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THE PROBLEM OF THE RELATIONSHIP OF THE DEBYE TEMPERATURE OF THE METAL WITH THE BASIC PHYSICAL PROPERTIES OF THE ELEMENTS

E.Yu. Shachneva[*], V.Ya. Khentov

Federal State Budgetary Educational Institution of Higher Education South-Russian State Polytechnic University, Novocherkassk, Russia

Abstract. The paper deals with the interaction of man and nature, as well as the problem of the occurrence of man-made waste. This is confirmed in the processes of transfer of matter, which affects the process of diffusion of elements. A relationship has been established between the physical properties of crystals and the Debye temperature for Group I s-element halides. High values of the correlation coefficients are presented. The graphical dependence of the values of the heats of sublimation with the Debye temperature of the metal element is presented. This suggests a possible mechanism for the transfer of the considered metals in nature.

Keywords: *technosphere, man-made waste, Debye temperature, metal concentration, correlation coefficient.*

Corresponding Author: *E.Yu. Shachneva, Federal State Budgetary Educational Institution of Higher Education South-Russian State Polytechnic University, 132, Prosveshcheniya Str., Novocherkassk, 346428, Russia, e-mail: evgshachneva@yandex.ru*

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1. Introduction

The concept of technosphere comes from the Greek root techne (art and craft) and sphaira (sphere). The technosphere is a part of the biosphere that has undergone changes as a result of human activity. It (the technosphere) has an artificial origin, i.e. it was created by human.

The ideas about the biosphere, which is considered as a single system, were developed by academician V.I. Vernadsky (Bird *et al*., 1974). The influence of man on nature is enormous. The consequences of this influence are not always beneficial for a person. All this served as the basis for Vernadsky's creation of the doctrine of the noosphere. The concept of the noosphere is nothing but the sphere of the mind. In addition, the concept of «environment» is used in ecology, which is a system. According to the aggregate state of the substance, the atmosphere, hydrosphere and lithosphere are distinguished.

The interaction of man and nature should lead to the sustainable development of the technosphere, new high-tech technologies should be created without serious consequences for man and nature. In this regard, we should talk about physical and chemical problems of the environment. These are various impacts of industrial and agricultural human activities on the atmosphere, hydrosphere and lithosphere, resulting in a huge amount of man-made waste.

Evolutionary processes in nature have led to the establishment of the distribution of chemical elements (Fig. 1) (Khentov, 2005).

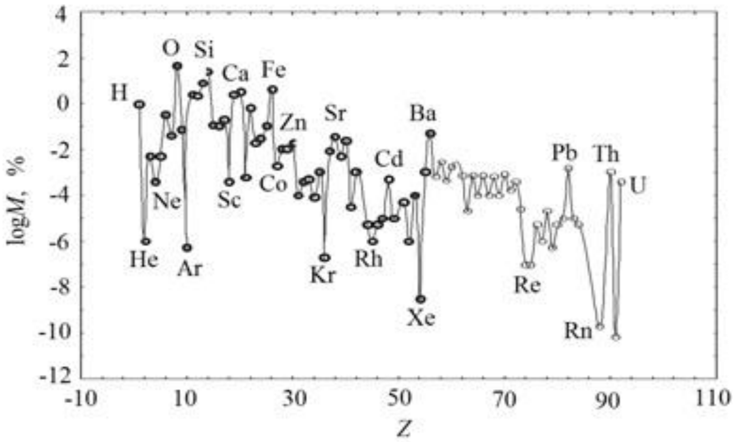

Fig. 1. The dependence of the logarithm of the average content of elements in the earth's crust logM on the ordinal number of the element Z

The content of metal elements in waste is comparable to mineral deposits. Therefore, an industrially developed society is faced with the task of developing waste recycling technology.

The problem of waste accumulation is one of the most acute problems of our time. In Russia, about 7 billion are recorded annually. tons of waste. It is possible to dispose of only 2 billion, i.e. 28%. According to other sources, only 5% of waste, mainly metallurgical slags, can be disposed of.

The formation of technogenic waste is associated with various physico-chemical processes occurring in a particular industrial sector. The development of science and technology constantly leads to the production and use of new functional materials, the development of new technological processes that use various chemicals. The most unpleasant moment in man-made human activity is the formation of a significant amount of a wide variety of waste in industrial and agricultural production. Of course, it is impossible to completely exclude their education. Only a conscious understanding of the processes of their formation will help reduce accumulation and outline ways to use them.

