ELECTRONIC STRUCTURE AND MECHANICAL PROPERTIES OF DODECABORIDES RARE EARTH METALS

Odintsov V.V., Koren E.V.[(1)]
Kherson State University, Kherson, 40 let Octyabrya 27, 73013, Ukraine, V.1tsov@mail.ru;
[(1)]Kherson State Agrarian University, Kherson, R.Luxembourg 23, 73006, Ukraine,
koren2205@yandex.ua

Dodecaborides rare earth metals with a structure of UB_{12} - YB_{12}, TbB_{12}, DyB_{12}, HoB_{12}, ErB_{12}, TmB_{12}, YbB_{12}, LuB_{12}, ZrB_{12} are poorly studied class of refractory compounds. The mechanical properties of these phases are virtually unexplored, which naturally limits their practical use in the presence of a high chemical resistance to acids and mixtures thereof, high melting point (2500 ÷ 2900K), small thermal expansion ($4 \cdot 10^{-6}$ K^{-1}), significant characteristic temperatures (800÷1000K), large radii of neutron absorption and high thermal conductivity [1].

In the present work we have on known relations Frenkel, which have been improved Frantsevich I.N., Koester [2,3,4], were evaluated modulus of elasticity, shear and Poisson's ratio, as well as static and dynamic experimental methods defined module of elasticity (Young's modulus) dodekaborides phases. The calculated and experimental values of the mechanical characteristics coincide numerically are: Young's modulus (E) 250, 200, 190, 190, 195, 197, 198, 190, 200 GPa, a shear modulus (G) 195, 160, 150, 160, 160, 160, 156, 170, 154 GPa, Poisson's ratio (μ) 0,31; 0,36; 0,37; 0,34; 0,30; 0,33; 0,35; 0,36; 0,39 respectively borides for YB_{12}, TbB_{12}, DyB_{12}, HoB_{12}, ErB_{12}, TmB_{12}, YbB_{12}, LuB_{12}, ZrB_{12}.

Considerably smaller (twice) values of these characteristics in comparison with those of pure boron (E_B=390GPa, G_B=320GPa [5], μ=0,39) can be associated with features of the electronic structure of dodekaborides phases.

In borides $MeB_{x>2}$ to form the three-dimensional structure of the complexes of boron requires a greater number of valence electrons than that which is present in the boron in connection with which the B-B bond in this compound borides, and as dodecaborides earth metals, carried out valence sd and even f-electrons in the metal. Complicating the structural elements of boron, observed at the transition from the lower to the higher borides, leads to increased stiffness of the crystal lattice.

Possibly, the mechanical properties dodecaborides defined their crystalline structure. Dodecaborides are formed in the cubic structure type of NaCl, where the role of Na - atoms of the rare earth metal atoms as role atoms of Cl - groups B_{12}. Having two cubic sublattice rare earth metal and B_{12} groups, apparently reduce the strength properties dodecaborides by sliding one on the other grating. In pure boron all define rigid covalent bonds B-B. In the case of dodecaborides phases atoms of rare earth metals are a plasticizer similarity reducer basic strength, mechanical characteristics dodecaborides phases.

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