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TITANIUM CHEMICAL NATURE FEATURES WHICH DETERMINE ITS MOST IMPORTANT PERFORMANCE PROPERTIES IN LINEAR ENGINE-GENERATOR

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ABSTRACT

Among the metals based on homonuclear chemical compounds of d-elements Ti, Zr and Hf (4-ep group of D.I. Mendeleev's periodic system) the choice of titanium as a primary structural material is justified for the manufacture of a reversible reciprocating electric machine translator with the capacity of 10-20 kW operating in harsh environments. This is due to the fact that the increase of metallicity degree of their homonuclear bonds Me---Me in the row titanium - zirconium - hafnium increases the density (γ) at a slight change of the thermal conductivity (λ), with a simultaneous decrease of thermal expansion ratio - TER ($\alpha \cdot 10^6$). Thus, the first property provides the possibility for the manufacture of lightweight parts and units for the assembly of a reversible reciprocating electric machine translator, which has a sufficiently high refractoriness (Tm. = 1668 °C) and corrosion resistance, especially taking into account the presence of a protective oxide film on titanium surface with very close TER.

Keywords: titanium, chemical bonding, structure, properties, electrical machine.

INTRODUCTION

The selection of material for the manufacture of any product and structure and is determined by a complex of required performance properties imposed on them, which in its turn is based on physical-chemical properties of the materials constituting the desired structure. At that the set of these properties is defined by a specific material structure.

During the development of a reversible reciprocating electric machine prototype with the capacity of 10-20 kW for the operation in harsh environments the use of new magnetic materials is required for the application as permanent magnets in a movable part of an electric machine, operating at the temperature of 150 °C in an aggressive environment. It is necessary to use the film materials which are applied as wear-resistant and antifriction coatings for frictional the contact surfaces, as well as structural metal materials combining strength, low density (lightness) and resistance to corrosive environments at elevated temperatures.

The purpose of this paper is to justify the choice of titanium and its alloys as a primary structural material for the manufacture of a reversible reciprocating electric machine translator with the capacity of 10-20 kW for harsh operating conditions.

TITANIUM AND ITS ALLOYS CHOICE JUSTIFICATION AS MAIN STRUCTURAL MATERIAL FOR TRANSLATOR MANUFACTURE

Among the metals based on d-elements of the IV-th PS group titanium differs from zirconium and hafnium by lower density (4.50, 6.50 and 13,1 g / cm3 respectively) [1], determining the possibility of its use for the lightweight machine parts in combination with a relatively high refractoriness (Tm = 1668 °C).

Therefore, it was interesting to reveal the fundamental causes of these beneficial properties combination in metallic titanium and determine the effectiveness of its use on this basis as a structural material, and to outline the prospects of its performance improvement with glassy coating use. A unified model of chemical bonding [2,3] can be used as the basis for the problem solution. This model allows to assess the impact of a fine chemical structure of any metal (e.g. titanium) or non-metallic (titanium oxide) substance and the material based on it. This model is represented by the formulas (1) and (2) for a pure metal, respectively – Ti_M (as a homonuclear compound with Ti --- Ti bonds) and titanium oxide - TiO_2 (as a heteronuclear compound with Ti - O bonds).

In this model [2-7] the total wave function of generalized (valence) electrons (GE) for the heteronuclear bond is calculated as follows:

$$\psi_{GE} = c_1\psi_{cov} + c_2\psi_{met} + c_3\psi_{ion}, \qquad (1)$$

where c_1, c_2 and c_3 are the factors determining the share of connection elements (components): covalent (C_K), metallic (C_M) and ionic (C_H), equal to the sum of one or 100 %. At that only a covalent chemical bond component (C_K), responsible for the maximum localization of GE on axis Y, connecting the centers of element nuclei may be equal to 100, but it cannot be decreased to 0 %. At the same time a metallic and ion components responsible for GE delocalization and the electron density as a whole, along the axes X and Y respectively, cannot achieve 100% of values in a chemical compound but can be equal to zero.

For example, during the transition from heteronuclear to homonuclear relations C_H becomes equal to 0 and the equation (1) is simplified to

$$\psi_{GE} = c_1\psi_{cov} + c_2\psi_{met} \qquad (2)$$

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The methods and results of these two or three chemical components calculation in a homo- or a heteronuclear relation are presented in [2-7] and summarized in the monograph [8].

The influence of ratio of homonuclear (Formula 2) and heteronuclear (Formula 1) components of relations on some substance properties and the materials based on these substances is demonstrated by the table data.