As a result of evolutionary processes in nature, an equilibrium has developed in the distribution of chemical elements. It can be disrupted mainly as a result of human activity. An important role in this is played by the transfer of matter. The phenomenon of transfer is a complex concept associated with the transfer of energy or mass from one part of an inhomogeneous system to another part. Transfer phenomena occur in any aggregate state of matter. They are especially noticeable in the gaseous and liquid phases.

The phenomenon of transfer is associated with nonequilibrium processes. Such processes are considered as a sequence of states. Moreover, within this sequence, not all states are equilibrium. Therefore, the system parameters should change over a certain period of time. This is possible due to the occurrence of flows associated with the transfer of heat, mass, electric charge, etc. Such processes that bring the system to an equilibrium state are called transfer phenomena.

Such processes as environmental pollution, the creation of difficult conditions at work, the occurrence of emergencies, climate change are associated with the transfer of substances. In this regard, it is interesting to consider the mechanisms of the transfer phenomenon, which are associated with the formation of composition and environmental pollution.

Three main mechanisms are responsible for the transfer phenomena: transfer phenomena at the molecular level (viscosity; electrical conductivity; physical evaporation; sublimation; diffusion and condensation); mechanical processes (dispersion of matter and accumulation of liquid in microlayers); chemical processes (complex formation; weathering of igneous rocks; redox processes occurring in man-made waste). One can also imagine three variants of the transfer phenomena – the transfer of the amount of motion (viscous flow); energy transfer (thermal conductivity and convection); transfer of matter (diffusion). A number of publications of the authors (Khentov *et al.*, 2005; Shachneva *et al.*, 2020; Shachneva *et al.*, 2019; Shachneva & Khentov, 2016) are devoted to the study of this problem, which most fully characterize the processes considered in the course of the study.

2. Research methods

The experimental part was processed by the method of dispersive, correlation and multiple regression analysis with the exception of insignificant members of the regression equations (Shachneva *et al.*, 2019; Vernadsky, 2004). The reliability of the multiple regression equations parameters was checked by dispersive analysis and the Student's criterion (Fernández & Grimvall, 1989).

3. The discussion of the results

The Debye temperature is an important integral parameter of a solid. The most important physical properties of crystalline substances are associated with the Debye temperature (Diyou *et al.*, 2019; Dhingra *et al.*, 2021; Ibrahim, 1988; Xing & Jia 2020). In this connection, the results of determining physical properties for the same type of chemical elements in the Debye temperature function are described with high reliability by a polynomial of the first degree (Table 1).

For group I s-element halides, a reliable relationship has been established between the physical properties of crystals and the Debye temperature. Table 2 shows the dependences of the interionic distances on the Debye temperature of the metal θ for the halides of s-elements of group I.

Figure 2 shows the dependence of the dissociation energy of a diatomic molecule of s-group I fluorides as a function of the Debye temperature of the metal.

Figure 3 shows the dependence of the viscosity of group I s-elements measured at 500°C on the Debye temperature of the metal.

Figure 4 shows the dependence of the thermal conductivity of s-elements of group I, measured at 500°C, on the Debye temperature of the metal.

The results obtained indicate that the most important physical properties of crystalline substances, such as the dissociation energy of a diatomic molecule, viscosity and thermal conductivity are closely related to the value of the Debye temperature of a metal element. High values of correlation coefficients are noted. With increasing values of the Debye temperature, the numerical values of the parameters under consideration increase. This suggests a possible mechanism of heavy metal transport in nature.

Table 1. Dependence of the physical properties of group I s-elements (Li, Na, K, Rb, Cs) on the Debye temperature θ, correlation coefficient R

Physical parameter	Regression equation	*R*
Density, g/cm^3	1,64464 – 0,003570	0,820
Melting point, °C	14639578 + 0,48650	0,997
Enthalpy of melting, kkcal/mol	0,3931 + 0,0020	0,980
Boiling point, °C	575,1245 + 2,19710	0,990
Enthalpy of evaporation, kkcal/mol	17,0555 + 0,0580	0,998
Heat capacity	32,114 – 0,02460	0,998
The binding energy of the elements, kkcal/mol	16,3129 + 0,06260	0,999
Coefficient of linear thermal expansion·10^{-6}, grad^{-1}	99,82824 – 0,16370	0,990
Compressibility·10^{-11}, cm^2/dyn	4,2679·10^{-11} – 1,1219·10^{-13}θ	0,860
Volumetric modulus of elasticity·10^{-11}, N/m^2	0,0103 + 0,00030	0,990
Lattice parameter, Å	6,06151 – 0,008050	0,950
Ionization energy, Ev	3,94031 + 0,004710	0,910
Fermi Energy, Ev	1,28594 + 0,010290	0,990
Electron output operation, eV	2,10625 + 0,000970	0,920
Surface tension·10^3, J/m^2	18,6814 + 1,10600	0,996
Hardness on the mineralogical scale	0,2561 + 0,00100	0,823
Young's modulus of elasticity, mJ/m^2	0,1444 + 0,0039*E*	0,999

