Change of Structure and Properties of System WC-Ti at Mechanical Activation

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Tungsten carbide is one of the most interesting representatives carbides transition of metals of maximum groups, which can have as cubic, and hexagonal crystallographic modification. In particular, cubic WC with structure as NaCl has rather wide area homogeneity on carbon and has high temperature melting, hardness and durability, and also propensity to formation double carbides with transitive 3d-metals. The data about peculiarities of the chemical bonding and changes in then electronic structure of the cubic WC at partial replacement of tungsten atoms by titanium atoms in the published literature has not enough for understanding of laws of formation properties of system "WC-Ti". Therefore in the given work the electronic structure and character of chemical bonding in carbide systems WC, $W_{1-x}Ti_xC$ is theoretically investigated. Recently presence lattice as C-, and W-vacancies in WC is shown. At mechanical activation in ball mill of powders WC and Ti, the size of a grain of which makes size about 1…5 micron, it is possible to expect solid-solid of reaction. Our estimations, carried out on basis of quantum-mechanical accounts of their electronic structure, show, that the mechanical properties of the given system can grow. The samples are investigated XRD by a method, analysis of areas coherent dispersion is carried out which are called to supervise changes of structure and properties during mechanical activation. Complex research of crystal and electronic structures of the given system allows to understand the laws of formation of physical properties of new materials.

Keywords: structure-physical properties relationships, tungsten compounds, x-ray powder diffractometry