For example, in CaO, the effective charge of the oxygen atom in the constrained state is $g = -1,22$ (in SiO₂ for Si $g_1 = +1.97$), and in the free

state for O $g = - 4.3$, and for Si, $g_1 = + 4.0$ [3,4]. Thus, in the broken chemical bond during milling two new ones are formed with an effective charge after neutralization in oxygen $g_{ef} = - 2.08$ ($4.3 - 1.22$), in Si $g_{ef} = + 2.03$ ($4.0 - 1, 97$).

Quantitatively and qualitatively, milling of the clinker leads to an increase in the activity of the surface of the cement grains, where there are many effective charges of different signs, which should approach each other by a distance of less than 0.4 nm [5] and interact. The convergence process is facilitated by the conductors [6], but there is an opinion [7] that "the entire inorganic part of the surrounding nature and all minerals are semiconductors."

However, the mechanism of their action in relation to the construction materials science has not been studied. It is known that the whole process of creating concrete is chemical-physical. Chemical part (synthesis) is instantaneous, at a speed of 10^{-8} – 10^{-10} seconds [8], and the remaining 28 days (according to regulatory documents), during which a concrete grade is achieved, we assign to physical processes, i.e. convergence of positive and negative charges up to the moment of their synthesis and the formation of a sufficient number of new particles in order to obtain the required brand of concrete.

The technologist should be working specifically with this process of convergence between + and -, reducing its duration, most likely, by means of facilitating (increasing the speed) of the passage of electrons in the environment of the freshly formed concrete. But in order to do that it is necessary to study the thermodynamic characteristics of the raw material, mainly of the binding agent, and subsequently of all kinds of additives, both in cement and in the water of mixture mixing.

However, the technologists evaluate the quality of the binding agent not

according to the energy characteristics of its components (conductors, semiconductors or dielectrics), but by their mineralogical or chemical composition.

With this in mind, we calculate the values (g_{ef}) and the number (%) of effective charges and the mass ($m \cdot 10^{-24}$) of the main minerals, oxides and atoms of portland cement grade 400, table 1.

Table 1

Characteristics of the mineralogical and chemical composition of portland cement grade 400

mineral				oxide			atom	
type	%	$m \cdot 10^{-24}$	g_{ef}	type	$m \cdot 10^{-24}$	g_{ef}	type	g_{ef}
$3CaOSiO_2$	52,1	378	-8,2	CaO	56,1	-8,2	Ca	+36,4
$2CaOSiO_2$	23,1	285	-7,6	SiO_2	99,6	-7,6	Si	+8
$3CaOAl_2O_3$	7,5	448	-9,7	Al_2O_3	169	-9,7	Al	+13,6
$4CaOAl_2O_3Fe_2O_3$	13,3	806	-16	Fe_2O_3	265	-16,1	Fe	+8,6
$CaSO_4 \cdot 2H_2O$	3,2	285	-7,7	SO_3	133	-9,2	S	+5,2
				H_2O	29,9	-2,3	O	-125

In our calculations, we use the reference data of effective charges of atomic nuclei [3, 4]. As a result, we find out that the effective charges in their valence state equal zero, i.e. minerals and cement oxides are electrically neutral [6] and it will require energy to activate them.

If in our calculations we take into account the effective charges of

atoms in their free state, all the minerals and oxides of the cement are negatively charged, i.e. repel each other. This ensures good conservation of cement in time, but in the absence of positive charges it causes deceleration in the creation of concrete – there is no synthesis. And only at the atomic level, Table 1, compared with minerals and oxides, the total amount of effective charges is maximum – 198 pcs: 73 of them are positively and 125 negatively charged, ready for synthesis and creation of concrete. Even when there are 1.8 times more of the negatively charged atoms than positive ones.

But is it really possible to turn dry grains of cement into atoms? Then cement becomes powdered, dispersed in a dry air environment, negatively charged grains. In this case, their electric charges are identified with matter. Electrons and the nucleus of atoms are tangible and therefore the more there are of them, the more matter accumulates in the cement.

The technologist needs to know the maximum of charges and that chemical energy of interatomic bonds which cement can accumulate. In one resource [6], the calculation of the amount of minerals in 1 kg of the M500 cement at 100% hydration of grains with a size of up to 20 μm is given. Continuing this calculation, we can find out the number of atoms in these minerals. According to the reference data [1], we find the effective charges of atoms in the free state. Putting it all together, we determine the electrical capacity of the cement. It includes approximately $164 \cdot 10^{24}$ pcs. of the positive effective charges and $136 \cdot 10^{24}$ pcs. of the negatively charged ones. The value of this lies in the knowledge of the relationship between the charges of different signs. Effective charges have no dimensionality and therefore the value of the charges is abstract. According to the total value of the energy of interatomic chemical bonds in 1 kg of cement, the calculations [6] lead to the figure $n = 86448 - 19803 = 65645$, approximately $66000 \cdot 1024$ kJ.

For standard cement, this is the maximum of the transmitter capacity, but it can be multiplied by introducing substances with more powerful charges in the raw material for cement production, with additives to the water of mixing the concrete mix, and using a reserve of non-hydrated grains of cement larger than 20 mm.

The mass of an atom or mineral, Table 1, is a measure of the energy of chemical bonds. It varies widely, 2.8 times for minerals, and 4.7 times for oxides. This difference disrupts the homogeneity of the chemical affinity of neighboring solid bodies: minerals, crystals, oxides. Their different resilience leads to different thermal fluctuations, and they in turn lead to defects in the structure and loss of the basic properties of the final product.

Thanks to the separate grinding of the various components, significant energy savings per unit of production are obtained by grinding and significantly improve the quality of the cement.

In addition to reducing water demand, it is possible to adjust the setting time of cement, as well as lower the temperature of hydration and increase strength.

Conclusions.

Thus, taking into account the characteristics of the system and structural organization of cement properties allows to solve:

1. Cement is an energy accumulator and its transmitter. The accumulation happens due to the conscious selection of atoms with an increase in their charge and their number with the ever more fine grinding or the introduction of energy-intensive additives. The task of the technologist is to increase the energy capacity of cement grains by all available means.

2. Cement as an energy transmitter requires the study of its

composition, taking into account the electrical characteristics: conductor, semiconductor and dielectric. The number of each of them is the acceleration or slowing down of the synthesis of charges of different signs.

3. It is impossible to consciously create a new building material or product with predetermined properties, without taking into account the natural essence of the raw material, semi-finished product and product: their electronic structure and build. It is recommended to evaluate the quality of the binding agent not only in terms of chemical and mineralogical compositions, but also taking into account its thermodynamic characteristics.

4. The technology of accumulation of charges, the acquisition of sufficient energy capacity of cement and its transfer to the receiver are built, being subject to a more detailed research and financial support.

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