Table 2. Correlation dependence, correlation coefficient R

Correlation dependence	***R***	**Halides**
L = 3,1537 – 0,0053θ	0,999	LiF, NaF, KF, RbF, CsF
L = 3,6212 – 0,0053θ	0,999	LiCl, NaCl, KCl, RbCl, CsCl
L = 3,7825 – 0,0053θ	0,999	LiBr, NaBr, KBr, RbBr, CsBr
L = 4,0108 – 0,0053θ	0,998	LiI, NaI, KI, RbI, CsI

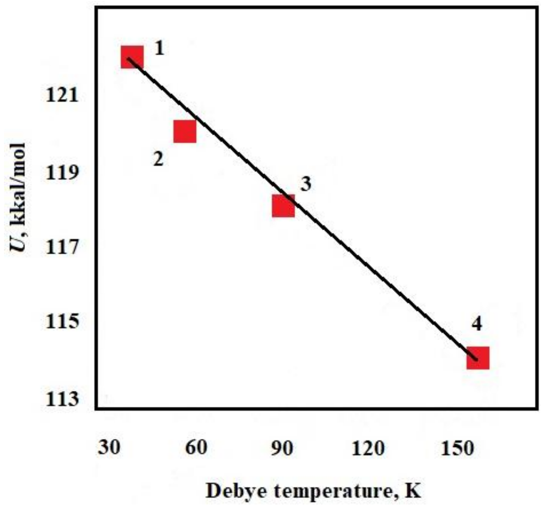

Fig. 2. The dependence of the dissociation energy on the Debye temperature of the metal 1 – CsF, 2 – RbF, 3 – KF, 4 – NaF. Correlation coefficient 0.995

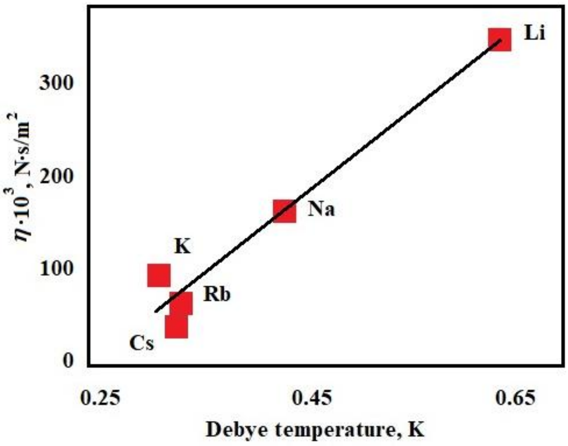

Fig. 3. Dependence of viscosity on the Debye temperature of the metal.
Correlation coefficient 0.979

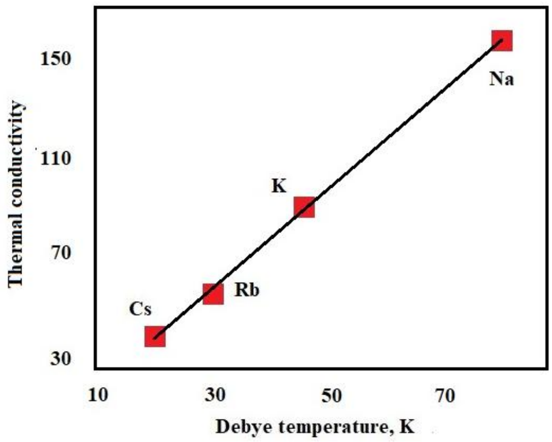

Fig. 4. Dependence of thermal conductivity on the Debye temperature of the metal.
Correlation coefficient 0.999

In the phenomena of transfer, an important role is assigned to the structural element. The nature of the structural element is chosen depending on the physical property under consideration. The transfer of matter during evaporation refers to liquid systems, during sublimation - to a solid body. These questions concern the transition of a substance from a liquid or solid state to a gaseous state.