The table shows that interesting homonuclear relations E_A-E_A in metals and non-metallic molecular compounds such as O_2 are characterized by two chemical relation components (covalent and metallic one), and heteronuclear E_A-E_B of TiO_2 type - by three corresponding components (covalent, metallic and ionic one). At that the pure metals based on homonuclear chemical compounds of d-elements Ti, Zr, and Hf (the 4-th group of the periodic system), are characterized predominantly by metal bonds ($C_M > C_K$). On the contrary the covalence dominates over metallicity in O_2 molecule ($C_K > C_M$). At that the following is found when the properties of metallic materials formed by these elements are compared. The density (γ) increases with metallicity icrease (from top to bottom) in the following row: Ti - Zr - Hf at small change in thermal conductivity (λ), and the coefficient of thermal expansion - CTE ($\alpha \cdot 10^6$) decreases. It is logically explained by GE localization - delocalization change in their relationships. After all, C_M increase and C_K decrease in homonuclear E-E relation, due to GE delocalization and electronic density decrease in internuclear space, the "pack" of atomic element cores becomes easier relative to each other (matter density increases), the heat transfer is somewhat simplified respectively (λ increases).

Table-1. The properties of substances and materials with mainly metallic, covalent or covalent - ionic bond of elements in material microstructure.

Chemical bond substance and characteristics (Cк/Cм/Cи), in %	γ, g/cm³	$\alpha \cdot 10^6$, K⁻¹ (TER)	λ, Wt/(m·K)
Homonuclear, mainly metallic or covalent bond			
Metal – $Ti_м$ Ti --- Ti (35,6/64,4)	4,5	7,5	22,00
Metal – $Zr_м$ Zr--- Zr (33,1/66,9)	6,5	6,3	21,40
Metal – $Hf_м$ Hf --- Hf (32,7/67,3)	13,3	Less than 6	23,00
Molecule – O_2 O=O (89,4/10,6)	2,0	-	0,27
Heteronuclear, mainly covalent-ionic bond			
Oxide - TiO_2 Ti -O (40,1/24,1/35,8)	4,0-5,1	7,1	34,70

As for TER value reduction ($\alpha \cdot 10^6$), the higher material thermal conductivity is (λ), the faster its retraction from the volume of material the less substance is consumed on material expansion. That is, a denser material structure provides a greater heat conductivity and lesser ability to machine part extension at temperature increase (TER).

The latter property can be explained not only by the properties of the metal itself, but by the presence of oxide film TiO_2 on titanium surface, which also has a high corrosion resistance. The titanium oxide due to Cк growth, lesser metallicity (table) and the appearance of an ion component in Ti - O bond must have a greater resistance to oxidation (Cк grows and Cм falls), strength (as Cк grows and Cи appears additionally, which leads to an additional shortening E-O bond strengthening). Thus, the titanium oxide film has almost the same density as the metal titanium, but has a much higher thermal conductivity. High protective properties of TiO_2 oxide film may be attributed to its minimum porosity (high continuity) and an optimum thickness, determined by chemical structure specificity of a developed oxide film. A too thin film will have insufficient anti-corrosion protective properties, and a too thick film will flake off rapidly due to a difference in thermal expansion coefficients of an oxide film and metallic titanium in severe operating conditions at elevated temperatures, resulting in a sharp reduction of its protective properties and equipment damage.

The table values shows that the density (4,0-5,1 and 4.5) and TER (7.5 and 7.1) of titanium and titanium oxide, forming a film on its surface, do not differ greatly. This is based on a higher thermal conductivity of the latter, should provide a greater stability of titanium oxide film in service conditions at elevated temperatures and in aggressive media (water vapors, hydrocarbons, carbon oxides, etc.). Moreover, titanium compared with zirconium and hafnium has a higher elasticity modulus (E = 116 GPa), according to Mohs hardness (6,0) and although a lesser ultimate strength value σ_B (220 MPa respectively, in comparison with 330 MPa for zirconium), but sufficient for detailed use of a reversible reciprocating electric machine [7-8]. And taking into account the high spread of titanium in the Earth crust that exceeds the spread of zirconium and hafnium by several orders [1], it is clear that the efficiency of its practical application due to the availability of raw materials and affordability is more appropriate.

CONCLUSIONS

Based on the above stated information one may conclude that it is reasonable to choose titanium and its alloys as the primary structural material for the manufacture of a reversible reciprocating electric machine translator with the power of 10-20 kW for heavy duty.

SUMMARY

Thus, for the first time the article reveals the direct dependence of metal structure and properties formed by d-element compounds of the 4th group in D.I. Mendeleev's periodic system, oxygen and titanium oxide on the chemical component ratio of homo- and heteronuclear bonds of the elements which constitute them. The peculiarities of Ti --- Ti, O = O and Ti - O chemical bond elements are revealed in their homonuclear and heteronuclear compounds, compared with chemical homonuclear compounds of Zr and Hf, which consist in a different number of chemical components (two or three ones) and their relationships, which determine the density (γ), the thermal conductivity (λ) and the thermal expansion coefficient (TEC).

Thus it is proved that among the considered range of metals, titanium has a set of necessary considered properties which ensure the expediency of part manufacture from it for the machines operating at elevated temperatures and in aggressive environments.

CONFLICT OF INTEREST

The author confirms that the presented data do not contain any conflict of interest.

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