ABSTRACT

Master dissertation: 102 pages, 16 tables, 35 figures, 73 references.

MODELING, STRUCTURE, ENTROPY, ALLOY, AB – INITIO, PSEUDOPOTENTIAL, ATOM, FLAPW, ENERGY

The object of research: model structure with BCC cell.

Purpose of research: theoretical research of atomic structure and interatomic interaction in crystalline structures that modeling a multicomponent TiZrHfCoNiCu alloy.

Methods of research: ab – initio methods for calculation the atomic and electronic structure of crystals FLAPW (Wien2k package) and the Pseudopotential method (Quantum Espresso).

Research results and novelty: the atomic structure of the model structure $Ti_9Zr_9Hf_9Co_9Ni_9Cu_9$ of symmetry B2 is calculated. It is established that the lengths of interatomic bonds differ considerably from the lengths in ideal lattice of BCC type which leads to larger displacements of atoms from ideal positions. It is showed that the reason of distortion of the crystalline lattice of the structure $Ti_9Zr_9Hf_9Co_9Ni_9Cu_9$ is strong interatomic interaction of Ti atoms with Co, Ni and Cu atoms. The characteristic feature of these interactions is much smaller length of bonds Ti – B (B = Co, Ni, Cu) compared to the length of bonds Zr – B and Hf – B. Binding energy of the atoms Co, Ni and Cu in model structures A_8B_8 (A = Ti, Zr, Hf; B = Co, Ni, Cu) were calculated by pseudopotential method. It is established that in all structures atom Co has the highest binding energy (-8,1 -8,5 eV) and atom Cu has the lowest energy (-5,1 -5,4 eV).

Field of application: aerospace, machine building and instrument making.