The processes of melting, boiling and sublimation occur with energy costs, which are called the enthalpy of melting, the enthalpy of boiling and the enthalpy of sublimation. Melting, boiling and sublimation temperatures correspond to these concepts. Table 3 shows the values of temperatures and enthalpies of melting, boiling, sublimation, as well as Debye temperature θ (K) for a number of chemical elements.

Table 4 shows the values of the heat of sublimation of fluorides of group I s-elements and the Debye temperature of the metal. According to these data, for lithium, sodium, potassium, rubidium and caesium fluorides, the dependence of the heat of sublimation of crystals on the Debye temperature of the metal θ was found (correlation coefficient 0.94): $Q = 203,3745 + 0,23020\theta$.

Table 3. Temperatures (°C) of melting, boiling, sublimation, energy (kJ/mol) of melting, boiling and sublimation, θ

Element	Melting temperature	Boiling temperature, sublimation temperature	Enthalpy of melting	Boiling enthalpy, enthalpy of sublimation	θ
Potassium	63,5	761	2,33	76,6	91
Lithium	180,54	1347	3	138	344
Sodium	97,9	886	2,6	90,1	156
Rubidium	39,49	686,04	2,19	70	56
Caesium	28,5	672	2,1	67	40

Table 4. The heat of sublimation of crystals, the Debye temperature of the metal θ

Crystals	Sublimation heat, kJ/mol	θ, K
LiF	278	344
NaF	244	158
KF	238	91
RbF	225	56
CsF	190	38

Table 5 shows the sublimation heats of group I s-elements and the Debye temperatures of metals θ.

Table 5. The heat of sublimation of s-elements, the Debye temperature of the metal θ

Metals	Sublimation heat, kJ/mol	θ, K
Li	135,13	344
Na	98,05	158
K	79,27	91
Cs	68,38	38

Figure 5 shows the dependence of the sublimation heat of group I s-elements on the Debye temperature of the metal (correlation coefficient 0.998).

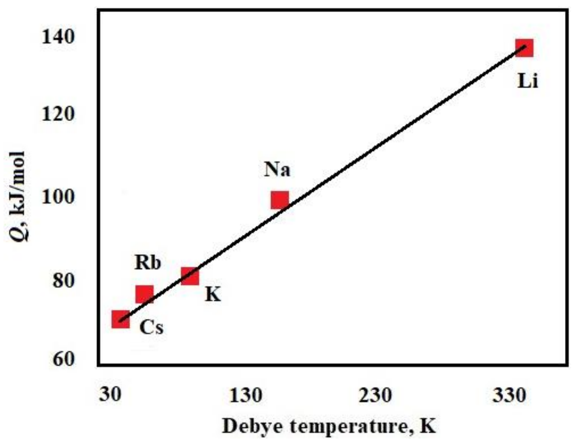

Fig. 5. Dependence of the sublimation heat on the Debye temperature of the metal

Thus, it was found that the value of the sublimation heats is closely related to the Debye temperature of the metal element. With an increase in the Debye temperature values, the numerical value of the sublimation heat decreases (for a group of elements). This suggests a possible mechanism of transfer of the metals in question in nature.

4. Conclusion

Describing all the above phenomena, we can draw the following conclusion. The technosphere is a single system, the human influence on which is very great. In this connection, the consideration of the processes of interaction between man and nature is of undoubted importance from a scientific point of view. Exposure leads to the appearance of man-made waste, so the problem of waste accumulation is one of the most urgent. Based on this, we can say that the problem of the transfer of matter and its mechanisms is also very interesting. The Debye temperature considered in the course of the study is an important integral parameter of a solid that determines the physical properties of the components.

The results obtained during the study indicate that the most important physical properties of substances are closely related to the value of the Debye temperature of the metal element. At the same time, high values of correlation coefficients were noted, which suggests a possible mechanism of heavy metal transport in nature. Within the framework of the study, the processes of melting, boiling and sublimation were studied. The values of the enthalpy of melting, the enthalpy of boiling and the enthalpy of sublimation are determined. These concepts correspond to melting, boiling and sublimation temperatures, as well as Debye temperatures. It is found that the value of the sublimation heats is closely related to the Debye temperature of the metal element. With an increase in the Debye temperature values, the numerical value of the sublimation heat decreases (for a group of elements). This allows us to assume a possible mechanism of transfer of the metals in question in nature and to consider the transfer phenomena.

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