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INFLUENCE OF THE CRYSTALLINE STRUCTURE ON THE MECHANICAL PROPERTIES OF DODECABORIDES OF RARE-EARTH METALS AND ZIRCONIUM

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For the first time, we determine the modulus of elasticity (Young's modulus), the shear modulus, and the coefficient of transverse deformation (Poisson's ratio) for hot-pressed dodecaborides by using the basic thermal characteristics of the dodecaborides of rare-earth metals and zirconium YB_{12}, TbB_{12}, DyB_{12}, HoB_{12}, ErB_{12}, TmB_{12}, YbB_{12}, LuB_{12}, and ZrB_{12} and the experimental methods of static and dynamic investigations. The numerical and experimental values of the mechanical parameters coincide. The modulus of elasticity of dodecaborides is approximately twice smaller than for pure boron and does not increase, as theoretically predicted, in the sequence $MeB_4 \rightarrow MeB_6 \rightarrow MeB_{12}$. This fact can be explained by the structural features of the crystal lattice of dodecaboride phases, the lengths of the B–B, Me–B, and Me–Me bonds, and the forces of interaction between the atoms in these phases.

Keywords: dodecaborides of rate-earth metals and zirconium, mechanical characteristics, Young's modulus, shear modulus, Poisson's ratio, crystal lattice, bond length, interaction forces.

In the contemporary branches of industry (chemistry, metallurgy, machine building, radio electronics, aircraft and spacecraft construction, nuclear and defense technologies), traditional metals and their numerous alloys fail to satisfy new requirements to the chemical stability, density, and physicomechanical properties, especially under the conditions of high mechanical loads, high temperatures, and the action of corrosive media. The scientific progress, as well as the economic and ecological requirements determine, to a significant extent, the properties of structural materials used in manufacturing various types of commercial products. The problem of creation of new classes of structural materials based of rare-earth metals (REM), carbon, silicon, boron, and other elements in the form of carbides, silicides, borides, and compositions of these compounds explains the necessity of profound scientific investigations of the physicochemical and mechanical properties of these materials. It is clear that the dodecaboride phases of REM and zirconium with structures of the UB_{12} type definitely belong to the indicated class of materials.

The physicochemical properties of these refractory compounds and, especially, their mechanical and strength characteristics are studied insufficiently [1–4]. Here, it is necessary to mention only the paper [5] in which it is shown that the bending strength of YB_{12} is equal to 165 GPa (and the porosity of the specimens sintered in vacuum is 22–26%). In addition, in [2], one can find the computed values of Young's modulus for the dodecaborides of REM.

The aim of the present work is to study the principal mechanical properties of cubic dodecaborides with the UB_{12} structure, namely, to perform the numerical analysis (by using the well-known formulas) of Young's and

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shear moduli and Poisson's ratio, to experimentally determine Young's modulus by the static and dynamic methods, and to establish the relationship between these characteristics and the specific features of the crystalline structures of dodecaboride phases and the influence of metal atoms on the mechanical properties of dodecaborides.

Materials and Procedure of Investigations

For the first time, we perform systematic investigations of the mechanical characteristics, such as the modulus of elasticity (Young's modulus) E, the shear modulus G, and the coefficient of transverse deformation (Poisson's ratio) μ for single-phase dodecaboride phases of YB_{12}, TbB_{12}, DyB_{12}, HoB_{12}, ErB_{12}, TmB_{12}, YbB_{12}, LuB_{12}, and ZrB_{12}. These phases were obtained by the method of thermal reduction of REM oxides by boron in a vacuum [6] and sintering of the powders of the corresponding borides in the argon atmosphere in crucibles made of zirconium diboride on a charge of coarse boride powder at 2100–2200°K. The porosity of sintered materials was equal to 15–20%. The specimens for investigations were cut out in an electric-spark discharge machine in the form of parallelepipeds $(10 \times 2.5 \times 0.5)$ mm in size.

Prior to the experimental investigations of the mechanical properties of dodecaborides, we computed them according to the well-known (Frenkel', Frantsevich, and Köster–Frantsevich) formulas by using the coefficient of thermal expansion α, the characteristic temperature Θ, the melting temperature T_{melt}, the velocity of sound, etc. [6–8].

According to the Frenkel' formula, we obtain

$$\alpha = \frac{nk}{nR^3E}, \qquad E = \frac{nk}{\alpha nR^3}.$$

By the Frantsevich formula, we get

$$\Theta_D = \frac{1.6818 \cdot 10^3 \sqrt{E}}{M^{1/3}\gamma^{1/6}}, \qquad E = \frac{\Theta^2 M^{2/3}\gamma^{1/3}}{1.6818^2 \cdot 10^6}.$$

At the same time, the Köster–Frantsevich formula gives

$$f(\mu) = \left(\left(\frac{1+\mu}{3(1-\mu)}\right)^{3/2} + 2\left(\frac{2(1+\mu)}{3(1-2\mu)}\right)^{3/2}\right), \qquad f(\mu) = \frac{3.34 \cdot 10^7 T_{\text{melt}}^{3/2}}{A\gamma^{1/2} C V^{3/2} \Theta^3}.$$

For the shear modulus, we can write $G = \gamma \upsilon_m^2$, where

$$\upsilon_m = \frac{\Theta_D}{\frac{h}{k}\sqrt[3]{\frac{3nN\gamma}{4\pi M}}}, \qquad \Theta_D = \frac{h}{k}\left(\frac{3nN\gamma}{4\pi M}\right)^{1/3} \upsilon_m,$$

k is the Boltzmann constant, γ is density, M is the molecular weight, υ_m is the velocity of sound in the material, Θ_D is the characteristic temperature, h is the Plank constant, n is the arithmetic mean of the principal quantum numbers of elementary substances in the compound, and N is the number of atoms in the molecule.